Scientific Notebook No. 170E: Total Performance Assessment (TPA) 3.2 Development (April 3, 1996 through September 16, 2003)

# SCIENTIFIC NOTEBOOK

# 170-9E

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# INITIAL ENTRIES

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**Objective**: Document activities related to the development of the TPA code Version 4.0. This section is focused in the required changes to the failt module.

12/20/99

## Weld corrosion

There is some discussion between NRC and CNWRA staff about wether or not corrosion along the welds should be included in the basecase. According to the present modeling, after the relative humidity exceeds a superior threshold, a film of water develops on the waste package (WP) surface. The relative humidity is only function of the WP temperature. If we assume that welding enhances the corrosion rate, then initial failure of the WPs occurs, invariably, along the welds. However, we decided not to include any model for the corrosion along the welds for the following reasons:

**1)** The longitudinal weld and circumferential weld in the middle of the WP (i.e., the WP will be made of two attached cylinders) will be solution annealed, which, according to Darrell Dunn and Gustavo Cragnolino, may not change the properties of the base metal. That is to say, the solution annealed welds may be as corrosion resistant as the base metal. The only weak welds are circumferential welds on flat ends of the WP, which will be in a vertical position when located in the drifts.

**2)** Experimental data indicates that the passive dissolution rate of the welded materials is similar to that measured for the base metal. The critical potential for localized corrosion in weld materials has been found to be less by ~100 mV, which is not sufficient guarantee a significant

contribution to the WP failure time.[1] Current TPA computations indicate that the corrosion potential is of the order of 0.1 $V_{SHE}$, while the critical potential for the presence of localized corrosion is of the order of 1 $V_{SHE}$. for Alloy 22. Thus, a difference of 100 mV between the critical potential for welds and the critical potential for the base metal is not expected to contribute significantly to WP failure time. Further testing with welded materials will be performed by the CLST KTI to assess the feasibility of welds to be a relevant contributor to the WP failure time. Experimental data gathered so far indicates that this may not be the case.

**3)** The flux of water will be severely hindered due to the location of the welds and their limited surface. Thus, in the event of failure along the welds, the available area for water infiltration and release of the radionuclides is very limited. The expected contribution to the performance of the system may be quite limited.

Thus, because of the above points, we decided not to include treatment of the welds in the present TPA code. However, auxiliary analyses will attempt to quantify the contribution of the welds to the performance of the system. In case of finding that the welds may be an important contributor to the performance of the system, a weld model will be introduced at a later time (i.e., not in TPA 4).

12/21/99

## Radiolysis

The main result of water radiolysis is the production of oxidants such as $H_2O_2$, which increase the corrosion potential by supplying to the environment with an easily reducible species in addition to dissolved $O_2$ and $H_2O$. Narasi Sridhar proposed that rather than performing detailed computations (which so far are impossible to be accomplished due to our limited understanding in the phenomenon) the computed corrosion potential is increased by a term, $\Delta E$, computed as

$$\Delta E = \Delta E_o e^{-\lambda t} \qquad [1]$$

where $t$ is the time variable. The decaying constant, $\lambda$, is an ad hoc parameter intended to simulate the expected decrease in the radiation levels from the spent fuel and, consequently, in the steady-state concentration of $H_2O_2$. The CLST KTI will suggest a value for the constant $\Delta E_o$ based on experimental data, and a value for $\lambda$ based on educated estimates.

---

[1] D. Dunn, Y.-M. Pan, and G. Cragnolino, CNWRA 99-004, pages 3-1– 5
PMPR No. FY2000-2, December 10, 1999, page 5

The following parameters will be declared in the tpa.inp file

DeltaPotentialDueToRadiolysis[V] → $\Delta E_o$
DecayingConstantRadiolysis[1/yr] → $\lambda$

The proposed change in the failt.f module is explained as follows. Let $E_{corr}^{old}$ represent the corrosion potential as computed in the TPA code Version 3.3. We propose to compute the corrosion potential for Version 4 as

$$E_{corr} = E_{corr}^{old} + \Delta E_o e^{-\lambda t} \qquad [2]$$

In case of not requiring to include the presence of radiolysis, then it will be possible to set $\Delta E_o = 0$.

12/22/99

## EDA II

The enhanced design alternative (EDA) II requires us to modify the code to allow for the incorporation of new materials. Currently, the failt module is designed model the situation in which the outer layer is made of carbon steel, and the inner layer of Alloy 22. It is desirable to allow the user the freedom to select the materials and define them in the tpa.inp file. Currently, the following properties have been identified as "hard-wired" in the failt.f module:

Densities of the outer and inner overpack
Molecular weights of the inner and outer overpack

These four parameters are used to transform current densities into corrosion rates. Further detail is next provided. Notation:

| | |
|---|---|
| $Z_j$ | oxidation state of the j-th alloy component |
| $f_j$ | weight fraction of the j-th alloy component |
| $W_j$ | molecular weight if the j-th alloy component [kg/mol] |
| $F$ | Faraday's constant = $9.64867 \times 10^4$ C/mol |
| $i$ | current density [A $m^{-2}$] |
| $\rho$ | Alloy density [kg $m^{-3}$] |

Assuming stoichiometric dissolution (or congruent dissolution) of the alloy components, it can be

proved that the relationship between the current density, $i$, and the corrosion rate, $CR$, is[2]

$$CR = \frac{i}{F\sum_j \frac{z_j f_j}{W_j}\rho} \qquad [3]$$

The *Equivalent Molecular Weight, EW*, for an alloy is defined as

$$EW = \frac{1}{\sum_j \frac{z_j f_j}{W_j}} \qquad [4]$$

The Equivalent Molecular Weight has units of kg/mol. The Equivalent Molecular Weight for the alloys in the EDA II will be defined by the user in the tpa.inp file. In the failt module, the following formula will be implemented to transform current densities into corrosion rates:

$$CR = \frac{i\ EW}{F\rho} \qquad [5]$$

No other "hard-wired" parameters in the failt.f have been identified. The following parameters will be introduced to the tpa.inp file:

DensityOuterOverpack[kg/m^3]
DensityInnerOverpack[kg/m^3]
EquivalentWeightOuterOverpack[kg/mol]
EquivalentWeightInnerOverpack[kg/mol]

The names of the parameters are self explanatory.

In the current version of the TPA code, mechanical failure of the outer overpack induced by thermal embrittlement of the pressure vessel carbon steel required the existence of cracks, which could lead to brittle failure, and residual stresses generated by welding or other manufacturing processes. As a simplification and using a conservative approach, corrosion pits are considered as cracks despite the different aspect ratio. This approach is justified because carbon steels are prone

[2] See the Scientific Notebook 355, pages 39-42 for details in the deduction of this equation

to localized corrosion in alkaline aqueous environments as those expected to contact the WPs. The fracture toughness was regarded as invariant in time because the repository temperatures, in the VA design, were not sufficiently high to enhance the thermal embrittlement. For the materials selected in the EDA II mechanical failure due to brittle fracture may not be feasible for both alloy 22 and Type 316L SS due to the high ductility of both materials. There is no embrittlement process that can be envisioned as possible for inducing mechanical failure under the current environmental conditions, with the exception of high loads resulting from seismic events that may promote plastic collapse. Nonetheless, the TPA code 4.0 will incorporate the same mechanical failure model as the existing in TPA 3.3. To avoid unnecessary changes in the code, values of the yield strength for alloy 22 and type 316L SS will be used whereas high values of fracture toughness, typical of ductile materials, will be assigned. In this manner, brittle failure will not occur in the TPA simulations. Adequate values of the yield strength and fracture toughness will be selected by the CLST KTI.

The last change related to the EDA II is related to the way localized corrosion of the inner and outer overpack is treated in the TPA code. Localized corrosion of carbon steel is described by

$$P = A t^n \qquad [6]$$

$P$ penetration depth [m]
$t$ time [yr]

$A$ and $n$ are two parameters defined in the tpa.inp file as CoefForLocCorrOfOuterOverpack and ExponetForLocCorrOfOuterOverpack, respectively.

Localized corrosion of Alloy 22 is described by

$$P = A t \qquad [7]$$

where $P$ and $t$ have the same meaning, and $A$ is defined in the tpa.inp file as LocalizedCorrRateOfInnerOverpack[m/yr]. Clearly Equation [7] can be obtained from Equation [6] by setting $n = 1$, and choosing an appropriate value for $A$.

We decided to use Equation [6] to describe both the localized corrosion of the outer and inner overpack. Different values of $A$ and $n$ will be selected for each case. Although Equation [6] is not an equation of general validity it has been decided to continue with its use for two reasons:

**1)** Results of the TPA code Version 3.3 will be easily reproduced, by an appropriate selection of parameters, and

**2)** the consensus is to continue with the use of constant for the penetration rate for Alloy 22, which

can be simulated by setting $n = 1$. In case of the SS 316 proposed in the EDA II, DOE has mentioned that it will not take any credit for the corrosion protection provided by this material. However, we may decide to evaluate the protection provided by this material, and Equation [6] will provide us with some limited capability to do so.

Two new parameters will be introduced in the tpa.inp:

CoefForLocCorrOfInnerOverpack
ExponentForLocCorrOfInnerOverpack

The name of these parameters is self explanatory.

1/5/2000

## Drip Shield

A meeting with NRC staff (Richard Codell, David Esh, and Tae Ahn), and CNWRA staff (Gustavo Cragnolino, Sitakanta Mohanty, Sean Brossia, and Osvaldo Pensado) was carried out to discuss an scheme to include the presence of the drip shield (DS) in the TPA model. A detailed modeling of the drip shield is not feasible for several reasons: incompleteness of experimental data, limited understanding of the degradation mechanisms, uncertainty in the environment, and uncertainty in the design. Instead of providing a detail mechanism, in the tpa.inp file a new variable will be created

DripShieldFailureTime[yr]

which will represent the a distribution function for the failure time of the drip shield. It was proposed to correlate this distribution function with the failure time for the WP. However, there is not any strong reason to support or deny this correlation. For the sake of simplicity, it was decided to let this variable as an independent variable.

This distribution function will affect the radionuclide release. Thus, water infiltration into the WP will occur only if both the DS and the WP have failed. Richard Codell is in charge of modifying the releaset.f module. In this section, only the modifications to the failt module will be discussed.

In the TPA model, the corrosion mechanisms are partially determined by the relative humidity (RH). The RH is not function of amount of water infiltrated into the drifts. The RH is defined as function of the temperature. If the DS is designed to limit the amount of water seeping

into the WP, then the RH humidity with or without the DS is the same, unless the temperature is disturbed by the presence of the DS. Sitakanta Mohanty is evaluating the effect in the temperature distribution by the presence of the DS. This evaluation is performed outside the failt.f module. No change in the failt module is necessary to accomplish that. Mohanty's analysis will be summarized in the form of a new data file.

During the meeting it was agreed that one of the consequences of the DS may be a limitation in the amount of salts contacting the WP. In the TPA model, this will be reflected in a change in the chloride concentration in contact with the WP. We decided to model this in the manner next described.

In the TPA code, the chloride concentration computed with multiflo is multiplied by a sampled parameter (uniform distribution with 0 and 1 as boundaries) called ChlorideMultFactor in the tpa.inp file. This algorithm will be replaced by the following scheme:

If the DS is intact (i.e., current time < DripShieldFailureTime[yr]) then use ChlorideMultFactorIntactDripShield. After failure of the DS (i.e., current time > DripShieldFailureTime[yr]) then use ChlorideMultFactor. Thus, a new parameter will be defined in the tpa.inp file:

ChlorideMultFactorIntactDripShield

We have decided to set this parameter equal to 1, but this choice may change.

01/11/2000

## Implementation of the changes to the failt module

The changes above discussed were implemented in the failt.f module. The following parameters have been introduced:

| *tpa.inp name* | *tpanames.dbs name* |
|---|---|
| CoefForLocCorrOfInnerOverpack | IO-CofLC |
| ExponentForLocCorrOfInnerOverpack | IO-ExpLC |
| ChlorideMultFactorIntactDripShield | ChloriDS |
| DripShieldFailureTime[yr] | DSFailTi |
| DensityOuterOverpack[kg/m^3] | OO-Densy |
| DensityInnerOverpack[kg/m^3] | IO-Densy |
| EquivalentWeightOuterOverpack[kg/mol] | OO-EqWei |

| | |
|---|---|
| EquivalentWeightInnerOverpack[kg/mol] | IO-EqWei |
| DeltaPotentialDueToRadiolysis[V] | DelPRadi |
| DecayingConstantRadiolysis[1/yr] | DecCRadi |

The following parameter has been deleted

| | |
|---|---|
| LocalizedCorrRateOfInnerOverpack[m/yr] | crate2 |

since this parameter can be made equivalent to CoefForLocCorrOfInnerOverpack. This variable has not yet been deleted from the tpanames.dbs file. All of the parameters have been already defined.

The files to be modified were provided by Ron Janetzke. A back-up of Janetke's files is located at **/home/opensado/tpa4/source/**, in **Vulcan**. All of the directories and files mentioned in this section are located in Vulcan, unless otherwise indicated. The notation ~/ is equivalent to **/home/opensado/**

---

All the directories referred to in this section are located in **Vulcan.**

**~/ = /home/opensado/**

---

The following unix instructions were used to copy Janetzke's files:

```
>>cp /net/scratchy1/export/home/janetzke/tpa/dev/*  ~/tpa4/source/
>>cp /net/scratchy1/export/home/janetzke/tpa/dev/codes/*  ~/tpa4/source/codes/
>>cp /net/scratchy1/export/home/janetzke/tpa/dev/data/*  ~/tpa4/source/data/
```

The modified files (i.e., those incorporating the DS, radiolysis and EDA II changes) can be found at ~/tpa4/ebsfail/. The changes can be easily located, since they are enclosed by the labels OPR and ENDOPR. The file tpanames.dbs does not contain such labels, but this file has also been modified. Plenty of *readme* files are located at the directory ~/tpa4, which should be enough to follow the development and testing stage.

The files in the directory ~/tpa4/source have been copied to the directory ~/tpa4/tpa4/. The modified files in the ~/tpa4/ebsfail/ directory have also been copied to the corresponding subdirectory in the ~/tpa4/source and compiled there with the available *Makefile* files.

In order to run the modified version of the tpa code, in its modified version, the following shell commands were used:

---

```
>>setenv TPA_TEST /home/opensado/tpa4/tpa4
```

>>setenv TPA_DATA /home/opensado/tpa4/tpa4

# Testing

Testing is thoroughly documented at ~/tpa/testfailt/ in the *readme* files. Testing was performed on the independent module failt.f and the whole TPA code. The failt.f module requires the following files in order to run: chldmf.dat, ebstrhc.inp, and ebsfail.inp. The file ebsfail.inp is an input file, where all the failt.f module constants are specified. The files chldmf.dat and ebstrhc.inp are data files containing the chloride concentration, the temperature, and the relative humidity. These files were copied to the ~/tpa/testfailt/ directory. The following unix commands were employed:

```
>>cp ~/tpa4/ebsfail/failt.e .
>>cp ~/tpa4/test1/ebsfail.inp .
>>cp ~/tpa4/test1/ebstrhc.inp .
>>cp ~/tpa4/test1/chlrdmf.dat .
>>cp ebsfail.inp ebsfail.inp.ref
```

The file ebsfail.inp.ref is used as reference input file throughout the testing phase. Here we reproduce a copy of such a file:

**ebsfail.inp.ref**

```
\example input file for ebsfail
|
\simulation time
  10000.00                ! tend: simulation time leng
\                               ! when iflag=1 (defined later)
\
 5.6820  1.8020           ! wplen,wpdia: wp length and
 0.1000E+00  0.2000E-01       ! cthick1,cthick2: wp layers
|
\choose source of temperature data
2, 1                    ! iflag(1:emp.equation,2:tab
1                               ! nset (temp.-rel hum. relationship to use
49.9999999                      ! timintv (used when iflag=2)
|
\other temperature parameters
0.                              ! age of fuel (not used in this version)
|
```

```
\Dry oxidation of wp outer overpack
 0.1375E+02              ! grainr: metal grain radius
25                      ! nseries (terms in the infi
 0.7000E-03             ! gbthick [micrometer]
 0.1000E-04             ! constant1: used in the dry
|
\evaporation-condensation
 0.5500E+00  0.7869E+00     ! humdc1, humdc2: crit. rel.
 0.2287E-02             ! filmthk: thickness of wate
 0.9990E+03             ! ctemp: boiling point of wa
|
\Corrosion Parameters(Ep: pitting potential [mVshe]; Erp: re
-584.8                  ! xipto: outer overpack Ep i
3.92                    ! pttemo: temp. coef. of out
-24.5                   ! slpto: outer overpack Ep s
-1.1                    ! slpttemo: temp. coef. of o
-0.6203E+03             ! xirpo: outer overpack Erp
 0.4700E+00             ! rptemo: temp. coef. of out
-0.9520E+02             ! slrpo: outer overpack Erp
 0.8800E+00             ! slrptemo: temp. coef. of o
200.                    ! xipti: inner overpack Ep i
0.                      ! pttemi: temp. coef. of inn
-240.                   ! slpti: inner overpack Ep s
0.                      ! slpttemi: temp. coef. of i
 0.1066E+04             ! xirpi: inner overpack Erp
 0.0000E+00             ! rptemi: temp. coef. of inn
 0.0000E+00             ! slrpi: inner overpack Erp
 0.0000E+00             ! slrptemi: temp. coef. of i
 0.7500E+00  0.5000E+00     ! betaox1, betahy1: beta kin
\                           for oxygen and water for WP outer overpack
 0.7500E+00  0.5000E+00     ! betaox2, betahy2: beta kin
\                           oxygen and water for WP inner overpack
 0.3800E+13  0.1600E+00     ! rkox1 [c*m/y/mol], rkhy1 [
 0.3730E+05  0.2500E+05     ! gox1 [J/mol], ghy1 [J/mol]
 0.3000E+11  0.3200E+01     ! rkox2 [c*m/y/m], rkhy2 [c/
 0.4000E+05  0.2500E+05     ! gox2 [J/mol], ghy2 [J/mol]
 0.3150E+06  0.0  0.0       ! aa(1,1) [C/m2/yr], aa(1,2)
 0.5879E+05  0.0  0.0       ! aa(2,1) [C/m2/yr], aa(2,2)
-0.4600E+00              ! eexpt: measured galvanic c
 0.5891E-02              ! rcoef: coef. for loc. corr
```

```
 0.4500E+00                ! rexpont: exponet for loc.
OPR 1/13/2000
 0.2500E-03                ! rcoef2: coef. for loc. cor
 0.1000E+01                ! rexpont2: exponent for loc
ENDOPR
 0.1160E-04                ! cratehac:humd.air corr.rt.
 0.0000E+00                ! xcouple, efficiency of gal
 0.0000E+00                ! xread: factor for defining
3.e-1                     ! clconc: chloride conc. [mo
 0.3000E-03                ! clcrit1: crit. chloride co
 0.1000E+01                ! clcrit2: crit. chloride co
 0.1383E+01                ! cfactor: factor for changi
 0.2100E+00  0.9000E+01        ! xgas: oxygen part.pr.[atm]
 0.0000E+00  0.1000E+01  0.1000E+01 althk: scale thick;taus:
OPR 1/13/2000
 0.1000E+01                ! cfactor2: factor for chang
 0.0000E+00                ! failtimds: failure time of
 0.0000E+00   0.7000E-04       !deltaEo and lamb: Radiolysi
0.786000E+04 0.814000E+04 0.279250E-01 0.255422E-01 !dense1 dense2 wtmol1 wtmol2
ENDOPR
|
\Mechanical failure data
 0.2050E+03  0.1400E+01        ! yieldstr: yield strength [
 0.2500E+03                ! dkic: fracture toughness [
|
\Runge-kutta control parameters
1.e-3, 1.e0                     ! dtini, dtmax
1.e-2, 1.e-30                   ! errrel (same as eps), errabs (same as tin
|
\end
```

We adopted the following Notation:

**corrode.outLABEL** is the failt.e output of **ebsfail.inpLABEL**

Thus, corrode.out.ref is the output of runnig failt.e with the inputfile ebsfail.inp.ref.

The testing was divided into three phases, testing related to the DS changes, to the radiolysis changes, and to the EDA II changes. Plots made with Matlab are used to perform the testing. In

order to reproduce the plots, at Matlab prompt, change the directory to point at ~/tpa4/testfailt/ and type runX (where X is a number or a label) and the appropriate plot will be displayed. The files containing the information of the plots are located at ~/tpa4/testfailt/ and are named runX.m and runX.mat. All of the matlab computations are thoroughly documented at ~/tpa4/testfailt/handy.m. The testing phase is next discussed.

1/14/2000

### DS testing

This section documents testing of the failt.f module concering the drip shield (DS) changes. Further documentation can be found at ~/tpa4/testfailt/*readmeDS*. In the modified failt.f the chloride concentration is multiplied by the adequate factor (cfactor1 or cfactor2) depending on whether the drip shield is intact or has failed. The input to the code is the failure time of the DS and the multiplication factors cfactor1 and cfactor2 (these are represented in the tpa.inp file by ChlorideMultFactor and ChlorideMultFactorIntactDripShield, respectively).

The failt.f module does not produce any output file including the chloride concentration affected by the cfactor. Thus, it is necessary to devise other means to verify the consistency in the code changes. The following premise has been used for that purpose.

**Premise**: the chloride flag in the corrode.out file equals 1 only if the relative humidity is above humdc2= 0.7869, and the chloride concentration exceeds the critical concentration of the material under degradation (either the outer or inner overpack).

In Runs 1 – 5, we exploit the above fact to test the changes to failt.f. We manipulate the input data to force the concentration flag to be 0 or 1 at certain times. These times are compared with the times at which the chloride concentration exceeds or is below the critical concentration, and the time at which the film of water is formed. The two sets of times must agree completely. Indeed we found this to be the case.

Rather than explaining in detail all of the actions, the unix shell commands are presented, which will shorten the discussion.

**Run1**

```
>>cp ebsfail.inp.ref ebsfail.inp
```

Changes to ebsfail.inp:

```
0.0             ! cfactor2: factor for chang
```

1.0000E+04 ! failtimds: failure time of

These changes are designed to set [Cl]=0 throughout the simulation period (10,000 yr). Thus, according with our premise, the chloride flag in corrode.out must equal zero at all times. Note that the failure time for the drip shield (failtimds) is equal to 10,000 yr, which means that throughout the simulation period the chloride multiplication factor is cfactor2 = 0.

```
>>failt.e
>>cp ebsfail.inp ebsfail.inp1
>>cp corrode.out corrode.out1
```

The expected output was produced. See ~/tpa4/testfailt/corrode.out1.

**Run2**

```
>>cp ebsfail.inp.ref ebsfail.inp
```

Changes to ebsfail.inp:

```
0.0          ! cfactor: factor for changi
0.0          ! failtimds: failure time of
```

This is a similar situation to that in Run 1. In this case the drip shield is initially failed, so that the relevant chloride multiplication factor is cfactor = 0. Since cfactor (Run 2) = cfacto2 (Run 1) = 0, the output files (corrode.out) must be identical for these runs.

```
>>failt.e
>>cp ebsfail.inp ebsfail.inp2
>>cp corrode.out corrode.out2
```

Effectively, the file corrode.out2 is identical to corrode.out1 as revealed by the following shell command:

```
>>diff corrode.out1 corrode.out1
```

No differences were reported by the above command, as expected.

**Run3**

```
>>cp ebsfail.inp.ref ebsfail.inp
```

Changes to ebsfail.inp:

```
50.0            ! cfactor2: factor for chang
1.0e+4            ! failtimds: failure time of

>>failt.e
>>cp ebsfail.inp ebsfail.inp3
>>cp corrode.out corrode.out3
```

**Expected output**: I computed a plot with Matlab (run3.m), displayed as Figure 1. The chloride concentration is above the critical concentration for both the inner and outer overpack during the wet time after ~1800 yr and before ~7000 yr. Thus, the chloride flag column in the corrode.out file must be zero outside of this period, and one within this period. This is exactly the content of the corrode.out3 file. Type run3 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display this figure. See the file ~/tpa4/testfailt/ handy.m for details in the Matlab computation for the generation of the plots.

