# SCIENTIFIC NOTEBOOK
# NUMBER 185, VOLUME 7

by

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The entries in this notebook #185, Volume 7, document activities conducted during the period Oct 1, 1998 to Dec. 31, 1998, under the EVAL KT/ (Proj. # 20-1402-561).

**11/10/98**

**Below is a copy of an email from S. Mohanty advising of the availability of TPA 3.2 code:**

Date: 11/6/98
"
Sender: Sitakanta Mohanty
"
To: #SA-WO_TECH, #DIRS-MGRS
"
Priority: Normal
"
Subject: how to use tpa3.2 code (revised)

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Please disregard my previous memo

---

The TPA Version 3.2 code and data files are now available for use. The new set up protocol is easier than what we had for TPA code versions 3.1.1-4. Please use the following procedure for a quick start.

Log onto a SUN work-station using your account number and password. If you are a former TPA code user, remove the directory tparun (or TPARUN). The following commands will set up the new environment:

"rm -r tparun" and hit "enter"
"/solapps/bin/setuptpa" and hit "enter"

At this point, log out and log back in. To run the TPA code, go to the directory tparun and execute the code by using the following command lines.

"cd tparun" and hit "enter"
"tpa.e" and hit "enter"

Please call me or Ron if you have difficulties with executing the code. Contact Ray if you have problem setting up the environment.

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The following is the site where you can access TPA code outputs for selected cases, including three 1000-realization runs. These 1000-realization runs are for (1) nominal case, (2) with faulto, and (3) with volcano. Please read the README file in /tpa. This directory is located on bigbend. If you have problem accessing

it, please contact Ray.

**12/10/98**

**Below is a copy of an email from Rob Rice, advising that he has completed running TPA 3.2 with and without invoking EBSFILT, a new module designed to simulate the presence of cementitious inverts in the repository.**

"
Date: 12/7/98
"
Sender: Robert Rice
To: Roberto Pabalan
cc: Sitakanta Mohanty, Gordon Wittmeyer
Priority: Normal
Subject: TPA runs with new invert properties

---

Bobby,

I have completed two runs using the Environment III Kds and the invert properties you provided in Tables 1 and 2 of your August 24, 1998 memo. These runs were performed (1) with the ebsfilt module and (2) bypassing the ebsfilt module. The output files are currently in my temp directory on bigbend at /bscr0/rrice/invert/ebsfilt (run ebsfilt) and /bscr0/rrice/invert/bypass (bypass ebsfilt). I would suggest copying these files to your site since /bscr0/ is cleaned weekly.

If you have any questions about these runs, please get in touch with me.

Thanks,

Rob

note: I did a little bit of snooping through the results and found that it looks like ebsfilt runs only four times in the 250 realizations (because of the average flow rate through the simulation time compared to invert permeability issue that we discussed earlier)

**For the record, the following is a copy of my memo regarding recommended values for invert properties:**

**DATE:** August 24, 1998

**TO:** S. Mohanty

**FROM:** R. Pabalan

**SUBJECT:** Base-case input parameters for concrete invert in EBSFILT model

Per Bret Leslie's request, the values of hydraulic, sorption, and other parameters pertinent to the concrete invert that is modeled in the EBSFILT addition to TPA 3.2 are listed in the attached tables. Also given are references for the listed values. Please contact me if you have any questions or comments.

cc: G. Wittmeyer
E. Pearcy
W. Murphy
B. Leslie

**Table 1. Radionuclide Kds cement environments for use with EBSFILT model of TPA 3.2. Values were taken mostly from Campbell and Krupka (1997) and also from Bradbury and Sarott (1995). For TPA 3.2 base-case, values in column-3 are recommended.**

| Element | Kd ($m^3$/kg) for cement Environment II[1] | Kd ($m^3$/kg) for cement Environment III[1] |
|---|---|---|
| Am | 5 | 0.5 |
| Np | 2 | 0.2 |
| I | 0.005 | 0.001 |
| Tc | 0 | 0 |
| Cl | 0.001 | 0 |
| Cm | 5[2] | 1[2] |
| U | 1 | 0.1 |
| Pu | 5 | 0.5 |
| Th | 5 | 0.5 |
| Ra | 0.1 | 0.1 |
| Pb | 0.5[2] | 0.05[2] |
| Cs | 0.02[2] | 0.02[2] |
| Ni | 0.1 | 0.01 |
| C | 0.1 | 0.01 |
| Se | 0.0001[2] | 0[2] |
| Nb | 1 | 0.1 |

[1]Environment II corresponds to the time period when the dissolution of portlandite buffers the pH of the system to about 12.5 (Campbell and Krupka, 1997). Environment III corresponds to the time period when the solubility of CSH phases buffers the pH to values between 12.5 and 10.5. Environment I (Kd values for which are not listed here) corresponds to the initial high pH, high ionic strength environment (pH>12.5) created by leaching of NaOH and KOH from the cement matrix.

[2]Values taken from Bradbury and Sarott (1995).

**Table 2. Porosity, permeability, diffusion coefficient, and thickness of concrete invert**

| Parameter | Value | Reference |
|---|---|---|
| InvertRockPorosity | 0.30 | Green et al. (1995) |
| InvertThickness[m] | 0.75 | Snell (1997)* |
| InvertDiffusionCoefficient[m^2/yr] | 4.4e-5 | Clifton et al. (1991) |
| InvertMatrixPermeability[m^2] | 2.0e-17, 2.0e-18 | Green et al. (1995) |

*Letter report of R.D. Snell (Manager, Engineering and Integration Operations, M&O Contractor) to S.J. Brocoum (Assistant Manager for Licensing, U.S. DOE), dated March 25, 1997, "Transmittal of Subsurface Engineered Barrier (EB) Segment Design, Deliverable RP120M3E, WBS 1.2.4.7," LV.RD.DGM.3/97.007.

**REFERENCES:**


Bradbury, M. H., and F.A. Sarott. 1995. *Sorption Databases for the Cementitious Near-Field of a L/ILW Repository for Performance Assessment.* PSI 95-06. Villigen, Switzerland: Paul Scherrer Institute.

Campbell, A.C., and K.M. Krupka. 1997. Application of geochemical data and modeling in performance assessments of low-level radioactive waste disposal facilities. Symposium on Hydrogeologic and Geochemical Aspects of Waste Disposal. Waste Management '97, March 4, 1997, Tucson, Arizona.

Clifton, J.R., L.I. Knab, E.J. Garboczi, L.X. Xiong. 1991. *Chloride Ion Diffusion in Low Water-to-Solid Cement Pastes.* NUREG/CR-5727. Washington, DC: U.S. Nuclear Regulatory Commission.

Green, R.T., F.T. Dodge, S.J. Svedeman, R.D. Manteufel, G. Rice, K.A. Meyer, and R.G. Baca. 1995. Thermally Driven Moisture Redistribution in Partially Saturated Porous Media. NUREG/CR-6348. Washington DC: U.S. Nuclear Regulatory Commission.


**The Kd values were converted by Rob Rice to Rf values, as discussed in the following email from Rob Rice:**

```
Date:              12/10/98
"
Sender:              Robert Rice
To:               Roberto Pabalan
cc:               Sitakanta Mohanty, Gordon Wittmeyer, Ronald Janetzke
Priority:              Normal
Subject:             Invert Retardation Factors
               ------------------------------------------------------------

               Bobby,
```

As per our discussion this afternoon at 1:15, I am sending to you the EXCEL file with the Environment II and Environment III Kd and Rd values. The Environment III Rds were used in the two runs that I have supplied to you (running ebsfilt and bypassing ebsfilt).

Please contact me if you have any questions regarding this information.

Thanks,

Rob

## Rds for Cement
## Environment II

Rd = 1 + [bulk density * Kd / porosity]

porosity = 0.3
bulk density = 1800 kg/m^3

| Element | Kd (m^3/kg) | Rd - |
|---|---|---|
| Am | 5 | 30001 |
| Np | 2 | 12001 |
| I | 0.005 | 31 |
| Tc | 0 | 1 |
| Cl | 0.001 | 7 |
| Cm | 5 | 30001 |
| U | 1 | 6001 |
| Pu | 5 | 30001 |
| Th | 5 | 30001 |
| Ra | 0.1 | 601 |
| Pb | 0.5 | 3001 |
| Cs | 0.02 | 121 |
| Ni | 0.1 | 601 |
| C | 0.1 | 601 |
| Se | 0.0001 | 1.6 |
| Nb | 1 | 6001 |

- Kds from 8/24/98 memo from R. Pabalan to S. Mohanty
- porosity and bulk density from R. Pabalan 11/11/98

## Rds for Cement Environment III

Rd = 1 + [bulk density * Kd / porosity]

porosity = 0.3
bulk density = 1800 kg/m^3

| Element | Kd (m^3/kg) | Rd - |
|---|---|---|
| Am | 0.5 | 3001 |
| Np | 0.2 | 1201 |
| I | 0.001 | 7 |
| Tc | 0 | 1 |
| Cl | 0 | 1 |
| Cm | 1 | 6001 |
| U | 0.1 | 601 |
| Pu | 0.5 | 3001 |
| Th | 0.5 | 3001 |
| Ra | 0.1 | 601 |
| Pb | 0.05 | 301 |
| Cs | 0.02 | 121 |
| Ni | 0.01 | 61 |
| C | 0.01 | 61 |
| Se | 0 | 1 |
| Nb | 0.1 | 601 |

- Kds from 8/24/98 memo from R. Pabalan to S. Mohanty
- porosity and bulk density from R. Pabalan 11/11/98

**Note that the values of matrix permeability used in the TPA 3.2 runs were in the range 2E-16 to 2E-18, instead of the 2E-17 to 2E-18 range recommended in the Aug. 24, 1998, memo from R. Pabalan to S. Mohanty. This change was done because a preliminary run by Rob Rice indicated that EBSFILT was not being called by the TPA 3.2 code because the mean flow rate was always larger than the invert matrix permeability, thus flow through the invert is unretarded.**