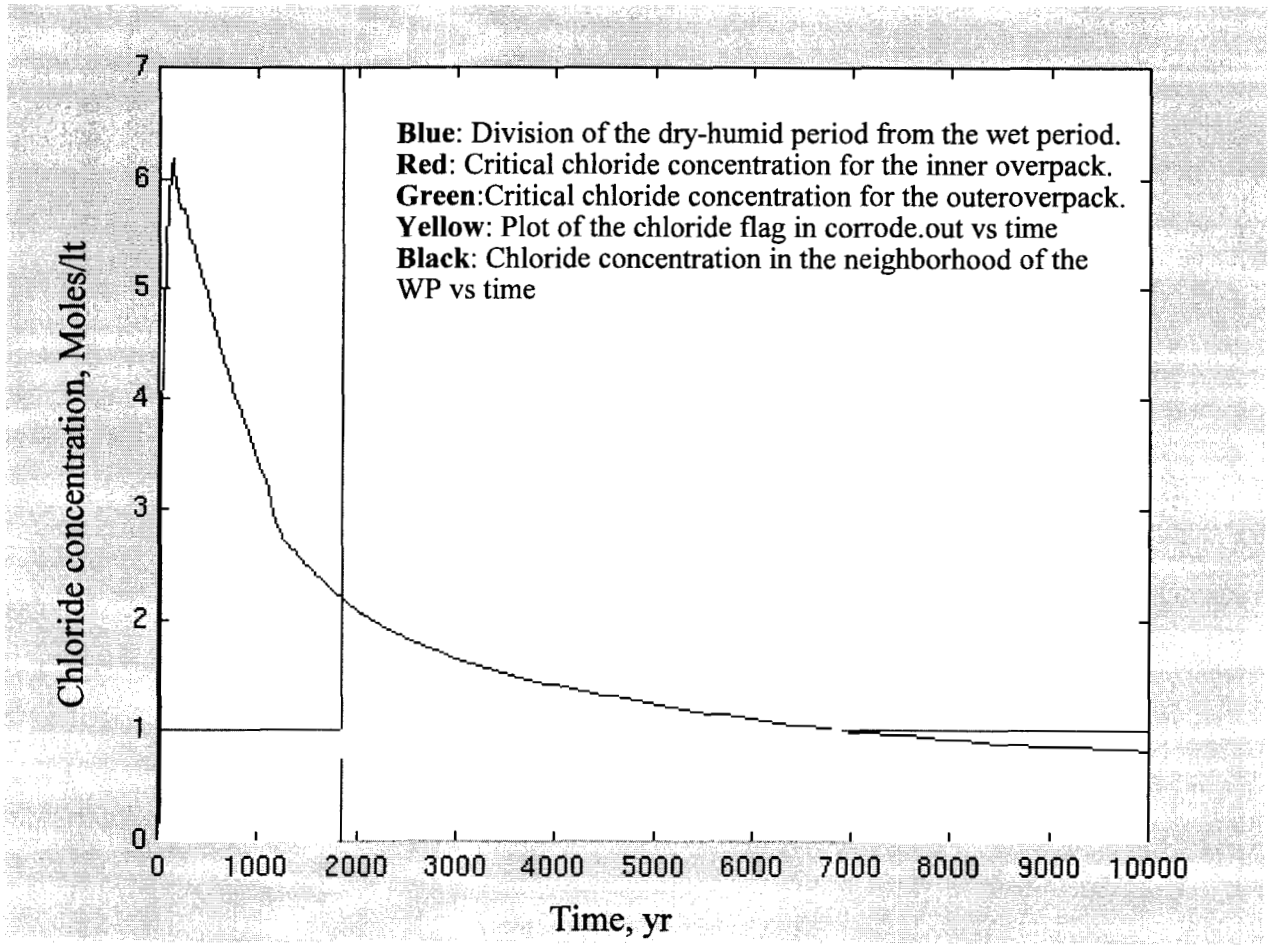


**Figure 1**: Plot presenting data of Run 3 (chloride concentration versus time, and chloride flag versus time). The yellow line represents the chloride flag(as defined in corrode.out3) versus time. The time region where this flag equals one is equivalent to the time region defined by the establishment of a wet environment, and the chloride concentration being above the critical chloride concentration.

**Run4**

```
>>cp ebsfail.inp.ref ebsfail.inp
```

Changes to ebsfail.inp:

```
100.0              ! cfactor: factor for changi
0.1000E+01              ! cfactor2: factor for chang
0.0000E+00              ! failtimds: failure time of

>>failt.e
>>cp ebsfail.inp ebsfail.inp4
>>cp corrode.out corrode.out4
```

**Expected output**: Since the drip shield is failed at time failtimds = 0, the chloride factor is cfactor = 100, the chloride concentration is above the critical concentration at all times. The Figure 2 shows that the chloride flag is 1 for time > 1800 yr. This is entirely consistent with our expectations. Type run4 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display this figure. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

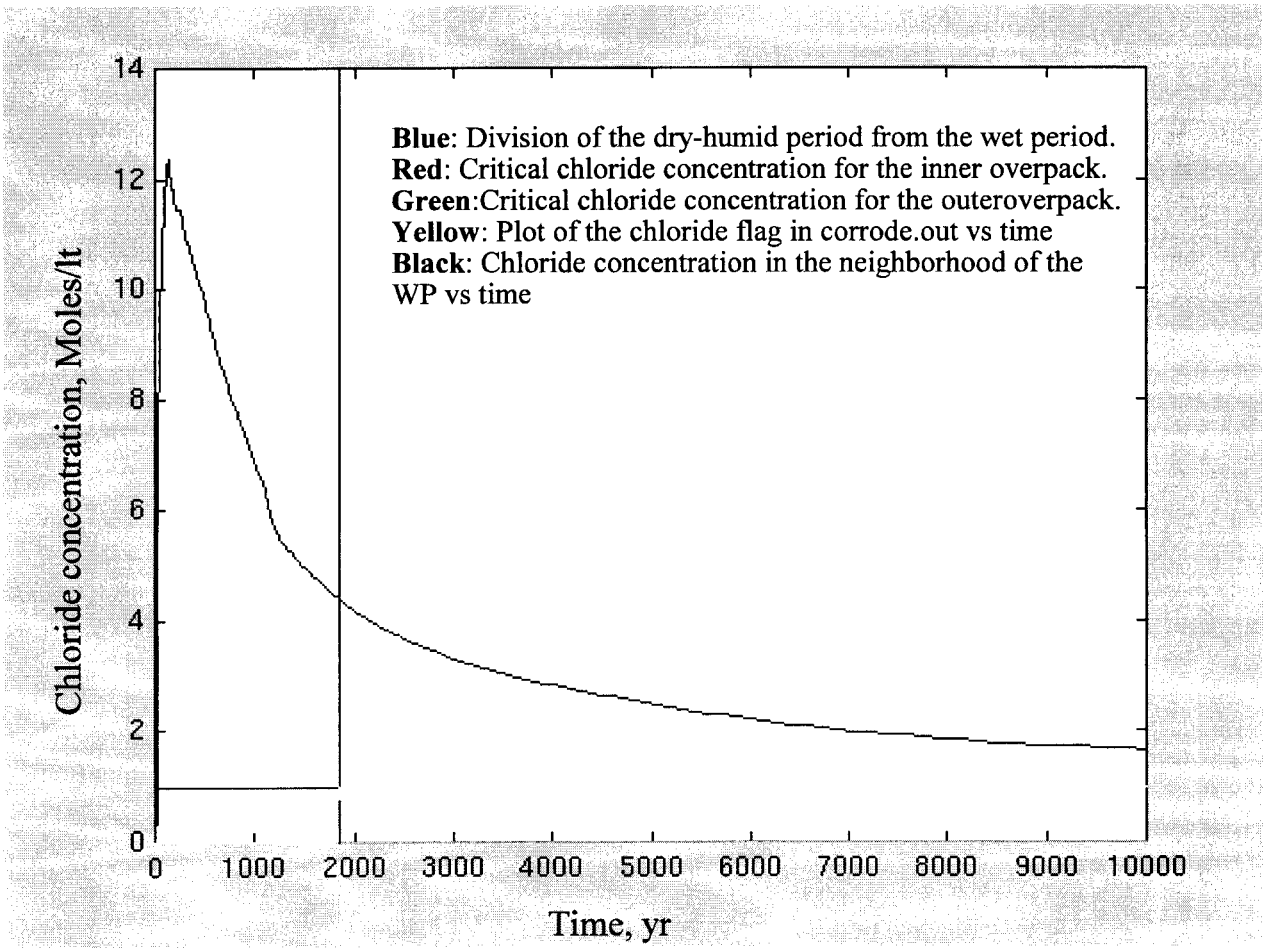


**Figure 2**: Plot presenting data of Run 4 (chloride concentration versus time, and chloride flag versus time). The yellow line represents the chloride flag(as defined in corrode.out4) versus time. The time region where this flag equals one is equivalent to the time region defined by the establishment of a wet environment, and the chloride concentration being above the critical chloride concentration (i.e., chloride flag = 1 for time > 1800 yr).

**Run5**

```
>>cp ebsfail.inp.ref ebsfail.inp

100.0            ! cfactor: factor for changi
50.0             ! cfactor2: factor for chang
8000.0           ! failtimds: failure time of

>>failt.e
>>cp ebsfail.inp ebsfail.inp5
>>cp corrode.out corrode.out5
```

**Expected output**: In this case it is expected that the concentration will fall below the critical concentration after ~7000 yr, and then will exceed the critical chloride concentration, after failure of the DS at failtimds = 8000 yr. Thus the cloride flag will be zero within 7000 yr and 8000 yr. The yellow line in Figure 3 readily shows this. Type run5 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display this figure. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

## CONCLUSION

We found consistent and predictable results. We conclude that the changes to the failt module concerning the drip shield perform as desired.

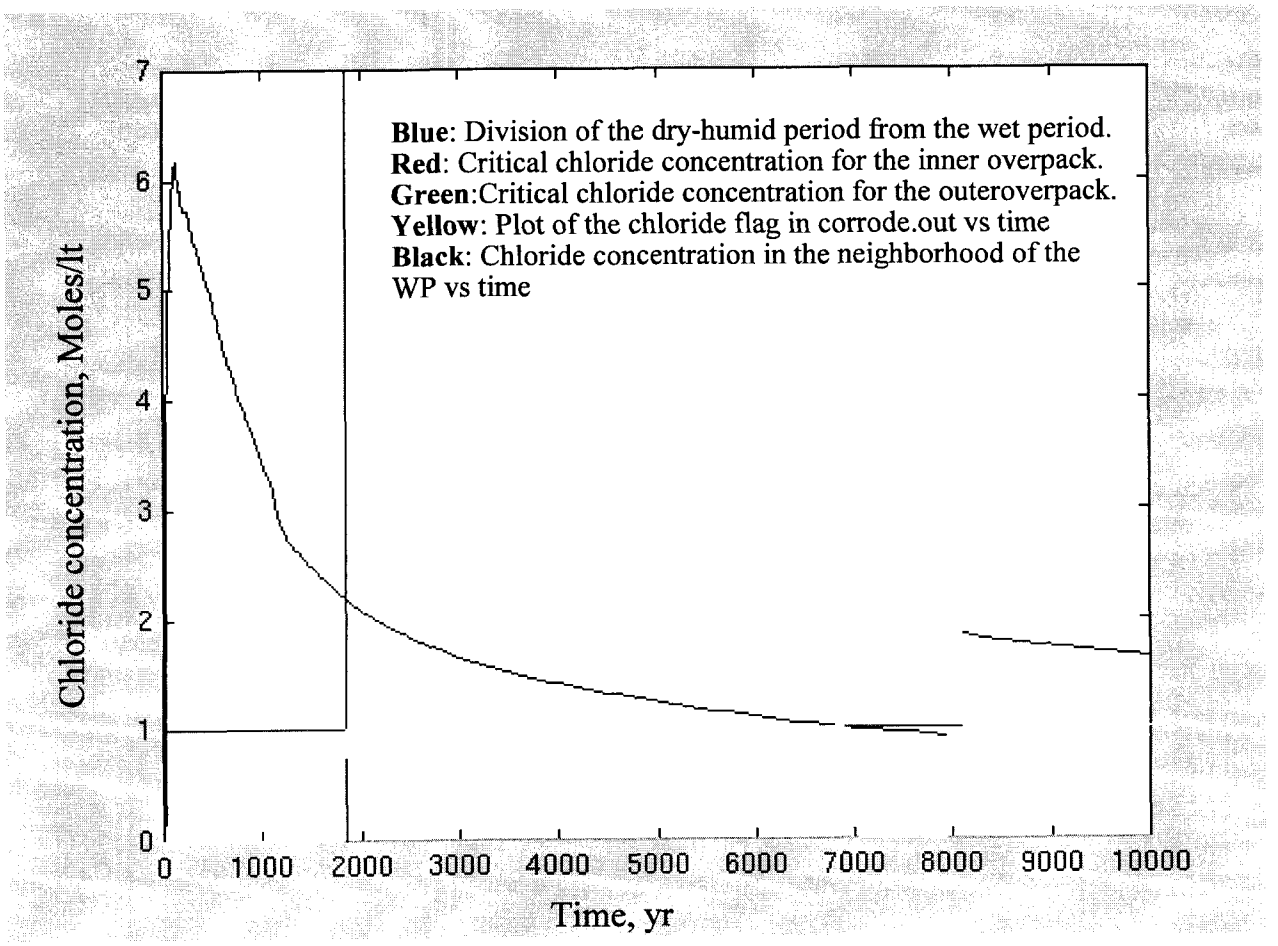


**Figure 3**: Plot presenting data of Run 5 (chloride concentration versus time, and chloride flag versus time). The yellow line represents the chloride flag(as defined in corrode.out5) versus time. The time region where this flag equals one is equivalent to the time region defined by the establishment of a wet environment, and the chloride concentration being above the critical chloride concentration. At 8000 yr the chloride concentration exceeds the critical chloride concentration because of failure of the drip shield.

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## Radiolysis testing

Testing of the failt module concerning the changes to simulate radiolysis are documented in this section. Radiolysis is simulated by an increase in the corrosion potential, described by Equation [1]. The time is measured with respect to time of the waste emplacement. Runs 6 and 7 were used to test the changes. After testing we concluded that the changes are working as intended.

**Run 6**

```
>>cp ebsfail.inp.ref ebsfail.inp
```

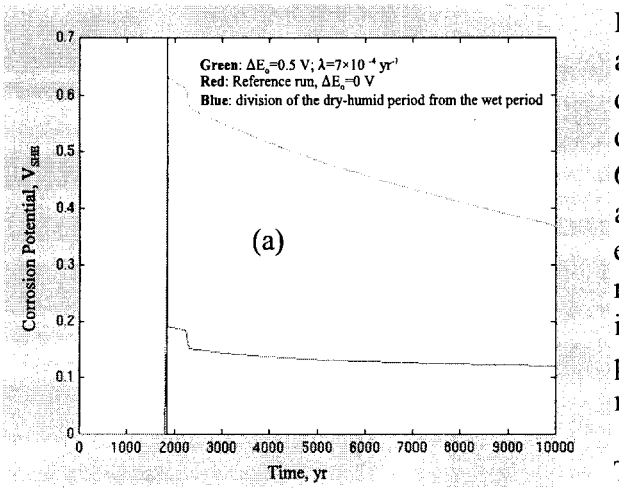
Changes to ebsfail.inp

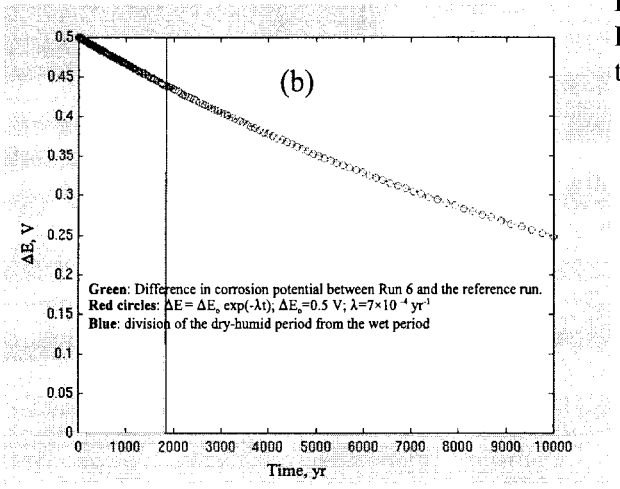
```
0.5   0.7000E-04        !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp6
>>cp corrode.out corrode.out6
```

In the reference run deltaEo = 0. In run 6 the corrosion potential exceeds that of the reference run by deltaE=deltaEo*exp(-lamb*time) (see Equation [1]). This can be visualized in Figure 4. Figure 4-a: corrosion potential Vs time for run6 and reference run. Figure 4-b: comparison of deltaE=deltaEo*exp(-lamb*time) and the difference in the corrosion potential between Run 6 and the reference run. Both curves are identical, as expected. Figure 4-c: penetration depth for run6 and the reference run. Both penetration depths are identical, since the increase in the corrosion potential does not suffice to change the corrosion mode.

Type run6a (or run6b or run6c) at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 4. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

We can conclude that the implemented formulas are working in the manner they are intended to work. However, another run is performed to verify that the increase in the corrosion potential can change the corrosion mode.



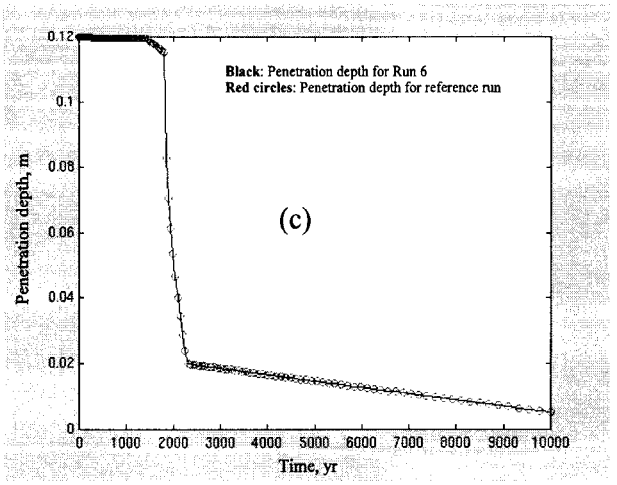




**Figure 4**: (a) corrosion potential Vs time for Run 6 and reference run. (b) Comparison of deltaE=deltaEo*exp(-lamb*time) and the difference in the corrosion potential between Run 6 and the reference run. Both curves are identical, after the establishment of the wet conditions, as expected. (c) Penetration depth for run6 and the reference run. Both penetration depths are identical, since the increase in the corrosion potential is not enough to change the corrosion mode.

The agreement between the curve computed via Equation [1] and the computed curve with the data of Run 6 and the reference run is a good indication that the failt.f changes are performing as expected.

**Run 7**

```
>>cp ebsfail.inp.ref ebsfail.in

30.0                ! cfactor: factor for changi
1.5  0.7000E-04     !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp7
>>cp corrode.out corrode.out7
```

In this run it is noted that the corrosion potential for Run 7 exceeds that of the reference run by exactly deltaE=deltaEo*exp(-lamb*time). This can be visualized in Figure 5. Figure 5-a: corrosion potential Vs time for run7 and reference run. Figure 5-b: comparison of deltaE=deltaEo*exp(-lamb*time) and the difference in the corrosion potential between run6 and the reference run. Both curves are identical, in the wet period, as expected. Figure 5-c: penetration depth for run7 and the reference run. We have adjusted the chloride concentration and the corrosion potential, so that the inner layer displays localized corrosion. In this run we note that failure is produced quite immediately after failure of the outer layer, as expected.

Type run7a (or run7b or run7c) at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 5. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

## CONCLUSION

The modifications to the failt concerning radiolysis are performing as intended.

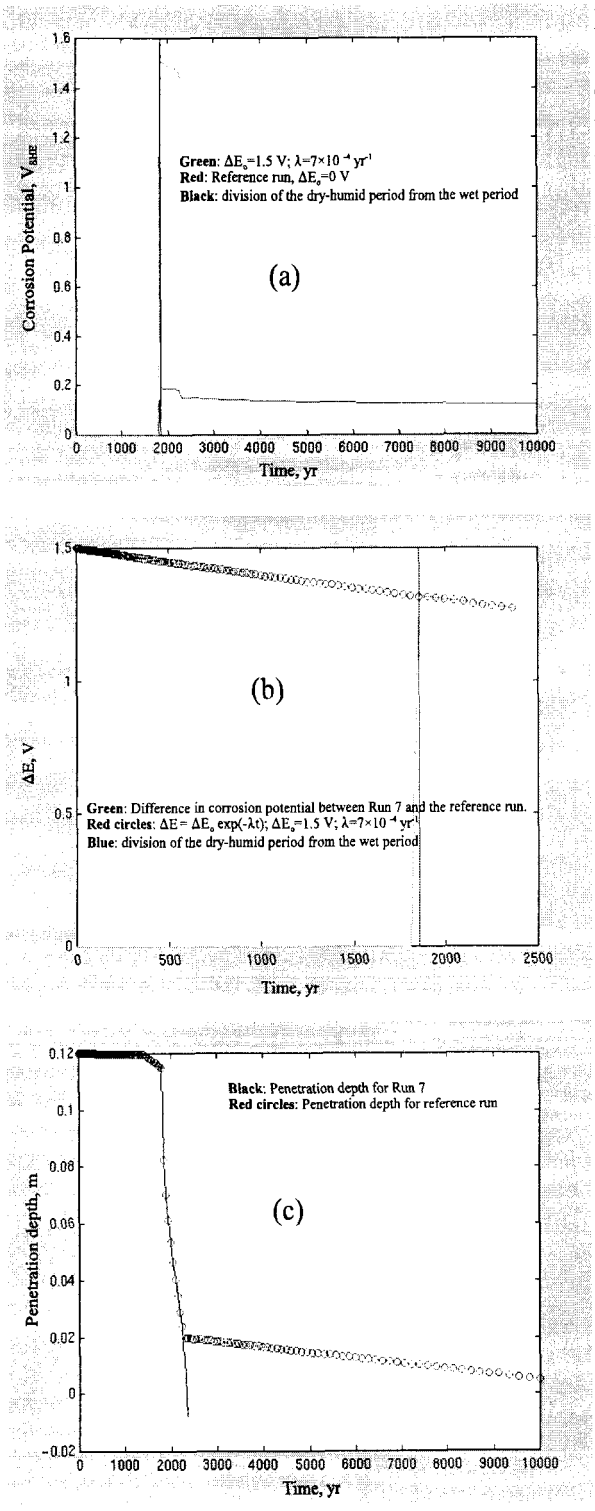



**Figure 5**: (a) Corrosion potential Vs time for Run 7 and reference run. (b) Comparison of deltaE=deltaEo*exp(-lamb*time) and the difference in the corrosion potential between Run 7 and the reference run. Both curves are identical, in the wet period, as expected. (c) Penetration depth for Run 7 and the reference run. The chloride concentration and the corrosion potential have been adjusted so that the inner layer displays localized corrosion. In Run 7 it is noted that failure is produced almost immediately after failure of the outer layer, as expected.

The agreement between the curve computed via Equation [1] and the computed curve with the data of Run 7 and the reference run is a good indication that the failt.f changes are performing as expected.

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## EDA II Testing

Hard-wire in parameters were put as user defined parameters. These are the densities of inner and outer layers, and equivalent molecular weights of inner and outer layers. On top of the above, the localized corrosion for the inner layer is described by the formula defined as Equation [6] (the outer layer uses this formula already).

It was first verified that the changes are capable of reproducing old computations (i.e., before-change computations). Data in the directories ~/tpa4/failt1 and ~/tpa4/failt2 are aimed to verify that.

failt1 --> run of the modified failt module.
failt2 --> run of the non-modified failt module (original code).

The file ~/tpa4/failt1/ebsfail.inp was designed to reproduce the file ~/tpa4/failt2/corrode.out (i.e., the output file of the non-modified code). For that aim, the following parameter values were adopted:

rcoef2 = 0.25E-3 (i.e., the same value of the constant crate2 in ~/tpa/failt2/ebsfail.inp – m $yr^{-1}$ )
rexpont2 = 1 (we have discussed that by choosing $n = 1$, Equation [6] reduces to Equation [7])
failtimds = 0 (the drip shield is initially failed, no drip shield protection)
deltaEo = 0 (no radiolysis effects)
dense1 = 7.60E+3 (density of carbon steel)
dense2 = 8.40E+3 (density of Alloy 22)
wtmol1 = 0.2792E- 1 (equivalent molecular weight of carbon steel – kg/mol )
wtmol2 = 0.0255422222222222222 (equivalent molecular weight of Alloy 22 – kg/mol )

All of the other parameters in ~/tpa/failt1/ebsfail.inp and ~/tpa/failt2/ebsfail.inp are identical. Therefore both input files represent the same situation, and the corresponding output files must be identical. We determined that this statement is true, and thus, the modified failt module is capable of reproducing old computations.

The shell command

>> diff ~/tpa/failt1/corrode.out ~/tpa/failt2/corrode.out

does not reveal any difference in the output files.

**Run 8**

Objective: verify that the formula for the penetration represented as Equation [6] is performing as expected for the inner and outer layer.

```
>>cp ebsfail.inp.ref ebsfail.inp

6.02E-05                ! rcoef2: coef. for loc. cor
0.7                ! rexpont2: exponent for loc
100.0                ! cfactor: factor for changi
1.5   0.7000E-04       !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp8
>>cp corrode.out corrode.out8
```

Figure 6 displays the expected penetration depth (blue line computed with Matlab, neglecting dry and humid air corrosion) and the computed penetration depth (green circles) with the modified failt.f module. The agreement is reasonable; however, further testing is needed to verify that the observed deviation is not due to other unforseen causes.

Type run8 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 6. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

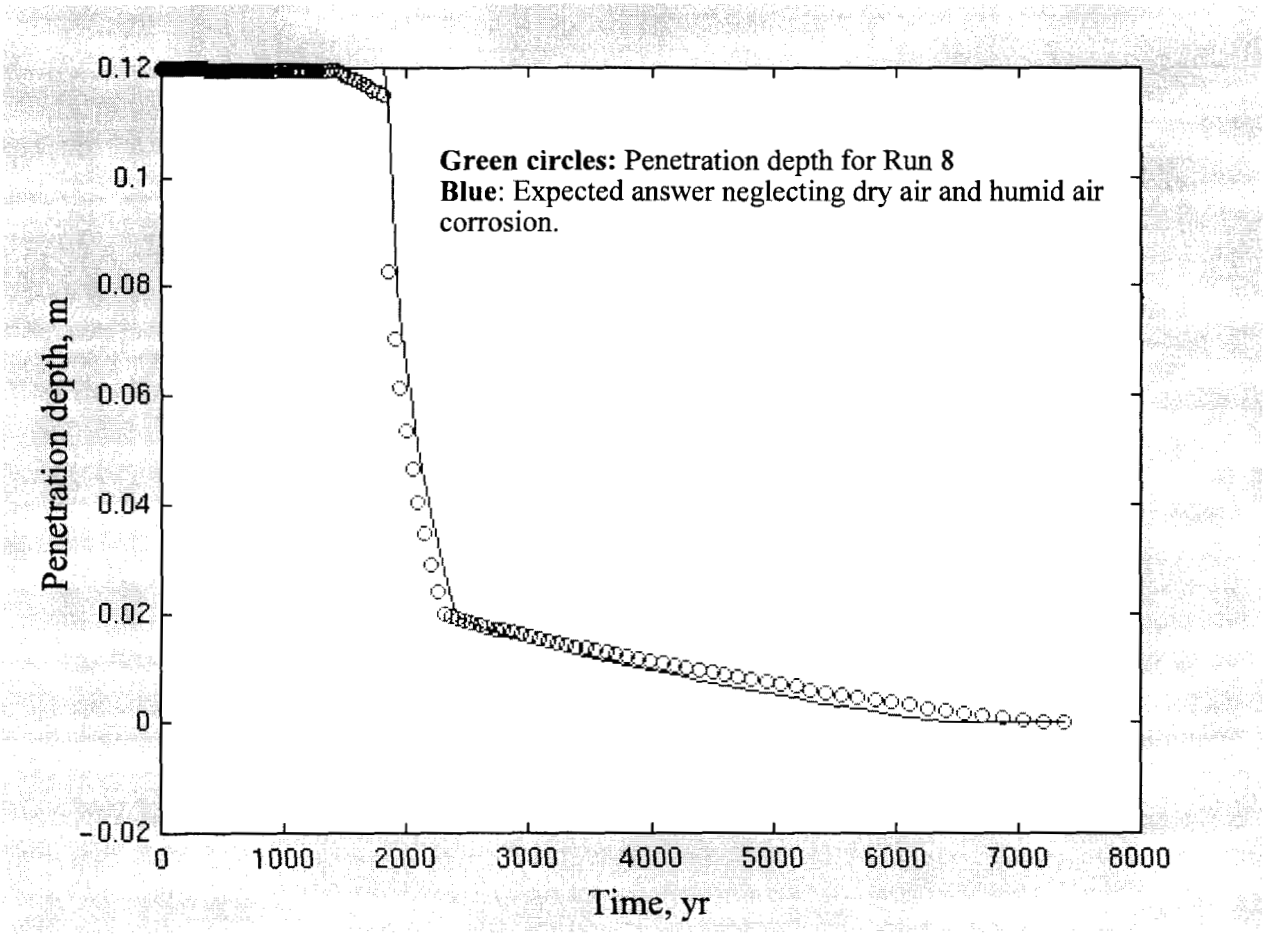



**Figure 6**: Penetration depth versus time for Run 8. Reasonable agreement was found between the expected and the computed output.

**Run 9**

Objective: same objective of Run 8.

```
>>cp ebsfail.inp.ref ebsfail.inp

4.4668E-03              ! rcoef: coef. for loc. corr
9.3525E-03              ! rcoef2: coef. for loc. cor
0.10000               ! rexpont2: exponent for loc
100.0               ! cfactor: factor for changi
2  0.7000E-04       !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp9
>>cp corrode.out corrode.out9
```

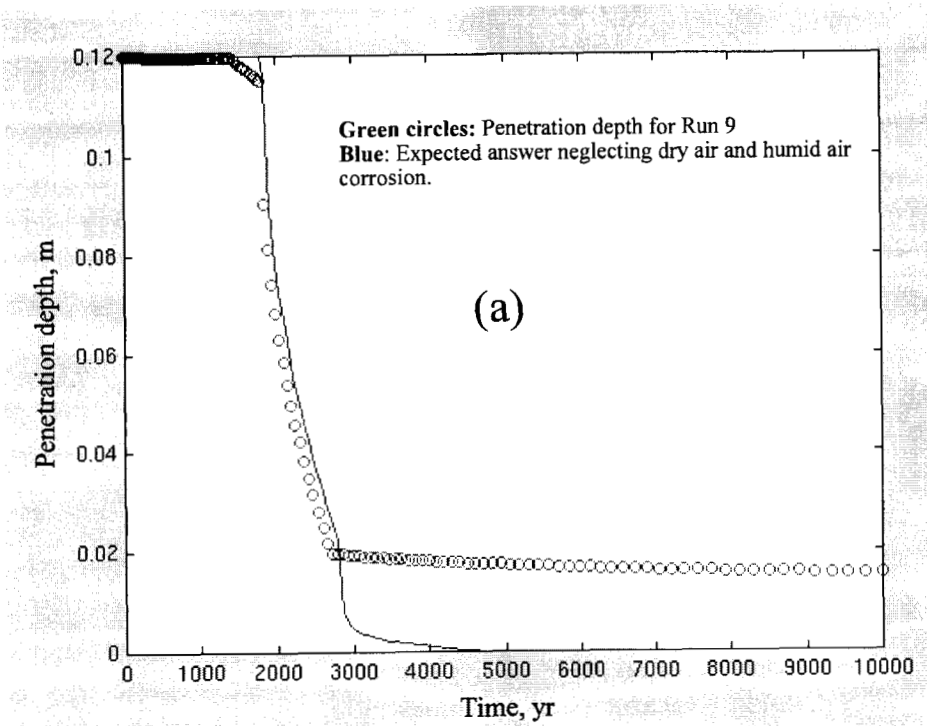
**ERROR FOUND!!!**

The expected output is quite different from the computed output!!! See Figure 7-a, which shows the expected (blue line) and the failt.f-computed (green circles) penetration depth versus time. Note that the divergence occurs in the localized corrosion of the inner layer. The reason of the divergence is that in failt.f the time in Equation [6] is measured with respect of the time at which wet conditions are established. For the outer layer this approach is correct, but it is not for the inner layer. For this layer, the time in Equation [6] must be measured with respect to the failure time of the outer layer.

The blue line Figure 7-b was computed with Matlab accounting for the above mistake. The agreement is excellent, which indicates that the divergence is entirely due to measuring the time with respect to a wrong origin of coordinates.

The failt.f module was modified to correct the mistake. Runs 10 and 11 are intended to verify the consistency of the change.

Type run9a (or run9b) at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 7. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.



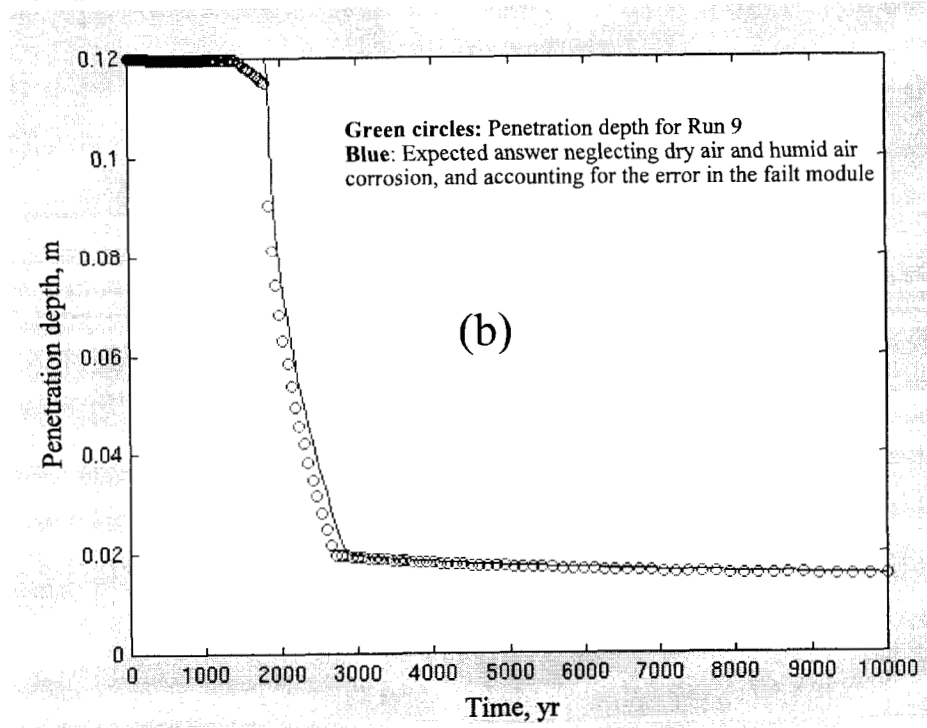




**Figure 7**: (a) Penetration depth versus time. Note that the divergence occurs in the localized corrosion of the inner layer time region. The reason of the divergence is that in failt.f the time in Equation [6] is measured with respect of the time at which wet conditions are established. For the outer layer this approach is correct, but it is not for the inner layer. For this layer, the time in Equation [6] must be measured with respect to the failure time of the outer layer.

(b) The blue line in was computed with Matlab accounting for the mistake explained in (a). The agreement is excellent, which indicates that the divergence is entirely due to measuring the time with respect to a wrong origin of coordinates.

**Run 10**

The failt.f module has been modified to solve the mistake presented in Figure 7.
Objective: same objective of Run8, and Run9

```
>>cp ebsfail.inp.ref ebsfail.inp

4.4668E-03              ! rcoef: coef. for loc. corr
9.3525E-03              ! rcoef2: coef. for loc. cor
0.10000               ! rexpont2: exponent for loc
100.0               ! cfactor: factor for changi
2   0.7000E-04       !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp10
>>cp corrode.out corrode.out10
```

Figure 8 displays the penetration depth versus time. The differences are entirely due to the non consideration of humid air corrosion in the Matlab computations.

Type run10 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 8. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

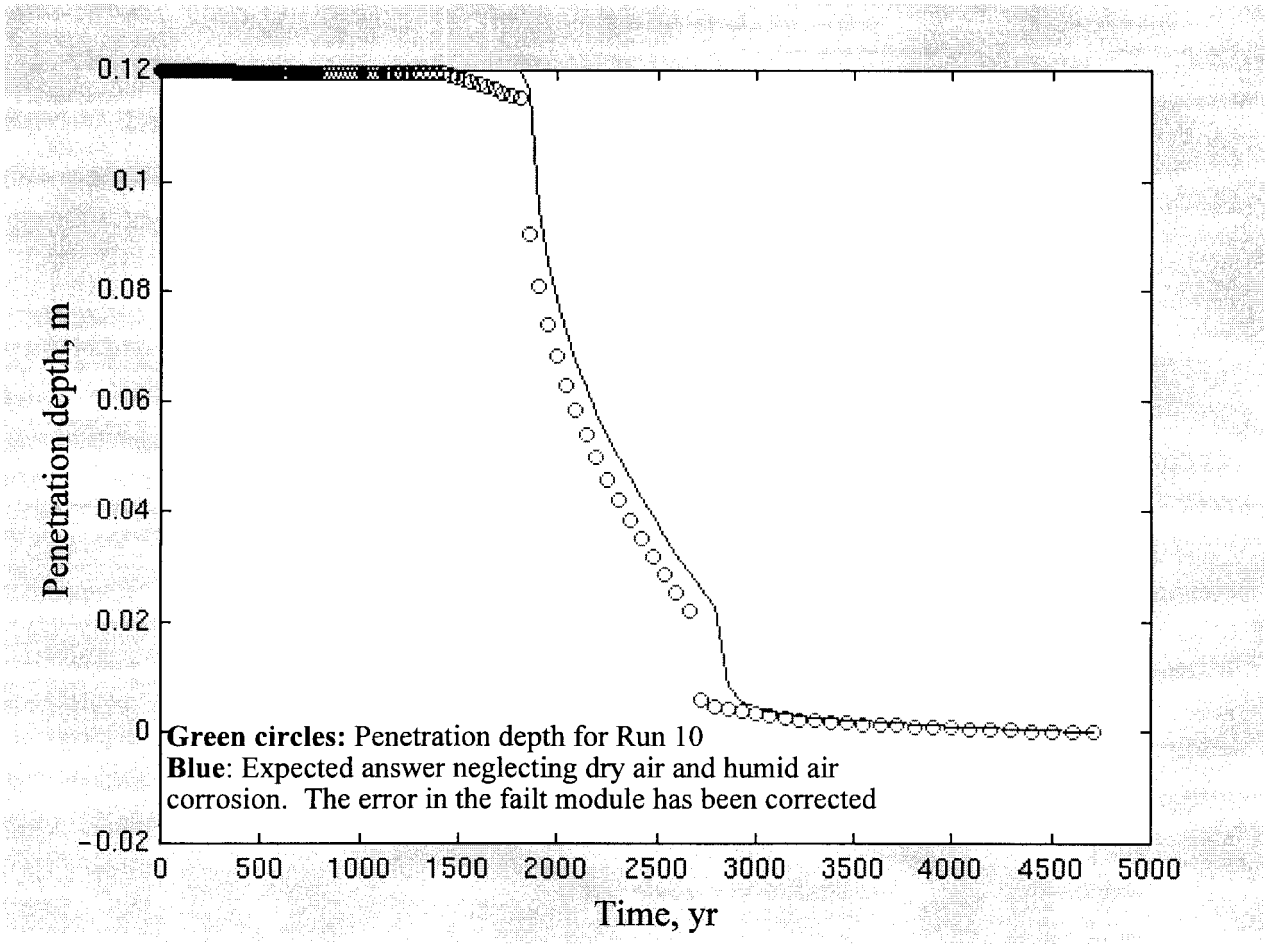



**Figure 8**: Penetration depth versus time for Run 10. The correction to the failt.f module provides consistent results.

**Run11**

More computations to verify that the correction to the failt module is satisfactory

```
>>cp ebsfail.inp.ref ebsfail.inp

1.0456e-3              ! rcoef: coef. for loc. corr
0.6              ! rexpont: exponet for loc.
7.3628E-05              ! rcoef2: coef. for loc. cor
0.7              ! rexpont2: exponent for loc
100.0              ! cfactor: factor for changi
2.0  0.7000E-04      !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp11
>>cp corrode.out corrode.out11
```

Figure 9 displays the penetration depth versus time. The differences are entirely due to the non consideration of humid air corrosion in the Matlab computations.

Type run11 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 9. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

**Partial conclusion**

An error in the implementation of the formulas in the failt module was discovered. The error was corrected. Figures 8 and 9 display penetration depths versus time, obtained with the corrected module, and they are quite consistent with the expected penetration depths, with deviations due to the disregard of humid air corrosion in the Matlab computations.

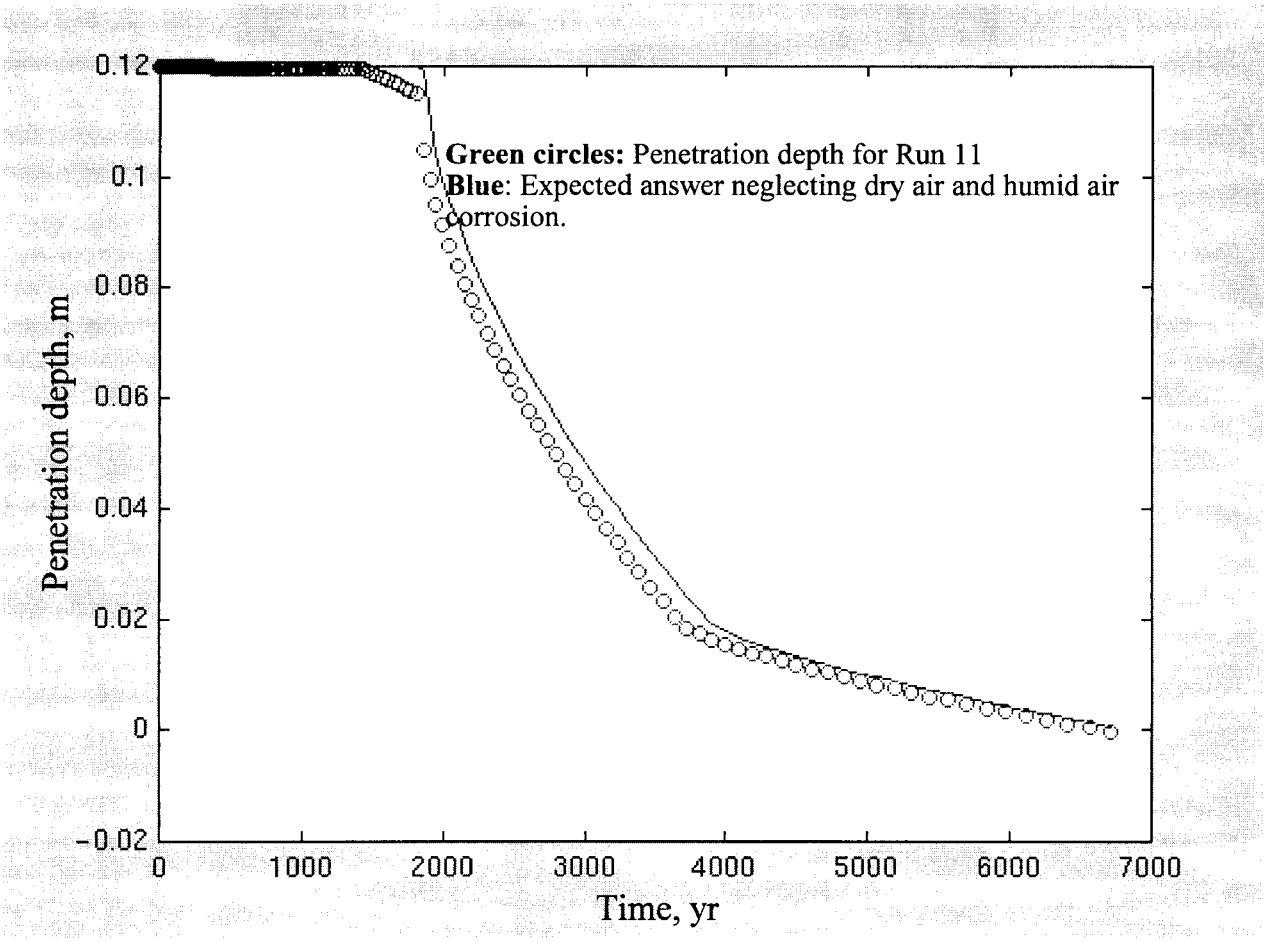



**Figure 9**: Penetration depth versus time for Run 11. The correction to the failt.f module provides consistent results.

Two other parameters that are now defined by the user are the density and the equivalent molecular weight for the inner and outer overpack. Those are used to transform current densities into corrosion rates. The following runs test that these new user-defined constants are well treated in the failt.f module.

We have already verified that it is possible to reproduce old results (see ~/tpa4/failt1 and ~/tpa/failt2, discussed above too). Thus, we have good indication that the changes are performing as desired. The next runs provide further indication that this is indeed the case.

The density and the equivalent weight are parameters only used in the general corrosion mode.

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**Run 12**

>>cp ebsfail.inp.ref ebsfail.inp

0.393E+04 0.407E+04 0.5585E-01 0.510844E-01 !dense1 dense2 wtmol1 wtmol2

Densities and molecular weights are multiplied by 2. According to Equation [5], this change does not affect the corrosion rate (same factor in the numerator and denominator of Equation [5]). Therefore, the contents in corrode.out must be identical to those of the reference run.

>>failt.e
>>cp ebsfail.inp ebsfail.inp12
>>cp corrode.out corrode.out12

The command

>> diff corrode.out12 corrode.out.ref

does not reveal differences. This is perfectly consistent with our expectations.

Note that only the inner layer corrodes by general corrosion. We need to verify that the conversion factor (to transform a current density into a corrosion rate) for the outer layer is working well too. Runs 13 and 14 take care of that.

**RUNS 13 and 14**
**Run 13**

```
>>cp ebsfail.inp.ref ebsfail.inp

0.1000E+01              ! clcrit1: crit. chloride co
```

The critical chloride concentration for the outer layer is set so high, that localized corrosion is never produced.

```
>>failt.e
>>cp ebsfail.inp ebsfail.inp13
>>cp corrode.out corrode.out13
```

**Run 14**

```
>>cp ebsfail.inp.ref ebsfail.inp

0.1000E+01              ! clcrit1: crit. chloride co
```

Same critical chloride concentration as that for Run 13.

```
2.358E+04 0.814E+04 0.83775E-01 0.255422E-01 !dense1 dense2 wtmol1 wtmol2
```

The density and molecular weight for the outer layer are multiplied by 3:

```
>>cp ebsfail.inp ebsfail.inp14
>>cp corrode.out corrode.out14
```

The only corrosion mode for the outer layer in Runs 13 and 14 is general corrosion. Both files, corrode.out13 and corrode.out14, must be identical. Indeed, we found that the shell command

```
>>diff corrode.out13 corrode.out14
```

does not reveal any difference in the files.

We conclude that the conversion factor to transform current densities into corrosion rates is working perfectly.

## OVERALL CONCLUSION

The changes to the failt.f module to account for the EDA II are performing as expected.

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I realized that in case the outer layer fails under dry air or humid air conditions, the equation describing localized corrosion for the inner layer will have wrong time coordinates. In that formula time must be measured with respect to the initial formation of the film of water, as opposed to the failure time of the outer layer. Although this is a remote possibility (that the outer layer will fail under dry or humid air conditions) the failt module has been modified to make it consistent with this possibility.

The failt.f module was modified to account for the above possibility. The modification defines the origin of time coordinates for Equation [6] applied to the inner layer as

$$t_o = \max(t_W, t_{OL}) \qquad [8]$$

$t_o$ origin of coordinates
$t_W$ time for the establishment of wet conditions
$t_{OL}$ failure time of the outer layer

Thus, the time in Equation [6] is measured with respect to $t_W$ in the case of the outer layer degradation, and with respect to $t_o$ in case of the inner layer degradation.

Further tests are needed to verify the consistency in the above change to the failt.f module.

**Run 15**

```
>> cp ebsfail.inp.ref ebsfail.inp

Changes to ebsfail.inp
0.5   0.7869E+00       ! humdc1, humdc2: crit. rel.
0.7000E-04                ! cratehac:humd.air corr.rt.
1.0456e-3               ! rcoef: coef. for loc. corr
0.6               ! rexpont: exponet for loc.
7.3628E-05                ! rcoef2: coef. for loc. cor
0.7               ! rexpont2: exponent for loc
100.0               ! cfactor: factor for changi
2.0   0.7000E-04      !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp15
```

```
>>cp corrode.out corrode.out15
```

In this case the time for the localized corrosion formula, Equation [6], for the inner layer is measured with respect to the failure time of the outer layer. Figure 10 readily shows this. The agreement between the expected penetration depth and the computed penetration depth is excellent.

In the Run 16, we present a situation where the time is measured with respect to the wetting time, $t_W$.

Type run15 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 10. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

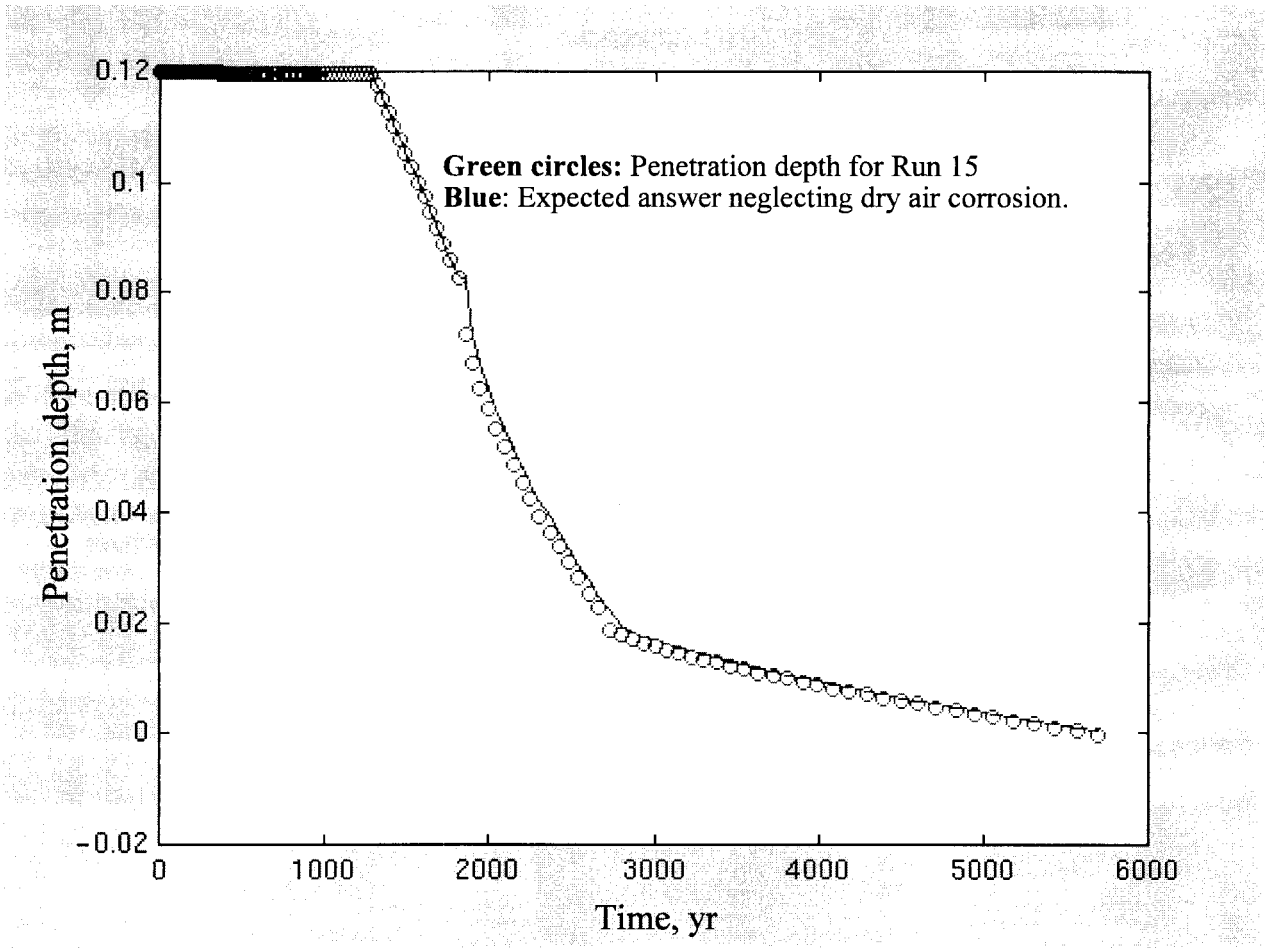


**Figure 10**: Penetration depth versus time. The agreement between the expected answer and the computed answer is excellent. The objective of this figure is to check that the formula for localized corrosion of the inner layer measures the time with respect to an adequate initial time. In this case the initial time is the failure time for the outer layer.

**Run 16**

```
>>cp ebsfail.inp.ref ebsfail.inp

0.4   0.7869E+00       ! humdc1, humdc2: crit. rel.
1.4711e-04               ! cratehac:humd.air corr.rt.
1.0456e-3               ! rcoef: coef. for loc. corr
0.6              ! rexpont: exponet for loc.
7.3628E-05               ! rcoef2: coef. for loc. cor
0.7              ! rexpont2: exponent for loc
100.0              ! cfactor: factor for changi
2.0   0.7000E-04       !deltaEo and lamb: Radiolysi

>>failt.e
>>cp ebsfail.inp ebsfail.inp16
>>cp corrode.out corrode.out16
```

In this case the time for the localized corrosion formula for the inner layer is measured with respect to the wetting time, $t_W$. Figure 11 readily shows this. The agreement between the expected penetration depth and the computed penetration depth is excellent.