**The following is the input file used by Rob Rice for the case where the EBSFILT switch is "on".**

```
title
~
 Input file tpa.inp as
supplied with TPA Version
3.2 Code.
~
 Base case data set Rev 3.2
7/16/98
~
**
~
**          ***>>>  GLOBAL
PARAMETERS   <<<***
**
**
**          ***>>>
Disruptive Scenario flags
<<<***
**
iflag
VolcanismDisruptiveScenario
Flag(yes=1,no=0)
0
**
iflag
FaultingDisruptiveScenarioF
lag(yes=1,no=0)
0
**
iflag
SeismicDisruptiveScenarioFl
ag(yes=1,no=0)
1
**
**
**          ***>>> Subarea
Size  <<<***
**
```

```
**
** Number and Location Of
SubAreas[m] Based On
Fig3.4-1 in TSPA95
**subarea
**1
**ZONE T="ONE RECTANGULAR
ZONE SUBAREA", F=POINT
**        547405.7
4076362.2
**        548469.3
4076362.2
**        548469.3
4079237.8
**        547405.7
4079237.8
**        547405.7
4076362.2
subarea
7
ZONE T="Subarea
1",I=5,F=POINT
547472.0, 4079323.7
548069.2, 4079136.5
547847.3, 4077816.2
547318.4, 4077934.0
547472.0, 4079323.7
ZONE T="Subarea
2",I=5,F=POINT
548069.2, 4079136.5
548609.7, 4078968.6
548547.9, 4077654.1
547847.3, 4077816.2
548069.2, 4079136.5
ZONE T="Subarea
3",I=5,F=POINT
547318.4, 4077934.0
547847.3, 4077816.2
548322.7, 4077192.2
547474.7, 4077281.6
547318.4, 4077934.0
ZONE T="Subarea
4",I=5,F=POINT
547847.3, 4077816.2
548547.9, 4077654.1
548504.8, 4077170.0
548322.7, 4077192.2
547847.3, 4077816.2
ZONE T="Subarea
5",I=5,F=POINT
547474.7, 4077282.6
547887.3, 4077238.1
547995.0, 4076338.9
547670.4, 4076435.5
547474.7, 4077282.6
ZONE T="Subarea
6",I=5,F=POINT
547887.3, 4077238.1
548322.7, 4077192.2
548319.5, 4076220.2
547995.0, 4076338.9
547887.3, 4077238.1
ZONE T="Subarea
7",I=5,F=POINT
548322.7, 4077192.2
548504.8, 4077170.0
548473.1, 4076533.7
548319.5, 4076220.2
548322.7, 4077192.2
**
iconstant
StartAtSubarea
1
**
iconstant
StopAtSubarea
7
**
**
**          ***>>> Nuclides
and Chains  <<<***
**
**  5/25/1998 tpa3.2 new
parameter section
**
**  Nuclides can be
eliminated from the
basecase set.
**  However, if additional
nuclides (Pu242, Am242m,
Pu238, Cm243,
**  U235, Pa231, Ac227,
Pu241, U233, Th229, Cm244,
U236, U232, Sm151,
**  Cs137, Sn126, Sn121m,
Ag108m, Pd107, Mo93, Zr93,
Sr90, or Ni63)
**  are added to the
basecase set, then
corresponding RDs, KDs,
**  solubilities, gap
fractions, and correlations
must be added.
**
iflag
CheckNuclidesAndChains(yes=
1,no=0)
0
**
aqueousnuclides
**   number of nuclides,
number of chains
20
13
**
**   chain 1
2
Cm246
U238
**   chain 2
3
Cm245
Am241
Np237
**   chain 3
2
Am243
Pu239
**   chain 4
1
Pu240
**   chain 5
4
U234
Th230
Ra226
Pb210
**   chain 6
1
Cs135
**   chain 7
1
I129
**   chain 8
1
Tc99
**   chain 9
1
Ni59
**   chain 10
1
C14
**   chain 11
1
Se79
**   chain 12
1
Nb94
**   chain 13
1
Cl36
**
endofnuclides
**
**
**          ***>>>
Parameter Sampling  <<<***
**
**  5/25/1998 tpa3.2 new
parameter;option to conduct
direct-release only
calculation
**
iflag
DirectReleaseOnlyFlag(yes=1
,no=0)
0
**
constant
SeedForRandomNumber
188910452.0
**
iflag
LatinHypercubeSampling(yes=
1,no=0)
1
**
iconstant
NumberOfRealizations
250
**
iconstant
StartAtRealization
1
**
iconstant
StopAtRealization
0
**
**
**          ***>>>
Simulation Times  <<<***
**
**  6/2/1998 tpa3.2 4 new
parameters; calculations at
two time periods
**
constant
DurationOfCompliancePeriod[
yr]
1.0e4
**
constant
```

```
MaximumTime[yr]
5.0e4
**
** Sum of pre- and post-
compliance time steps must
not exceed 201
**
iconstant
NumberOfTimeStepsInComplian
cePeriod
101
**
constant
RatioOfLastToFirstTimeStepI
nCompliancePeriod
100.0
**
**  Next two parameters
ignored if MaximumTime[yr]
=
DurationOfCompliancePeriod[
yr]
**
iconstant
NumberOfTimeStepsAfterCompl
iancePeriod
100
**
constant
RatioOfLastToFirstTimeStepA
fterCompliancePeriod
100.0
**
**
**    ***>>>  Output Print
Options  <<<***
**
iconstant
OutputMode(0=None,1=All,2=U
serDefined)
0
**
iconstant
UserDefinedLowerRealization
Appended
1
**
iconstant
UserDefinedUpperRealization
Appended
1
**
**  5/25/1998 tpa3.2 new
parameter
**
** Select Append Files
**   0 = append all files
**   1 = uzflow.ech and
uzflow.rlt only
**   2 = nfenv.ech and
nfenv.rlt only
**   3 = ebsfail.ech and
ebsfail.rlt only
**   4 = seismo.ech and
seismo.rlt only
**   5 = faulto.ech and
faulto.rlt only
**   6 = volcano.ech and
volcano.rlt only
**   7 = ebsrel.ech and
ebsrel.rlt only
**   8 = uzft.ech and
uzft.rlt only
**   9 = szft.ech and
szft.rlt only
**   10 = dcagw.ech and
dcagw.rlt only
**   11 = ashplumo.ech and
ashplumo.rlt only
**   12 = ashrmovo.ech and
ashrmovo.rlt only
**   13 = dcags.ech and
dcags.rlt only
**   14 = ashplume.cum only
**   15 = failt.cum only
**   16 = nefiiuz.cum only
**   17 = releaset.cum only
**
iconstant
SelectAppendFiles
0
**
**
**          ***>>> UZFLOW
<<<***
**
uniform
ArealAverageMeanAnnualInfil
trationAtStart[mm/yr]
1.0, 10.0
**
uniform
MeanAveragePrecipitationMul
tiplierAtGlacialMaximum
1.5, 2.5
**
uniform
MeanAverageTemperatureIncre
aseAtGlacialMaximum[degC]
-10, -5
**
constant
TimeStepForClimate[yr]
500.0
**
constant
StandardDeviationOfMAPAbout
MeanInOneTimePeriod[mm/yr]
0.0
**
constant
StandardDeviationOfMATAbout
MeanInOneTimePeriod[degC]
0.0
**
constant
CorrelationBetweenMAPAndMAT
-0.8
**
iconstant
ClimatePerturbationSet
1
**
**
**          ***>>> NFENV
<<<***
**
iflag
TabularTemperatureRHFlag(ye
s=1,no=0)
0
**
iconstant
nsetUsedToPickTempRHDataSet
1
**
**  6/2/98 tpa3.2  name
change for  UseReflux2
**
iconstant
SelectRefluxModel(1,2,3)
3
**
constant
LengthOfRefluxZone[m]
20
**
constant
MaximumFluxInRefluxZone[m/s
]
1.0e-9
**
constant
PerchedBucketVolumePerSAare
a[m3/m2]
0.5
**
constant
Reflux2Thickness
100.0
**
constant
Reflux2Porosity
0.14
**
constant
Reflux2SatInit
0.9
**
constant
Reflux2SatResid
0.1
**
constant
Reflux2Period
100.0
**
constant
Reflux2LossI
0.1
**
constant
Reflux2LossD
0.1
**
constant
WPLength[m]
5.682
**
constant
WPDiameter[m]
1.802
**
constant
EmplacementDriftDiameter[m]
5.0
**
constant
WPSpacingAlongEmplacementDr
ift[m]
19.0
**
```

```
**  6/4/98 tpa3.2: Next 4
new parameters specific to
reflux3 model
**
constant
WPUnitCellWidth[m]
22.5
**
loguniform
FractionOfCondensateRemoved
[1/yr]
1.0e-8, 1.0
**
uniform
FractionOfCondensateTowardR
epository[1/yr]
0.0, 1.0
**
loguniform
FractionOfCondensateTowardR
epositoryRemoved[1/yr]
1.0e-8, 1.0
**
constant
DensityOfWaterAtBoiling[kg/
m^3]
960.5
**
constant
EnthalpyOfPhaseChangeForWat
er[J/kg]
2.4e6
**
uniform
TemperatureGradientInVicini
tyOfBoilingIsotherm[K/m]
1.0, 100.0
**
constant
ArealMassLoading[MTU/acre]
83.0
**
constant
WastePackagePayload[MTU]
9.76
**
constant
AgeOfWaste[yr]
26.0
**
constant
AmbientRepositoryTemperatur
e[C]
20.0
**
constant
MassDensityofYMRock[kg/m^3]
2580.0
**
constant
SpecificHeatofYMRock[J/(kg-
K)]
840.0
**
uniform
ThermalConductivityofYMRock
[W/(m-K)]
1.8, 2.2
**
constant
EmissivityOfDriftWall[-]
0.8
**
constant
EmissivityOfWastePackage[-]
0.7
**
constant
ThermalConductivityOfFloor[
W/(m-C)]
0.6
**
constant
EffectiveThermalConductivit
yOfUnbackfilledDrift[W/(m-
C)]
0.90
**
constant
TimeOfBackfillEmplaced[yr]
100001.0
**
constant
EffectiveThermalConductivit
yOfBackfill[W/(m-C)]
0.60
**
constant
ThermalConductivityOfInnerS
tainlessSteelWall[W/m-C]
15.0
**
constant
ThermalConductivityOfOuterC
arbonSteelWall[W/m-C]
50.0
**
constant
EffectiveThermalConductivit
yOfBasket&SFinWP[W/(m-C)]
1.0
**
constant
ElevationOfRepositoryHorizo
n[m]
1072.0
**
constant
ElevationOfGroundSurface[m]
1400.0
**
**
**          ***>>>  EBSFAIL
<<<***
**
constant
OuterWPThickness[m]
0.1
**
constant
InnerWPThickness[m]
0.02
**
constant
MetalGrainRadius[micrometer
]
13.75
**
constant
GrainBoundaryThickness[micr
ometer]
7.0e-4
**
constant
DryOxidationConstant
0.00001
**
constant
CriticalRelativeHumidityHum
idAirCorrosion
0.55
**
normal
CriticalRelativeHumidityAqu
eousCorrosion
0.75, 0.85
**
uniform
ThicknessOfWaterFilm[m]
0.001, 0.003
**
constant
BoilingPointOfWater[C]
97.0
**
constant
OuterOverpackErpIntercept
-620.3
**
constant
TempCoefOfOuterPackErpInter
cept
0.47
**
constant
OuterOverpackErpSlope
-95.2
**
constant
TempCoefOfOuterPackErpSlope
0.88
**
uniform
InnerOverpackErpIntercept
1040.0,   1240.0
**48.5, 148.5  >>> 625 <<<
**
constant
TempCoefOfInnerPackErpInter
cept
0.0
**
constant
InnerOverpackErpSlope
0.0
**-160.8   >>> 625 <<<
**
constant
TempCoefOfInnerPackErpSlope
0.0
**
constant
OuterWPBetaKineticsParamete
rforOxygen
0.75
**
constant
OuterWPBetaKineticsParamete
rforWater
0.5
**
constant
```

```
InnerWPBetaKineticsParamete
rforOxygen
0.75
**
constant
InnerWPBetaKineticsParamete
rforWater
0.5
**
constant
OuterWPRateConstantforOxyge
nReduction[coulomb-
m/mole/yr]
3.8e12
**
constant
OuterWPRateConstantforWater
Reduction[coulomb-m/m^2/yr]
1.6e-1
**
constant
OuterWPActivationEnergyforO
xygenReduction[J/mole]
37300.0
**
constant
OuterWPActivationEnergyforW
aterReduction[J/mole]
25000.0
**
constant
InnerWPRateConstantforOxyge
nReduction[coulomb-
m/mole/yr]
3.0e10
**
constant
InnerWPRateConstantforWater
Reduction[coulomb-m/m^2/yr]
3.2
**
constant
InnerWPActivationEnergyforO
xygenReduction[J/mole]
40000.0
**
constant
InnerWPActivationEnergyforW
aterReduction[J/mole]
25000.0
**
constant
AA_1_1[C/m2/yr]
3.15e5
**
uniform
AA_2_1[C/m2/yr]
2.0e4, 6.3e4
**
constant
MeasuredGalvanicCouplePoten
tial
-0.46
**
uniform
CoefForLocCorrOfOuterOverpa
ck
8.66e-4, 8.66e-3
**
constant
ExponetForLocCorrOfOuterOve
rpack
0.45
**
constant
HumidAirCorrosionRate[m/yr]
1.16e-5
**
constant
LocalizedCorrRateOfInnerOve
rpack[m/yr]
2.5e-4
**
constant
FractionalCouplingStrength
0.0
**
constant
FactorForDefiningChoiceOfCr
itPotential
0.0
**
constant
CritChlorideConcForFirstLay
er[moL/L]
3.0e-4
**
constant
CritChlorideConcForSecondLa
yer[moL/L]
1.0
**3.0e-2  >>> 625 <<<
**
uniform
ChlorideMultFactor
1.0, 30.0
**
constant
ReferencepH
9.0
**
constant
WPsurfaceScaleThickness[m]
0.0
**
constant
TortuosityOfScaleonWP
1.0
**
constant
PorosityOfScaleonWP
1.0
**
constant
YieldStrength[MPa]
205.0
**
constant
SafetyFactor
1.4
**
constant
FractureToughness[MPa-
m**0.5]
250.0
**
**
**          ***>>> SEISMO
<<<***
**
hazardcurve
SeismicHazardCurveforSEISMO
10
0.05 180.0
0.10 500.0
0.15 1200.0
0.20 2400.0
0.25 4400.0
0.30 7800.0
0.35 11000.0
0.40 20000.0
0.45 30000.0
0.50 44000.0
**
constant
WeightPercentageOfRockFallT
hatHitsWPforSEISMO
1.0
**
constant
WeightOfWPforSEISMO[N]
1.27D05
**
constant
WPStiffnessforSEISMO[Pa*m]
1.21D10
**
constant
WPModulusOfElasticityforSEI
SMO[Pa]
2.07D11
**
normal
RockModulusOfElasticityforS
EISMO[Pa]
2.76D10, 4.14D10
**
constant
WPPoissonRatioforSEISMO[]
0.2D0
**
normal
RockPoissonRatioforSEISMO[]
0.15, 0.25
**
constant
RockFallingDistanceforSEISM
O[m]
2.0D0
**
constant
WPFallingDistanceforSEISMO[
m]
0.3D0
**
iconstant
WPNumberofSupportPairforSEI
SMO
2
**
constant
WPSupportStiffnessforSEISMO
[pa*m]
5.5D09
**
constant
DistributionJointSpacing1fo
rSEISMO
5.0D-03
**
constant
```

```
DistributionJointSpacing2fo
rSEISMO
5.0D-03
**
constant
DistributionJointSpacing3fo
rSEISMO
5.0D-03
**
constant
DistributionJointSpacing4fo
rSEISMO
0.629D0
**
constant
DistributionJointSpacing5fo
rSEISMO
0.356D0
**
normal
SEISMOJointSpacing1[m]
0.466, 0.600
**
normal
SEISMOJointSpacing2[m]
0.333 0.466
**
normal
SEISMOJointSpacing3[m]
0.20, 0.333
**
normal
SEISMOJointSpacing4[m]
0.06, 0.20
**
normal
SEISMOJointSpacing5[m]
0.03, 0.06
**
**  5/28/1998 tpa3.2 new
value (smh)
**
constant
WPUltimateStrength[N/m^2]
4.5D08
**
constant
GrainDensityforTSw2SEISMO[]
2.55
**
**  5/28/1998 tpa3.2 new
values next 60