Type run16 at a Matlab prompt window (pointing at the ~/tpa4/testfailt/ directory) to display the plots in Figure 11. See ~/tpa4/testfailt/handy.m for details in the Matlab computation for the generation of the plots.

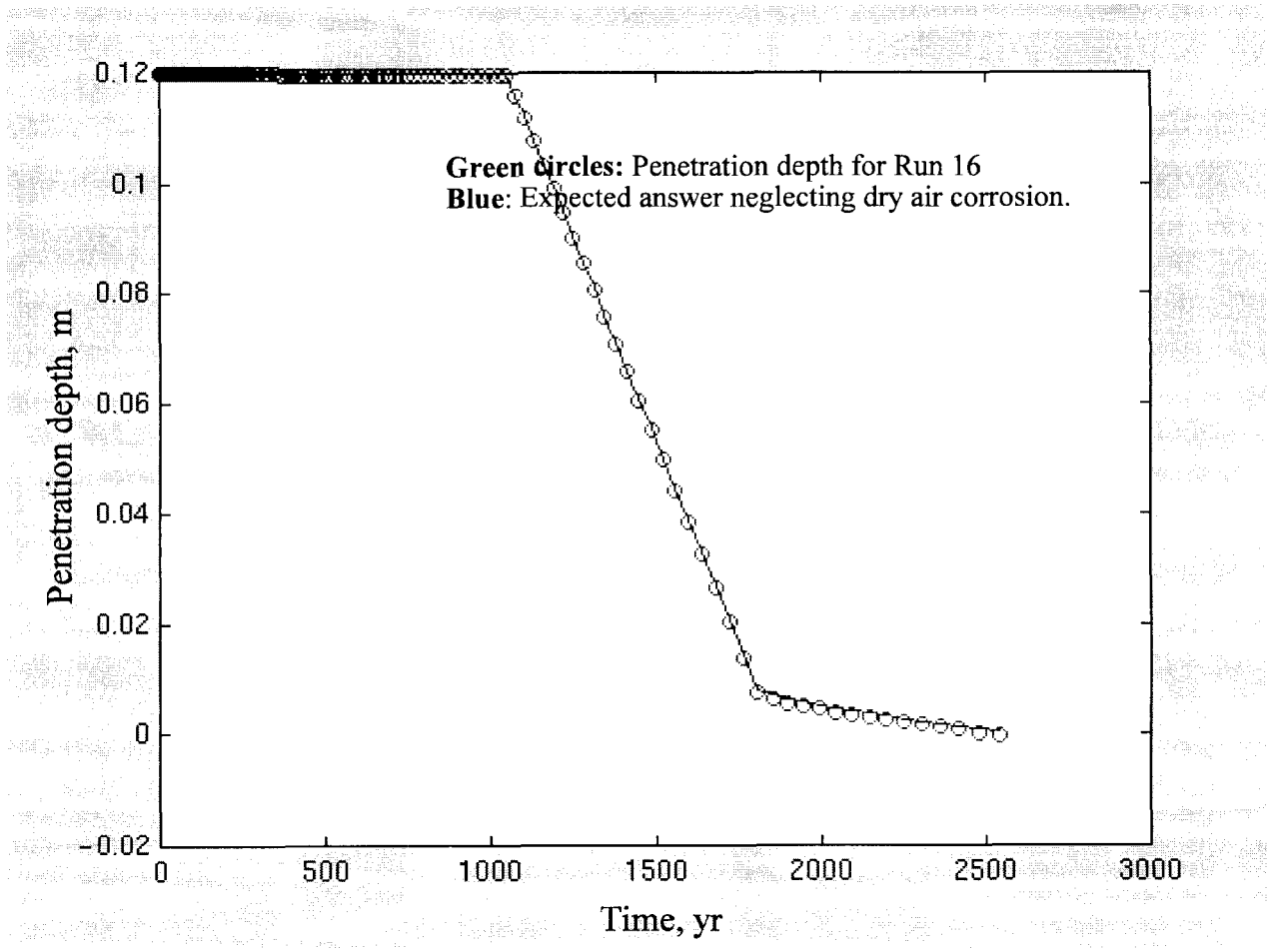


**Figure 11**: Penetration depth versus time. The agreement between the expected answer and the computed answer is excellent. The objective of this figure is to check that the formula for localized corrosion of the inner layer measures the time with respect to an adequate initial time. In this case the initial time is the wetting time (the time at which wet conditions are established).

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**CONCLUSIONS 2**

The time in the formula for localized corrosion is measured with respect to the failure time of the outer layer, or with respect to the wetting time, whichever happens at the latest time.

Testing of the failt module is now complete.

# OVERALL CONCLUSION

Changes to the failt.f module concerning the EDA II, the drip shield, and radiolysis have been completes, and the changes have been tested. The testing phase has revealed some problems that have been corrected. In the author's opinion the failt.f module is performing as expected.

# Testing of ebsfail.f

The module ebsfail.f is a module that reads data from the tpa.inp file assembles the input file ebsfail.inp to be used by failt.e (the executable of the failt.f module). The ebsfail.f module has been modified to read the following new parameters from the tpa.inp file:

| *tpa.inp name* | *tpanames.dbs name* |
|---|---|
| CoefForLocCorrOfInnerOverpack | IO-CofLC |
| ExponentForLocCorrOfInnerOverpack | IO-ExpLC |
| ChlorideMultFactorIntactDripShield | ChloriDS |
| DripShieldFailureTime[yr] | DSFailTi |
| DensityOuterOverpack[kg/m^3] | OO-Densy |
| DensityInnerOverpack[kg/m^3] | IO-Densy |
| EquivalentWeightOuterOverpack[kg/mol] | OO-EqWei |
| EquivalentWeightInnerOverpack[kg/mol] | IO-EqWei |
| DeltaPotentialDueToRadiolysis[V] | DelPRadi |
| DecayingConstantRadiolysis[1/yr] | DecCRadi |

Besides, the following parameter has been deleted

| | |
|---|---|
| LocalizedCorrRateOfInnerOverpack[m/yr] | crate2 |

since this parameter can be made equivalent to CoefForLocCorrOfInnerOverpack. This variable has not yet been deleted from the tpanames.dbs file. All of the parameters have been already defined in prior sections.

The modified files are located at ~/tpa4/ebsfail/. These files have been copied to the appropriate subdirectories in ~/tpa4/tpa4/, and compiled there with the available *Makefile* files prepared by R. Janetzke. All the other files in ~/tpa4/tpa4/ are identical to those located at ~/tpa4/source/ (i.e., those files provided by R. Janetzke).

## First test

The first test with the whole TPA code was to validate that old basecase results with the TPA code Version 3.3 are reproduced. The directory ~/tpa4/bc33/ contains a run or TPA 3.3, with the same input file as ~/tpa4/source/tpa.inp, plus the changes next presented:

tpa.inp file details

```
iconstant
StopAtSubarea
2

iconstant
NumberOfRealizations
3

iconstant
OutputMode(0=None,1=All,2=UserDefined)
1
**
iconstant
UserDefinedLowerRealizationAppended
1
**
iconstant
UserDefinedUpperRealizationAppended
3
```

The TPA_TEST and TPA_DATA paths were defined with the following commands:

```
>>setenv TPA_TEST /home/opensado/tpa4/source
>>setenv TPA_DATA /home/opensado/tpa4/source
```

The TPA code was run and the results are stored in the directory ~/tpa4/bc33.

Data in the directory ~/tpa4/test1/ contain a simulation of the data in ~/tpa4/bc33/ with the TPA code compiled in the directory ~/tpa4/tpa4/.

The tpa.inp input file is the same as ~/tpa4/ebsfail/tpa.inp, with the following changes:

```
iconstant
StopAtSubarea
2

iconstant
NumberOfRealizations
3
```

```
iconstant
OutputMode(0=None,1=All,2=UserDefined)
1
**
iconstant
UserDefinedLowerRealizationAppended
1
**
iconstant
UserDefinedUpperRealizationAppended
3

**OPR
constant
CoefForLocCorrOfInnerOverpack
2.5e-4
**
constant
ExponentForLocCorrOfInnerOverpack
1.0

**No drip shield protection
constant
DripShieldFailureTime[yr]
0.0

**No radiolysis present
constant
DeltaPotentialDueToRadiolysis[V]
0.0
```

The following shell commands were used to define the TPA paths:

```
>>setenv TPA_TEST /home/opensado/tpa4/tpa4
>>setenv TPA_DATA /home/opensado/tpa4/tpa4
```

The TPA code was run in the directory ~/tpa4/test1.

I found negligible differences in the corrode.out, failt.out, and failt.cum in the ~/tpa4/test1 and

~/tpa4/bc33. The reason of the differences is due to the parameter

constant
EquivalentWeightInnerOverpack[kg/mol]
0.02554222222

which is passed on to ebsfail.inp with just six digits after the decimal point. This small difference causes the difference between these data in ~/tpa4/test1/ and ~/tpa4/bc33/. Nonetheless, the differences are negligible.

Note that in ~/tpa4/failt1/ and ~/tpa4/failt2/, where the failt module is tested by itself and more relevant digits for the constants can be defined, the modified and the original code produce identical results. Thus, the above differences are indeed entirely due to the limited digits available for the constants in the ebsfail.inp file.

**Therefore, we conclude that the new version of the code, with the failt.f changes, is capable of reproducing old results.**

1/19/2000

## Second test

Another run of the TPA code in ~/tpa4/tpa4/ was performed to verify that the ebsfail.f module is reading well the data in the tpa.inp file, and passed on to the ebsfail.inp file.

The following shell commands were used to define the paths

>>setenv TPA_TEST /home/opensado/tpa4/tpa4
>>setenv TPA_DATA /home/opensado/tpa4/tpa4

The tpa.inp file in the first test, with some extra modifications, was utilized.

>> cp ../test1/tpa.inp .

The modifications to the tpa.inp file are next described:

iconstant
StopAtSubarea
2

```
iconstant
NumberOfRealizations
3

iconstant
OutputMode(0=None,1=All,2=UserDefined)
1
**
iconstant
UserDefinedLowerRealizationAppended
1
**
iconstant
UserDefinedUpperRealizationAppended
3

**OPR
uniform
DripShieldFailureTime[yr]
2.0e+3, 10.0e+3

constant
DeltaPotentialDueToRadiolysis[V]
0.5

constant
DecayingConstantRadiolysis[1/yr]
0.0001
```

After running the modified TPA code, the file cp.tpa was reviewed to verify that the new 9 constants were properly read.

Relevant contents of the cp.tpa file:

```
2.500000000000000E-04 = CoefForLocCorrOfInnerOverpack
1.000000000000000E+00 = ExponentForLocCorrOfInnerOverpack
1.000000000000000E+00 = ChlorideMultFactorIntactDripShield
7.860000000000000E+03 = DensityOuterOverpack[kg/m^3]
8.140000000000000E+03 = DensityInnerOverpack[kg/m^3]
2.792500000000000E-02 = EquivalentWeightOuterOverpack[kg/mol]
```

2.554222200000000E-02 = EquivalentWeightInnerOverpack[kg/mol]
5.000000000000000E-01 = DeltaPotentialDueToRadiolysis[V]
1.000000000000000E-04 = DecayingConstantRadiolysis[1/yr]

The above numbers are entirely consistent with the data in the tpa.inp file. The 10th variable is the DripShieldFailureTime[yr]. This was assigned the 15th position in the file samplpar.abb (variable DSFailTi).

The file samplpar.res assigns the following values for the three realizations:

0.3866122E+04
0.7647757E+04
0.5670638E+04

which clearly lie within the defined limits (2000 and 10000 yr). The contents in the ebsfail.inp are perfectly consistent with the above constants. Note that ebsfail.inp contains information of only the last realization, and thus the failure time taken for the drip shield is 0.5670638E+04.

We reproduce here the ebsfail.inp file.

---

```
\example input file for ebsfail
|
\simulation time
  10000.00                  ! tend: simulation time leng
\                                 ! when iflag=1 (defined later)
\
 5.6820  1.8020              ! wplen,wpdia: wp length and
 0.1000E+00  0.2000E-01        ! cthick1,cthick2: wp layers
|
\choose source of temperature data
2, 1                      ! iflag(1:emp.equation,2:tab
1                                 ! nset (temp.-rel hum. relationship to use
49.9999999                        ! timintv (used when iflag=2)
|
\other temperature parameters
0.                                ! age of fuel (not used in this version)
|
\Dry oxidation of wp outer overpack
 0.1375E+02                ! grainr: metal grain radius
25                        ! nseries (terms in the infi
```

```
 0.7000E-03                ! gbthick [micrometer]
 0.1000E-04                ! constant1: used in the dry
|
\evaporation-condensation
 0.5500E+00  0.8217E+00      ! humdc1, humdc2: crit. rel.
 0.2898E-02                ! filmthk: thickness of wate
 0.9990E+03                ! ctemp: boiling point of wa
|
\Corrosion Parameters(Ep: pitting potential [mVshe]; Erp: re
-584.8                     ! xipto: outer overpack Ep i
3.92                      ! pttemo: temp. coef. of out
-24.5                     ! slpto: outer overpack Ep s
-1.1                      ! slpttemo: temp. coef. of o
-0.6203E+03                ! xirpo: outer overpack Erp
 0.4700E+00                ! rptemo: temp. coef. of out
-0.9520E+02                ! slrpo: outer overpack Erp
 0.8800E+00                ! slrptemo: temp. coef. of o
200.                      ! xipti: inner overpack Ep i
0.                        ! pttemi: temp. coef. of inn
-240.                     ! slpti: inner overpack Ep s
0.                        ! slpttemi: temp. coef. of i
 0.1066E+04                ! xirpi: inner overpack Erp
 0.0000E+00                ! rptemi: temp. coef. of inn
 0.0000E+00                ! slrpi: inner overpack Erp
 0.0000E+00                ! slrptemi: temp. coef. of i
 0.7500E+00  0.5000E+00      ! betaox1, betahy1: beta kin
\                            for oxygen and water for WP outer overpack
 0.7500E+00  0.5000E+00      ! betaox2, betahy2: beta kin
\                            oxygen and water for WP inner overpack
 0.3800E+13  0.1600E+00      ! rkox1 [c*m/y/mol], rkhy1 [
 0.3730E+05  0.2500E+05      ! gox1 [J/mol], ghy1 [J/mol]
 0.3000E+11  0.3200E+01      ! rkox2 [c*m/y/m], rkhy2 [c/
 0.4000E+05  0.2500E+05      ! gox2 [J/mol], ghy2 [J/mol]
 0.3150E+06  0.0  0.0       ! aa(1,1) [C/m2/yr], aa(1,2)
 0.5879E+05  0.0  0.0       ! aa(2,1) [C/m2/yr], aa(2,2)
-0.4600E+00                ! eexpt: measured galvanic c
 0.5891E-02                ! rcoef: coef. for loc. corr
 0.4500E+00                ! rexpont: exponet for loc.
OPR 1/13/2000
 0.2500E-03                ! rcoef2: coef. for loc. cor
```

```
 0.1000E+01                ! rexpont2: exponent for loc
ENDOPR
 0.1160E-04                ! cratehac:humd.air corr.rt.
 0.0000E+00                ! xcouple, efficiency of gal
 0.0000E+00                ! xread: factor for defining
3.e-1                      ! clconc: chloride conc. [mo
 0.3000E-03                ! clcrit1: crit. chloride co
 0.1000E+01                ! clcrit2: crit. chloride co
 0.1345E+02                ! cfactor: factor for changi
 0.2100E+00  0.9000E+01        ! xgas: oxygen part.pr.[atm]
 0.0000E+00  0.1000E+01  0.1000E+01 althk: scale thick;taus:
OPR 1/13/2000
 0.1000E+01                ! cfactor2: factor for chang
 0.5671E+04                ! failtimds: failure time of
 0.5000E+00   0.1000E-03       !deltaEo and lamb: Radiolysi
0.786000E+04 0.814000E+04 0.279250E-01 0.255422E-01  !dense1
ENDOPR
|
\Mechanical failure data
 0.2050E+03  0.1400E+01        ! yieldstr: yield strength [
 0.2500E+03                ! dkic: fracture toughness [
|
\Runge-kutta control parameters
1.e-3, 1.e0                     ! dtini, dtmax
1.e-2, 1.e-30                   ! errrel (same as eps), errabs (same as tin
|
\end
```

**It is evident that the ebsfail.f module is properly reading the data in tpa.inp and passing it to ebsfail.inp. We conclude that the modifications to the ebsfail.f module are performing as expected.**

## Title: Test to changes to the releaset module

### TPA Test Plan

Osvaldo Pensado 3/2/00

**Test name**: Test of changes described in PA-SCR-296 to the releaset module.
**Anticipated start date**: 3/2/00
**Anticipated completion date**: 3/6/00
**Amount of your time available to perform this test**: 20 hr
**Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50):** 80/20
**Output files to be checked**: trelease.out, ebsnef.dat, relcum.out, relfrac.out, maxrel.dat, inv1000.out
**Input files to be checked for proper data transfer to the program**: ebsrel.inp

**Disposition of documentation (storage medium, physical location, and access method)**:
Electronic files are located in vulcan, at
/home/opensado/tpa4/testreleaset/
/home/opensado/tpa4/tparel
Multiple *readme* files are included therein for the easy reading of the computations.

**Functional Test Descriptions**:

**Process-level tests**:

The radionuclide release is only function of the number of waste packages failed, the wet fraction, and the failure time. It is not function of the failure type. It is also function of the water contact mode. With that in mind, several runs having the same number of waste packages failed, the same wet fraction, and the same failure time, must have the same output files.

**System-level tests**:

The TPA code will be run to determine that the flags defining the water contact mode for each failure type are appropriately mapped into the file ebsrel.inp. The output files trelease.out, ebsnef.dat, relcum.out, relfrac.out, maxrel.dat, and inv1000.out produced by a TPA run must coincide with runs of the isolated module releaset.f

**Reasonableness Test Description**:

Runs of the releaset.f module for TPA 3.3 and TPA 4.0beta having the same numbers in the ebsrel.inp files (with the exception of the new flags), must produce identical output files, if all of the water contact flags are adequately selected.

**Objective**: Test changes to the releaset module by Rob Rice (PA-SCR-296). The changes include the addition of flags to define the water contact mode (bathtub or flowthrough) as function of the failure type. Testing includes process and system level testing. Testing is performed at the process level (testing of the releaset.e module) and at the system level (testing of the whole tpa code).

The computations are documented at /home/opensado/tpa4/ in Vulcan. Multiple *readme* files are therein included to facilitate the reading of the computations.

**In the following discussion, all of the mentioned directories are located in Vulcan, in /home/opensado/tpa4/**

Needed files for the releaset module to run: ebsrel.inp, ebstrh.dat, ebsflo.dat, ebspac.nuc. The files ebstrh.dat, ebsflo.dat, and ebspac.nuc were obtained from /tpa40betaRun/. Output files by releaset.e: trelease.out, ebsnef.dat, relcum.out, relfrac.out, maxrel.dat, inv1000.out. The most important output files is ebsnef.dat. According to Rob Rice, the other files are not used by the tpa system.

## Relevant files at /testreleaset/

tpa.inp --> reference input file. A tpa run of the beta version was completed to generate necessary input files. The tpa run data are located at ../tpa40betaRun/

ren --> shell instructions to run releaset.e and rename the output files from releaset.e. A given prefix is added to the output files. The files ebsfail.inp and ebstrh.dat are returned to the original values in ebsfail.inp.ref and ebstrh.dat.ref

dif --> shell instructions to make an easy run of the UNIX diff instruction

ebsrel.inp.ref –> reference file used in the computations.

3/2/00

## Testing Assumptions

The number of WP failed due to corrosion and the failure time are not indicated in the file ebsrel.inp. The reason is that once a WP is failed, it is assumed that all of the WPs for that subarea are failed. The way releaset.e determines whether or not corrosion failure has been produced is by looking at the third number, counting from bottom to top, of the file ebstrh.dat. If this number equals the simulation time, then no corrosion failure is produced. All of the other WPs (i.e., those that have not failed due to juvenile failures, faulting, igneous activity, or seismicity) fail due to corrosion otherwise. The fourth row in ebsrel.inp contains the total number of WPs for the subarea. The total

number of WP failed due to corrosion is computed as this number minus the number of WPs failed due to any other reason.

In the folder /releasetRef/ there are a couple of runs of the releaset.e module for TPA 3.3. One of the runs is with the bathtub model, and another with the flowthrough model. The parameters in the input files were adjusted so that most the numbers are identical to the input files herein considered. If the changes to the releaset.e module are adequate, then old results can be reproduced with the new module.

**Premise 1**

If the bathtub and flowthrough models are appropriately implemented in the releaset module for TPA 3.3, then these two models will be well implemented in the modified releaset module if the results coincide with those obtained with the old (for TPA 3.3) releaset module when the water contact mode is selected to be exclusively bathtub or flowthrough (i.e., no mixture of contact models).

**Premise 2**

The radionuclide release is only function of the number of waste packages failed, the wet fraction, and the failure time. It is not function of the failure type. It is also function of the water contact mode. With that in mind, several runs having the same number of waste packages failed, the same wet fraction, and the same failure time, must have the same output files. That can easily be identified with the UNIX shell command diff.

**Testing plan**

The test plan is aimed at the validation of Premises 1 and 2. In order to validate premise 1, several runs of the releaset.e module for tpa 3.3 were run. Runs for the new releaset.e module should produce equivalent results, provided the input file ebsrel.inp is adequately selected.

To test premise 2, several runs having exactly the same number of failed WP, the same fraction of wetted fuel, and the same failure time should produce identical output files.

**Test A1**

```
>>cp ebsrel.inp.ref ebsrel.inp
>>ren A1    # releaset.e is run, and the relevant input and output files are renamed with a
        prefix A1

>>diff A1ebsnef.dat ../releasetRef/BTebsnef.dat
```

The above instruction does not reveal any difference, meaning that the bath tub

computations are consistent with the computations of the releaset.e module for TPA 3.3. This is consistent with Premise 1.

**Test A2**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.00000E+00 8.0      ! sftimef,isconf:  faulting fail time [yr] & WPs affected
9.32450E-01  0       ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
```

>>ren A2  # releaset.e is run, and the relevant input and output files are renamed with a prefix A2.
>>diff A1ebsnef.dat A2ebsnef.dat
>>diff A1relfrac.out A2relfrac.out

All of the other output files, trelease.out, relcum.out, maxrel.out, inv1000.out are identical too. Since Run A1 and A2 have the same # of failed WP, the same release mode (bathtub), and the same wet fraction, the output files, ebsnef.dat and relfrac.out, identical for both runs, as expected. Result consistent with Premise 2.

**Test A3**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.00000E+00 8.0      ! sftimev,isconv:  volcano fail time [yr] & WPs affected
9.32450E-01  0       ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
```

>>ren A3
>>diff A1ebsnef.dat A3ebsnef.dat
>>diff A1relfrac.out A3relfrac.out

Since Run A1 and A3 have the same # of failed WP, the same release mode (bathtub), and the same wet fraction, the output files, ebsnef.dat and relfrac.out, identical for both runs, as expected. All of the other output files, trelease.out, relcum.out, maxrel.out, inv1000.out are identical too.

**Test A4**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.0 8.0       ! seismt1,seismp1: first  seismic failure time [yr] & WP affected
9.32450E-01  0      ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
```

>>ren A4
>>diff A1ebsnef.dat A4ebsnef.dat
>>diff A1relfrac.out A4relfrac.out

All of the other output files, trelease.out, relcum.out, maxrel.out, inv1000.out are identical too. No difference revealed, as expected.

**Test A5**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

0.00000E+00 0.0 ! defect,idefect: initially defective time [yr] & WPs affected
0.0 8.0 ! seismt2,seismp2: second seismic failure time [yr] & WP affected
9.32450E-01 0 ! wetfrac(5),iwatcont(5): seim2 fail ht fract of wet SF and water contact

>>ren A5
>>diff A1ebsnef.dat A5ebsnef.dat
>>diff A1relfrac.out A5relfrac.out

Identical output. All of the other output files, trelease.out, relcum.out, maxrel.out, inv1000.out are identical too.

**Test A6**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

0.00000E+00 0.0 ! defect,idefect: initially defective time [yr] & WPs affected
0.0 8.0 ! seismt3,seismp3: third seismic failure time [yr] & WP affected
9.32450E-01 0 ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact

>>renA6
>>diff A1ebsnef.dat A6ebsnef.dat
>>diff A1relfrac.out A6relfrac.out

No difference revealed, as expected. All of the other output files, trelease.out, relcum.out, maxrel.out, inv1000.out are identical too.

**Test A7**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

0.00000E+00 0.0 ! defect,idefect: initially defective time [yr] & WPs affected
0.0 8.0 ! seismt4,seismp4: fourth seismic failure time [yr] & WP affected
9.32450E-01 0 ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact

>>diff A1ebsnef.dat A7ebsnef.dat
>>diff A1relfrac.out A7relfrac.out

No difference revealed, as expected. All of the other output files, trelease.out, relcum.out, maxrel.out, inv1000.out are identical too.

**Test A8**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
8.0   1.08314E-01    ! xcon: # of WP; sawetfrac: wetted subarea
0.00000E+00 0.0       ! defect,idefect:  initially defective time [yr] & WPs affected
9.32450E-01  0       ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact
```

Changes to ebstrh.dat

0.0 instead of 10000.00, third row from bottom to top.
This change is used to define failure of the corrosion failed WP at t=0 yr

>>diff A1ebsnef.dat A8ebsnef.dat
>>diff A1relfrac.out A8relfrac.out

>>diff A1inv1000.out A8inv1000.out ---> revealed differences. This output file is not used by the tpa system.

**Premise 2 is violated when WP failed due to corrosion are considered.**

All of the other output files, trelease.out, relcum.out, maxrel.out are identical.

The fact that A1relfrac.out and A8relfrac.out are identical poses another inconsistency, taking into account that A1inv1000.out and A8inv1000.out are different. The data in relfract.out are computed on the basis of data in ebsnef.dat and inv1000.out, and it should be different for both realizations, but it is not.

This issue must be further investigated.

**PARTIAL CONCLUSION**: The file A8inv1000.out differs from the expected answer. Based on this observation, A8relfrac.out was expected to be different from A1relfrac.out, but it is not. This issue must be further investigated. Premise 2 is partially violated in Run A8.

**TEST OF THE FLOWTHROUGH MODEL FLAGS**

Test B1
Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
9.32450E-01  1      ! wetfrac(1),iwatcont(1): init def ht fract of wet SF and water contact
```

```
>>diff B1ebsnef.dat ../releasetRef/FTebsnef.dat
```

The above instruction does not reveal any difference, meaning that the flowthrough computations are consistent with the computations of the releaset.e module for TPA 3.3. This is consistent with Premise 1.

Furthermore

```
>>diff A1inv1000.out B1inv1000.out
```

does not reveal any difference. This result is surprising. In principle the amount of radionuclides in the groundwater are function of the contact mode, and this is not revealed above. Probably the reason is that in the bathtub model the time to achieve the maximum wetting fraction from the failure time is negligible compared to failure period (i.e., from the failure time to the maximum simulation time).

**Test B2**
Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.00000E+00 8.0      ! sftimef,isconf:  faulting fail time [yr] & WPs affected
9.32450E-01  1      ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
```

```
>>diff B1ebsnef.dat B2ebsnef.dat
>>diff B1relfrac.out B2relfrac.out
```

No difference revealed, as expected. Consistent with Premise 2.

**Test B3**
Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.00000E+00 8.0      ! sftimev,isconv:  volcano fail time [yr] & WPs affected
9.32450E-01  1      ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
```

```
>>diff B1ebsnef.dat B3ebsnef.dat
```

>>diff B1relfrac.out B3relfrac.out

No difference revealed, as expected. Consistent with Premise 2.
The results are also consistent with Premise 3.

**Test B4**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.0 8.0      ! seismt1,seismp1: first  seismic failure time [yr] & WP affected
9.32450E-01  1     ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
```

>>diff B1ebsnef.dat B4ebsnef.dat
>>diff B1relfrac.out B4relfrac.out

No difference revealed, as expected. Consistent with Premise 2.

**Test B5**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.0 8.0      ! seismt2,seismp2: second seismic failure time [yr] & WP affected
9.32450E-01  1     ! wetfrac(4),iwatcont(4): seim2 fail ht fract of wet SF and water contact
```

>>diff B1ebsnef.dat B5bsnef.dat
>>diff B1relfrac.out B5elfrac.out

No difference revealed, as expected. Consistent with Premise 2.
The results are also consistent with Premise 3.

**Test B6**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)

```
0.00000E+00 0.0      ! defect,idefect:  initially defective time [yr] & WPs affected
0.0 8.0      ! seismt3,seismp3: third  seismic failure time [yr] & WP affected
9.32450E-01  1     ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact
```

>>diff B1ebsnef.dat B6bsnef.dat
>>diff B1relfrac.out B6elfrac.out

No difference revealed, as expected. Consistent with Premise 2.

**Test B7**

Changes to ebsrel.inp (the base input file is ebsrel.inp.ref)
0.00000E+00 0.0 ! defect,idefect: initially defective time [yr] & WPs affected
0.0 8.0 ! seismt4,seismp4: fourth seismic failure time [yr] & WP affected
9.32450E-01 1 ! wetfrac(7),iwatcont(7): seim4 fail ht fract of wet SF and water contact

>>diff B1ebsnef.dat B7bsnef.dat
>>diff B1relfrac.out B7elfrac.out

No difference revealed, as expected. Consistent with Premise 2.

**Test B8**

8.0 1.08314E-01 ! xcon: # of WP; sawetfrac: wetted subarea
0.00000E+00 0.0 ! defect,idefect: initially defective time [yr] & WPs affected
9.32450E-01 1 ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact

Changes to ebstrh.dat
0.0 instead of 10000.00, third row from bottom to top.
This change is used to define failure of the corrosion failed WP at t=0 yr

>>diff B1ebsnef.dat B8ebsnef.dat

Does not reveal differences, as expected.

>>diff B1relfrac.out B8relfrac.out

**The above instruction reveals differences. There is something wrong.**

Furthermore,

>>diff B1inv1000.out B8inv1000.out --> **revealed differences**
>>diff B1maxrel.dat B8maxrel.dat --> **revealed differences**
>>diff B1relcum.out B8relcum.out ---> same
>>diff B1trelease.out B8trelease.out --> same

The file inv1000.out is used in the computation of the fractional release rate (relfrac.out). Thus, being B1inv1000.out different from B8inv1000.out, the output in relfrac.out must be different for runs B1 and B8.

The numbers on the third column (1000-yr inventory, Ci) of the file B8inv1000.out are lower than the numbers on B1inv1000.out by a factor of 174.25. Similarly, the data in B1maxrel.dat and B8maxrel.dat differ by the same factor of 174.25. Thus, the difference is due to the same issue.

**Premise 2 is violated. The expected output is not produced.**

In ../releasetRef/ (where the releaset module for TPA 3.3 is considered) I did another run of releaset.e with pure corrosion failure (8 WP failing in total at t = 0 yr). I labeled this case as FC in that directory.

diff ../releasetRef/FCebsnef.dat B8ebsnef.dat
diff ../releasetRef/FCrelfrac.out B8relfrac.out

Both instructions above did not reveal any difference in the data. Therefore, if there is a mistake in the implementation it is a mistake that was there for version 3.3 of the TPA code.

Note that

>>diff A8inv1000.out B8inv1000.out

does not reveal any difference. This is surprising due to the existence of a different water contact mode for the two runs. Note also that inv1000.out for Run B1 and run B8 are different, which is inconsistent (violates Premise 2).

**CONCLUSION:**

**Differences were found in intermediate output files. However, these files are not used by the TPA system. Further testing is needed to verify that the differences do not impact the output. The secondary output files should also be modified since the user has access to data there reported.**

**TEST C, multiple failure modes and water contact modes.**

**Test C1**
Changes to ebsrel.inp
1000 20 ! defect,idefect: initially defective time [yr] & WPs affected

```
1000 20      ! sftimev,isconv:  volcano fail time [yr] & WPs affected
2000 30      ! seismt2,seismp2: second seismic failure time [yr] & WP affected
2000 30      ! seismt4,seismp4: fourth seismic failure time [yr] & WP affected

0.8  0     ! wetfrac(1),iwatcont(1): init def ht fract of wet SF and water contact
0.8  0     ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
0.7  0     ! wetfrac(5),iwatcont(5): seim2 fail ht fract of wet SF and water contact
0.7  0     ! wetfrac(7),iwatcont(7): seim4 fail ht fract of wet SF and water contact

>>diff C1ebsnef.dat ../releasetRef/C1ebsnef.dat
>>diff C1relfrac.out ../releasetRef/relfrac.out
>>diff C1trelease.out ../releasetRef/trelease.out
>>diff C1relcum.out ../releasetRef/relcum.out
>>diff C1maxrel.dat ../releasetRef/maxrel.dat
>>diff C1inv1000.out ../releasetRef/inv1000.out
```

No difference was revealed by the above instructions, which means that the output files are consistent with computations carried out with the releaset.e for TPA 3.3. Result consistent with Premise 1.

**Test C2**

Changes to ebsrel.inp

```
1000 20      ! sftimef,isconf:  faulting fail time [yr] & WPs affected
1000 20      ! seismt1,seismp1: first  seismic failure time [yr] & WP affected
2000 30      ! seismt3,seismp3: third  seismic failure time [yr] & WP affected
2000 30      ! seismt4,seismp4: fourth seismic failure time [yr] & WP affected
0.8  0     ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
0.8  0     ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
0.7  0     ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact
0.7  0     ! wetfrac(7),iwatcont(7): seim4 fail ht fract of wet SF and water contact
```

No difference in the output files from C1 and C2 runs was obtained, as expected. Result consistent with Premise 2.

**Test C3**

Changes to ebsrel.inp

```
100   1.08314E-01    ! xcon: # of WP; sawetfrac: wetted subarea
1000 20      ! sftimef,isconf:  faulting fail time [yr] & WPs affected
1000 20      ! seismt1,seismp1: first  seismic failure time [yr] & WP affected
2000 30      ! seismt3,seismp3: third  seismic failure time [yr] & WP affected
```

0.8 0 ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
0.8 0 ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
0.7 0 ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact
0.7 0 ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact

Change to ebstrh.dat
Line 205: 2000.0000

>>ren C3
>>diff C1ebsnef.dat C3ebsnef.dat ---> no difference revealed
>>diff C1relfrac.out C3relfrac.out --> **DIFFERENCES**
>>diff C1trelease.out C3trelease.out --> no difference
>>diff C1relcum.out C3relcum.out ---> no difference
>>diff C1maxrel.dat C3maxrel.dat ---> **DIFFERENCES**
>>diff C1inv1000.out C3inv1000.out --> **DIFFERENCES**

The differences is the above files is due to the differences in inv1000.out. The reason for the difference is not yet well understood.

Osvaldo Pensado talked to Sitakanta Mohanty about this issue. The explanation offered is that during modification of the ebsrel module, little attention was paid to the generation of the secondary output files, if these were not used by the TPA system. If that is the case, I suggest adding a little note to the TPA manual, Appendix E, saying exactly that. Otherwise users may utilize data that are not well validated. The data that need this note are relfrac.out, maxrel.dat, inv1000.out, and probably trelease.out and relcum.out too.

Comparison with data generated by releaset.e of TPA 3.3:

>>diff ../releasetRef/C3ebsnef.dat C3ebsnef.dat
>>diff ../releasetRef/C3relfrac.out C3relfrac.out
>>diff ../releasetRef/C3trelease.out C3trelease.out
>>diff ../releasetRef/C3relcum.out C3relcum.out
>>diff ../releasetRef/C3maxrel.dat C3maxrel.dat
>>diff ../releasetRef/C3inv1000.out C3inv1000.out

All of the above instructions revealed no difference. The output files for releaset.e for TPA 3.3 and 4.0 are identical. Thus, the problem is a carry-over from prior implementations of the code.

**CONCLUSION**

The data in ebsnef.dat are adequate. The flags implemented by R. Rice are well implemented.

Secondary output files are generated that do not contain the expected data (relfrac.out, maxrel.dat, inv1000.out). These files are not used by the tpa system. The releaset.e module for TPA 3.3 had that same problem. This problem was not generated by the addition of the flags by R. Rice.

---

So far I have proved that the results are consistent with the prior version (3.3) of the TPA code. What remains to be proved is that results are consistent for mixed failure modes. For that aim, I will make seval runs with different contact modes within a run. The realizations will be chosen to produce the same output.

**Run D1**

```
0.00000E+00 10      ! defect,idefect:  initially defective time [yr] & WPs affected
1000 50       ! sftimev,isconv:  volcano fail time [yr] & WPs affected
2000 100       ! seismt2,seismp2: second seismic failure time [yr] & WP affected
4000 200       ! seismt4,seismp4: fourth seismic failure time [yr] & WP affected
0.1  0      ! wetfrac(1),iwatcont(1): init def ht fract of wet SF and water contact
0.2  1      ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
0.3  0      ! wetfrac(5),iwatcont(5): seim2 fail ht fract of wet SF and water contact
0.4  1      ! wetfrac(7),iwatcont(7): seim4 fail ht fract of wet SF and water contact
```

**Run D2**

Changes to ebsfail.inp

```
360   1.08314E-01    ! xcon: # of WP; sawetfrac: wetted subarea
0 0       ! defect,idefect:  initially defective time [yr] & WPs affected
0  10       ! sftimef,isconf:  faulting fail time [yr] & WPs affected
1000 50       ! seismt1,seismp1: first  seismic failure time [yr] & WP affected
2000 100       ! seismt3,seismp3: third  seismic failure time [yr] & WP affected

0.1  0      ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
0.2  1      ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
0.3  0      ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact
0.4  1      ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact
```

ebstrh.dat, line 205: 4000.00

>>diff D1ebsnef.dat D2ebsnef.dat

No differences were detected by the above instruction. Diferences were detected in the relfrac.out, inv1000.out, and maxrel.dat files.

**Run D3**

0.00000E+00 10 ! defect,idefect: initially defective time [yr] & WPs affected

1000 50 ! sftimev,isconv: volcano fail time [yr] & WPs affected
2000 100 ! seismt2,seismp2: second seismic failure time [yr] & WP affected
4000 200 ! seismt3,seismp3: third seismic failure time [yr] & WP affected

0.1 0 ! wetfrac(1),iwatcont(1): init def ht fract of wet SF and water contact
0.2 1 ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
0.3 0 ! wetfrac(5),iwatcont(5): seim2 fail ht fract of wet SF and water contact
0.4 1 ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact

No differences in the output D1 and D3 output files were detected.

**03/05/00**

## CONCLUSION

The implementation of the contact mode flags for failure type is adequate. The most important file is the file ebsnef.dat. Other files must not be used. This note must be written to the manual. Otherwise, the code must be reviewed so that we make sure that all of the output files contain consistent data. The next step is to carry out some testing of the TPA system as a whole. What is needed is the verification that the flags are well passed from the tpa.inp file, into the ebsrel.inp file. This is documented in the directory /tparel/

---

## TESTING OF THE WHOLE TPA SYSTEM

We have tested the good performance of the releaset.e module. We have found inconsistent output files that need to be modified. The primary output file passed to other parts of the system is entirely consistent. Therefore, although some files seem to have inconsistent results, they do not affect the flow of data within the TPA system. They are of concern, however, because the user may decide to use data that are incorrect.

This testing phase verifies that data are well read from the tpa.inp file, and passed on to ebsrel.inp. The output files must be consistent with those obtained by the isolated run of the releaset.e module.

**Testing plan**

Several runs of the tpa4beta with diverse selection of the water contact mode flags are carried out. The flags in the ebsrel.inp file must be well mapped accordingly, and the output file in the tpa run must be consistent with the output files in the releaset run.

The six flags, added by R. Rice, to define the water contact mode as function of the failure mode are

WaterContactMode_Initial(0=BathTub,1=FlowThrough)
WaterContactMode_Faulting(0=BathTub,1=FlowThrough)
WaterContactMode_Volcanic(0=BathTub,1=FlowThrough)
WaterContactMode_SeismicInterval1(0=BathTub,1=FlowThrough)
WaterContactMode_SeismicInterval2(0=BathTub,1=FlowThrough)
WaterContactMode_SeismicInterval3(0=BathTub,1=FlowThrough)
WaterContactMode_SeismicInterval4(0=BathTub,1=FlowThrough)
WaterContactMode_Corrosion(0=BathTub,1=FlowThrough)

**Location of the testing files**
The files for this testing phase are located in Vulcan, at
/home/opensado/tpa4/tparel

This directory contains four subdirectories:
ref –> run of the reference tpa.inp file
releaset –> run of the releaset module
t1 –> run of the t1 case, defined by tpa.inp1
t2 –> run of the t2 case, defined by tpa.inp2
t3 –> run of the t3 case, defined by tpa.inp3

tpa.inp --> reference file for the computations in the subdirectories. 1 subarea, 1 realization

**Testing**
tpa.inp1

WaterContactMode_Initial(0=BathTub,1=FlowThrough) --> 0
WaterContactMode_Faulting(0=BathTub,1=FlowThrough) --> 1
WaterContactMode_Volcanic(0=BathTub,1=FlowThrough) --> 0
WaterContactMode_SeismicInterval1(0=BathTub,1=FlowThrough) --> 1
WaterContactMode_SeismicInterval2(0=BathTub,1=FlowThrough) --> 0
WaterContactMode_SeismicInterval3(0=BathTub,1=FlowThrough) --> 1
WaterContactMode_SeismicInterval4(0=BathTub,1=FlowThrough) --> 0
WaterContactMode_Corrosion(0=BathTub,1=FlowThrough) --> 1

```
>>cp tpa.inp1 t1/tpa.inp
>>cd t1
>>$TPA_TEST/tpa.e
```

The file t1/ebsrel.inp contains the following data

```
\Fuel leaching model paramters and water contact mode (bathtub=0, flowthru=1)
1.29052E-01  0      ! wetfrac(1),iwatcont(1): init def ht fract of wet SF and water contact
7.59571E-01  1      ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
1.63517E-01  0      ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
6.98734E-01  1     ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
 8.57395E-01  0     ! wetfrac(5),iwatcont(5): seim2 fail ht fract of wet SF and water contact
6.56664E-01  1     ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact
4.32742E-01  0     ! wetfrac(7),iwatcont(7): seim4 fail ht fract of wet SF and water contact
6.65776E-01  1      ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact
```

The flags are entirely consistent with the expectations.

tpa.inp2, directory: t2

```
WaterContactMode_Initial(0=BathTub,1=FlowThrough)  --> 1
WaterContactMode_Faulting(0=BathTub,1=FlowThrough)  --> 0
WaterContactMode_Volcanic(0=BathTub,1=FlowThrough)  --> 1
WaterContactMode_SeismicInterval1(0=BathTub,1=FlowThrough) --> 0
WaterContactMode_SeismicInterval2(0=BathTub,1=FlowThrough)  --> 1
WaterContactMode_SeismicInterval3(0=BathTub,1=FlowThrough)  --> 0
WaterContactMode_SeismicInterval4(0=BathTub,1=FlowThrough) --> 1
WaterContactMode_Corrosion(0=BathTub,1=FlowThrough) --> 0
```

The file tpa.inp2 was copied to t2/tpa.inp and the tpa code was run.

The file t2/ebsrel.inp contains the following data, which is consistent with the expectations.

```
1.29052E-01  1      ! wetfrac(1),iwatcont(1): init def ht fract of wet SF and water contact
7.59571E-01  0      ! wetfrac(2),iwatcont(2): fau fail ht fract of wet SF and water contact
1.63517E-01  1      ! wetfrac(3),iwatcont(3): vol fail ht fract of wet SF and water contact
6.98734E-01  0     ! wetfrac(4),iwatcont(4): seim1 fail ht fract of wet SF and water contact
8.57395E-01  1     ! wetfrac(5),iwatcont(5): seim2 fail ht fract of wet SF and water contact
6.56664E-01  0     ! wetfrac(6),iwatcont(6): seim3 fail ht fract of wet SF and water contact
4.32742E-01  1     ! wetfrac(7),iwatcont(7): seim4 fail ht fract of wet SF and water contact
6.65776E-01  0      ! wetfrac(8),iwatcont(8): cor fail ht fract of wet SF and water contact
```

tpa.inp3, directory: t3

```
WaterContactMode_Initial(0=BathTub,1=FlowThrough)  --> 0

constant
SFWettedFraction_Initial_1
1.29052E-01
```

The file tpa.inp2 was copied to t3/tpa.inp and the tpa code was run. The file t3/ebsnef.dat was compared to ref/ebsnef.dat. Both files are identical, as expected.

As an additional check-up, the data in releaset/t3ebsnef.dat must be identical to t3/ebsnef.dat Effectively, the instruction

>>diff t3/ebsnef.dat releaset/t3ebsnef.dat

does not reveal any difference. This means that releaset.e module is running well within the tpa system.

3/7/00
**CONCLUSION**

The ebsrel module is reading the flags in tpa.inp and passing them to ebsfail.inp. The output of the releaset.e within the tpa system is consistent with the output of releaset.e as a stand-alone module. The only caveat is that secondary output files of the releaset.e module, other than ebsnef.dat, are not validated, and these data should not be used. The reader must be made aware of that.

## Test Results

Osvaldo Pensado 3/15/00

Several runs of the releaset module were completed. The runs were selected in such a manner that the same number of WP failed, the same spent fuel wet fraction, and the same failure time were chosen. The only output data file used by the tpa system is ebsnef.dat. This file displayed always identical (and, therefore, consistent) results for all of the realizations. The same output file is generated with the releaset module for tpa 3.3, when the input data in ebsrel.inp is adequately selected.

Other output files did not display consistent data, such as relfrac.out, maxrel.dat, inv1000.out (these files are not used by the tpa system), specially when the WP are failed due to corrosion. I found that the releaset.e module for TPA 3.3 had that same problem. Thus, this problem was not generated by the addition of the flags by R. Rice. This problem needs to be addressed.

With respect to the system level testing, no problem was found. The flags in tpa.inp are well mapped into ebsrel.inp. Results of a single module realization are identical to the results of the TPA run.

Printed: September 19, 2003
Osvaldo
Pensado

# Title: seismo module, modified equation for the average radius

## Test Plan

Osvaldo Pensado 3/6/00

**Test name**: Test of changes described in PA-SCR-302 to the releaset module.
**Anticipated start date**: 3/6/00
**Anticipated completion date**: 3/11/00
**Amount of your time available to perform this test**: 20 hr
**Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50):** 0/100
**Output files to be checked**: wpsfail.res
**Input files to be checked for proper data transfer to the program**: tpa.inp

**Disposition of documentation (storage medium, physical location, and access method)**:
Electronic files are located in vulcan, at
/home/opensado/tpa4/testseismo/
Multiple *readme* files are included therein for the easy reading of the computations.

**Functional Test Descriptions**:

**Process-level tests**: N/A

**System-level tests**:

Equations (4-43) and (4-47) in the TPA manual for version 3.2 can be made invariant for several choices of the WPDiameter. The average radius, $R_{ave}$, is function of the WP diameter. If the average radius is well computed, the output of several realizations having identical values of $P_{dyn}$ and $p$, as defined by Equations (4-43) and (4-47), must be identical, provided that the only failure mode is seismicity. Another restriction is that the WPModulusOfElasticityforSEISMO is kept constant. The failure criterion for the WP in the SEISMO mudule is that if the impact energy exceeds a constant, then failure of the WP is produced. The impact energy is function of the impact stress, $p$, and the WP Young modulus, $E_{wp}$ Therefore, if several runs have the same value of $p$ and $E_{wp}$, the number of WPs failed for these runs must be identical.

**Reasonableness Test Description**:

A run TPA 3.3 code having exactly the same SEISMO parameters as a run of the TPA 4.0beta code must produce similar results. The results are not necessarily identical because of the different way in which the average radius is computed, and because the subarea geometry and number of WPs is different. However, the results are not expected to display significant differences.

**Objective**: Test changes to the seismo module by R. Janetzke (PA-SCR-302). The average radius of the canister is computed by

$$R_{ave} = (WPDiameter - WPWall) / 2 \qquad [9]$$

Originally, the above equation was implemented without a parenthesis.

The computations are documented at the following location in Vulcan

/home/opensado/tpa4/testseismo/

Multiple *readme* files are therein included to facilitate the reading of the computations.

**In the following discussion, all of the mentioned directories are located in Vulcan, at /home/opensado/tpa/seismo/**

3/7/00

The following changes were made to the tpa.inp.ref file to guarantee that the WP do not fail due to corrosion:

Subarea 1, one single realization.

constant
AA_1_1[C/m2/yr]
1e-1

constant
AA_2_1[C/m2/yr]
1e-1

constant
CoefForLocCorrOfOuterOverpack
1e-8

constant
ExponetForLocCorrOfOuterOverpack
1

constant
CoefForLocCorrOfInnerOverpack
1e-8

constant
RockModulusOfElasticityforSEISMO[Pa]
3.45D10

constant
RockFallingDistanceforSEISMO[m]
10.0D0

constant
WPPoissonRatioforSEISMO[]
0.7D0

constant
DefectiveFractionOfWPs/cell
0.0

Commands to make sure that the tpa 4.0 beta version is run:

**>>setenv TPA_TEST /solapps/cnwra/A_tpa4.0beta**
**>>setenv TPA_DATA /solapps/cnwra/A_tpa4.0beta**

Assumptions:

**Premise**:

Equations (4-43) and (4-47) in the TPA manual for version 3.2 can be made invariant for several choices of the WPDiameter. The average radius is function of the WP diameter. If the average radius is well computed, the output of several realizations having identical values of $P_{dyn}$ and $p$, as defined by Equations (4-43) and (4-47), must be identical, provided that the only failure mode is seismicity. Another restriction is that the WPModulusOfElasticityforSEISMO is kept constant. The failure criterion is that if the impact energy exceeds a constant, then the WP is considered failed. The impact energy is function of the impact stress, p, and the WP Young modulus, $E_{wp}$. The equation is

$$Energy = \frac{p^2}{2E_{wp}} \qquad [10]$$

Thus, if p is invariant, and $E_{wp}$ (WPModulusOfElasticityforSEISMO) is also invariant, two different realizations must produce the same output.

See the Scientific Notebook 355, pages 67 – 71, to determine how $P_{dyn}$, $p$, and Energy were forced to be invariant for several selections of WPDiameter. See the file constants.xls for the arithmetic operations. Here we summarize the main equations

$h$ –> RockFallingDistanceforSEISMO[m]
$k_b$ –> WPSupportStiffnessforSEISMO[pa*m]
$d$ –> WPDiameter[m]
$E_{wp}$ –> WPModulusOfElasticityforSEISMO[Pa]
$E_{rock}$ –> RockModulusOfElasticityforSEISMO[Pa]
$\mu_{wp}$ –> WPPoissonRatioforSEISMO[]
$t$ = outer overpack thickness + inner overpack thickness

Let $\xi$ be a real such that

$$1 < \xi < \frac{1}{\left(1-\mu_{wp}^{\ 2}\right)^3} \qquad [11]$$

them, the following transformation preserves the energy defined as Equation [2]:

$$\begin{aligned} h' &= \xi h \\ k_b' &= k_b / \xi \\ d' &= \frac{1}{\sqrt[3]{\xi}}(d-t)+t \\ E_{rock}' &= E_{rock}\frac{d'}{d} \\ \mu_{wp}' &= \sqrt{1-\left(1-\mu_{wp}^{\ 2}\right)\frac{d}{d'}} \end{aligned} \qquad [12]$$

In the deduction of the above transformation it was used the fact that the average radius $R_{ave}$ is computed as indicated in Equation [1].

**Contents of the folder /testseismo/**
ref –> TPA run of a reference case
A1, A2, A3, A4 –> run of a specific case, computed on the basis of the transformation defined in Equation [4].
constants.xls –> excel file used to do the computations
constants.txt –> same information as constants.xls, but in a text format
tpa.inp.ref –> tpa.inp file used as reference file.

**Run ref**

Run of the tpa.inp.ref. Data used as reference data.

**Run A1**

WPDiameter[m] 1.455004
RockFallingDistanceforSEISMO[m] 20
WPSupportStiffnessforSEISMO[pa*m] 2.75E+09
WPPoissonRatioforSEISMO[] 0.606937389
RockModulusOfElasticityforSEISMO[Pa] 2.7856630312E+10

The instruction
>>diff wpsfail.res ../ref/wpsfail.res
does not reveal any difference, as expected. The same number of WP failed due to seismicity are produced.

**Run A2**

WPDiameter[m] 1.179593603
RockFallingDistanceforSEISMO[m] 40
WPSupportStiffnessforSEISMO[pa*m] 1.38E+09
WPPoissonRatioforSEISMO[] 0.470001241
RockModulusOfElasticityforSEISMO[Pa] 2.2583784296E+10

The instruction
>>diff wpsfail.res ../ref/wpsfail.res
does not reveal any difference, as expected. The same number of WP failed due to seismicity are produced.

**Run A3**

WPDiameter[m] 0.999278886

RockFallingDistanceforSEISMO[m] 70
WPSupportStiffnessforSEISMO[pa*m] 7.86E+08
WPPoissonRatioforSEISMO[] 0.283402195
RockModulusOfElasticityforSEISMO[Pa] 1.9131588001E+10

The instruction
>>diff wpsfail.res ../ref/wpsfail.res
does not reveal any difference, as expected. The same number of WP failed due to seismicity are produced.

**Run A4**

WPDiameter[m] 1.045640272
RockFallingDistanceforSEISMO[m] 60
WPSupportStiffnessforSEISMO[pa*m] 9.17E+08
WPPoissonRatioforSEISMO[] 0.347984957
RockModulusOfElasticityforSEISMO[Pa] 2.0019194999E+10

The instruction
>>diff wpsfail.res ../ref/wpsfail.res
does not reveal any difference, as expected. The same number of WP failed due to seismicity are produced.

**CONCLUSION**

Consistent results were found that point toward the adequacy of the seismo mudule.

3/14/00

**REASONABLENES TEST**

A run TPA 3.3 code having exactly the same SEISMO parameters as a run of the TPA 4.0beta code must have more WPs failed due to seismicity. The $R_{ave}$ computed with TPA 3.3 is greater than the $R_{ave}$ computed with TPA 4.0beta. This implies a greater $P_{dyn}$ and greater energy for the TPA 3.3 case. In the end more WPs have to fail due to seismicity in TPA 3.3, but not many more.

>>cd /home/tpa4/testseismo/
>>setenv TPA_TEST /solapps/cnwra/A_tpa3.3
>>setenv TPA_DATA /solapps/cnwra/A_tpa3.3
>>mk dir B1
>>cd B1
>>cp $TPA_TEST/tpa.inp .

After that, all of the SEISMO parameters in ../tpa.inp.ref were copied to the tpa.inp file. The following adjustments were further made to make the tpa.inp file consistent with ../tpa.inp.ref.

constant
AA_1_1[C/m2/yr]
1e-1

constant
AA_2_1[C/m2/yr]
1e-1

constant
CoefForLocCorrOfOuterOverpack
1e-8

constant
ExponetForLocCorrOfOuterOverpack
1

constant
LocalizedCorrRateOfInnerOverpack[m/yr]
1e-8

constant
RockModulusOfElasticityforSEISMO[Pa]
3.45D10

constant
RockFallingDistanceforSEISMO[m]
10.0D0

constant
WPPoissonRatioforSEISMO[]
0.7D0

constant
DefectiveFractionOfWPs/cell
0.0

After the above changes, the tpa code 3.3 was run.

Indeed, this run has more WPs failed at several time steps, indicated in wpsfail.res, but not many. At times the WPs failed are 3 and 4. The file ../ref/wpsfail.res never has more than 2 wp failed at any timestep. Therefore effectively the TPA 3.3 code produces more failure of the WP due to seismicity than the TPA 4.0beta, but not many more.

**CONCLUSION**

The average radius as defined in Equation [1] produces less WPs to fail due to corrosion, compared to results with the TPA 3.3. The results are comparable though.

## Test Results

Osvaldo Pensado, 3/15/00

The results were consistent with the expectations. Several runs were completed with different values of the WP diameter, Poisson ratio, support stiffness, and rock fall height distance, selected in such a manner that the impact energy was the same for all of the runs. The number of WPs failed due to seismicity for these runs was the same, as expected. This indicates that the implementation of the SEISMO equations is adequate, in particular the equation for the computation of the average radius.

A comparison with a run of tpa 3.3 revealed similar results. The results cannot be identical because of the different way in which the average radius is computed, and because the subarea geometry and number of WPs is different.

## Title: Changes to gentpa module

### Test Plan

Osvaldo Pensado 3/22/00

**Test name**: Test of changes described in PA-SCR-310 to the gentpa module.
**Anticipated start date**: 3/21/00
**Anticipated completion date**: 3/22/00
**Amount of your time available to perform this test**: 16 hr
**Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50):** 20/80
**Output files to be checked**: genv.out, gmedia.out, gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat, dcf.cum
**Input files to be checked for proper data transfer to the program**: tpa.inp, gdefault.inp

**Disposition of documentation (storage medium, physical location, and access method)**:
Electronic files are located in Vulcan, at
/home/opensado/tpa4/test310/
/home/opensado/tpa4/tpa4betaKRun/
Multiple *readme* files are included therein for the easy reading of the computations.

A floppy disk containing the relevant data in the above directories is attached, including also a copy of the scientific notebook documenting the test.

**Summary of changes described in PA-SCR-310**

Change I: Introduction of six inhalation rate parameters in tpa.inp [InhalationRate(1-6)]
The value of this inhalation rate is mapped into gdefault.inp as the RINH parameter. The value selected is defined by the selection of the age group (ReceptorAgeGroup in tpa.inp).

Change II: Creation of a new append file dcf.cum containing the data in gw_cb_ad.dat and gw_pb_ad.dat

Change III: Update of the header in gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat

**Functional Test Descriptions**:

**Process-level tests**:

Run the stand alone codes envin.e and env.e to generate the output files genv.out and gmedia.out. The input file to these stand alone codes defined by the variables in tpa.inp is gdefault.inp. If gdefault.inp is the same for several runs, then these tpa runs must have the same

genv.out and gmedia.out files.

**System-level tests**:

Track the mapping of each of the six InhalationRate parameters defined in tpa.inp into gdefault.inp. Verify that the output files by the tpa code genv.out and gmedia.out coincide with the output files generated by the stand-alone codes envin.e and env.e.

Verify that data in dcf.cum indeed contain single realization data contained in gw_cb_ad.dat, gw_pb_ad.dat.

Verify that the new header in gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat does not affect the numerical data.

**Reasonableness Test Description**:

Comparable output files genv.out and gmedia.out must be produced by TPA 4 beta and TPA 4 beta K. The results cannot be identical since data files defining exposition pathways have been updated after the release of TPA 4 beta. The results must be comparable.

Similarly, data in gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat must be comparable.

Osvaldo Pensado 3/20/00
Test of the changes dercribed in PA-SCR-310, implemented by M. Smith.
The changes are related to the GENTPA

The home directory for the present discussion is located in Vulcan at
**/home/opensado/tpa4/test310/**
In the following unix shell commands, assume that the unix terminal is pointing at such directory.