parameters(replacing
seismo.dat)
**
constant
FractionAreaForGroundMotion
1
0.05
**
constant
FractionAreaForGroundMotion
2
0.12
**
constant
FractionAreaForGroundMotion
3
0.17
**
constant
FractionAreaForGroundMotion
4
0.23
**
constant
FractionAreaForGroundMotion
5
0.28
**
constant
FractionAreaForGroundMotion
6
0.34
**
constant
FractionAreaForGroundMotion
7
0.4
**
constant
FractionAreaForGroundMotion
8
0.46
**
constant
FractionAreaForGroundMotion
9
0.5
**
constant
FractionAreaForGroundMotion
10
0.54
**
** rwr 7/8/98 modify the
VerticalExtentOfRockFall
names by adding "_"
constant
VerticalExtentOfRockFall1_1
[m]
0.0
**
constant
VerticalExtentOfRockFall1_2
[m]
0.0
**
constant
VerticalExtentOfRockFall1_3
[m]
0.0
**
constant
VerticalExtentOfRockFall1_4
[m]
0.0
**
constant
VerticalExtentOfRockFall1_5
[m]
0.0
**
constant
VerticalExtentOfRockFall1_6
[m]
0.0
**
constant
VerticalExtentOfRockFall1_7
[m]
0.0
**
constant
VerticalExtentOfRockFall1_8
[m]
0.0
constant
VerticalExtentOfRockFall1_9
[m]
0.0
**
constant
VerticalExtentOfRockFall1_1
0[m]
0.0
**
uniform
VerticalExtentOfRockFall2_1
[m]
0.5 0.6
**
uniform
VerticalExtentOfRockFall2_2
[m]
0.5 1.0
**
uniform
VerticalExtentOfRockFall2_3
[m]
0.5 1.1
**
uniform
VerticalExtentOfRockFall2_4
[m]
0.5 1.2
**
uniform
VerticalExtentOfRockFall2_5
[m]
0.5 1.3
**
uniform
VerticalExtentOfRockFall2_6
[m]
0.5 1.4
**
uniform
VerticalExtentOfRockFall2_7
[m]
0.5 1.45
**
uniform
VerticalExtentOfRockFall2_8
[m]
0.5 1.5
**
uniform
VerticalExtentOfRockFall2_9
[m]
0.5 1.65
**
uniform
VerticalExtentOfRockFall2_1
0[m]
0.0 1.8
**
uniform
VerticalExtentOfRockFall3_1
[m]
0.5 1.0
**
uniform
```

```
VerticalExtentOfRockFall3_2
[m]
0.5 2.0
**
uniform
VerticalExtentOfRockFall3_3
[m]
0.5 2.5
**
uniform
VerticalExtentOfRockFall3_4
[m]
0.5 3.0
**
uniform
VerticalExtentOfRockFall3_5
[m]
0.5 3.5
**
uniform
VerticalExtentOfRockFall3_6
[m]
0.5 4.0
**
uniform
VerticalExtentOfRockFall3_7
[m]
0.5 4.5
**
uniform
VerticalExtentOfRockFall3_8
[m]
0.5 5.0
**
uniform
VerticalExtentOfRockFall3_9
[m]
0.5 5.7
**
uniform
VerticalExtentOfRockFall3_1
0[m]
0.5 6.5
**
uniform
VerticalExtentOfRockFall4_1
[m]
0.5 2.7
**
uniform
VerticalExtentOfRockFall4_2
[m]
0.5 5.5
**
uniform
VerticalExtentOfRockFall4_3
[m]
0.5 6.0
**
uniform
VerticalExtentOfRockFall4_4
[m]
0.5 6.5
**
uniform
VerticalExtentOfRockFall4_5
[m]
0.5 7.0
**
uniform
VerticalExtentOfRockFall4_6
[m]
0.5 7.5
**
uniform
VerticalExtentOfRockFall4_7
[m]
0.5 8.0
**
uniform
VerticalExtentOfRockFall4_8
[m]
0.5 8.5
**
uniform
VerticalExtentOfRockFall4_9
[m]
0.5 9.3
**
uniform
VerticalExtentOfRockFall4_1
0[m]
0.5 10.0
**
uniform
VerticalExtentOfRockFall5_1
[m]
0.5 4.7
**
uniform
VerticalExtentOfRockFall5_2
[m]
0.5 9.33
**
uniform
VerticalExtentOfRockFall5_3
[m]
0.5 9.7
**
uniform
VerticalExtentOfRockFall5_4
[m]
0.5 10.0
**
uniform
VerticalExtentOfRockFall5_5
[m]
0.5 10.7
**
uniform
VerticalExtentOfRockFall5_6
[m]
0.5 11.33
**
uniform
VerticalExtentOfRockFall5_7
[m]
0.5 12.0
**
uniform
VerticalExtentOfRockFall5_8
[m]
0.5 12.66
**
uniform
VerticalExtentOfRockFall5_9
[m]
0.5 13.3
**
uniform
VerticalExtentOfRockFall5_1
0[m]
0.5 14.0
**
**  5/28/1998 tpa3.2 two
new parameters introduced
**
constant
WPYieldPoint[]
0.002
**
constant
WPPlasticElongation[]
0.02
**
**
**          ***>>>  EBSREL
<<<***
**
** rwr 7/8/98 modify flow
model flag
iflag
FlowModelFlag(0=BathTub,1=F
lowThrough)
0
**
lognormal
FowFactor
0.01, 3.0
**
lognormal
FmultFactor
0.01, 0.2
**
uniform
SubAreaWetFraction
0.0, 1.0
**
**  5/21/98 tpa3.2: New
parameter; nonzero initial
failure times
**
constant
InitialFailureTime[yr]
0.0
**
uniform
DefectiveFractionOfWPs/cell
1.0e-4,  1.0e-2
**
**  6/2/1998 tpa3.2 5 new
parameters; number of
SEISMO inservals not to
exceed 4
**
iconstant
NumberOfSEISMOWPFailureInte
rvals
4
**
constant
BeginningOfSEISMOWPFailureI
nterval1[yr]
0.0
**
constant
BeginningOfSEISMOWPFailureI
nterval2[yr]
2000.0
**
constant
```

```
BeginningOfSEISMOWPFailureI
nterval3[yr]
5000.0
**
constant
BeginningOfSEISMOWPFailureI
nterval4[yr]
10000.0
**
constant
WPInternalVolume[m3]
4.83
**
constant
FlowOnsetTemperature[C]
999.
**
constant
SFDensity[kg/m3]
10600.
**
iconstant
SurfaceAreaModel
1
**
iconstant
IModel
2
**
constant
OxygenPartialPressure[atm]
0.21
**
constant
NegativeLog10CarbonateConce
ntration[mol/L]
3.71
**
constant
UserLeachRate[kg/yr/m2]
2.5e-6
**
constant
RD_Invert_Cm
6.00e3
**
constant
RD_Invert_Pu
3.00e3
**
constant
RD_Invert_U
6.01e2
**
constant
RD_Invert_Am
3.00e3
**
constant
RD_Invert_Np
1.20e3
**
constant
RD_Invert_Th
3.00e3
**
constant
RD_Invert_Ra
6.01e2
**
constant
RD_Invert_Pb
3.01e2
**
constant
RD_Invert_Cs
1.21e2
**
constant
RD_Invert_I
7.00e0
**
constant
RD_Invert_Tc
1.0
**
constant
RD_Invert_Ni
6.10e1
**
constant
RD_Invert_Cl
1.0
**
constant
RD_Invert_C
6.10e1
**
constant
RD_Invert_Se
1.0
**
constant
RD_Invert_Nb
6.01e2
**
constant
GapFractionForCM246
0.0
**
constant
GapFractionForU238
0.0
**
constant
GapFractionForCM245
0.0
**
constant
GapFractionForAM241
0.0
**
constant
GapFractionForNP237
0.0
**
constant
GapFractionForAM243
0.0
**
constant
GapFractionForPU239
0.0
**
constant
GapFractionForPU240
0.0
**
constant
GapFractionForU234
0.0
**
constant
GapFractionForTH230
0.0
**
constant
GapFractionForRA226
0.0
**
constant
GapFractionForPB210
0.0
**
constant
GapFractionForCS135
0.06
**
constant
GapFractionForI129
0.06
**
constant
GapFractionForTC99
0.01
**
constant
GapFractionForNI59
0.0
**
constant
GapFractionForCL36
0.12
**
constant
GapFractionForC14
0.1
**
constant
GapFractionForSE79
0.06
**
constant
GapFractionForNB94
0.0
**
normal
InitialRadiusOfSFParticle[m
]
7.0e-4,  3.0e-3
**
constant
RadiusOfSFGrain[m]
1.25e-5
**
constant
CladdingCorrectionFactor
1.0
**
normal
SubGrainFragmentRadiusAfter
TransFrac[m]
5.0e-7,  2.0e-6
**
constant
ThicknessOfCladding[m]
6.1e-4
**
constant
SFC-14InventoryPerKgSF[ci]
7.2e-4
**
constant
```

```
CladC-
14InventoryPerKgSF[ci]
4.89e-4
**
constant
ZyrOxideAndCrudC-
14InvPerKgSF[ci]
2.48e-5
**
constant
GapAndGrainBoundaryInventor
yPerKgSF[ci]
6.2e-6
**
uniform
SolubilityAm[kg/m3]
2.4e-8,  2.4e-4
**
logtriangular
SolubilityNp[kg/m3]
1.2e-3,  3.4e-2,  2.4e-1
**
constant
Solubility_I[kg/m3]
1.29e2
**
constant
SolubilityTc[kg/m3]
9.93e1
**
constant
SolubilityCl[kg/m3]
3.6e1
**
constant
Solubility_C[kg/m3]
1.4e1
**
constant
Solubility_U[kg/m3]
7.6e-3
**
constant
SolubilityCm[kg/m3]
2.4e-4
**
uniform
SolubilityPu[kg/m3]
2.4e-6, 2.4e-4
**
constant
SolubilityTh[kg/m3]
2.3e-4
**
constant
SolubilityRa[kg/m3]
2.3e-5
**
constant
SolubilityPb[kg/m3]
6.6e-5
**
constant
SolubilityCs[kg/m3]
1.35e2
**
constant
SolubilityNi[kg/m3]
1.1e-1
**
constant
SolubilitySe[kg/m3]
7.9e1
**
constant
SolubilityNb[kg/m3]
9.3e-7
**
**  6/2/1998 tpa3.2 next
parameter replaced with 44
new parameters
**
SFWettedFraction_(failureki
nd)_subarea
**
uniform
SFWettedFraction_Initial_1
0.0, 1.0
**
uniform
SFWettedFraction_Initial_2
0.0, 1.0
**
uniform
SFWettedFraction_Initial_3
0.0, 1.0
**
uniform
SFWettedFraction_Initial_4
0.0, 1.0
**
uniform
SFWettedFraction_Initial_5
0.0, 1.0
**
uniform
SFWettedFraction_Initial_6
0.0, 1.0
**
uniform
SFWettedFraction_Initial_7
0.0, 1.0
**
uniform
SFWettedFraction_FAULTO
0.0, 1.0
**
uniform
SFWettedFraction_VOLCANO
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_1
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_2
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_3
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_4
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_5
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_6
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO1_7
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_1
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_2
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_3
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_4
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_5
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_6
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO2_7
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_1
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_2
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_3
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_4
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_5
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_6
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO3_7
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO4_1
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO4_2
0.0, 1.0
**
```

```
uniform
SFWettedFraction_SEISMO4_3
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO4_4
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO4_5
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO4_6
0.0, 1.0
**
uniform
SFWettedFraction_SEISMO4_7
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
1
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
2
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
3
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
4
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
5
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
6
0.0, 1.0
**
uniform
SFWettedFraction_Corrosion_
7
0.0, 1.0
**
**  7/4/1998 tpa3.2 four
new parameters for invert
**
iflag
InvertBypass(0=ebsfilt,1=by
pass-ebsfilt)
0
**
constant
InvertRockPorosity
0.3
**
constant
InvertThickness[m]
0.75
**
constant
InvertDiffusionCoefficient[
m^2/yr]
4.4e-5
**
lognormal
InvertMatrixPermeability[m^
2]
2.0e-18, 2.0e-16
**
**
**           ***>>>  UZFT
<<<***
**
constant
UnsaturatedZoneMinimumVeloc
ityChangeFactor[Fraction]
0.4
**
constant
MatrixLongitudinalDispersiv
ity[FractionOfLayer]
0.1
**
constant
FractureLongitudinalDispers
ivity[FractionOfLayer]
0.1
**
lognormal
MatrixKD_TSw_Am[m3/kg]
4.2e+00  3.8e+06
**
lognormal
MatrixKD_CHnvAm[m3/kg]
1.3e+01  1.2e+07
**
lognormal
MatrixKD_CHnzAm[m3/kg]
1.2e+01  1.1e+07
**
lognormal
MatrixKD_PPw_Am[m3/kg]
9.5e+00  8.7e+06
**
lognormal
MatrixKD_UCF_Am[m3/kg]
1.0e+01  9.1e+06
**
lognormal
MatrixKD_BFw_Am[m3/kg]
4.1e+00  3.7e+06
**
lognormal
MatrixKD_UFZ_Am[m3/kg]
3.9e+00  3.5e+06
**
lognormal
MatrixKD_TSw_Np[m3/kg]
1.6e-06  2.2e-01
**
lognormal
MatrixKD_CHnvNp[m3/kg]
4.8e-06  6.6e-01
**
lognormal
MatrixKD_CHnzNp[m3/kg]
4.4e-06  6.0e-01
**
lognormal
MatrixKD_PPw_Np[m3/kg]
3.6e-06  5.0e-01
**
lognormal
MatrixKD_UCF_Np[m3/kg]
3.8e-06  5.2e-01
**
lognormal
MatrixKD_BFw_Np[m3/kg]
1.5e-06  2.1e-01
**
lognormal
MatrixKD_UFZ_Np[m3/kg]
1.5e-06  2.0e-01
**
constant
MatrixKD_TSw_I[m3/kg]
0.0
**
constant
MatrixKD_CHnvI[m3/kg]
0.0
**
constant
MatrixKD_CHnzI[m3/kg]
0.0
**
constant
MatrixKD_PPw_I[m3/kg]
0.0
**
constant
MatrixKD_UCF_I[m3/kg]
0.0
**
constant
MatrixKD_BFw_I[m3/kg]
0.0
**
constant
MatrixKD_UFZ_I[m3/kg]
0.0
**
constant
MatrixKD_TSw_Tc[m3/kg]
0.0
**
constant
MatrixKD_CHnvTc[m3/kg]
0.0
**
constant
MatrixKD_CHnzTc[m3/kg]
0.0
**
constant
MatrixKD_PPw_Tc[m3/kg]
0.0
**
constant
MatrixKD_UCF_Tc[m3/kg]
0.0
**
constant
MatrixKD_BFw_Tc[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Tc[m3/kg]
0.0
**
constant
```

```
MatrixKD_TSw_Cl[m3/kg]
0.0
**
constant
MatrixKD_CHnvCl[m3/kg]
0.0
**
constant
MatrixKD_CHnzCl[m3/kg]
0.0
**
constant
MatrixKD_PPw_Cl[m3/kg]
0.0
**
constant
MatrixKD_UCF_Cl[m3/kg]
0.0
**
constant
MatrixKD_BFw_Cl[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Cl[m3/kg]
0.0
**
constant
MatrixKD_TSw_Cm[m3/kg]
0.0
**
constant
MatrixKD_CHnvCm[m3/kg]
0.0
**
constant
MatrixKD_CHnzCm[m3/kg]
0.0
**
constant
MatrixKD_PPw_Cm[m3/kg]
0.0
**
constant
MatrixKD_UCF_Cm[m3/kg]
0.0
**
constant
MatrixKD_BFw_Cm[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Cm[m3/kg]
0.0
**
lognormal
MatrixKD_TSw_U[m3/kg]
4.2e-10  1.1e+00
**
lognormal
MatrixKD_CHnvU[m3/kg]
1.3e-09  3.3e+00
**
lognormal
MatrixKD_CHnzU[m3/kg]
1.2e-09  3.0e+00
**
lognormal
MatrixKD_PPw_U[m3/kg]
9.6e-10  2.5e+00
**
lognormal
MatrixKD_UCF_U[m3/kg]
1.0e-09  2.6e+00
**
lognormal
MatrixKD_BFw_U[m3/kg]
4.1e-10  1.0e+00
**
lognormal
MatrixKD_UFZ_U[m3/kg]
3.9e-10  1.0e+00
**
lognormal
MatrixKD_TSw_Pu[m3/kg]
2.3e-02  2.2e+01
**
lognormal
MatrixKD_CHnvPu[m3/kg]
7.1e-02  6.7e+01
**
lognormal
MatrixKD_CHnzPu[m3/kg]
6.5e-02  6.1e+01
**
lognormal
MatrixKD_PPw_Pu[m3/kg]
5.3e-02  5.0e+01
**
lognormal
MatrixKD_UCF_Pu[m3/kg]
5.6e-02  5.2e+01
**
lognormal
MatrixKD_BFw_Pu[m3/kg]
2.3e-02  2.1e+01
**
lognormal
MatrixKD_UFZ_Pu[m3/kg]
2.2e-02  2.1e+01
**
lognormal
MatrixKD_TSw_Th[m3/kg]
4.8e-05  2.5e+03
**
lognormal
MatrixKD_CHnvTh[m3/kg]
1.5e-04  7.6e+03
**
lognormal
MatrixKD_CHnzTh[m3/kg]
1.3e-04  6.9e+03
**
lognormal
MatrixKD_PPw_Th[m3/kg]
1.1e-04  5.7e+03
**
lognormal
MatrixKD_UCF_Th[m3/kg]
1.1e-04  5.9e+03
**
lognormal
MatrixKD_BFw_Th[m3/kg]
4.7e-05  2.4e+03
**
lognormal
MatrixKD_UFZ_Th[m3/kg]
4.5e-05  2.3e+03
**
loguniform
MatrixKD_TSw_Ra[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_CHnvRa[m3/kg]
0.050, 0.10
**
loguniform
MatrixKD_CHnzRa[m3/kg]
1.0, 5.0
**
loguniform
MatrixKD_PPw_Ra[m3/kg]
0.1, 0.5
**
loguniform
MatrixKD_UCF_Ra[m3/kg]
0.1, 0.5
**
loguniform
MatrixKD_BFw_Ra[m3/kg]
0.1, 0.5
**
loguniform
MatrixKD_UFZ_Ra[m3/kg]
0.1, 0.5
**
loguniform
MatrixKD_TSw_Pb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_CHnvPb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_CHnzPb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_PPw_Pb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_UCF_Pb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_BFw_Pb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_UFZ_Pb[m3/kg]
0.10, 0.50
**
loguniform
MatrixKD_TSw_Cs[m3/kg]
0.020, 1.0
**
loguniform
MatrixKD_CHnvCs[m3/kg]
0.010, 0.10
**
loguniform
MatrixKD_CHnzCs[m3/kg]
0.50, 5.0
**
loguniform
MatrixKD_PPw_Cs[m3/kg]
0.020, 1.0
**
loguniform
MatrixKD_UCF_Cs[m3/kg]
```

```
0.020, 1.0
**
loguniform
MatrixKD_BFw_Cs[m3/kg]
0.020, 1.0
**
loguniform
MatrixKD_UFZ_Cs[m3/kg]
0.020, 1.0
**
loguniform
MatrixKD_TSw_Ni[m3/kg]
5.0e-6, 0.50
**
loguniform
MatrixKD_CHnvNi[m3/kg]
1.0e-6, 0.10
**
loguniform
MatrixKD_CHnzNi[m3/kg]
5.0e-6, 0.50
**
loguniform
MatrixKD_PPw_Ni[m3/kg]
5.0e-6, 0.50
**
loguniform
MatrixKD_UCF_Ni[m3/kg]
5.0e-6, 0.50
**
loguniform
MatrixKD_BFw_Ni[m3/kg]
5.0e-6, 0.50
**
loguniform
MatrixKD_UFZ_Ni[m3/kg]
5.0e-6, 0.50
**
constant
MatrixKD_TSw_C[m3/kg]
0.0
**
constant
MatrixKD_CHnvC[m3/kg]
0.0
**
constant
MatrixKD_CHnzC[m3/kg]
0.0
**
constant
MatrixKD_PPw_C[m3/kg]
0.0
**
constant
MatrixKD_UCF_C[m3/kg]
0.0
**
constant
MatrixKD_BFw_C[m3/kg]
0.0
**
constant
MatrixKD_UFZ_C[m3/kg]
0.0
**
loguniform
MatrixKD_TSw_Se[m3/kg]
3.0e-7, 0.030
**
loguniform
MatrixKD_CHnvSe[m3/kg]
2.0e-7, 0.020
**
loguniform
MatrixKD_CHnzSe[m3/kg]
1.5e-7, 0.015
**
loguniform
MatrixKD_PPw_Se[m3/kg]
3.0e-7, 0.030
**
loguniform
MatrixKD_UCF_Se[m3/kg]
3.0e-7, 0.030
**
loguniform
MatrixKD_BFw_Se[m3/kg]
3.0e-7, 0.030
**
loguniform
MatrixKD_UFZ_Se[m3/kg]
3.0e-7, 0.030
**
constant
MatrixKD_TSw_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_CHnvNb[m3/kg]
0.10, 1.0
**
constant
MatrixKD_CHnzNb[m3/kg]
0.10, 1.0
**
constant
MatrixKD_PPw_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_UCF_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_BFw_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_UFZ_Nb[m3/kg]
0.10, 2.0
**
constant
FractureRD_TSw_Am
1.0
**
constant
FractureRD_CHnvAm
1.0
**
constant
FractureRD_CHnzAm
1.0
**
constant
FractureRD_PPw_Am
1.0
**
constant
FractureRD_UCF_Am
1.0
**
constant
FractureRD_BFw_Am
1.0
**
constant
FractureRD_UFZ_Am
1.0
**
constant
FractureRD_TSw_Np
1.0
**
constant
FractureRD_CHnvNp
1.0
**
constant
FractureRD_CHnzNp
1.0
**
constant
FractureRD_PPw_Np
1.0
**
constant
FractureRD_UCF_Np
1.0
**
constant
FractureRD_BFw_Np
1.0
**
constant
FractureRD_UFZ_Np
1.0
**
constant
FractureRD_TSw_I
1.0
**
constant
FractureRD_CHnvI
1.0
**
constant
FractureRD_CHnzI
1.0
**
constant
FractureRD_PPw_I
1.0
**
constant
FractureRD_UCF_I
1.0
**
constant
FractureRD_BFw_I
1.0
**
constant
FractureRD_UFZ_I
1.0
**
constant
FractureRD_TSw_Tc
1.0
**
constant
FractureRD_CHnvTc
1.0
```

```
**
constant
FractureRD_CHnzTc
1.0
**
constant
FractureRD_PPw_Tc
1.0
**
constant
FractureRD_UCF_Tc
1.0
**
constant
FractureRD_BFw_Tc
1.0
**
constant
FractureRD_UFZ_Tc
1.0
**
constant
FractureRD_TSw_Cl
1.0
**
constant
FractureRD_CHnvCl
1.0
**
constant
FractureRD_CHnzCl
1.0
**
constant
FractureRD_PPw_Cl
1.0
**
constant
FractureRD_UCF_Cl
1.0
**
constant
FractureRD_BFw_Cl
1.0
**
constant
FractureRD_UFZ_Cl
1.0
**
constant
FractureRD_TSw_Cm
1.0
**
constant
FractureRD_CHnvCm
1.0
**
constant
FractureRD_CHnzCm
1.0
**
constant
FractureRD_PPw_Cm
1.0
**
constant
FractureRD_UCF_Cm
1.0
**
constant
FractureRD_BFw_Cm
1.0
**
constant
FractureRD_UFZ_Cm
1.0
**
constant
FractureRD_TSw_U
1.0
**
constant
FractureRD_CHnvU
1.0
**
constant
FractureRD_CHnzU
1.0
**
constant
FractureRD_PPw_U
1.0
**
constant
FractureRD_UCF_U
1.0
**
constant
FractureRD_BFw_U
1.0
**
constant
FractureRD_UFZ_U
1.0
**
constant
FractureRD_TSw_Pu
1.0
**
constant
FractureRD_CHnvPu
1.0
**
constant
FractureRD_CHnzPu
1.0
**
constant
FractureRD_PPw_Pu
1.0
**
constant
FractureRD_UCF_Pu
1.0
**
constant
FractureRD_BFw_Pu
1.0
**
constant
FractureRD_UFZ_Pu
1.0
**
constant
FractureRD_TSw_Th
1.0
**
constant
FractureRD_CHnvTh
1.0
**
constant
FractureRD_CHnzTh
1.0
**
constant
FractureRD_PPw_Th
1.0
**
constant
FractureRD_UCF_Th
1.0
**
constant
FractureRD_BFw_Th
1.0
**
constant
FractureRD_UFZ_Th
1.0
**
constant
FractureRD_TSw_Ra
1.0
**
constant
FractureRD_CHnvRa
1.0
**
constant
FractureRD_CHnzRa
1.0
**
constant
FractureRD_PPw_Ra
1.0
**
constant
FractureRD_UCF_Ra
1.0
**
constant
FractureRD_BFw_Ra
1.0
**
constant
FractureRD_UFZ_Ra
1.0
**
constant
FractureRD_TSw_Pb
1.0
**
constant
FractureRD_CHnvPb
1.0
**
constant
FractureRD_CHnzPb
1.0
**
constant
FractureRD_PPw_Pb
1.0
**
constant
FractureRD_UCF_Pb
1.0
**
constant
FractureRD_BFw_Pb
1.0
**
```

```
constant
FractureRD_UFZ_Pb
1.0
**
constant
FractureRD_TSw_Cs
1.0
**
constant
FractureRD_CHnvCs
1.0
**
constant
FractureRD_CHnzCs
1.0
**
constant
FractureRD_PPw_Cs
1.0
**
constant
FractureRD_UCF_Cs
1.0
**
constant
FractureRD_BFw_Cs
1.0
**
constant
FractureRD_UFZ_Cs
1.0
**
constant
FractureRD_TSw_Ni
1.0
**
constant
FractureRD_CHnvNi
1.0
**
constant
FractureRD_CHnzNi
1.0
**
constant
FractureRD_PPw_Ni
1.0
**
constant
FractureRD_UCF_Ni
1.0
**
constant
FractureRD_BFw_Ni
1.0
**
constant
FractureRD_UFZ_Ni
1.0
**
constant
FractureRD_TSw_C
1.0
**
constant
FractureRD_CHnvC
1.0
**
constant
FractureRD_CHnzC
1.0
**
constant
FractureRD_PPw_C
1.0
**
constant
FractureRD_UCF_C
1.0
**
constant
FractureRD_BFw_C
1.0
**
constant
FractureRD_UFZ_C
1.0
**
constant
FractureRD_TSw_Se
1.0
**
constant
FractureRD_CHnvSe
1.0
**
constant
FractureRD_CHnzSe
1.0
**
constant
FractureRD_PPw_Se
1.0
**
constant
FractureRD_UCF_Se
1.0
**
constant
FractureRD_BFw_Se
1.0
**
constant
FractureRD_UFZ_Se
1.0
**
constant
FractureRD_TSw_Nb
1.0
**
constant
FractureRD_CHnvNb
1.0
**
constant
FractureRD_CHnzNb
1.0
**
constant
FractureRD_PPw_Nb
1.0
**
constant
FractureRD_UCF_Nb
1.0
**
constant
FractureRD_BFw_Nb
1.0
**
constant
FractureRD_UFZ_Nb
1.0
**
lognormal
MatrixPermeability_TSw_[m2]
0.2e-19, 0.2e-17
**
lognormal
MatrixPermeability_CHnv[m2]
0.2e-14, 0.2e-12
**
lognormal
MatrixPermeability_CHnz[m2]
0.5e-18, 0.5e-16
**
lognormal
MatrixPermeability_PPw_[m2]
0.1e-17, 0.1e-15
**
lognormal
MatrixPermeability_UCF_[m2]
0.3e-18, 0.3e-16
**
lognormal
MatrixPermeability_BFw_[m2]
0.2e-19, 0.2e-17
**
lognormal
MatrixPermeability_UFZ_[m2]
1.8e-18,  2.1e-16
**
constant
MatrixPorosity_TSw_
0.12
**
constant
MatrixPorosity_CHnv
0.33
**
constant
MatrixPorosity_CHnz
0.32
**
constant
MatrixPorosity_PPw_
0.28
**
constant
MatrixPorosity_UCF_
0.28
**
constant
MatrixPorosity_BFw_
0.12
**
constant
MatrixPorosity_UFZ_
0.12
**
constant
MatrixBeta_TSw_
1.5
**
constant
MatrixBeta_CHnv
1.3
**
constant
MatrixBeta_CHnz
2.3
**
constant
```

```
MatrixBeta_PPw_
1.5
**
constant
MatrixBeta_UCF_
1.4
**
constant
MatrixBeta_BFw_
1.7
**
constant
MatrixBeta_UFZ_
2.3
**
constant
MatrixGrainDensity_TSw_[kg/
m3]
2460.0
**
constant
MatrixGrainDensity_CHnv[kg/
m3]
2260.0
**
constant
MatrixGrainDensity_CHnz[kg/
m3]
2400.0
**
constant
MatrixGrainDensity_PPw_[kg/
m3]
2540.0
**
constant
MatrixGrainDensity_UCF_[kg/
m3]
2420.0
**
constant
MatrixGrainDensity_BFw_[kg/
m3]
2570.0
**
constant
MatrixGrainDensity_UFZ_[kg/
m3]
2630.0
**
lognormal
FracturePermeability_TSw_[m
2]
8.0e-15, 8.0e-11
**
lognormal
FracturePermeability_CHnv[m
2]
8.0e-15, 8.0e-11
**
lognormal
FracturePermeability_CHnz[m
2]
6.0e-15, 6.0e-11
**
lognormal
FracturePermeability_PPw_[m
2]
6.0e-15, 6.0e-11
**
lognormal
FracturePermeability_UCF_[m
2]
6.0e-15, 6.0e-11
**
lognormal
FracturePermeability_BFw_[m
2]
3.0e-15, 3.0e-11
**
lognormal
FracturePermeability_UFZ_[m
2]
1.0e-13, 1.0e-11
**
loguniform
FracturePorosity_TSw_
1.0e-3, 1.0e-2
**
loguniform
FracturePorosity_CHnv
1.0e-3, 1.0e-2
**
loguniform
FracturePorosity_CHnz
1.0e-3, 1.0e-2
**
loguniform
FracturePorosity_PPw_
1.0e-3, 1.0e-2
**
loguniform
FracturePorosity_UCF_
1.0e-3, 1.0e-2
**
loguniform
FracturePorosity_BFw_
1.0e-3, 1.0e-2
**
loguniform
FracturePorosity_UFZ_
1.0e-3, 1.0e-2
**
constant
FractureBeta_TSw_
3.0
**
constant
FractureBeta_CHnv
3.0
**
constant
FractureBeta_CHnz
3.0
**
constant
FractureBeta_PPw_
3.0
**
constant
FractureBeta_UCF_
3.0
**
constant
FractureBeta_BFw_
3.0
**
constant
FractureBeta_UFZ_
3.0
**
constant
InletArea__1SubArea[m2]
5.4e5
**
constant
InletArea__2SubArea[m2]
5.4e5
**
constant
InletArea__3SubArea[m2]
5.4e5
**
constant
InletArea__4SubArea[m2]
5.4e5
**
constant
InletArea__5SubArea[m2]
5.4e5
**
constant
InletArea__6SubArea[m2]
5.4e5
**
constant
InletArea__7SubArea[m2]
5.4e5
**
constant
TSw_Thickness_1SubArea[m]
33.0
**
constant
CHnvThickness_1SubArea[m]
0.0
**
constant
CHnzThickness_1SubArea[m]
163.0
**
constant
PPw_Thickness_1SubArea[m]
34.0
**
constant
UCF_Thickness_1SubArea[m]
67.0
**
constant
BFw_Thickness_1SubArea[m]
0.0
**
constant
UFZ_Thickness_1SubArea[m]
0.0
**
constant
TSw_Thickness_2SubArea[m]
116.0
**
constant
CHnvThickness_2SubArea[m]
0.0
**
constant
CHnzThickness_2SubArea[m]
154.0
**
constant
PPw_Thickness_2SubArea[m]
39.0
**
```

```
constant
UCF_Thickness_2SubArea[m]
20.0
**
constant
BFw_Thickness_2SubArea[m]
0.0
**
constant
UFZ_Thickness_2SubArea[m]
0.0
**
constant
TSw_Thickness_3SubArea[m]
20.0
**
constant
CHnvThickness_3SubArea[m]
0.0
**
constant
CHnzThickness_3SubArea[m]
122.0
**
constant
PPw_Thickness_3SubArea[m]
40.0
**
constant
UCF_Thickness_3SubArea[m]
158.0
**
constant
BFw_Thickness_3SubArea[m]
0.0
**
constant
UFZ_Thickness_3SubArea[m]
0.0
**
constant
TSw_Thickness_4SubArea[m]
110.0
**
constant
CHnvThickness_4SubArea[m]
0.0
**
constant
CHnzThickness_4SubArea[m]
132.0
**
constant
PPw_Thickness_4SubArea[m]
34.0
**
constant
UCF_Thickness_4SubArea[m]
57.0
**
constant
BFw_Thickness_4SubArea[m]
0.0
**
constant
UFZ_Thickness_4SubArea[m]
0.0
**
constant
TSw_Thickness_5SubArea[m]
20.0
**
constant
CHnvThickness_5SubArea[m]
113.0
**
constant
CHnzThickness_5SubArea[m]
0.0
**
constant
PPw_Thickness_5SubArea[m]
38.0