```
setenv TPA_TEST  /home/janetzke/tpa40betaK
setenv TPA_DATA  /home/janetzke/tpa40betaK
setenv ori $TPA_DATA
cp $TPA_TEST/codes/env* .
cp ../tpa4betaKRun/FILENAME.DAT .
cp ../tpa4betaKRun/ggenii.inp .
cp ../tpa4betaKRun/grmdlib.dat .
cp ../tpa4betaKRun/gftrans.inp .
cp ../tpa4betaKRun/gbioac1.dat .
cp ../tpa4betaKRun/ggamen.dat .
cp ../tpa4betaKRun/genv.in .
cp ../tpa4betaKRun/gdefault.inp .
cp ../tpa4betaKRun/gdosinc2.dat .
cp ../tpa4betaKRun/ggrdf.dat .
```

**Input files for envin.e**: FILENAME.DAT, ggenii.inp, grmdlib.dat, gftrans.inp, gbioac1.dat, ggamen.dat, gdefault.inp, gdosinc2.dat, ggrdf.dat
**Output files from envin.e**: fort.1, gwork.buf, ggenii.out

**Input files for env.e**: genv.in
**Output files for env.e**: genv.out, gmedia.out

**Important variable**
ReceptorAgeGroup(1=Nfnt,2Tod,3PTeen,4Teen,5Adlt,6AdltFGR11)

By changing the above variable the parameter RINH – Chronic Breathing (cm3/s) – is adjusted in gdefault.inp

## TEST PLAN

**Change I**
Change *ReceptorAgeGroup* in tpa.inp and see that the appropriate value of RINH is mapped into gdefault.inp

The results must be consistent with the prior version of the TPA code when ReceptorAgeGroup=6. The two most important output files are genv.out and gmedia.out. This takes care of the reasonableness testing.

**Change II**
Verify that data in dcf.cum indeed contain single realization data contained in gw_cb_ad.dat, gw_pb_ad.dat.

**Change III**
Verify that the new header in gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat does not affect the numerical data. A run of the 4beta version must produce comparable numbers as a run of the 4betaK version.

**Reference Run**
A reference run of the TPA4betaK version, 1 single realization, 1 subarea, is located at
../tpa4betaKRun/
Data in this location will be used as reference data.

---

3/21/00

## HEADER TEST

```
mkdir beta
setenv TPA_TEST  /home/janetzke/tpa40beta
setenv TPA_DATA  /home/janetzke/tpa40beta
setenv ori $TPA_DATA
diff beta/tpa.inp ../tpa4betaKRun/tpa.inp  > difBetaK
```

After that the tpa.inp file for the *beta* run was modified so that the differences between the above tpa.inp files were minimized. Certainly the tpa.inp file for *betaK* has more variables and it is not possible to make both input files identical. Most of the entries are identical, though.

```
cd beta
$TPA_TEST/tpa.e
diff gw_cb_ad.dat ../../tpa4betaKRun/gw_cb_ad.dat  > difcb_ad
```

```
diff gw_cb_ci.dat ../../tpa4betaKRun/gw_cb_ci.dat > difcb_ci
diff gw_pb_ad.dat ../../tpa4betaKRun/gw_pb_ad.dat > difpb_ad
diff gw_pb_ci.dat ../../tpa4betaKRun/gw_pb_ci.dat > difpb_ci
```

***gw_cb_ad.dat***
Besides the difference in the header, minor differences were noted in the DCF for Np237, I129, Tc99 Important differences are displayed in the Cl36 for "dir exp" and "ing crop" of the order of 40 %. I talked to Pat LaPlante about this issue and he told me that the reason is the the data files have been modified. The new data files impact the radionuclide pathways. The most affected radionuclide is Cl36. Pat is reporting this issue in his testing.

**The header is well written and is not affecting the data.**

***gw_cb_ci.dat***
The old and new data are identical. The header is well written.

***gw_pb_ad.dat***
Important differences are displayed under the row for milk ingestion ("ing milk"). LaPlante told me that the reason is an update in the data files, and that such differences are expected.

***gw_pb_ci.dat***
The old and new data are identical. The header is well written.

## Conclusion

The header does not affect the data in gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat. In all cases the header is well written. Differences in the files gw_cb_ci.dat and gw_pb_ci.dat are noted when compared to the beta version of the tpa code. According to LaPlante these differences are expected, and due to the use of new data files. LaPlante is reporting these issues as part of his testing results (addressing PA-SCR-30).

---

3/21/00
### Introduction of inhalation rates for six age groups

Test Plan:
Need to check the mapping of the InhalationRate variables from tpa.inp into gdefault.inp. Need to check consistency between betaK and beta versions. The output files to be compared are genv.out, gmedia.out.

**mkdir A1**
cp tpa.inpBetaK A1/tpa.inp
cd A1

Changes to tpa.inp
ReceptorAgeGroup --> 1
InhalationRate1 --> 270.0

$TPA_TEST/tpa.e
cd ..
diff A1/genv.out ../tpa4betaKRun/genv.out
diff A1/gmedia.out ../tpa4betaKRun/gmedia.out
diff A1/gdefault.inp gdefault.inp

The above instructions do not reveal any difference, as expected. The last instruction means that data from tpa.inp are appropriately mapped into gdefault.inp.

**Consistency Check**

diff A1/genv.out beta/genv.out

The above instruction revealed minor differences. The differences are due to the choice of different data files.

diff A1/gmedia.out beta/gmedia.out

Differences are noted in the "Surface Soil mCi/m2" column. The radiocuclides that display different surface soil concentrations are Cl36, Tc99, I129, Np237, and Pa233. The most important difference is in the Cl concentration, differing in more than two significant digits. According to LaPlante these differences are expected, and due to the use of new data files. LaPlante is reporting these issues as part of his testing results (addressing PA-SCR-301).

**mkdir A2**
cp tpa.inpBetaK A2/tpa.inp
cd A2

Changes to tpa.inp
ReceptorAgeGroup --> 2
InhalationRate2 --> 270.0

```
$TPA_TEST/tpa.e

cd ..
diff A2/genv.out ../tpa4betaKRun/genv.out
diff A2/gmedia.out ../tpa4betaKRun/gmedia.out
diff A2/gdefault.inp gdefault.inp
```

The above instructions do not reveal any difference, as expected. The last instruction means that data from tpa.inp are appropriately mapped into gdefault.inp.

```
mkdir A3
cp tpa.inpBetaK A3/tpa.inp
cd A3
```

Changes to tpa.inp
ReceptorAgeGroup --> 3
InhalationRate3 --> 270.0

```
$TPA_TEST/tpa.e
cd ..
diff A3/genv.out ../tpa4betaKRun/genv.out
diff A3/gmedia.out ../tpa4betaKRun/gmedia.out
diff A3/gdefault.inp gdefault.inp
```

The above instructions do not reveal any difference, as expected. The last instruction means that data from tpa.inp are appropriately mapped into gdefault.inp.

```
mkdir A4
cp tpa.inpBetaK A4/tpa.inp
cd A4
```

Changes to tpa.inp
ReceptorAgeGroup --> 4
InhalationRate4 --> 270.0

```
$TPA_TEST/tpa.e
cd ..
diff A4/genv.out ../tpa4betaKRun/genv.out
diff A4/gmedia.out ../tpa4betaKRun/gmedia.out
diff A4/gdefault.inp gdefault.inp
```

The above instructions do not reveal any difference, as expected. The last instruction means that data from tpa.inp are appropriately mapped into gdefault.inp.

**mkdir A5**
cp tpa.inpBetaK A5/tpa.inp
cd A5

Changes to tpa.inp
ReceptorAgeGroup --> 5
InhalationRate5 --> 270.0

$TPA_TEST/tpa.e
cd ..
diff A5/genv.out ../tpa4betaKRun/genv.out
diff A5/gmedia.out ../tpa4betaKRun/gmedia.out
diff A5/gdefault.inp gdefault.inp

The above instructions do not reveal any difference, as expected. The last instruction means that data from tpa.inp are appropriately mapped into gdefault.inp.

**Partial Conclusion**
The InhalationRateX parameters are well mapped into the file gdfault.inp. The output files genv.out and gmedia.out contain consistent data for all of the realizations.

**Second phase of Testing for Change I**

IinhalationRateX is selected as 52.0 (X=1,..,6)

**mkdir B1**
cp tpa.inpBetaK B1/tpa.inp
cd B1

Changes to tpa.inp
ReceptorAgeGroup --> 1
InhalationRate1 --> 52.0

$TPA_TEST/tpa.e
cd ..
cat B1/gdefault.inp | grep RINH
diff B1/gdefault.inp gdefault.inp

The only difference is in the RINH row, which displays 52.0, as expected. Data are well mapped from tpa.inp into gdefault.inp

**mkdir B2**
cp tpa.inpBetaK B2/tpa.inp
cd B2

Changes to tpa.inp
ReceptorAgeGroup --> 2
InhalationRate2 --> 52.0

$TPA_TEST/tpa.e
cd ..
diff B1/genv.out B2/genv.out
diff B1/gmedia.out B2/gmedia.out
diff B1/gdefault.inp B2/gdefault.inp

The above instructions do not display differences, as expected. It is necessarily true that data are well mapped from tpa.inp into gdefault.inp.

**mkdir B3**
cp tpa.inpBetaK B3/tpa.inp
cd B3

Changes to tpa.inp
ReceptorAgeGroup --> 3
InhalationRate3 --> 52.0

$TPA_TEST/tpa.e
cd ..
diff B1/genv.out B3/genv.out
diff B1/gmedia.out B3/gmedia.out
diff B1/gdefault.inp B3/gdefault.inp

The above instructions do not display differences, as expected. It is necessarily true that data are well mapped from tpa.inp into gdefault.inp.

**mkdir B4**
cp tpa.inpBetaK B4/tpa.inp
cd B4

Changes to tpa.inp
ReceptorAgeGroup --> 4
InhalationRate4 --> 52.0

```
$TPA_TEST/tpa.e
cd ..
diff B4/genv.out B1/genv.out
diff B4/gmedia.out B1/gmedia.out
diff B4/gdefault.inp B1/gdefault.inp
```

The above instructions do not display differences, as expected. It is necessarily true that data are well mapped from tpa.inp into gdefault.inp.

```
mkdir B5
cp tpa.inpBetaK B5/tpa.inp
cd B5
```

Changes to tpa.inp
ReceptorAgeGroup --> 5
InhalationRate5 --> 52.0

```
$TPA_TEST/tpa.e
cd ..
diff B5/genv.out B1/genv.out
diff B5/gmedia.out B1/gmedia.out
diff B5/gdefault.inp B1/gdefault.inp
```

The above instructions do not display differences, as expected. It is necessarily true that data are well mapped from tpa.inp into gdefault.inp.

```
mkdir B6
cp tpa.inpBetaK B6/tpa.inp
cd B6
```

Changes to tpa.inp
ReceptorAgeGroup --> 6
InhalationRate6 --> 52.0

```
$TPA_TEST/tpa.e
cd ..
```

```
diff B6/genv.out B1/genv.out
diff B6/gmedia.out B1/gmedia.out
diff B6/gdefault.inp B1/gdefault.inp
```

The above instructions do not display differences, as expected. It is necessarily true that data are well mapped from tpa.inp into gdefault.inp.

**CONCLUSION**

The InhalationRateX parameters are well mapped from tpa.inp into gdefault.inp. The output files affected by such a change (genv.out and gmedia.out) provide quite consistent results. Differences are noted between this version (4 beta K) and the beta version because of the selection of different input data files. Pat LaPlante has reported and explained the reason for this difference in the testing plan and test results addressing PA-SCR-301

---

## Testing of dcf.cum

```
mkdir dcf1
cp tpa.inpBetaK dcf1/tpa.inp
```

Modifications to tpa.inp
1 subarea
5 realizations
Start append: realization 1
Stop append: realization 5

Data for the last realization in dcf.cum was compared to data in gw_cb_ad.dat and gw_pb_ad_dat. New data files were assembled with data in dcf.cum: gw_cb_ad.dat5 and gw_pb_ad_dat5. The data were identical to the found in gw_cb_ad.dat and gw_pb_ad_dat, as expected. Data between the 2nd and 4th realization was copied to dcf.cum24