**
constant
UCF_Thickness_5SubArea[m]
158.0
**
constant
BFw_Thickness_5SubArea[m]
32.0
**
constant
UFZ_Thickness_5SubArea[m]
0.0
**
constant
TSw_Thickness_6SubArea[m]
53.0
**
constant
CHnvThickness_6SubArea[m]
125.0
**
constant
CHnzThickness_6SubArea[m]
0.0
**
constant
PPw_Thickness_6SubArea[m]
26.0
**
constant
UCF_Thickness_6SubArea[m]
136.0
**
constant
BFw_Thickness_6SubArea[m]
0.0
**
constant
UFZ_Thickness_6SubArea[m]
0.0
**
constant
TSw_Thickness_7SubArea[m]
121.0
**
constant
CHnvThickness_7SubArea[m]
0.0
**
constant
CHnzThickness_7SubArea[m]
114.0
**
constant
PPw_Thickness_7SubArea[m]
43.0
**
constant
UCF_Thickness_7SubArea[m]
63.0
**
constant
BFw_Thickness_7SubArea[m]
0.0
**
constant
UFZ_Thickness_7SubArea[m]
0.0
**
**
**            ***>>>  SZFT
<<<***
**
constant
MixingZoneDispersionFractio
n
0.01
**
constant
DispersionFraction_STFF
0.01
**
constant
DispersionFraction_SAV
0.1
**
constant
MinimumResidenceTime_STFF[y
r]
10.0
**
constant
MinimumResidenceTime_SAV[yr
]
10.0
**
constant
FractureRD_STFF_Am
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
lognormal
AlluviumMatrixRD_SAV_Am
7.5e4, 6.8e10
**
constant
FractureRD_STFF_Np
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
lognormal
AlluviumMatrixRD_SAV_Np
1.0, 3.9e3
**
constant
FractureRD_STFF_I
1.0
**
loguniform
AlluviumMatrixRD_SAV_I
1.0, 4.0
**
constant
FractureRD_STFF_Tc
```

```
1.0
**
loguniform
AlluviumMatrixRD_SAV_Tc
1.0, 30.0
**
constant
FractureRD_STFF_Cl
1.0
**
constant
AlluviumMatrixRD_SAV_Cl
1.0
**
constant
FractureRD_STFF_Cm
1.0
**
constant
AlluviumMatrixRD_SAV_Cm
1.0
**
constant
FractureRD_STFF_U
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
lognormal
AlluviumMatrixRD_SAV_U
1.0, 1.9e4
**
constant
FractureRD_STFF_Pu
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
lognormal
AlluviumMatrixRD_SAV_Pu
4.2e2, 3.9e5
**
constant
FractureRD_STFF_Th
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
lognormal
AlluviumMatrixRD_SAV_Th
1.9, 4.5e7
**
constant
FractureRD_STFF_Ra
1.0
**
loguniform
AlluviumMatrixRD_SAV_Ra
2.0e3, 8.0e3
**
constant
FractureRD_STFF_Pb
1.0
**
loguniform
AlluviumMatrixRD_SAV_Pb
2.0e3, 8.0e3
**
constant
FractureRD_STFF_Cs
1.0
**
loguniform
AlluviumMatrixRD_SAV_Cs
9.0e4, 1.0e5
**
constant
FractureRD_STFF_Ni
1.0
**
loguniform
AlluviumMatrixRD_SAV_Ni
1.0, 8.0e3
**
constant
FractureRD_STFF_C
1.0
**
constant
AlluviumMatrixRD_SAV_C
1.0
**
constant
FractureRD_STFF_Se
1.0
**
loguniform
AlluviumMatrixRD_SAV_Se
1.0, 500.0
**
constant
FractureRD_STFF_Nb
1.0
**
loguniform
AlluviumMatrixRD_SAV_Nb
2.0e3, 3.0e4
**
loguniform
FracturePorosity_STFF
1.e-3, 1.e-2
**
uniform
AlluviumMatrixPorosity_SAV
1.e-1, 1.5e-1
**
constant
ImmobileRD_STFF_Am
1.8e4
**
constant
ImmobileRD_STFF_Np
19.0
**
constant
ImmobileRD_STFF_I
1.0
**
constant
ImmobileRD_STFF_Tc
1.0
**
constant
ImmobileRD_STFF_Cl
1.0
**
constant
ImmobileRD_STFF_Cm
1.0
**
constant
ImmobileRD_STFF_U
37.0
**
constant
ImmobileRD_STFF_Pu
1.8e3
**
constant
ImmobileRD_STFF_Th
1.8e4
**
constant
ImmobileRD_STFF_Ra
5.4e3
**
constant
ImmobileRD_STFF_Pb
5.4e3
**
constant
ImmobileRD_STFF_Cs
9.0e3
**
constant
ImmobileRD_STFF_Ni
1.8e3
**
constant
ImmobileRD_STFF_C
1.0
**
constant
ImmobileRD_STFF_Se
55.0
**
constant
ImmobileRD_STFF_Nb
1.8e4
**
constant
ImmobilePorosity_STFF
0.01
**
constant
DiffusionRate_STFF
0.0
**
**
**          ***>>>   DCAGW
<<<***
**
constant
DistanceToReceptorGroup[km]
[should_be_10_or_20]
20.0
**
uniform
WellPumpingRateAtReceptorGr
oup10km[gal/day]
1.35e4, 2.64e5
**
uniform
WellPumpingRateAtReceptorGr
oup20km[gal/day]
4.5e6, 1.3e7
**
```

```
uniform
PlumeThickness5km[m]
10.0, 100.0
**
uniform
AquiferThickness5km[m]
300.0, 700.0
**
uniform
MixingZoneThickness20km[m]
50.0, 200.0
**
**
**          ***>>> FAULTO
<<<***
**
finiteexponential
TimeOfNextFaultingEventinRe
gionOfInterest[yr]
100.0, 10000.0, 2.0e-5
**
userdistribution
ThresholdDisplacementforFau
ltDisruptionOfWP[m]
4
0.1
0.2
0.3
0.4
**
uniform
XLocationOfFaultingEventInR
egionOfInterest[m]
547400.0, 548600.0
**
uniform
YLocationOfFaultingEventInR
egionOfInterest[m]
4076200.0, 4079040.0
**
constant
ProbabilityForNWOrientation
OfFaults
0.05
**
uniform
RNtoDetermineFaultOrientati
on
0.0, 1.0
**
constant
NWFaultStrikeOrientationMea
suredfromNorthClockwise[deg
rees]
-32.5
**
constant
NEFaultStrikeOrientationMea
suredfromNorthClockwise[deg
rees]
10.0
**
constant
NWFaultTraceLength[m]
4000.0
**
constant
NEFaultTraceLength[m]
4000.0
**
beta
NWFaultZoneWidth[m]
0.5, 275.0, 1.25, 15.0
**
beta
NEFaultZoneWidth[m]
0.5, 365.0, 1.25, 15.0
**
lognormal
NWAmountOfLargestCredibleDi
splacement[m]
5.41e-2, 3.3e-1
**
lognormal
NEAmountOfLargestCredibleDi
splacement[m]
5.41e-2, 3.3e-1
**
constant
NWCumulativeDisplacementRat
e[mm/yr]
0.00005
**
constant
NECumulativeDisplacementRat
e[mm/yr]
0.00005
**
**
**          ***>>> VOLCANO
<<<***
**
finiteexponential
TimeOfNextVolcanicEventinRe
gionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**
constant
XLocationInRegionOfInterest
[m]
548000.0
**
constant
YLocationInRegionOfInterest
[m]
4078000.0
**
uniform
RNtoDetermineIfExtrusiveOrI
ntrusiveVolcanicEvent
0.0, 1.0
**
constant
FractionOfTimeVolcanicEvent
IsExtrusive
0.999
**
uniform
AngleOfVolcanicDikeMeasured
FromNorthClockwise[degrees]
0.0, 15.0
**
uniform
LengthOfVolcanicDike[m]
2000.0, 11000.0
**
uniform
WidthOfVolcanicDike[m]
1.0, 10.0
**
uniform
DiameterOfVolcanicCone[m]
24.6, 77.9
**
**
**          ***>>> ASHPLUMO
<<<***
**
constant
DensityOfAirAtSTP[g/cm3]
0.00129
**
constant
ViscosityOfAirAtSTP[g/cm-s]
0.00018
**
constant
ConstantRelatingFallTimeToE
ddyDiffusivity[cm2/s5/2]
400.0
**
constant
MaximumParticleDiameterForP
articleTransport[cm]
10.d0
**
constant
MinimumFuelParticulateSize[
cm]
0.0001
**
constant
ModeFuelParticulateSize[cm]
0.001
**
constant
MaximumFuelParticulateSize[
cm]
0.01
**
constant
MinimumAshDensityForVariati
onWithSize[g/cm3]
1.2
**
constant
MaximumAshDensityForVariati
onWithSize[g/cm3]
2.0
**
constant
MinimumAshLogdiameterForDen
sityVariation
-2.0
**
constant
MaximumAshLogdiameterForDen
sityVariation
-1.0
**
constant
ParticleShapeParameter
0.5
**
constant
IncorporationRatio
0.3
**
constant
WindDirection[degrees]
-90.0
**
exponential
```

```
WindSpeed[cm/s]
0.00083
**
loguniform
VolcanicEventDuration[s]
6.13e4, 7.24e6
**
loguniform
VolcanicEventPower[W]
2.57e9, 3.55e11
**
constant
VolcanicColumnConstantBeta
10.0
**
logtriangular
AshMeanParticleLogDiameter[
d_in_cm]
0.01, 0.1, 1.0
**
constant
AshParticleSizeDistribution
StandardDeviation
1.0
**
**
**          ***>>> ASHRMOVO
<<<***
**
constant
RelativeRateOfBlanketRemova
l[1/yr]
0.0001
**
constant
FractionOfPrecipitationLost
ToEvapotranspiration
0.68
**
constant
FractionOfIrrigationLostToE
vapotranspiration
0.5
**
constant
AnnualPrecipitation[m/yr]
0.085
**
constant
AnnualIrrigation[m/yr]
1.52
**
constant
FractionOfYearSoilIsSaturat
edDueToPrecipitation
0.0054
**
constant
FractionOfYearSoilIsSaturat
edDueToIrrigation
0.2
**
constant
AshBulkDensity[g/cm3]
1.4
**
constant
AshVolumetricMoistureFracti
onAtSaturation
0.4
**
constant
DepthOfTheRootingZone[m]
0.15
**
constant
KdOfUraniumInVolcanicAsh[cm
3/g]
35.0
**
constant
KdOfCuriumInVolcanicAsh[cm3
/g]
4000.0
**
constant
KdOfPlutoniumInVolcanicAsh[
cm3/g]
550.0
**
constant
KdOfAmericiumInVolcanicAsh[
cm3/g]
1900.0
**
constant
KdOfThoriumInVolcanicAsh[cm
3/g]
3200.0
**
constant
KdOfRadiumInVolcanicAsh[cm3
/g]
500.0
**
constant
KdOfLeadInVolcanicAsh[cm3/g
]
270.0
**
constant
KdOfProtactiniumInVolcanicA
sh[cm3/g]
550.0
**
constant
KdOfActiniumInVolcanicAsh[c
m3/g]
450.0
**
constant
KdOfNeptuniumInVolcanicAsh[
cm3/g]
5.0
**
constant
KdOfSamariumInVolcanicAsh[c
m3/g]
245.0
**
constant
KdOfCesiumInVolcanicAsh[cm3
/g]
280.0
**
constant
KdOfIodineInVolcanicAsh[cm3
/g]
1.0
**
constant
KdOfTinInVolcanicAsh[cm3/g]
130.0
**
constant
KdOfSilverInVolcanicAsh[cm3
/g]
55.0
**
constant
KdOfPaladiumInVolcanicAsh[c
m3/g]
55.0
**
constant
KdOfTechnetiumInVolcanicAsh
[cm3/g]
0.1
**
constant
KdOfMolybdenumInVolcanicAsh
[cm3/g]
10.0
**
constant
KdOfNiobiumInVolcanicAsh[cm
3/g]
160.0
**
constant
KdOfZirconiumInVolcanicAsh[
cm3/g]
600.0
**
constant
KdOfStrontiumInVolcanicAsh[
cm3/g]
15.0
**
constant
KdOfSeleniumInVolcanicAsh[c
m3/g]
150.0
**
constant
KdOfNickelInVolcanicAsh[cm3
/g]
400.0
**
constant
KdOfChlorineInVolcanicAsh[c
m3/g]
0.0
**
constant
KdOfCarbonInVolcanicAsh[cm3
/g]
5.0
**
constant
SolubilityOfUraniumInVolcan
icAsh[moles/liter]
4.5e-5
**
constant
SolubilityOfCuriumInVolcani
cAsh[moles/liter]
1.0e-6
**
constant
SolubilityOfPlutoniumInVolc
anicAsh[moles/liter]
5.0e-6
```

```
**
constant
SolubilityOfAmericiumInVolc
anicAsh[moles/liter]
1.0e-6
**
constant
SolubilityOfThoriumInVolcan
icAsh[moles/liter]
3.2e-9
**
constant
SolubilityOfRadiumInVolcani
cAsh[moles/liter]
1.0e-7
**
constant
SolubilityOfLeadInVolcanicA
sh[moles/liter]
3.2e-7
**
constant
SolubilityOfProtactiniumInV
olcanicAsh[moles/liter]
3.2e-8
**
constant
SolubilityOfActiniumInVolca
nicAsh[moles/liter]
1.0e-6
**
constant
SolubilityOfNeptuniumInVolc
anicAsh[moles/liter]
1.0e-4
**
constant
SolubilityOfSamariumInVolca
nicAsh[moles/liter]
5.0e-6
**
constant
SolubilityOfCesiumInVolcani
cAsh[moles/liter]
1.0
**
constant
SolubilityOfIodineInVolcani
cAsh[moles/liter]
1.0
**
constant
SolubilityOfTinInVolcanicAs
h[moles/liter]
5.0e-8
**
constant
SolubilityOfSilverInVolcani
cAsh[moles/liter]
1.0
**
constant
SolubilityOfPaladiumInVolca
nicAsh[moles/liter]
9.5e-4
**
constant
SolubilityOfTechnetiumInVol
canicAsh[moles/liter]
1.0
**
constant
SolubilityOfMolybdenumInVol
canicAsh[moles/liter]
1.0
**
constant
SolubilityOfNiobiumInVolcan
icAsh[moles/liter]
1.0e-8
**
constant
SolubilityOfZirconiumInVolc
anicAsh[moles/liter]
3.2e-10
**
constant
SolubilityOfStrontiumInVolc
anicAsh[moles/liter]
1.3e-4
**
constant
SolubilityOfSeleniumInVolca
nicAsh[moles/liter]
1.0
**
constant
SolubilityOfNickelInVolcani
cAsh[moles/liter]
2.0e-3
**
constant
SolubilityOfChlorineInVolca
nicAsh[moles/liter]
1.0
**
constant
SolubilityOfCarbonInVolcani
cAsh[moles/liter]
1.0
**
**
**          ***>>>   DCAGS
<<<***
**
constant
DistanceCutoffForDoseConver
sionDualityInDCAGS[km]
19.99
**
loguniform
AirborneMassLoadForVolcanis
mDoseCalculation[g/m3]
1.0e-4, 1.0e-2
**
constant
OccupancyFactorForVolcanism
DoseCalculation[-]
0.24
**
constant
DepthOfResuspendableLayer[c
m]
0.3
**
**
**          ***>>>
CORRELATED PARAMETERS
<<<***
**
correlateinputs
SubAreaWetFraction
ArealAverageMeanAnnualInfil
trationAtStart[mm/yr]
0.631
**
correlateinputs
SubAreaWetFraction
MatrixPermeability_TSw_[m2]
-0.623
**
correlateinputs
FowFactor
ArealAverageMeanAnnualInfil
trationAtStart[mm/yr]
-0.224
**
correlateinputs
FowFactor
MatrixPermeability_TSw_[m2]
0.13
**
correlateinputs
FowFactor
SubAreaWetFraction
-0.366
**
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Pu
0.964
**
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_U
0.346
**
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Np
0.837
**
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Th
0.112
**
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_U
0.489
**
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_Np
0.881
**
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_Th
0.109
**
correlateinputs
AlluviumMatrixRD_SAV_Np
AlluviumMatrixRD_SAV_Th
0.260
**
correlateinputs
AlluviumMatrixRD_SAV_Np
AlluviumMatrixRD_SAV_U
0.610
**
correlateinputs
```

```
AlluviumMatrixRD_SAV_Th          0.165                          endoffile
AlluviumMatrixRD_SAV_U           **
```

**Note that according to Rob Rice, one should not compare the results from his two runs with those of the 1,000-vector runs that S. Mohanty is referring to in his 11/6/98 email. Several parameters are different, including number of vectors (250 in Rice's runs), invert properties (including Kds for the invert), and spent fuel gap fraction (which was revised subsequent to the 1,000-vector runs). One should compare instead the two runs that Rice made, one with the EBSFILT switch "off" and the other with the switch "on."**

**S. Mohanty said that one can use the EBSFILT module to simulate an altered repository horizon layer. One can increase the thickness of the layer in EBSFILT, but one should make commensurate decreases in the TSw layer (in all seven subareas) to make the overall thickness of the UZ constant.**

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**12/11/98**

In previous sensitivity analyses for CANE (see, for example, notebook #185, volumes 5, p. 119), a measure of sensitivity that was used was TOTAL RELEASE, values of which are in the output file relgwgs.res (third column). The values of total release were plotted against the values of the individual parameters of interest (if the parameters were sampled), such as matrix porosity/permeability and fracture porosity/permeability. Values of sampled parameters are in the output file samplpar.res.

For the two runs that were done by R. Rice, only the invert matrix permeability was allowed to be sampled, among the parameters in the EBSFILT module. Invert permeability is the 115th parameter that was sampled in the R. Rice runs, out of a total of 246 sampled parameters. A Fortran 90 code was written to extract values of invert permeability from samplpar.res. The source code is listed below:

```
C     Last change:  RTP  11 Dec 1998    4:35 pm

      PROGRAM READSAMPPAR
      IMPLICIT REAL (A-H,O-Z)
      DIMENSION PARVAL(1000)
C
      OPEN(UNIT=5,FILE='SAMPPAR.INP')
      OPEN(UNIT=6,FILE='SAMPPAR.OUT')
C
C     READ FROM INPUT FILE # OF REALIZATIONS, # OF SAMPLED PARAMETERS
      READ(5,*) NVECTOR, NSAMPPAR
C     WRITE TO OUTPUT FILE # OF REALIZATIONS, # OF SAMPLED PARAMETERS
      WRITE(6,*)'# OF REALIZATIONS: ',NVECTOR, '; # OF SAMPLED
     1 PARAMETERS: ',NSAMPPAR
C
C--CALCULATE NUMBER OF OUTPUT LINES PER REALIZATION. THERE ARE FIVE
C  VALUES LISTED PER LINE, PLUS ONE HEADER LINE PER REALIZATION.
C
      NLINES=(INT(NSAMPPAR/5) + (NSAMPPAR/5 - INT(NSAMPPAR/5))*5)
C
C     READ FROM INPUT FILE THE SAMPLE PARAMETER # OF INTEREST'
      READ(5,*) IPAR
C
C--READ VALUES OF SAMPLED PARAMETERS FOR EACH REALIZATION.
C  READ THE FIRST (HEADER) LINE BUT IGNORE VALUES.
C
      WRITE(6,*)'SAMPLED PAR # :',IPAR
      WRITE(6,*)'REALIZATION # ;','PAR. VALUE = '
      DO 20 H=1,NVECTOR
      READ(5,*)
      J=1
      DO 10 I=1,NLINES
      READ(5,*,END=10) PARVAL(J),PARVAL(J+1),PARVAL(J+2),PARVAL(J+3),
     1 PARVAL(J+4)
      J=J+5
10    CONTINUE
      WRITE(6,*)H,PARVAL(IPAR)
20    CONTINUE

      CLOSE(5)
      CLOSE(6)
      STOP
```

END

The following is the samppar.out file resulting from extracting invert permeability values from samplpar.res for the case where EBSFILT was switched to "on". This particular TPA 3.2 run will be referred to as case EBSFILT-1. Several of the values were checked by comparison with the values in the original samplpar.res file.

```
 # OF REALIZATIONS:  250 ;
# OF SAMPLED
PARAMETERS:  246
~
 SAMPLED PAR # : 115
~
 REALIZATION # ;PAR. VALUE
=
~
 1.00000000 1.22404202E-17
~
 2.00000000 9.00087071E-18
~
 3.00000000 5.14068796E-17
~
 4.00000000 8.47582129E-17
 5.00000000 1.25135503E-17
 6.00000000 4.87513287E-17
 7.00000000 1.51383896E-17
 8.00000000 3.08865006E-17
 9.00000000 2.58366804E-17
 10.0000000 1.73165695E-17
 11.0000000 1.99231893E-17
 12.0000000 2.32445495E-17
 13.0000000 4.58112608E-17
 14.0000000 2.06120802E-17
 15.0000000 3.12939995E-17
 16.0000000 5.24123904E-17
 17.0000000 4.31103010E-17
 18.0000000 2.36553207E-17
 19.0000000 4.01374106E-17
 20.0000000 1.18914600E-17
 21.0000000 2.02603399E-17
 22.0000000 1.85604798E-16
 23.0000000 2.73153203E-17
 24.0000000 3.71194785E-17
 25.0000000 2.00848204E-17
 26.0000000 1.76848105E-17
 27.0000000 1.14423696E-16
 28.0000000 1.43709595E-17
 29.0000000 2.25827404E-17
 30.0000000 4.05961286E-17
 31.0000000 1.26911798E-17
 32.0000000 2.42666899E-17
 33.0000000 1.31771700E-17
 34.0000000 1.48429306E-17
 35.0000000 1.58428199E-17
 36.0000000 2.59794898E-17
 37.0000000 9.90859473E-17
 38.0000000 2.67102592E-17
 39.0000000 6.84904306E-18
 40.0000000 5.84301128E-17
 41.0000000 1.10588498E-17
 42.0000000 2.80420316E-17
 43.0000000 8.15783139E-18
 44.0000000 1.95072399E-17
 45.0000000 2.12900805E-17
 46.0000000 9.91774169E-18
 47.0000000 4.78118294E-18
 48.0000000 9.78889425E-18
 49.0000000 6.70625630E-17
 50.0000000 6.04725690E-18
 51.0000000 1.14620697E-17
 52.0000000 2.89407898E-17
 53.0000000 6.37233408E-17
 54.0000000 1.44825594E-17
 55.0000000 3.25911808E-17
 56.0000000 1.40744599E-17
 57.0000000 1.31667804E-16
 58.0000000 9.74017165E-18
 59.0000000 1.90625493E-17
 60.0000000 4.11403704E-17
 61.0000000 1.35742597E-17
 62.0000000 5.64770798E-17
 63.0000000 2.52830798E-17
 64.0000000 2.28960500E-17
 65.0000000 6.44993007E-18
 66.0000000 1.45921393E-17
 67.0000000 2.24061506E-17
 68.0000000 3.93223598E-17
 69.0000000 1.65410000E-17
 70.0000000 7.25475696E-18
 71.0000000 9.12627129E-18
 72.0000000 1.47197204E-17
 73.0000000 4.67656287E-17
 74.0000000 2.10657301E-18
 75.0000000 1.27618202E-17
 76.0000000 1.02671304E-17
 77.0000000 3.95679298E-17
 78.0000000 4.63809897E-17
 79.0000000 4.40957709E-17
 80.0000000 2.48242494E-17
 81.0000000 2.04701807E-17
 82.0000000 1.86684093E-17
 83.0000000 2.56712393E-17
 84.0000000 2.28854902E-17
 85.0000000 5.51319394E-18
 86.0000000 1.68170004E-17
 87.0000000 1.50449595E-17
 88.0000000 5.56229133E-17
 89.0000000 1.52624799E-17
 90.0000000 3.14932805E-17
 91.0000000 7.13046811E-18
 92.0000000 1.11959996E-17
 93.0000000 1.39512001E-17
 94.0000000 8.63682439E-18
 95.0000000 9.30115961E-18
 96.0000000 1.59656198E-17
 97.0000000 7.01341461E-18
 98.0000000 1.08724198E-17
 99.0000000 6.26390005E-18
 100.000000 4.48979508E-17
 101.000000 2.96868306E-17
 102.000000 7.49047779E-17
 103.000000 3.93904979E-18
 104.000000 1.04915403E-17
 105.000000 3.42011489E-17
 106.000000 8.52468186E-18
 107.000000 2.85980491E-17
 108.000000 1.42124700E-17
 109.000000 3.39873393E-17
 110.000000 3.17214004E-17
 111.000000 3.78173907E-17
 112.000000 7.12987270E-17
 113.000000 3.01062906E-17
 114.000000 4.10185920E-18
 115.000000 2.35696596E-17
 116.000000 2.76761299E-17
 117.000000 2.17007194E-17
 118.000000 1.37829300E-17
 119.000000 1.09138897E-17
 120.000000 1.65757995E-17
 121.000000 4.73564309E-17
 122.000000 6.30032900E-17
 123.000000 1.15095201E-17
 124.000000 1.43431894E-17
 125.000000 2.41041208E-17
 126.000000 6.74525423E-17
 127.000000 1.57357298E-17
 128.000000 1.04096900E-17
 129.000000 8.84143661E-18
 130.000000 1.82896698E-17
 131.000000 2.63465595E-17
 132.000000 2.23605498E-17
 133.000000 2.82814805E-17
 134.000000 1.32761603E-17
 135.000000 3.55727997E-17
 136.000000 1.35042297E-17
 137.000000 1.91936706E-17
 138.000000 1.63771901E-17
 139.000000 1.67012199E-17
 140.000000 5.06160419E-18
 141.000000 1.17735702E-17
 142.000000 1.13078501E-17
 143.000000 1.06585903E-17
 144.000000 2.84476809E-17
 145.000000 1.37156298E-17
 146.000000 1.70241198E-17
 147.000000 3.33550193E-17
 148.000000 4.16470814E-17
 149.000000 5.71988280E-18
 150.000000 2.38062200E-17
 151.000000 4.97874485E-17
 152.000000 3.49873808E-17
 153.000000 1.96486100E-17
 154.000000 2.62889397E-17
 155.000000 1.02043796E-17
 156.000000 6.02184574E-17
 157.000000 1.53928700E-17
 158.000000 1.07555102E-17
 159.000000 1.55699198E-17
 160.000000 4.19806105E-17
 161.000000 2.94222287E-17
 162.000000 2.07846797E-17
 163.000000 7.44157404E-18
 164.000000 1.93453193E-17
 165.000000 6.59603912E-18
 166.000000 1.89502396E-17
 167.000000 3.68466313E-17
 168.000000 3.63698709E-17
```

| | | |
|---|---|---|
| 169.000000 1.30615599E-17 | 197.000000 3.88111985E-17 | 225.000000 2.21104104E-17 |
| 170.000000 2.18627393E-17 | 198.000000 8.78351577E-18 | 226.000000 1.60912106E-17 |
| 171.000000 2.43443804E-17 | 199.000000 4.81210899E-17 | 227.000000 2.67644197E-17 |
| 172.000000 7.74315003E-18 | 200.000000 3.32825508E-18 | 228.000000 3.08028395E-17 |
| 173.000000 1.74679700E-17 | 201.000000 4.95910494E-18 | 229.000000 3.37725403E-17 |
| 174.000000 4.36284296E-18 | 202.000000 8.07257719E-18 | 230.000000 1.23537596E-17 |
| 175.000000 2.54463107E-17 | 203.000000 3.29072399E-17 | 231.000000 3.28729913E-17 |
| 176.000000 1.20359999E-17 | 204.000000 7.90427820E-18 | 232.000000 6.19915025E-17 |
| 177.000000 3.22745791E-17 | 205.000000 8.22225387E-18 | 233.000000 1.33044003E-17 |
| 178.000000 2.20119494E-17 | 206.000000 4.42737703E-17 | 234.000000 3.45688109E-17 |
| 179.000000 5.37538590E-17 | 207.000000 2.03670495E-17 | 235.000000 3.81720493E-17 |
| 180.000000 5.35663305E-18 | 208.000000 7.34955202E-17 | 236.000000 3.62128886E-17 |
| 181.000000 1.00942703E-17 | 209.000000 1.84808494E-17 | 237.000000 2.49934806E-17 |
| 182.000000 2.76307706E-17 | 210.000000 1.55341392E-17 | 238.000000 2.09204697E-17 |
| 183.000000 2.70968603E-17 | 211.000000 1.79672794E-17 | 239.000000 1.24202401E-17 |
| 184.000000 1.28476899E-17 | 212.000000 9.25892790E-18 | 240.000000 3.53339595E-17 |
| 185.000000 9.46696961E-18 | 213.000000 1.77980300E-17 | 241.000000 1.16523899E-17 |
| 186.000000 1.75084705E-17 | 214.000000 5.77374913E-17 | 242.000000 3.06031515E-17 |
| 187.000000 1.87840607E-17 | 215.000000 1.82394301E-17 | 243.000000 7.58137336E-18 |
| 188.000000 9.12888832E-17 | 216.000000 8.43125015E-18 | 244.000000 2.11731304E-17 |
| 189.000000 5.93289504E-18 | 217.000000 1.97442602E-17 | 245.000000 3.01114402E-18 |
| 190.000000 9.54333079E-18 | 218.000000 2.33003097E-17 | 246.000000 8.28876928E-17 |
| 191.000000 1.81180794E-17 | 219.000000 5.42287996E-17 | 247.000000 7.92018885E-17 |
| 192.000000 1.20973601E-17 | 220.000000 7.32815931E-18 | 248.000000 9.70649928E-17 |
| 193.000000 2.45675405E-17 | 221.000000 1.62843606E-17 | 249.000000 3.83612388E-17 |
| 194.000000 4.28993303E-17 | 222.000000 5.05849896E-17 | 250.000000 2.14264693E-17 |
| 195.000000 2.99853700E-17 | 223.000000 6.36239699E-18 | |
| 196.000000 2.90672491E-17 | 224.000000 1.71533899E-17 | |

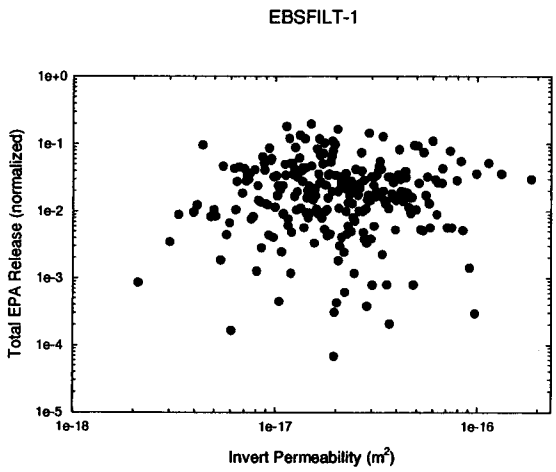
Below is a copy of the output file relgwgs.res from the TPA 3.2 run by R. Rice for the case where the EBSFILT switch was "on":

```
 Input file tpa.inp as supplied with TPA Version 3.2 Code.
~
 Base case data set Rev 3.2   7/16/98
~
 TPA 3.2, Job started: Fri Dec  4 16:37:43 1998
 EPA Groundwater, Ground Surface, and Total Release
 Normalized - Values for Each Vector
```