```
cd dcf1
$TPA_TEST/tpa.e
cd ..
diff dcf1/genv.out2  ../tpa4betaKRun/genv.out2
diff dcf1/gw_cb_ad.dat  ../tpa4betaKRun/gw_cb_ad.dat
diff dcf1/gw_pb_ad.dat  ../tpa4betaKRun/gw_pb_ad.dat
```

The above instruction did not reveal any difference. If genv.out is the same for two runs, and the

same age group is selected for two runs, then the dose conversion factors must be the same for the two runs, as seen above.

**mkdir dcf2**
cp dcf1/tpa.inp dcf2/

Changes to tpa.inp
1 subarea
5 realizations
Start append: realization 2
Stop append: realization 4

cd dcf2
$TPA_TEST/tpa.e
cd ..

The files dcf.cum and dcf.cum24 were compared according to diff dcf2/dcf.cum dcf1/dcf.cum24. The above instruction did not reveal any difference in the data. This indicates that the file dcf.cum has been constructed in a consistent manner.

**mkdir dcf3**
cp dcf1/tpa.inp dcf3/

Changes to tpa.inp
2 subarea
5 realizations
Start append: realization 1
Stop append: realization 5

cd dcf3
$TPA_TEST/tpa.e
cd ..
diff dcf1/dcf.cum dcf3/dcf.cum

The above instruction does not reveal differences. This is exppected since a single pair of files gw_cb_ad.dat and gw_pb_ad.dat is generated for all of the subareas.

## CONCLUSION

Several tests were performed to verify that the data in dcf.cum is adequate. Data in for the last realization in dcf.cum was compared to the data in the files gw_cb_ad.dat and gw_pb_ad.dat. The comparison revealed no difference, as expected.

Another run including 2 subareas and 5 realizations was completed. The contents of the file dcf.cum are identical to the dcf.cum file for the single subarea realizations.

Another run was completed by appending data between realizations 2 and 4. These data were compared to the appropriate data generated with the append instruction activated for the initial 5-realizations run. The data resulted identical.

The append file dcf.cum is working as intended. The validity of the data is subject to the validity of the data in gw_cb_ad.dat and gw_pb_ad.dat. Pat LaPlante has addressed this issue as part of another testing plan.

## Index of /home/opensado/tpa4/test310/

beta — Run of tpa4beta
*setenv TPA_TEST /home/janetzke/tpa40beta*
*setenv TPA_DATA /home/janetzke/tpa40beta*
*setenv ori $TPA_DATA*

difBeta — Output from diff ../tpa4betaRun/tpa.inp ../tpa4betaKRun/tpa.inp > difBetaK

tpa.inpBetaK — tpa.inp file for TPA 4 Beta K. It is used as a reference file in the computations.

tgenv.f and tgenv.x — Little program to delete the first two lines from genv.out

tgenv.inp — Input data to the tgenv.x program. It specifies, in four lines, the file to be modified, the output file, the number of lines to delete at the beginning, and the total number of lines in the original file.

A1,A2, A3, A4, A5 — Testing of introduction of InhalationRateX parameters

B1, B2, B3, B4, B5, B6 — Testing of introduction of InhalationRateX parameters

dcf1, dcf2, dcf3 — Testing of the new append file dcf.cum

gather.e — Little program to gather data between line1 and line2 of a file and drop it into an output file.
See /home/opensado/f77Library/gather.f for details. It uses the file gather.inp to run

gather.inp — Input file to gather.e

## Test Results

Osvaldo Pensado, 3/22/00

The three changes reported in PA-SCR-310 have been tested. The code tested is TPA 4.0 betaK. The new InhalationRate(1–6) are well mapped from tpa.inp into gdefault.inp. The output files genv.out and gmedia.out are influenced by the selection of this parameter. These files contain comparable data as those generated with TPA 4.0 beta. Differences are due to the update in the data files between beta and beta K versions. These differences have been addressed by Pat LaPlante and are reported elsewhere.

New headers have been added to the files gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat. The headers do not influence the correctness of the data. The data in these files is comparable to the data in these files generated with TPA 4.0 beta. Differences are due to the update in the data files between beta and beta K versions. These differences have been addressed by Pat LaPlante and are reported elsewhere.

Data are appropriately appended to dcf.cum. Single realization data were compared to data in this file with a 100 % agreement, thus indicating that the data in dcf.cum is adequate. The validity of these data rely on the validity of the data in gw_cb_ad.dat and gw_pb_ad.dat.

In summary, the changes reported in PA-SCR-310 are well implemented.

***This page formerly contained the statement page for the six month submittal of data to Quality Assurance in accordance with QAP-001.***

## Test Results

Osvaldo Pensado, 3/22/00

The three changes reported in PA-SCR-310 have been tested. The code tested is TPA 4.0 betaK. The new InhalationRate(1–6) are well mapped from tpa.inp into gdefault.inp. The output files genv.out and gmedia.out are influenced by the selection of this parameter. These files contain comparable data as those generated with TPA 4.0 beta. Differences are due to the update in the data files between beta and beta K versions. These differences have been addressed by Pat LaPlante and are reported elsewhere.

New headers have been added to the files gw_cb_ad.dat, gw_cb_ci.dat, gw_pb_ad.dat, gw_pb_ci.dat. The headers do not influence the correctness of the data. The data in these files is comparable to the data in these files generated with TPA 4.0 beta. Differences are due to the update in the data files between beta and beta K versions. These differences have been addressed by Pat LaPlante and are reported elsewhere.

Data are appropriately appended to dcf.cum. Single realization data were compared to data in this file with a 100 % agreement, thus indicating that the data in dcf.cum is adequate. The validity of these data rely on the validity of the data in gw_cb_ad.dat and gw_pb_ad.dat.

In summary, the changes reported in PA-SCR-310 are well implemented.

Osvaldo Pensado, 25/September/2000

Importance Analysis Notes. These notes will be added to scientific notebook 170-9e.

# ELEMENTS OF THE FILE ia.dat

BARRIER = 'BarrierBiosphereStudy'
**
**Component** = 'ComponentPrecipitationStudy'
**
parameter = 'WastePackageFlowMultiplicationFactor'
value = 1.0
**
parameter = 'SubAreaWetFraction'
value = 1.0
**

**Physical meaning**

No water focusing or diversion in the upper unsaturated zone. All of the waste packages are contacted by water.

This component is not well defined. It is intended to be combined with other components. It may be necessary to split this component into two subcomponents. In case other parameters controlling the extent of the water flux (hitting the drifts) are selected, they should be added to this section of the file ia.dat.

If WastePackageFlowMultiplicationFactor = 1, no focusing nor diversion.
If WastePackageFlowMultiplicationFactor>1, focusing.
If WastePackageFlowMultiplicationFactor<1, diversion.

SubAreaWetFraction (<1) is an efficiency factor. It is equivalent to Fwet in Appendix F. It is a measurement of the fraction of waste packages that are wet. If SubAreaWetFraction=1, all of the waste packages are wet and all of them release radionuclides after failure.

---

**
BARRIER = 'BarrierUpperUnsaturatedZoneStudy'
**
**Component** = 'ComponentTivaCanyonStudy'
**

THIS BARRIER MAY NOT BE WELL IMPLEMENTED. SEE NOTE ON February 13, 2001.

parameter = 'Reflux2SatInit'
value = 0.1 (equal to Reflux2SatResid. This causes the amount of water available for refluxing equal to zero. See Equation (5-25) in the TPA manual for version 4.0)
**
parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
value = 1.0e-10 (Very small conductivity. This selection causes the penetration distance, L, in equation (5-28) in the TPA manual for version 4.0 to be extremely large)
**
parameter = 'FractionOfCondensateRemoved[1/yr]'
value = 0.0 (no water removed after condensation)
**
parameter = 'FractionOfCondensateTowardRepository[1/yr]'
value =1.0 (all water goes back to the drifts)
**
parameter = 'FractionOfCondensateTowardRepositoryRemoved[1/yr]'
value = 0.0 (no water removed after reflux)
**
parameter = 'ChlorideMultFactor'
value = 0.0 (zero chloride concentration. Setting this number equal to zero does not cause any problem)
**
parameter = 'ChlorideMultFactorIntactDripShield'
value = 0.0 (zero chloride concentration. Setting this number equal to zero does not cause any problem)
**

**Physical meaning**
Unsaturated zone above the drift. The contribution to the performance of the system is in spreading in space and time the infiltration of water. The above parameters are aimed at eliminating the "reflux".

The selected values for Reflux2SatInit and ThermalConductivityofYMRock[W/(m-K)] eliminate the reflux.

The reflux parameters FractionOfCondensateRemoved[1/yr], FractionOfCondensateTowardRepository[1/yr], and FractionOfCondensateTowardRepositoryRemoved[1/yr] were suggested by Debra Hughson in her report Thermal Effects on Flow, Process-Level Sensitivity Analysis, Status Report CNWRA,

July 2000.

ChlorideMultFactor and ChlorideMultFactorIntactDripShield were set to equal zero. The chloride concentration in contact with the waste package is zero. If the UZ above the drift is removed, then there is no source for chloride.

When nullifying this component, the component ComponentPrecipitationStudy should also be nullified.

**In TPA 3.3 the following selections were made to remove the UZ**:
ElevationOfGroundSurface[m] = 1072.0 (Equal to ElevationOfRepositoryHorizon[m] for base case. This means that the repository horizon is brought to the surface)

MassDensityofYMRock[kg/m^3] = 1.0e-27 (very low mass density. Same value as importance analysis for TPA 3.2)

SpecificHeatofYMRock[J/(kg-K)] = 0.1 (very low specific heat. Same value as importance analysis for TPA 3.2)

ThermalConductivityofYMRock[W/(m-K)] = 1000.0 (very high thermal conductivity. Same value as importance analysis for TPA 3.2)

EmissivityOfDriftWall[-] = 0.4 (base case emissivity = 0.8. Same value as importance analysis for TPA 3.2. Same value as importance analysis for TPA 3.2)

ChlorideMultFactor = 0.0 (zero chloride concentration. Setting this number equal to zero does not cause any problem)

ChlorideMultFactorIntactDripShield = 0.0 (zero chloride concentration. Setting this number equal to zero does not cause any problem)

I do not have a good idea of why the above parameters were selected as such for TPA 3.3. It seems to me that such selection does not amount to removing the unsaturated zone (UZ).

---

**
BARRIER = 'BarrierLowerUnsaturatedZoneStudy'
**

Component = '**ComponentTSwStudy**'
**
parameter = 'Tsw_Thickness_XSubArea[m]' (X = 1, ..., No of subareas)
value = 0.0
**

**Physical meaning**
Topopah Springs, welded. Thickness of this zone equal to zero, therefore there is no retardation time.

**
Component = '**ComponentCHnvStudy**'
**
parameter = 'CHnvThickness_XSubArea[m]' (X = 1, ..., No of subareas)
value = 0.0
**

**Physical meaning**
Calico Hills, vitric. Thickness of this zone equal to zero, therefore there is no retardation time.

**
Component = '**ComponentCHnzStudy**'
**
parameter = 'CHnzThickness_1SubArea[m]' (X = 1, ..., No of subareas)
value = 0.0
**

**Physical meaning**
Calico Hills, zeolitic. Thickness of this zone equal to zero, therefore there is no retardation time.

**
Component = '**ComponentPPwStudy**'
**
parameter = 'PPw_Thickness_XSubArea[m]' (X = 1, ..., No of subareas)
value = 0.0
**

**Physical meaning**
Prow pass, welded. Thickness of this zone equal to zero, therefore there is no retardation time.

**

Component = '**ComponentUCFStudy**'
**
parameter = 'UCF_Thickness_XSubArea[m]' (X = 1, ..., No of subareas)
value = 0.0
**

**Physical meaning**
Upper Crater Flat. Thickness of this zone equal to zero, therefore there is no retardation time.

**
Component = 'ComponentBFwStudy'
**
parameter = 'BFw_Thickness_XSubArea[m]' (X = 1, .... No of subareas)
value = 0.0
**

**Physical meaning**
Bullfrog, welded. Thickness of this zone equal to zero, therefore there is no retardation time.

---

**
BARRIER = 'BarrierSaturatedZoneStudy'
**
Component = '**Component_STFF_SAV_Study**'
**
parameter = 'DistanceToTuffAlluviumInterface[km]'
value = 10.0 (Distance from repository foot print to tuff/alluvium interface)
**
parameter = 'DistanceToReceptorGroup[km][should_be_10_or_20]'
value = 10 (This makes the SZ to be composed just of tuff)
**
parameter = 'FractureRD_STFF_X' (X = Am, Np, I, Tc, Cl, Cm, U, Pu, Th, Ra, Pb, Cs, Ni, C, Se, Nb)
value = 1 (This causes no retardation)
**
parameter = 'ImmobileRD_STFF_X' (X = Am, Np, I, Tc, Cl, Cm, U, Pu, Th, Ra, Pb, Cs, Ni, C, Se, Nb)
value = 1 (This causes no retardation)
**
parameter = 'FracturePorosity_STFF'
value = 1.0e-4 (lower limit for base case: 1.0e-3, so this is a small selection. See comments at

end to see how this value was selected.)
**
parameter = 'DiffusionRate_STFF'
value = 0.0 (this avoids diffusion into the rock matrix)
**

**Physical meaning**

The saturated zone leg is forced to be composed just of tuff. Retardation factors are selected equal to one, and the diffusion coefficient is set equal to zero to avoid diffusion of contaminants into the rock matrix. The fracture porosity is selected very small to decrease the travel time in the SZ. Travel times of the order of years can be neglected compared to the thousands of years of the repository lifetime.

---

**
BARRIER = 'BarrierReceptorGroupStudy'
**
Component = **'ComponentWellWaterStudy'**
**
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value = 0.0
**
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value = 0.0
**

**Physical meaning**

No extra water is available for dilution of the radionuclides. This gives maximal concentrations.

---

**
SUBSYSTEM = 'SubsystemEngineeredStudy'
**
BARRIER = 'BarrierDriftStudy'
**
Component = '**ComponentBackfillStudy**'
parameter = 'EmplacementBackfillThickness[m]'
value = 0.0
**

**Physical meaning**

No backfill

**
Component = '**ComponentDripShieldStudy**'
**
parameter = 'DripShieldThickness[m]'
value = 0.0
**
parameter = 'DripShieldFailureTime[yr]'
value = 0.0
**

**Physical meaning**
No drip shield. The above parameters are independent of each other and have to be adjusted manually.

---

BARRIER = 'BarrierWastePackageStudy'
**
Component = '**ComponentInnerContainerStudy**'
parameter = 'InnerWPThickness[m]'
value = 0.0
**

**Physical meaning**
No outer waste package.

**
Component = '**ComponentOuterContainerStudy**'
parameter = 'OuterWPThickness[m]'
value = 0.0
**

**Physical meaning**
No inner waste package. Nullifying the outer and inner waste packages may require nullifying also the ComponentPrecipitationStudy.

# TESTING

## Selection of the porosity (FracturePorosity_STFF)

OPR 9/25/2000
Runs with TPA 4.0 were completed. Runs were performed at Vulcan: **/home/opensado/ia41/** and at Dakath: **d:\ia41**
Relevant output files are backed up at Dakath: **d:\osvaldo\pa\ia41**

Default tpa.inp for TPA 4.0 was selected. 1 subarea computations (1st subarea).

The following changes were made to tpa.inp:

InnerWPThickness[m] = 0
OuterWPThickness[m] = 0
DripShieldFailureTime[yr] = 0

DistanceToTuffAlluviumInterface[km] = 10
DistanceToReceptorGroup[km][should_be_10_or_20] = 10
DiffusionRate_STFF = 0.0

Several values of FracturePorosity_STFF were selected, from $10^{-6}$ to $10^{-1}$.

FracturePorosity_STFF = 1.0e-6

I got this error message

```
========================================
exec: calling szft
 ***>>> Error in uzft:aftnef
 Trouble in reading the "nef
 file nefii.dis
 - check the file nefii.dis
 - check for "nefmks" NORMAL
   at the end of the file ne
 - check that in the file ne
   "#RATES" .le. maxnumdis
   maxnumdis =       49999
========================================
```

I did a short analysis to select an adequate porosity, explained as follows.

Case 1: FracturePorosity_STFF = 1.0e-1
tpa1.inp totdose1.res

Case 2: FracturePorosity_STFF = 1.0e-2
tpa2.inp totdose2.res

Case 3: FracturePorosity_STFF = 1.0e-3
tpa3.inp totdose3.res

Case 4: FracturePorosity_STFF = 1.0e-4
tpa4.inp totdose4.res

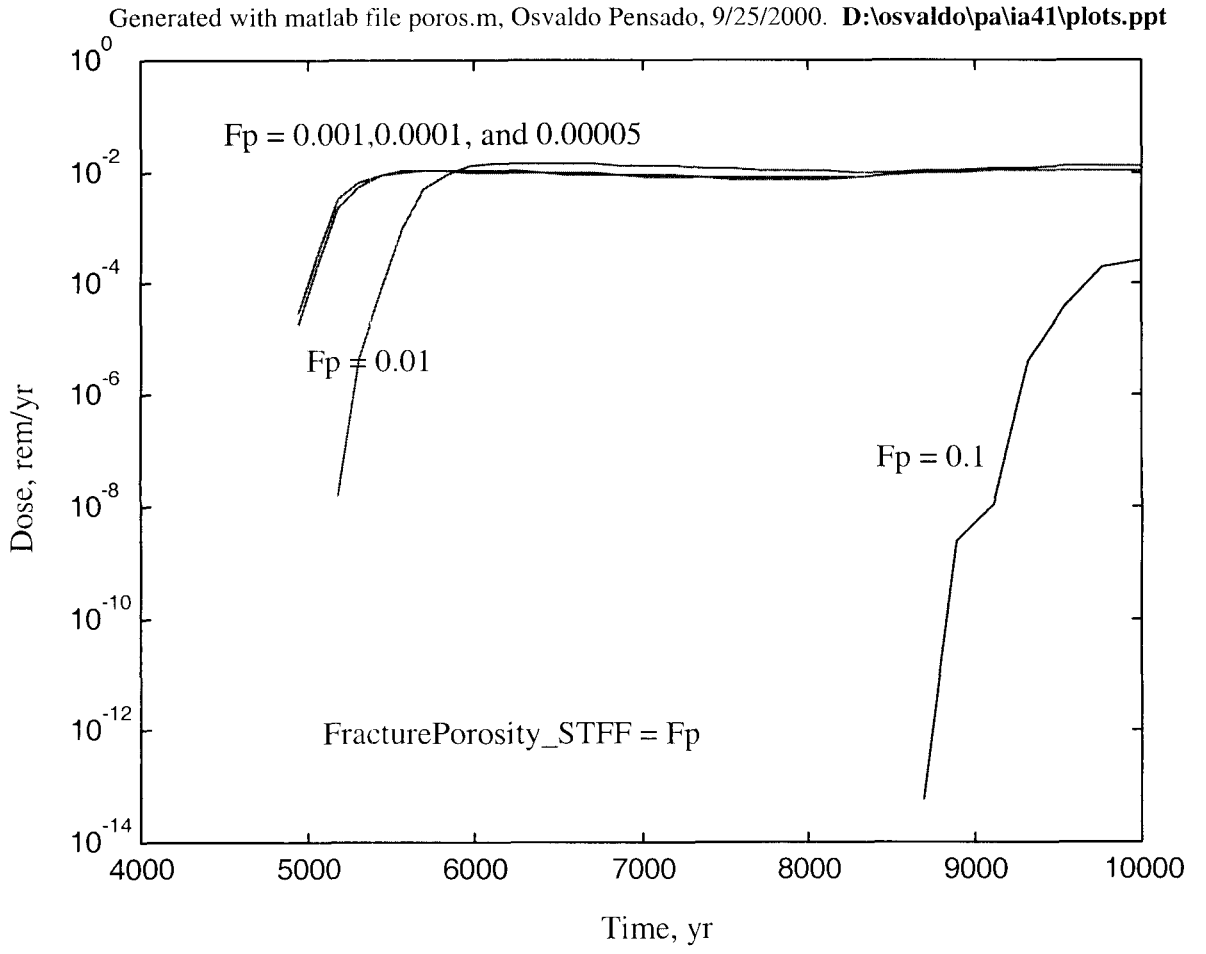
Case 5: FracturePorosity_STFF = 5.0e-5
tpa5.inp totdose5.res

For the case
FracturePorosity_STFF = 1.0e-5

The following error is produced:

```
---------------------------------------------
 exec: calling szft
  ***>>> Error in uzft:aftnefmks <<<***
 Number of times in "nefmks" output file
       nefii.dis exceeds maxnumdis.
 maxnumdis =   49999
 numtimnew =   90911
 ichainnum =   1
 Note: IEEE floating-point exception flags raised:
   Inexact;  Division by Zero;
 See the Numerical Computation Guide, ieee_flags(3M)
---------------------------------------
```

The following plot shows a comparison of the total dose versus time.




The results from the Cases 3, 4, and 5 are nearly identical. We can conclude that FracturePorosity_STFF = 1.0e-4 is an adequate selection.

Printed: September 19, 2003
Osvaldo
Pensado

# Removal of reflux (removal of unsaturated zone above the drifts)

OPR 9/26/2000
Runs with TPA 4.0 were completed. Runs were performed at Vulcan: **/home/opensado/ia41/**
Relevant output files are backed up at Dakath: **d:\osvaldo\pa\ia41**

Default tpa.inp for TPA 4.0 was selected. 1 subarea computations (1st subarea).

The following changes were made to tpa.inp:

InnerWPThickness[m] = 0
OuterWPThickness[m] = 0
DripShieldFailureTime[yr] = 0

FractionOfCondensateRemoved[1/yr]= 0.0
FractionOfCondensateTowardRepository[1/yr]= 1.0
FractionOfCondensateTowardRepositoryRemoved[1/yr]= 0.0

ThermalConductivityofYMRock[W/(m-K)]= 1.0e-10
Reflux2SatInit = 0.1

The input file tpa.inp, and the output files infilper.res and totdose.res and are backed up at d:\osvaldo\pa\ia41\ as tpa.inp, infilperUZ.res, and totdoseUZ.res, respectively. A copy of infilperUZ.res is included on Page 11. It is seen that the infiltration after reflux (4th column) is equivalent to the average infiltration (3rd column). No effort was placed on making the infiltration after diversion (5th column) equal to the infiltration after reflux. The reason is that the only element that is removed is the unsaturated zone. Diversion also occurs along the drifts, drip shield and the waste package.

Input file tpa.inp as supplied with TPA Version 4.0 Code.

Base case

TPA 4.0, Job started: Tue Sep 26 10:07:14 2000
Subarea Averaged Infiltration/Deep Percolation Including

After Reflux and Diversion - Values for Each Vector

| vector unitless | time yr | avinfil mm/yr | avreflux mm/yr | avdivert mm/yr |
|---|---|---|---|---|
| 1 | 0.0000E+00 | 8.1946E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.5694E+01 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 5.8078E+01 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 9.8894E+01 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 1.5034E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 2.1518E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 2.9690E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 3.9990E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 5.2972E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 6.9334E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 8.9957E+02 | 8.1946E+00 | 8.1946E+00 | 6.3475E-02 |
| 1 | 1.1595E+03 | 8.3323E+00 | 8.3323E+00 | 6.4541E-02 |
| 1 | 1.4871E+03 | 8.5134E+00 | 8.5085E+00 | 6.5906E-02 |
| 1 | 1.9000E+03 | 8.6098E+00 | 8.6098E+00 | 6.6691E-02 |
| 1 | 2.4204E+03 | 8.9225E+00 | 8.9225E+00 | 6.9113E-02 |
| 1 | 3.0764E+03 | 9.6489E+00 | 9.6489E+00 | 7.4739E-02 |
| 1 | 3.9031E+03 | 1.0056E+01 | 1.0056E+01 | 7.7891E-02 |
| 1 | 4.9451E+03 | 1.1221E+01 | 1.1218E+01 | 8.6896E-02 |
| 1 | 6.2584E+03 | 1.2550E+01 | 1.2550E+01 | 9.7207E-02 |
| 1 | 7.9137E+03 | 1.4872E+01 | 1.4869E+01 | 1.1518E-01 |
| 1 | 1.0000E+04 | 1.7511E+01 | 1.7511E+01 | 1.3564E-01 |

**NOTES**

I do not think that the implementation is perfect. There are some missing points. It is necessary to check the information in the following files:

infilper.res
dcagw.ech – Average annual precipitation
nfenv.ech – flux per waste package
nfenv.rlt – flux hitting waste packages (WPs) and flux missing waste packages. It seems that just a small fraction hits the WPs.
uzflow.rlt – flux per subarea
wpflow.dat – fow and fwet factors
wpflow.def – fow and fwet factors

I need more time to analyze the problem thoroughly. I need to verify that the average annual precipitation is the same as the near field infiltration. As of 9/26/2000 this analysis is incomplete. However, Debra Hughson has already done sensitivity analyses in Thermal Effects on Flow, Process-Level Sensitivity Analysis, Status Report CNWRA, July 2000. There she recommends to change the parameters

FractionOfCondensateRemoved[1/yr]
FractionOfCondensateTowardRepository[1/yr]
FractionOfCondensateTowardRepositoryRemoved[1/yr]

and that is already accomplished in the current implementation. It is not clear that Debra did the checking that I am here proposing.

Note the existence of the following tpa.inp variable
InvertBypass(0=ebsfilt,1=bypass-ebsfilt)
Selecting 1 bypasses the drift.

The routine
nfdrip in nfenv.f is in charge of computing the flux of water hitting WPs.

**February 13, 2001**

I discovered that the variable

ThermalConductivityofYMRock

is used in the thermal computations. If this parameter is fixed at a small value, refluxing is eliminated. However, this also has an effect on the rock temperature. The approach to eliminate the upper UZ is not adequate.

Refluxing is eliminated by letting L (defined in Eq 5-28 of the manual for TPA 4.0) go to infinity.

If the thermal conductivity of the rock goes to zero, L goes to infinity. Other possibilities are selecting

DensityOfWaterAtBoiling[kg/m^3]

or

EnthalpyOfPhaseChangeForWater[J/kg]

equal to huge values.

The enthalpy could also have an effect on the temperature distribution.

DensityOfWaterAtBoiling[kg/m^3] is only used within reflux3 but several times. Probably this density is a good selection. If none of these two choices work, then refluxing cannot be eliminated by changing parameters in tpa.inp.

**Run 41e**

The following operations on Vulcan: /home/opensado/ia41/ were performed.

**cp $TPA_DATA/tpa.inp 41etpa.inp**

To the file tpa41e.inp the following changes were applied

InnerWPThickness[m] = 0
OuterWPThickness[m] = 0
DripShieldFailureTime[yr] = 0

FractionOfCondensateRemoved[1/yr]= 0.0
FractionOfCondensateTowardRepository[1/yr]= 1.0
FractionOfCondensateTowardRepositoryRemoved[1/yr]= 0.0

Reflux2SatInit = 0.1

OutputMode(0=None,1=All,2=UserDefined) = 2
SelectAppendFiles = 3

StopAtSubarea = 1

Version 4.1e of the code was run. The following files were saved:
tpa.inp → 41etpa.inp
ebsfail.ech → 41eebsfail.ech : temperature records
infilper.res → 41einfilper.res : refluxing records
totdose.res → 41etotdose.res : dose rate records

**Run 6**

The following change was done to tpa.inp:

ThermalConductivityofYMRock[W/(m-K)]= 1.0e-10

The output files were saved as

6ebsfail.ech
6infilper.res
6totdose.res
6tpa.inp

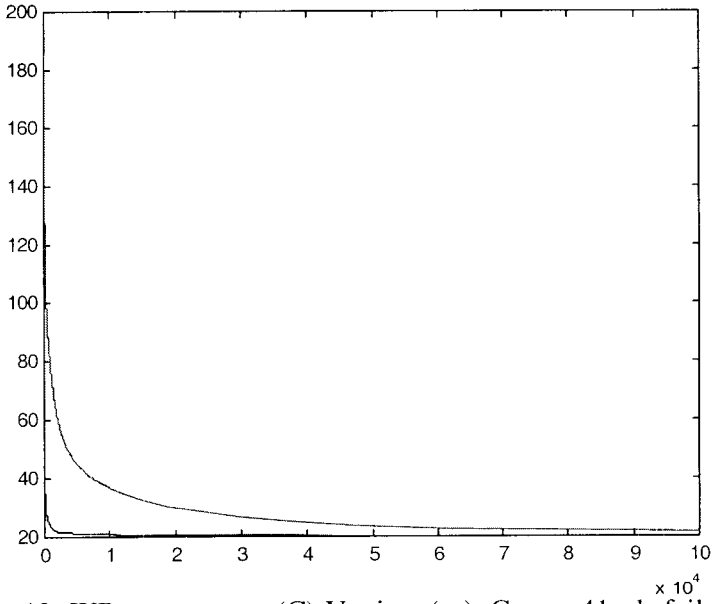



Figure 13: WP temperature (C) Vs time (yr). Green: 41eebsfail.ech. Blue: 6ebsfail.ech

The above figure shows that by changing ThermalConductivityofYMRock[W/(m-K)] the temperature is affected. Therefore, changing ThermalConductivityofYMRock[W/(m-K)] to eliminate refluxing is not an adequate choice.

**Run 7**

The following change was done to 41etpa.inp:

DensityOfWaterAtBoiling[kg/m^3]= 1.0e+10

The output files were saved as

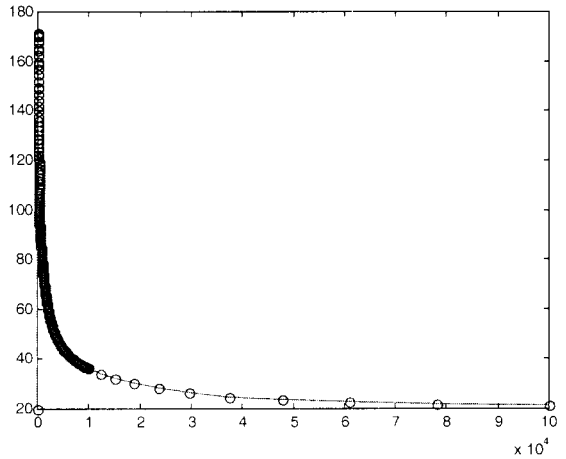



Figure 15: Repository temperature (C) Vs time (yr). Blue circles: 7ebsfail.ech. Green line: 41eebsfail.ech

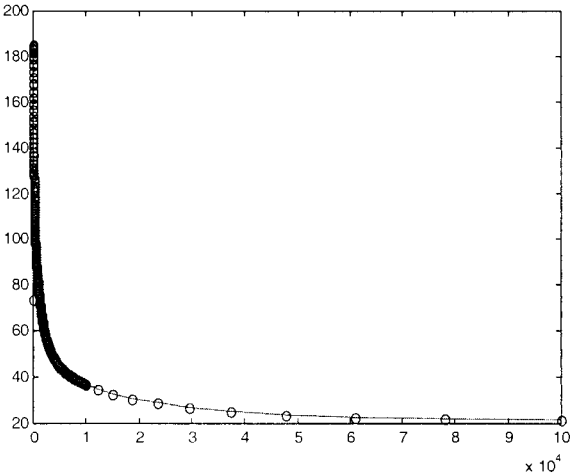



Figure 14: WP temperature (C) Vs time (yr). Blue circles: 7ebsfail.ech. Green line: 41eebsfail.ech

7ebsfail.ech
7infilper.res
7totdose.res

7tpa.inp

Therefore, changing the density of water does not change the temperature profile. The next page shows a copy of the file 7infilper.res

```
Input file tpa.inp as supplied with TPA Version 4.1e Code.
 Base case.
 TPA 4.1e, Job started: Tue Feb 13 15:56:04 2001
 Subarea Averaged Infiltration/Deep Percolation Including

 After Reflux and Diversion - Values for Each Vector
```

| vector | time | avinfil | avreflux | avdivert |
|---|---|---|---|---|
| unitless | yr | mm/yr | mm/yr | mm/yr |
| 1 | 0.0000E+00 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.5694E+01 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 5.8078E+01 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 9.8894E+01 | 1.2173E+01 | 1.2173E+01 | 9.4289E-02 |
| 1 | 1.5034E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 2.1518E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 2.9690E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 3.9990E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 5.2972E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 6.9334E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 8.9957E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 1.1595E+03 | 1.2377E+01 | 1.2377E+01 | 9.5874E-02 |
| 1 | 1.4871E+03 | 1.2646E+01 | 1.2639E+01 | 9.7901E-02 |
| 1 | 1.9000E+03 | 1.2790E+01 | 1.2790E+01 | 9.9067E-02 |
| 1 | 2.4204E+03 | 1.3254E+01 | 1.3254E+01 | 1.0267E-01 |
| 1 | 3.0764E+03 | 1.4333E+01 | 1.4333E+01 | 1.1102E-01 |
| 1 | 3.9031E+03 | 1.4938E+01 | 1.4938E+01 | 1.1571E-01 |
| 1 | 4.9451E+03 | 1.6668E+01 | 1.6665E+01 | 1.2908E-01 |
| 1 | 6.2584E+03 | 1.8642E+01 | 1.8642E+01 | 1.4440E-01 |
| 1 | 7.9137E+03 | 2.2091E+01 | 2.2088E+01 | 1.7109E-01 |
| 1 | 1.0000E+04 | 2.9496E+01 | 2.9481E+01 | 2.2836E-01 |
| 1 | 1.0000E+05 | 1.6612E+01 | 1.6612E+01 | 1.2867E-01 |