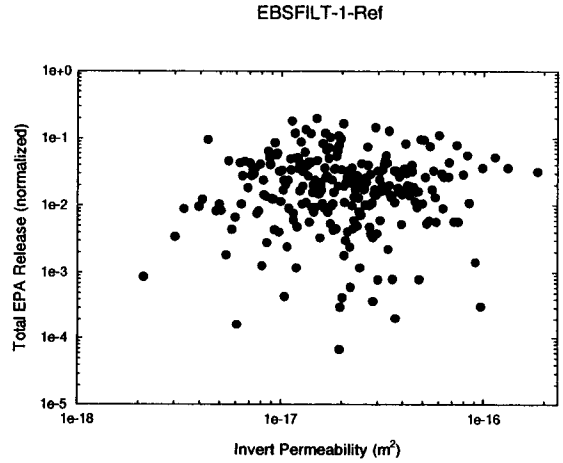
| vector unitless | gwepasum unitless | gsepasum unitless | epasum unitless |
|---|---|---|---|
| 1 | 3.4989E-02 | 0.0000E+00 | 3.4989E-02 |
| 2 | 1.2604E-02 | 0.0000E+00 | 1.2604E-02 |
| 3 | 2.5905E-02 | 0.0000E+00 | 2.5905E-02 |
| 4 | 5.1636E-03 | 0.0000E+00 | 5.1636E-03 |
| 5 | 8.7819E-02 | 0.0000E+00 | 8.7819E-02 |
| 6 | 9.4655E-02 | 0.0000E+00 | 9.4655E-02 |
| 7 | 4.6643E-02 | 0.0000E+00 | 4.6643E-02 |
| 8 | 3.2106E-02 | 0.0000E+00 | 3.2106E-02 |
| 9 | 1.7276E-02 | 0.0000E+00 | 1.7276E-02 |
| 10 | 7.1981E-02 | 0.0000E+00 | 7.1981E-02 |
| 11 | 3.3750E-02 | 0.0000E+00 | 3.3750E-02 |
| 12 | 2.6696E-02 | 0.0000E+00 | 2.6696E-02 |
| 13 | 1.1236E-02 | 0.0000E+00 | 1.1236E-02 |
| 14 | 1.1017E-02 | 0.0000E+00 | 1.1017E-02 |
| 15 | 1.6083E-02 | 0.0000E+00 | 1.6083E-02 |
| 16 | 5.3145E-03 | 0.0000E+00 | 5.3145E-03 |
| 17 | 1.9094E-02 | 0.0000E+00 | 1.9094E-02 |
| 18 | 2.7656E-02 | 0.0000E+00 | 2.7656E-02 |
| 19 | 1.5882E-02 | 0.0000E+00 | 1.5882E-02 |
| 20 | 1.1611E-03 | 0.0000E+00 | 1.1611E-03 |
| 21 | 1.6258E-01 | 0.0000E+00 | 1.6258E-01 |
| 22 | 2.9676E-02 | 0.0000E+00 | 2.9676E-02 |
| 23 | 4.7849E-03 | 0.0000E+00 | 4.7849E-03 |
| 24 | 3.2185E-02 | 0.0000E+00 | 3.2185E-02 |
| 25 | 4.2408E-04 | 0.0000E+00 | 4.2408E-04 |
| 26 | 9.8337E-03 | 0.0000E+00 | 9.8337E-03 |
| 27 | 5.1431E-02 | 0.0000E+00 | 5.1431E-02 |
| 28 | 1.9731E-02 | 0.0000E+00 | 1.9731E-02 |
| 29 | 4.4730E-03 | 0.0000E+00 | 4.4730E-03 |
| 30 | 3.4740E-02 | 0.0000E+00 | 3.4740E-02 |
| 31 | 1.0419E-02 | 0.0000E+00 | 1.0419E-02 |
| 32 | 2.0217E-02 | 0.0000E+00 | 2.0217E-02 |
| 33 | 1.3309E-01 | 0.0000E+00 | 1.3309E-01 |
| 34 | 9.2982E-03 | 0.0000E+00 | 9.2982E-03 |
| 35 | 1.6657E-02 | 0.0000E+00 | 1.6657E-02 |
| 36 | 1.0042E-02 | 0.0000E+00 | 1.0042E-02 |
| 37 | 3.5591E-02 | 0.0000E+00 | 3.5591E-02 |
| 38 | 7.3489E-02 | 0.0000E+00 | 7.3489E-02 |
| 39 | 1.8218E-02 | 0.0000E+00 | 1.8218E-02 |
| 40 | 5.6434E-03 | 0.0000E+00 | 5.6434E-03 |
| 41 | 4.9281E-02 | 0.0000E+00 | 4.9281E-02 |
| 42 | 1.0697E-02 | 0.0000E+00 | 1.0697E-02 |
| 43 | 2.3560E-02 | 0.0000E+00 | 2.3560E-02 |
| 44 | 6.7505E-05 | 0.0000E+00 | 6.7505E-05 |
| 45 | 4.0347E-03 | 0.0000E+00 | 4.0347E-03 |
| 46 | 1.1334E-02 | 0.0000E+00 | 1.1334E-02 |
| 47 | 8.2284E-03 | 0.0000E+00 | 8.2284E-03 |
| 48 | 3.2124E-02 | 0.0000E+00 | 3.2124E-02 |
| 49 | 2.6012E-02 | 0.0000E+00 | 2.6012E-02 |
| 50 | 1.6292E-04 | 0.0000E+00 | 1.6292E-04 |
| 51 | 7.6565E-03 | 0.0000E+00 | 7.6565E-03 |
| 52 | 1.7170E-02 | 0.0000E+00 | 1.7170E-02 |
| 53 | 2.6080E-02 | 0.0000E+00 | 2.6080E-02 |
| 54 | 7.9376E-03 | 0.0000E+00 | 7.9376E-03 |
| 55 | 4.6324E-02 | 0.0000E+00 | 4.6324E-02 |
| 56 | 4.3825E-02 | 0.0000E+00 | 4.3825E-02 |
| 57 | 3.5622E-02 | 0.0000E+00 | 3.5622E-02 |
| 58 | 3.9970E-03 | 0.0000E+00 | 3.9970E-03 |
| 59 | 1.9399E-02 | 0.0000E+00 | 1.9399E-02 |
| 60 | 8.2025E-02 | 0.0000E+00 | 8.2025E-02 |
| 61 | 2.7197E-02 | 0.0000E+00 | 2.7197E-02 |
| 62 | 3.2218E-02 | 0.0000E+00 | 3.2218E-02 |
| 63 | 2.4022E-02 | 0.0000E+00 | 2.4022E-02 |
| 64 | 1.3221E-02 | 0.0000E+00 | 1.3221E-02 |
| 65 | 2.7291E-02 | 0.0000E+00 | 2.7291E-02 |
| 66 | 2.0197E-02 | 0.0000E+00 | 2.0197E-02 |
| 67 | 3.5987E-02 | 0.0000E+00 | 3.5987E-02 |
| 68 | 5.1961E-03 | 0.0000E+00 | 5.1961E-03 |
| 69 | 1.1835E-01 | 0.0000E+00 | 1.1835E-01 |
| 70 | 3.3798E-02 | 0.0000E+00 | 3.3798E-02 |
| 71 | 1.2288E-02 | 0.0000E+00 | 1.2288E-02 |
| 72 | 2.3651E-02 | 0.0000E+00 | 2.3651E-02 |
| 73 | 9.2704E-03 | 0.0000E+00 | 9.2704E-03 |
| 74 | 8.5380E-04 | 0.0000E+00 | 8.5380E-04 |
| 75 | 1.9197E-02 | 0.0000E+00 | 1.9197E-02 |
| 76 | 2.3491E-02 | 0.0000E+00 | 2.3491E-02 |
| 77 | 1.4410E-02 | 0.0000E+00 | 1.4410E-02 |
| 78 | 1.5768E-02 | 0.0000E+00 | 1.5768E-02 |
| 79 | 3.9179E-02 | 0.0000E+00 | 3.9179E-02 |
| 80 | 7.1260E-03 | 0.0000E+00 | 7.1260E-03 |
| 81 | 1.7745E-03 | 0.0000E+00 | 1.7745E-03 |
| 82 | 4.4894E-03 | 0.0000E+00 | 4.4894E-03 |
| 83 | 1.7067E-02 | 0.0000E+00 | 1.7067E-02 |
| 84 | 5.9644E-03 | 0.0000E+00 | 5.9644E-03 |
| 85 | 4.5790E-02 | 0.0000E+00 | 4.5790E-02 |
| 86 | 2.6901E-02 | 0.0000E+00 | 2.6901E-02 |

| | | | |
|---|---|---|---|
| 87 | 1.9542E-01 | 0.0000E+00 | 1.9542E-01 |
| 88 | 1.6933E-02 | 0.0000E+00 | 1.6933E-02 |
| 89 | 1.4726E-02 | 0.0000E+00 | 1.4726E-02 |
| 90 | 1.9392E-02 | 0.0000E+00 | 1.9392E-02 |
| 91 | 2.7731E-02 | 0.0000E+00 | 2.7731E-02 |
| 92 | 3.3737E-02 | 0.0000E+00 | 3.3737E-02 |
| 93 | 1.1691E-01 | 0.0000E+00 | 1.1691E-01 |
| 94 | 6.3493E-02 | 0.0000E+00 | 6.3493E-02 |
| 95 | 8.5387E-02 | 0.0000E+00 | 8.5387E-02 |
| 96 | 1.0643E-02 | 0.0000E+00 | 1.0643E-02 |
| 97 | 4.2336E-02 | 0.0000E+00 | 4.2336E-02 |
| 98 | 9.1160E-03 | 0.0000E+00 | 9.1160E-03 |
| 99 | 4.2743E-02 | 0.0000E+00 | 4.2743E-02 |
| 100 | 1.8602E-02 | 0.0000E+00 | 1.8602E-02 |
| 101 | 3.7993E-03 | 0.0000E+00 | 3.7993E-03 |
| 102 | 5.6274E-03 | 0.0000E+00 | 5.6274E-03 |
| 103 | 9.5589E-03 | 0.0000E+00 | 9.5589E-03 |
| 104 | 2.0486E-02 | 0.0000E+00 | 2.0486E-02 |
| 105 | 1.9579E-02 | 0.0000E+00 | 1.9579E-02 |
| 106 | 2.7849E-03 | 0.0000E+00 | 2.7849E-03 |
| 107 | 1.4610E-02 | 0.0000E+00 | 1.4610E-02 |
| 108 | 9.2587E-03 | 0.0000E+00 | 9.2587E-03 |
| 109 | 1.2670E-01 | 0.0000E+00 | 1.2670E-01 |
| 110 | 3.3862E-02 | 0.0000E+00 | 3.3862E-02 |
| 111 | 1.7906E-02 | 0.0000E+00 | 1.7906E-02 |
| 112 | 5.6605E-03 | 0.0000E+00 | 5.6605E-03 |
| 113 | 7.8025E-04 | 0.0000E+00 | 7.8025E-04 |
| 114 | 1.2188E-02 | 0.0000E+00 | 1.2188E-02 |
| 115 | 2.5083E-02 | 0.0000E+00 | 2.5083E-02 |
| 116 | 3.7319E-03 | 0.0000E+00 | 3.7319E-03 |
| 117 | 3.3010E-02 | 0.0000E+00 | 3.3010E-02 |
| 118 | 5.6263E-03 | 0.0000E+00 | 5.6263E-03 |
| 119 | 8.8860E-03 | 0.0000E+00 | 8.8860E-03 |
| 120 | 2.5798E-02 | 0.0000E+00 | 2.5798E-02 |
| 121 | 1.5772E-02 | 0.0000E+00 | 1.5772E-02 |
| 122 | 8.9169E-03 | 0.0000E+00 | 8.9169E-03 |
| 123 | 6.0286E-03 | 0.0000E+00 | 6.0286E-03 |
| 124 | 1.5350E-02 | 0.0000E+00 | 1.5350E-02 |
| 125 | 1.2844E-02 | 0.0000E+00 | 1.2844E-02 |
| 126 | 4.2835E-02 | 0.0000E+00 | 4.2835E-02 |
| 127 | 2.0790E-02 | 0.0000E+00 | 2.0790E-02 |
| 128 | 4.4146E-04 | 0.0000E+00 | 4.4146E-04 |
| 129 | 4.0217E-02 | 0.0000E+00 | 4.0217E-02 |
| 130 | 3.4181E-02 | 0.0000E+00 | 3.4181E-02 |
| 131 | 2.1724E-02 | 0.0000E+00 | 2.1724E-02 |
| 132 | 9.8207E-03 | 0.0000E+00 | 9.8207E-03 |
| 133 | 3.2761E-03 | 0.0000E+00 | 3.2761E-03 |
| 134 | 1.0884E-02 | 0.0000E+00 | 1.0884E-02 |
| 135 | 7.8956E-04 | 0.0000E+00 | 7.8956E-04 |
| 136 | 3.9687E-02 | 0.0000E+00 | 3.9687E-02 |
| 137 | 1.0819E-01 | 0.0000E+00 | 1.0819E-01 |
| 138 | 3.5485E-02 | 0.0000E+00 | 3.5485E-02 |
| 139 | 6.6777E-02 | 0.0000E+00 | 6.6777E-02 |
| 140 | 8.3198E-03 | 0.0000E+00 | 8.3198E-03 |
| 141 | 5.0945E-02 | 0.0000E+00 | 5.0945E-02 |
| 142 | 1.7941E-01 | 0.0000E+00 | 1.7941E-01 |
| 143 | 2.4038E-03 | 0.0000E+00 | 2.4038E-03 |
| 144 | 3.7276E-04 | 0.0000E+00 | 3.7276E-04 |
| 145 | 4.3977E-02 | 0.0000E+00 | 4.3977E-02 |
| 146 | 7.7936E-03 | 0.0000E+00 | 7.7936E-03 |
| 147 | 4.2234E-02 | 0.0000E+00 | 4.2234E-02 |
| 148 | 2.9723E-02 | 0.0000E+00 | 2.9723E-02 |
| 149 | 4.3921E-03 | 0.0000E+00 | 4.3921E-03 |
| 150 | 4.9293E-03 | 0.0000E+00 | 4.9293E-03 |
| 151 | 1.0457E-02 | 0.0000E+00 | 1.0457E-02 |
| 152 | 1.2883E-02 | 0.0000E+00 | 1.2883E-02 |
| 153 | 3.0262E-04 | 0.0000E+00 | 3.0262E-04 |
| 154 | 2.5582E-02 | 0.0000E+00 | 2.5582E-02 |
| 155 | 1.6800E-02 | 0.0000E+00 | 1.6800E-02 |
| 156 | 1.0865E-01 | 0.0000E+00 | 1.0865E-01 |
| 157 | 1.4761E-02 | 0.0000E+00 | 1.4761E-02 |
| 158 | 2.3605E-02 | 0.0000E+00 | 2.3605E-02 |
| 159 | 3.2976E-03 | 0.0000E+00 | 3.2976E-03 |
| 160 | 1.9596E-02 | 0.0000E+00 | 1.9596E-02 |
| 161 | 1.4061E-02 | 0.0000E+00 | 1.4061E-02 |
| 162 | 2.9775E-03 | 0.0000E+00 | 2.9775E-03 |
| 163 | 3.5966E-02 | 0.0000E+00 | 3.5966E-02 |
| 164 | 7.7843E-02 | 0.0000E+00 | 7.7843E-02 |
| 165 | 4.4995E-02 | 0.0000E+00 | 4.4995E-02 |
| 166 | 6.3569E-02 | 0.0000E+00 | 6.3569E-02 |
| 167 | 2.0414E-04 | 0.0000E+00 | 2.0414E-04 |
| 168 | 1.0946E-02 | 0.0000E+00 | 1.0946E-02 |
| 169 | 6.1421E-02 | 0.0000E+00 | 6.1421E-02 |
| 170 | 2.3887E-03 | 0.0000E+00 | 2.3887E-03 |
| 171 | 7.9648E-03 | 0.0000E+00 | 7.9648E-03 |
| 172 | 8.1994E-03 | 0.0000E+00 | 8.1994E-03 |
| 173 | 5.3305E-03 | 0.0000E+00 | 5.3305E-03 |
| 174 | 9.4877E-02 | 0.0000E+00 | 9.4877E-02 |
| 175 | 2.1650E-02 | 0.0000E+00 | 2.1650E-02 |
| 176 | 4.7953E-03 | 0.0000E+00 | 4.7953E-03 |
| 177 | 3.9588E-02 | 0.0000E+00 | 3.9588E-02 |
| 178 | 2.1471E-02 | 0.0000E+00 | 2.1471E-02 |
| 179 | 5.1201E-03 | 0.0000E+00 | 5.1201E-03 |
| 180 | 1.8095E-03 | 0.0000E+00 | 1.8095E-03 |
| 181 | 3.3335E-02 | 0.0000E+00 | 3.3335E-02 |
| 182 | 2.8664E-02 | 0.0000E+00 | 2.8664E-02 |
| 183 | 9.8920E-03 | 0.0000E+00 | 9.8920E-03 |
| 184 | 3.1761E-02 | 0.0000E+00 | 3.1761E-02 |
| 185 | 5.6619E-02 | 0.0000E+00 | 5.6619E-02 |
| 186 | 1.0203E-01 | 0.0000E+00 | 1.0203E-01 |
| 187 | 5.3743E-02 | 0.0000E+00 | 5.3743E-02 |
| 188 | 1.4031E-03 | 0.0000E+00 | 1.4031E-03 |
| 189 | 6.6270E-03 | 0.0000E+00 | 6.6270E-03 |
| 190 | 5.9602E-02 | 0.0000E+00 | 5.9602E-02 |
| 191 | 4.2612E-03 | 0.0000E+00 | 4.2612E-03 |
| 192 | 5.1315E-02 | 0.0000E+00 | 5.1315E-02 |
| 193 | 1.1633E-03 | 0.0000E+00 | 1.1633E-03 |
| 194 | 1.3875E-02 | 0.0000E+00 | 1.3875E-02 |
| 195 | 3.2367E-02 | 0.0000E+00 | 3.2367E-02 |
| 196 | 1.4304E-01 | 0.0000E+00 | 1.4304E-01 |
| 197 | 3.1152E-02 | 0.0000E+00 | 3.1152E-02 |
| 198 | 5.1163E-02 | 0.0000E+00 | 5.1163E-02 |
| 199 | 7.8393E-04 | 0.0000E+00 | 7.8393E-04 |
| 200 | 8.8161E-03 | 0.0000E+00 | 8.8161E-03 |
| 201 | 1.0372E-02 | 0.0000E+00 | 1.0372E-02 |
| 202 | 1.2517E-03 | 0.0000E+00 | 1.2517E-03 |
| 203 | 5.4591E-02 | 0.0000E+00 | 5.4591E-02 |
| 204 | 4.0954E-02 | 0.0000E+00 | 4.0954E-02 |
| 205 | 1.4267E-02 | 0.0000E+00 | 1.4267E-02 |
| 206 | 3.1595E-02 | 0.0000E+00 | 3.1595E-02 |
| 207 | 1.9166E-02 | 0.0000E+00 | 1.9166E-02 |
| 208 | 7.7947E-02 | 0.0000E+00 | 7.7947E-02 |
| 209 | 3.5215E-02 | 0.0000E+00 | 3.5215E-02 |
| 210 | 2.1709E-02 | 0.0000E+00 | 2.1709E-02 |
| 211 | 1.0545E-02 | 0.0000E+00 | 1.0545E-02 |
| 212 | 4.3607E-03 | 0.0000E+00 | 4.3607E-03 |
| 213 | 2.3944E-02 | 0.0000E+00 | 2.3944E-02 |
| 214 | 1.2892E-02 | 0.0000E+00 | 1.2892E-02 |
| 215 | 1.5477E-02 | 0.0000E+00 | 1.5477E-02 |
| 216 | 1.3541E-02 | 0.0000E+00 | 1.3541E-02 |
| 217 | 9.6878E-02 | 0.0000E+00 | 9.6878E-02 |
| 218 | 1.6977E-02 | 0.0000E+00 | 1.6977E-02 |
| 219 | 7.4524E-02 | 0.0000E+00 | 7.4524E-02 |
| 220 | 2.9335E-02 | 0.0000E+00 | 2.9335E-02 |
| 221 | 9.1090E-03 | 0.0000E+00 | 9.1090E-03 |
| 222 | 9.3030E-02 | 0.0000E+00 | 9.3030E-02 |
| 223 | 1.0400E-02 | 0.0000E+00 | 1.0400E-02 |
| 224 | 5.0071E-02 | 0.0000E+00 | 5.0071E-02 |
| 225 | 6.0836E-04 | 0.0000E+00 | 6.0836E-04 |
| 226 | 8.2868E-02 | 0.0000E+00 | 8.2868E-02 |
| 227 | 3.9346E-02 | 0.0000E+00 | 3.9346E-02 |
| 228 | 5.9453E-03 | 0.0000E+00 | 5.9453E-03 |
| 229 | 2.2046E-03 | 0.0000E+00 | 2.2046E-03 |
| 230 | 1.6370E-02 | 0.0000E+00 | 1.6370E-02 |
| 231 | 1.6734E-02 | 0.0000E+00 | 1.6734E-02 |
| 232 | 2.9168E-02 | 0.0000E+00 | 2.9168E-02 |
| 233 | 3.9971E-02 | 0.0000E+00 | 3.9971E-02 |
| 234 | 1.4298E-02 | 0.0000E+00 | 1.4298E-02 |
| 235 | 1.5752E-02 | 0.0000E+00 | 1.5752E-02 |
| 236 | 3.2196E-02 | 0.0000E+00 | 3.2196E-02 |
| 237 | 4.1638E-02 | 0.0000E+00 | 4.1638E-02 |
| 238 | 2.0966E-02 | 0.0000E+00 | 2.0966E-02 |
| 239 | 4.2452E-02 | 0.0000E+00 | 4.2452E-02 |
| 240 | 1.3909E-02 | 0.0000E+00 | 1.3909E-02 |
| 241 | 1.1938E-01 | 0.0000E+00 | 1.1938E-01 |
| 242 | 2.3861E-02 | 0.0000E+00 | 2.3861E-02 |
| 243 | 7.5768E-03 | 0.0000E+00 | 7.5768E-03 |
| 244 | 2.6019E-02 | 0.0000E+00 | 2.6019E-02 |
| 245 | 3.4342E-03 | 0.0000E+00 | 3.4342E-03 |
| 246 | 5.4818E-02 | 0.0000E+00 | 5.4818E-02 |
| 247 | 2.8279E-02 | 0.0000E+00 | 2.8279E-02 |
| 248 | 2.8959E-04 | 0.0000E+00 | 2.8959E-04 |
| 249 | 2.6368E-02 | 0.0000E+00 | 2.6368E-02 |
| 250 | 3.0786E-02 | 0.0000E+00 | 3.0786E-02 |