```
~
~
"7infilper.res" 30 lines, 2404 characters
```

In the above file it is seen that the columns avinfil and avreflux have identical numbers. Therefore, refluxing is indeed being eliminated.

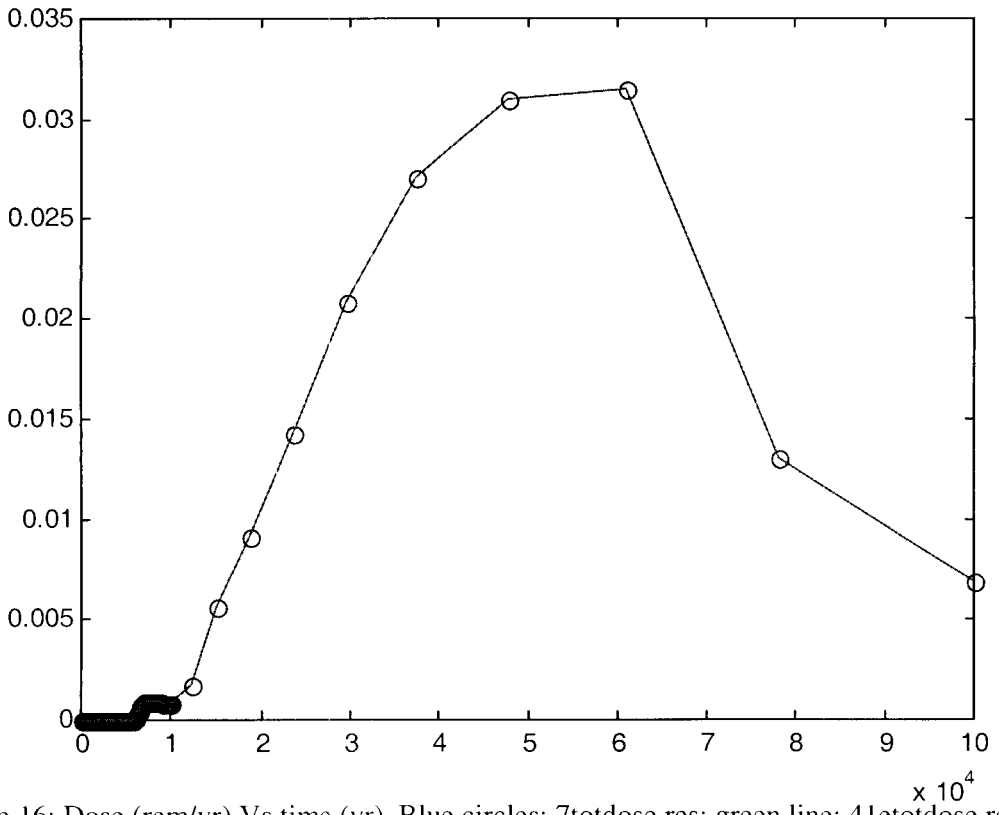
Input file tpa.inp as supplied with TPA Version 4.1e Code.
Base case.
TPA 4.1e, Job started: Tue Feb 13 14:06:25 2001
Subarea Averaged Infiltration/Deep Percolation Including

After Reflux and Diversion - Values for Each Vector

| vector | time | avinfil | avreflux | avdivert |
|---|---|---|---|---|
| unitless | yr | mm/yr | mm/yr | mm/yr |
| 1 | 0.0000E+00 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.5694E+01 | 1.2173E+01 | 1.1830E+01 | 9.1632E-02 |
| 1 | 5.8078E+01 | 1.2173E+01 | 1.2249E+01 | 9.4876E-02 |
| 1 | 9.8894E+01 | 1.2173E+01 | 1.0870E+01 | 8.4199E-02 |
| 1 | 1.5034E+02 | 1.2173E+01 | 1.1630E+01 | 9.0083E-02 |
| 1 | 2.1518E+02 | 1.2173E+01 | 1.2148E+01 | 9.4100E-02 |
| 1 | 2.9690E+02 | 1.2173E+01 | 1.2148E+01 | 9.4098E-02 |
| 1 | 3.9990E+02 | 1.2173E+01 | 1.2267E+01 | 9.5021E-02 |
| 1 | 5.2972E+02 | 1.2173E+01 | 1.2387E+01 | 9.5947E-02 |
| 1 | 6.9334E+02 | 1.2173E+01 | 1.2322E+01 | 9.5444E-02 |
| 1 | 8.9957E+02 | 1.2173E+01 | 1.2289E+01 | 9.5191E-02 |
| 1 | 1.1595E+03 | 1.2377E+01 | 1.2377E+01 | 9.5874E-02 |
| 1 | 1.4871E+03 | 1.2646E+01 | 1.2636E+01 | 9.7876E-02 |
| 1 | 1.9000E+03 | 1.2790E+01 | 1.2790E+01 | 9.9067E-02 |
| 1 | 2.4204E+03 | 1.3254E+01 | 1.3254E+01 | 1.0267E-01 |
| 1 | 3.0764E+03 | 1.4333E+01 | 1.4333E+01 | 1.1102E-01 |
| 1 | 3.9031E+03 | 1.4938E+01 | 1.4938E+01 | 1.1571E-01 |
| 1 | 4.9451E+03 | 1.6668E+01 | 1.6663E+01 | 1.2907E-01 |
| 1 | 6.2584E+03 | 1.8642E+01 | 1.8642E+01 | 1.4440E-01 |
| 1 | 7.9137E+03 | 2.2091E+01 | 2.2087E+01 | 1.7108E-01 |
| 1 | 1.0000E+04 | 2.9496E+01 | 2.9476E+01 | 2.2832E-01 |
| 1 | 1.0000E+05 | 1.6612E+01 | 1.6612E+01 | 1.2867E-01 |

~
~
"41einfilper.res" 30 lines, 2404 characters

Note that the avinfil column for the files 41einfilper.res and 7infilper.res are identical. We can conclude that the only effect of changing the water density is in the reflux computations.




The above plot shows that changing DensityOfWaterAtBoiling does not have any other effect on the dose. It only affects reflux phenomena.

Figure 16: Dose (rem/yr) Vs time (yr). Blue circles: 7totdose.res; green line: 41etotdose.res

**Run 8**

The following changes were done to 41etpa.inp:

MassDensityofYMRock[kg/m^3] = 1.0e-27 (very low mass density. Same value as importance analysis for TPA 3.2)

SpecificHeatofYMRock[J/(kg-K)] = 0.1 (very low specific heat. Same value as importance analysis for TPA 3.2)

ThermalConductivityofYMRock[W/(m-K)] = 1000.0 (very high thermal conductivity. Same value as importance analysis for TPA 3.2)

EmissivityOfDriftWall[-] = 0.4 (base case emissivity = 0.8. Same value as importance analysis for TPA 3.2. Same value as importance analysis for TPA 3.2)

This was the selection in TPA 3.2 to eliminate the UZ above the repository.

The output files were saved as
8ebsfail.ech
8infilper.res
8totdose.res
8tpa.inp

A copy of 8infilper.res is next supplied:

"8infilper.res" 30 lines, 2404 characters
Input file tpa.inp as supplied with TPA Version 4.1e Code.
Base case.
TPA 4.1e, Job started: Tue Feb 13 16:29:43 2001
Subarea Averaged Infiltration/Deep Percolation Including

After Reflux and Diversion - Values for Each Vector

| vector unitless | time yr | avinfil mm/yr | avreflux mm/yr | avdivert mm/yr |
|---|---|---|---|---|
| 1 | 0.0000E+00 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.5694E+01 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 5.8078E+01 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 9.8894E+01 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 1.5034E+02 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.1518E+02 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.9690E+02 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 3.9990E+02 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 5.2972E+02 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 6.9334E+02 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 8.9957E+02 | 1.2173E+01 | 5.9051E+01 | 4.5740E-01 |
| 1 | 1.1595E+03 | 1.2377E+01 | 1.2377E+01 | 9.5874E-02 |
| 1 | 1.4871E+03 | 1.2646E+01 | 1.2632E+01 | 9.7844E-02 |
| 1 | 1.9000E+03 | 1.2790E+01 | 1.2790E+01 | 9.9067E-02 |
| 1 | 2.4204E+03 | 1.3254E+01 | 1.3254E+01 | 1.0267E-01 |
| 1 | 3.0764E+03 | 1.4333E+01 | 1.4333E+01 | 1.1102E-01 |
| 1 | 3.9031E+03 | 1.4938E+01 | 1.4938E+01 | 1.1571E-01 |
| 1 | 4.9451E+03 | 1.6668E+01 | 1.6661E+01 | 1.2906E-01 |
| 1 | 6.2584E+03 | 1.8642E+01 | 1.8642E+01 | 1.4440E-01 |
| 1 | 7.9137E+03 | 2.2091E+01 | 2.2085E+01 | 1.7107E-01 |
| 1 | 1.0000E+04 | 2.9496E+01 | 2.9466E+01 | 2.2824E-01 |
| 1 | 1.0000E+05 | 1.6612E+01 | 1.6612E+01 | 1.2867E-01 |

~
"8infilper.res" 30 lines, 2404 characters

Note that the numbers under avinfil and avreflux columns are different. Therefore, the parameters in TPA 3.2 selected to get rid of the UZ above the repository are not an adequate choice.

**Run 9**

The following change was done to 41etpa.inp:
EnthalpyOfPhaseChangeForWater[J/kg] = 1.0e+20

The input and output files were saved as
9ebsfail.ech
9infilper.res

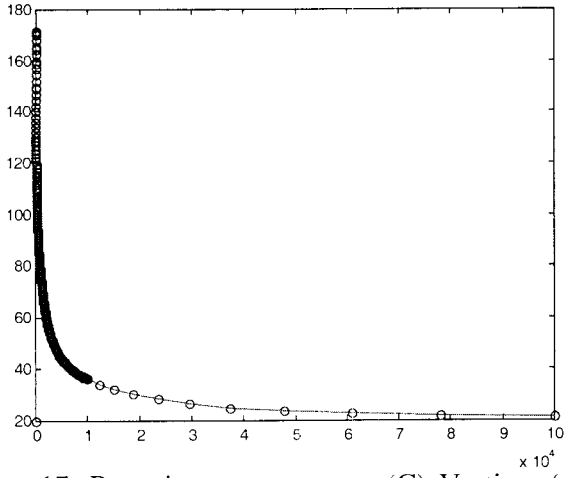



Figure 17: Repository temperature (C) Vs time (yr) Blue circles: 9ebsfail.ech. Green line: 41eebsfail.ech

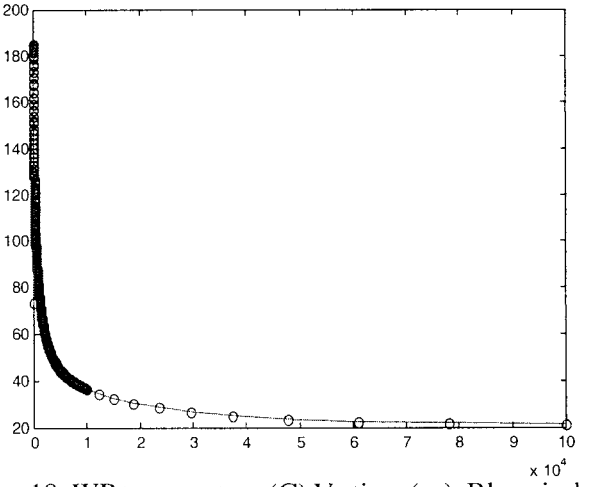



Figure 18: WP temperature (C) Vs time (yr). Blue circles: 9ebsfail.ech. Green line: 41eebsfail.ech

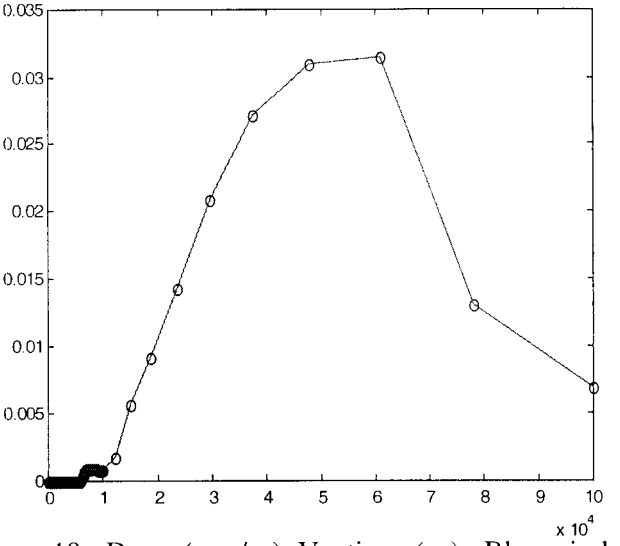



Figure 19: Dose (rem/yr) Vs time (yr). Blue circles: 7totdose.res; green line: 41etotdose.res

Note that the above results are identical to results of Run 41e. Furthermore, the output file 9infilper.res is

```
Input file tpa.inp as supplied with TPA Version 4.1e Code.
 Base case.
 TPA 4.1e, Job started: Tue Feb 13 16:41:17 2001
 Subarea Averaged Infiltration/Deep Percolation Including

 After Reflux and Diversion - Values for Each Vector
```

| vector | time | avinfil | avreflux | avdivert |
|---|---|---|---|---|
| unitless | yr | mm/yr | mm/yr | mm/yr |
| 1 | 0.0000E+00 | 1.2173E+01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 2.5694E+01 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 5.8078E+01 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 9.8894E+01 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 1.5034E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 2.1518E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 2.9690E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 3.9990E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 5.2972E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 6.9334E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 8.9957E+02 | 1.2173E+01 | 1.2173E+01 | 9.4290E-02 |
| 1 | 1.1595E+03 | 1.2377E+01 | 1.2377E+01 | 9.5874E-02 |
| 1 | 1.4871E+03 | 1.2646E+01 | 1.2639E+01 | 9.7901E-02 |
| 1 | 1.9000E+03 | 1.2790E+01 | 1.2790E+01 | 9.9067E-02 |
| 1 | 2.4204E+03 | 1.3254E+01 | 1.3254E+01 | 1.0267E-01 |
| 1 | 3.0764E+03 | 1.4333E+01 | 1.4333E+01 | 1.1102E-01 |
| 1 | 3.9031E+03 | 1.4938E+01 | 1.4938E+01 | 1.1571E-01 |
| 1 | 4.9451E+03 | 1.6668E+01 | 1.6665E+01 | 1.2908E-01 |
| 1 | 6.2584E+03 | 1.8642E+01 | 1.8642E+01 | 1.4440E-01 |
| 1 | 7.9137E+03 | 2.2091E+01 | 2.2088E+01 | 1.7109E-01 |
| 1 | 1.0000E+04 | 2.9496E+01 | 2.9481E+01 | 2.2836E-01 |
| 1 | 1.0000E+05 | 1.6612E+01 | 1.6612E+01 | 1.2867E-01 |

```
~
"9infilper.res" 30 lines, 2404 characters
```

Therefore by changing EnthalpyOfPhaseChangeForWater[J/kg] reflux can be eliminated without any additional consequence.

**Conclusion of computations on February 13, 2001:**

**
BARRIER = 'BarrierUpperUnsaturatedZoneStudy'
**
**Component** = 'ComponentTivaCanyonStudy'
**
THIS BARRIER MAY NOT BE WELL IMPLEMENTED. SEE NOTE ON February 13, 2001.

parameter = 'Reflux2SatInit'
value = 0.1 (equal to Reflux2SatResid. This causes the amount of water available for refluxing equal to zero. See Equation (5-25) in the TPA manual for version 4.0)
**
parameter = 'DensityOfWaterAtBoiling[kg/m^3]'
value = 1.0e+10 (Very high density. This selection causes the penetration distance, L, in equation (5-28) in the TPA manual for version 4.0 to be extremely large. Another possibility is selecting EnthalpyOfPhaseChangeForWater[J/kg] = 1.0e+20. Both selections have similar implications and are equally valid to eliminate refluxing. Test results reported above justify these selections. )
**
parameter = 'FractionOfCondensateRemoved[1/yr]'
value = 0.0 (no water removed after condensation)
**
parameter = 'FractionOfCondensateTowardRepository[1/yr]'
value =1.0 (all water goes back to the drifts)
**
parameter = 'FractionOfCondensateTowardRepositoryRemoved[1/yr]'
value = 0.0 (no water removed after reflux)
**
parameter = 'ChlorideMultFactor'
value = 0.0 (zero chloride concentration. Setting this number equal to zero does not cause any problem)
**
parameter = 'ChlorideMultFactorIntactDripShield'
value = 0.0 (zero chloride concentration. Setting this number equal to zero does not cause any problem)
**

Contents of disk submitted to QA records on 04/03/2001

Contents of 'D:\Osvaldo\PA\ia41'

| Name | Size | Type | Modified |
|---|---|---|---|
| 6infilper.res | 3KB | RES File | 2/13/01 4:25 PM |
| 6totdose.res | 14KB | RES File | 2/13/01 4:25 PM |
| 6tpa.inp | 60KB | INP File | 2/13/01 4:25 PM |
| 7ebsfail.ech | 20KB | ECH File | 2/13/01 4:59 PM |
| 7infilper.res | 3KB | RES File | 2/13/01 4:57 PM |
| 7totdose.res | 14KB | RES File | 2/13/01 5:16 PM |
| 7tpa.inp | 60KB | INP File | 2/13/01 4:57 PM |
| 8ebsfail.ech | 20KB | ECH File | 2/13/01 5:32 PM |
| 8infilper.res | 3KB | RES File | 2/13/01 5:32 PM |
| 8totdose.res | 14KB | RES File | 2/13/01 5:32 PM |
| 8tpa.inp | 60KB | INP File | 2/13/01 5:32 PM |
| 9ebsfail.ech | 20KB | ECH File | 2/13/01 5:45 PM |
| 9infilper.res | 3KB | RES File | 2/13/01 5:42 PM |
| 9totdose.res | 14KB | RES File | 2/13/01 5:44 PM |
| 9tpa.inp | 60KB | INP File | 2/13/01 5:42 PM |
| cpfiles | 1KB | File | 2/13/01 4:24 PM |
| ebsfail.ech | 20KB | ECH File | 2/13/01 4:24 PM |
| handy.m | 1KB | Matlab files | 2/13/01 6:30 PM |
| ia.dat | 8KB | DAT File | 2/13/01 6:11 PM |
| ia.f | 31KB | F File | 9/21/00 6:16 PM |
| iaComments.wpd | 507KB | Corel WordPerfect 8 ... | 2/13/01 6:54 PM |
| iaOsv.dat | 8KB | DAT File | 9/26/00 10:46 AM |
| ImportanceAnalysisTable.xls | 25KB | Microsoft Excel Work... | 7/28/00 6:05 PM |
| infilper.res | 3KB | RES File | 2/13/01 4:24 PM |
| infilperUZ.res | 3KB | RES File | 9/26/00 11:08 AM |
| mirror.bat | 1KB | MS-DOS Batch File | 2/13/01 6:41 PM |
| plots.ppt | 35KB | Microsoft PowerPoint... | 9/25/00 3:52 PM |
| poros.m | 1KB | Matlab files | 9/25/00 3:31 PM |
| readme.txt | 1KB | TXT File | 2/13/01 6:30 PM |
| totdose.res | 14KB | RES File | 2/13/01 4:24 PM |
| totdose1.res | 14KB | RES File | 9/25/00 3:24 PM |
| totdose2.res | 14KB | RES File | 9/25/00 3:00 PM |
| totdose3.res | 14KB | RES File | 9/25/00 3:01 PM |
| totdose4.res | 14KB | RES File | 9/25/00 3:01 PM |
| totdose5.res | 14KB | RES File | 9/25/00 3:02 PM |
| totdoseUZ.res | 13KB | RES File | 9/26/00 11:09 AM |
| tpa.inp | 61KB | INP File | 9/25/00 9:59 AM |
| tpa1.inp | 61KB | INP File | 9/25/00 12:15 PM |
| tpa2.inp | 61KB | INP File | 9/25/00 12:15 PM |
| tpa3.inp | 61KB | INP File | 9/25/00 12:19 PM |
| tpa4.inp | 61KB | INP File | 9/25/00 12:25 PM |
| tpa5.inp | 56KB | INP File | 9/25/00 2:52 PM |
| tpaUZ.inp | 56KB | INP File | 9/26/00 11:06 AM |

***This page formerly contained the statement page for the six month submittal of data to Quality Assurance in accordance with QAP-001.***

**Testing of TPA Code**

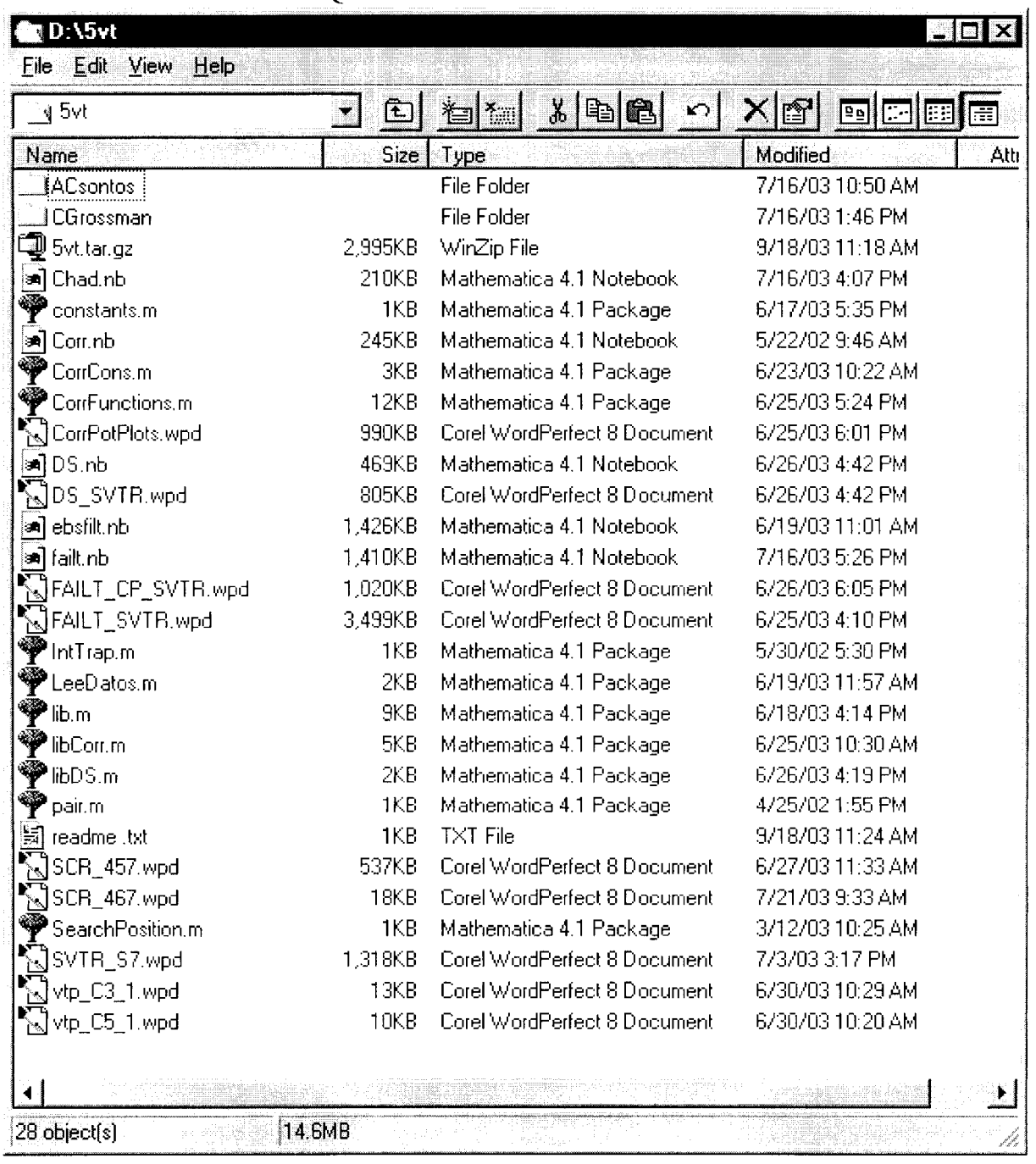
A series of software validation test reports were prepared to document validation testing of TPA 5.0. The following validation reports were written by Osvaldo Pensado, Christopher Grossman (NRC), Al Csontos (NRC), and David Esh (NRC).

Test IDs were identified in the Software Validation Testing Plan for TPA 5.0. A copy of this document must be available in the library and quality-assurance records. The above mentioned people were in charge of the following tests

S7 (transfer of data between DSFAILT and EXEC)
C3-1 and C5-1 (transfer of data between FAILT, WELDFAILT and EXEC)
C3-3 and C3-5 (comparison to simple computations of waste package and weld failure by general corrosion)
C3-4 (compare FAILT outputs to previously generated data)
C4-2 (drip shield failure by general corrosion)

The software validation test reports are complete documents that do not necessitate additional explanation. Some relevant data is attached in the form of a CD-R in case some of these tests need to be repeated in the future. The Mathematica notebooks (files with extension nb) are self-explanatory, with abundant notes, for future reproduction. The version of Mathematica used was 4.1. The files *.m are Mathematica package files containing scripts written in Mathematica language.

Contents of CD submitted to QA records on 9-19-2003



Entries into Scientific Notebook 170-9e for the period September 11, 2000 to April 3, 2001 have been made by

OAP 4/3/2001

Osvaldo Pensado Date

Entries into Scientific Notebook No. 170 for pages 95 to 121 have been made by

OAP 4/3/2001

Osvaldo Pensado Date

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

OAP 4/3/2001

Osvaldo Pensado Date

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.

James Winterle 11-09-05

Page form when received for review

JRW 11-9-05

121A JRW 11-9-05