Below is a plot of invert permeability vs total EPA (normalized) release for case EBSFILT-1:




For comparison, the results of the TPA 3.2 run by R. Rice with the EBSFILT switch set to "off" if plotted below. This TPA 3.2 run will be referred to as EBSFILT-1-Ref.




Microsoft Excel was used to compare the output for EBSFILT-1 and EBSFILT-1-Ref. Only four realizations (#s 4, 22, 179, and 248) had different values of total EPA release for the two cases. The differences ("on" value minus "off" value) in total EPA release are -0.00554, -0.0017, -0.00066, and -1.9E-05 for realization 4, 22, 179, and 248, respectively. The values of invert permeability in each realization are the same for EBSFILT-1 and EBSFILT-1-Ref because parameter sampling is done by the code prior to calling the EBSFILT module.

**12/14/98**

To check if the version of TPA 3.2 that Rob Rice used is the same as the version that I installed in the workstation "bigbend", I ran TPA 3.2 using the same tpa.inp file R. Rice used (with EBSFILT switched on). The program was allowed to run for a few iterations, then terminated. A comparison of total EPA release values from the new run versus R. Rice's results are as follows:

| New results | R. Rice results |
|---|---|
| 3.499E-02 | 3.499E-02 |
| 1.260E-02 | 1.260E-02 |
| 2.591E-02 | 2.591E-02 |
| 5.164E-03 | 5.164E-03 |
| 8.782E-02 | 8.782E-02 |
| 9.466E-02 | 9.466E-02 |
| 4.664E-02 | 4.664E-02 |

As shown, the results are the same.

**[The rest of this page is left blank]**

**12/15/98**

Ron Janetzke provided a new file of mean values parameters for TPA 3.2. I plan to use mean value parameters for my sensitivity analyses studying the potential effect of cementitious materials. Below is a copy of Janetzke's email transmitting a copy of the said file.

```
Date:              12/15/98
Sender:              Ronald Janetzke
To:               Roberto Pabalan, Ronald Janetzke
Priority:               Normal
Subject:               meaanvalues for new values of gap fraction, invert, and
faul
             ---------------------------------------------------------------
--
             --------------
             Bobby,

             This file does not have correlation relationships as most
tpa.inp
             files do.

             ron j
```

Ron suggested that I check the old tpa.inp file to determine if any of the invert properties have correlation parameters. He suspects there isn't, which means I don't have to modify the file he provided me with respect to the correlation relationships. However, I need to check if the invert properties are the ones that Rob Rice used, which in term are based on the values I provided to R. Rice.

Below is a copy of the mean values file that Janetzke provided:

```
title
 Input file tpa.inp as
supplied with TPA Version
3.2 Code.
 Base case data set Rev 3.2
7/16/98
** **
** ** This file was
automatically generated by
the TPA code
** ** and contains the mean
values of the sampled
parameters
** ** submitted for the run
on Tue Dec 15 11:13:12
1998.
** **
** **
**
**           ***>>>  GLOBAL
PARAMETERS   <<<***
**
**
**          ***>>>
Disruptive Scenario flags
<<<***
**
iflag
VolcanismDisruptiveScenario
Flag(yes=1,no=0)
0
**
iflag
FaultingDisruptiveScenarioF
lag(yes=1,no=0)
0
**
iflag
SeismicDisruptiveScenarioFl
ag(yes=1,no=0)
1
**
**
**          ***>>> Subarea
Size  <<<***
**
**
** Number and Location Of
SubAreas[m] Based On
Fig3.4-1 in TSPA95
**subarea
**1
**ZONE T="ONE RECTANGULAR
ZONE SUBAREA", F=POINT
**        547405.7
4076362.2
**        548469.3
4076362.2
**        548469.3
4079237.8
**        547405.7
4079237.8
**        547405.7
4076362.2
subarea
7
ZONE T="Subarea
1",I=5,F=POINT
547472.0, 4079323.7
548069.2, 4079136.5
547847.3, 4077816.2
547318.4, 4077934.0
547472.0, 4079323.7
ZONE T="Subarea
2",I=5,F=POINT
548069.2, 4079136.5
548609.7, 4078968.6
548547.9, 4077654.1
547847.3, 4077816.2
548069.2, 4079136.5
ZONE T="Subarea
3",I=5,F=POINT
547318.4, 4077934.0
547847.3, 4077816.2
548322.7, 4077192.2
```

```
547474.7, 4077281.6
547318.4, 4077934.0
ZONE T="Subarea
4",I=5,F=POINT
547847.3, 4077816.2
548547.9, 4077654.1
548504.8, 4077170.0
548322.7, 4077192.2
547847.3, 4077816.2
ZONE T="Subarea
5",I=5,F=POINT
547474.7, 4077282.6
547887.3, 4077238.1
547995.0, 4076338.9
547670.4, 4076435.5
547474.7, 4077282.6
ZONE T="Subarea
6",I=5,F=POINT
547887.3, 4077238.1
548322.7, 4077192.2
548319.5, 4076220.2
547995.0, 4076338.9
547887.3, 4077238.1
ZONE T="Subarea
7",I=5,F=POINT
548322.7, 4077192.2
548504.8, 4077170.0
548473.1, 4076533.7
548319.5, 4076220.2
548322.7, 4077192.2
**
iconstant
StartAtSubarea
1
**
iconstant
StopAtSubarea
7
**
**
**          ***>>> Nuclides
and Chains  <<<***
**
**  5/25/1998 tpa3.2 new
parameter section
**
**  Nuclides can be
eliminated from the
basecase set.
**  However, if additional
nuclides (Pu242, Am242m,
Pu238, Cm243,
**  U235, Pa231, Ac227,
Pu241, U233, Th229, Cm244,
U236, U232, Sm151,
**  Cs137, Sn126, Sn121m,
Ag108m, Pd107, Mo93, Zr93,
Sr90, or Ni63)
**  are added to the
basecase set, then
corresponding RDs, KDs,
**  solubilities, gap
fractions, and correlations
must be added.
**
iflag
CheckNuclidesAndChains(yes=
1,no=0)
0
**
aqueousnuclides
**   number of nuclides,
number of chains
20
13
**
**   chain 1
2
Cm246
U238
**   chain 2
3
Cm245
Am241
Np237
**   chain 3
2
Am243
Pu239
**   chain 4
1
Pu240
**   chain 5
4
U234
Th230
Ra226
Pb210
**   chain 6
1
Cs135
**   chain 7
1
I129
**   chain 8
1
Tc99
**   chain 9
1
Ni59
**   chain 10
1
C14
**   chain 11
1
Se79
**   chain 12
1
Nb94
**   chain 13
1
Cl36
**
endofnuclides
**
**
**          ***>>>
Parameter Sampling  <<<***
**
**  5/25/1998 tpa3.2 new
parameter;option to conduct
direct-release only calcula
**
iflag
DirectReleaseOnlyFlag(yes=1
,no=0)
0
**
constant
SeedForRandomNumber
188910452.0
**
iflag
LatinHypercubeSampling(yes=
1,no=0)
   0
**
iconstant
NumberOfRealizations
1000
**
iconstant
StartAtRealization
1
**
iconstant
StopAtRealization
0
**
**
**          ***>>>
Simulation Times  <<<***
**
**  6/2/1998 tpa3.2 4 new
parameters; calculations at
two time periods
**
constant
DurationOfCompliancePeriod[
yr]
1.0e4
**
constant
MaximumTime[yr]
5.0e4
**
** Sum of pre- and post-
compliance time steps must
not exceed 201
**
iconstant
NumberOfTimeStepsInComplian
cePeriod
101
**
constant
RatioOfLastToFirstTimeStepI
nCompliancePeriod
100.0
**
**  Next two parameters
ignored if MaximumTime[yr]
=
DurationOfCompliancePeriod[
**
iconstant
NumberOfTimeStepsAfterCompl
iancePeriod
100
**
constant
RatioOfLastToFirstTimeStepA
fterCompliancePeriod
100.0
**
**
**    ***>>>  Output Print
Options  <<<***
**
iconstant
OutputMode(0=None,1=All,2=U
serDefined)
0
```

```
**
iconstant
UserDefinedLowerRealization
Appended
1
**
iconstant
UserDefinedUpperRealization
Appended
1
**
**  5/25/1998 tpa3.2 new
parameter
**
** Select Append Files
**    0 = append all files
**    1 = uzflow.ech and
uzflow.rlt only
**    2 = nfenv.ech and
nfenv.rlt only
**    3 = ebsfail.ech and
ebsfail.rlt only
**    4 = seismo.ech and
seismo.rlt only
**    5 = faulto.ech and
faulto.rlt only
**    6 = volcano.ech and
volcano.rlt only
**    7 = ebsrel.ech and
ebsrel.rlt only
**    8 = uzft.ech and
uzft.rlt only
**    9 = szft.ech and
szft.rlt only
**    10 = dcagw.ech and
dcagw.rlt only
**    11 = ashplumo.ech and
ashplumo.rlt only
**    12 = ashrmovo.ech and
ashrmovo.rlt only
**    13 = dcags.ech and
dcags.rlt only
**    14 = ashplume.cum only
**    15 = failt.cum only
**    16 = nefiiuz.cum only
**    17 = releaset.cum only
**
iconstant
SelectAppendFiles
0
**
**
**          ***>>> UZFLOW
<<<***
**
constant
ArealAverageMeanAnnualInfil
trationAtStart[mm/yr]
     5.5000000000000
**
constant
MeanAveragePrecipitationMul
tiplierAtGlacialMaximum
     2.0000000000000
**
constant
MeanAverageTemperatureIncre
aseAtGlacialMaximum[degC]
    -7.5000000000000
**
constant
TimeStepForClimate[yr]
500.0
**
constant
StandardDeviationOfMAPAbout
MeanInOneTimePeriod[mm/yr]
0.0
**
constant
StandardDeviationOfMATAbout
MeanInOneTimePeriod[degC]
0.0
**
constant
CorrelationBetweenMAPAndMAT
-0.8
**
iconstant
ClimatePerturbationSet
1
**
**
**          ***>>> NFENV
<<<***
**
iflag
TabularTemperatureRHFlag(ye
s=1,no=0)
0
**
iconstant
nsetUsedToPickTempRHDataSet
1
**
**  6/2/98 tpa3.2  name
change for  UseReflux2
**
iconstant
SelectRefluxModel(1,2,3)
3
**
constant
LengthOfRefluxZone[m]
20
**
constant
MaximumFluxInRefluxZone[m/s
]
1.0e-9
**
constant
PerchedBucketVolumePerSAare
a[m3/m2]
0.5
**
constant
Reflux2Thickness
100.0
**
constant
Reflux2Porosity
0.14
**
constant
Reflux2SatInit
0.9
**
constant
Reflux2SatResid
0.1
**
constant
Reflux2Period
100.0
**
constant
Reflux2LossI
0.1
**
constant
Reflux2LossD
0.1
**
constant
WPLength[m]
5.682
**
constant
WPDiameter[m]
1.802
**
constant
EmplacementDriftDiameter[m]
5.0
**
constant
WPSpacingAlongEmplacementDr
ift[m]
19.0
**
**  6/4/98 tpa3.2: Next 4
new parameters specific to
reflux3 model
**
constant
WPUnitCellWidth[m]
22.5
**
constant
FractionOfCondensateRemoved
[1/yr]
     1.0000000000000D-04
**
constant
FractionOfCondensateTowardR
epository[1/yr]
    0.50000000000000
**
constant
FractionOfCondensateTowardR
epositoryRemoved[1/yr]
     1.0000000000000D-04
**
constant
DensityOfWaterAtBoiling[kg/
m^3]
960.5
**
constant
EnthalpyOfPhaseChangeForWat
er[J/kg]
2.4e6
**
constant
TemperatureGradientInVicini
tyOfBoilingIsotherm[K/m]
     50.500000000000
**
constant
ArealMassLoading[MTU/acre]
83.0
**
```

```
constant
WastePackagePayload[MTU]
9.76
**
constant
AgeOfWaste[yr]
26.0
**
constant
AmbientRepositoryTemperatur
e[C]
20.0
**
constant
MassDensityofYMRock[kg/m^3]
2580.0
**
constant
SpecificHeatofYMRock[J/(kg-
K)]
840.0
**
constant
ThermalConductivityofYMRock
[W/(m-K)]
     2.0000000000000
**
constant
EmissivityOfDriftWall[-]
0.8
**
constant
EmissivityOfWastePackage[-]
0.7
**
constant
ThermalConductivityOfFloor[
W/(m-C)]
0.6
**
constant
EffectiveThermalConductivit
yOfUnbackfilledDrift[W/(m-
C)]
0.90
**
constant
TimeOfBackfillEmplaced[yr]
100001.0
**
constant
EffectiveThermalConductivit
yOfBackfill[W/(m-C)]
0.60
**
constant
ThermalConductivityOfInnerS
tainlessSteelWall[W/m-C]
15.0
**
constant
ThermalConductivityOfOuterC
arbonSteelWall[W/m-C]
50.0
**
constant
EffectiveThermalConductivit
yOfBasket&SFinWP[W/(m-C)]
1.0
**
constant
ElevationOfRepositoryHorizo
n[m]
1072.0
**
constant
ElevationOfGroundSurface[m]
1400.0
**
**
**          ***>>>  EBSFAIL
<<<***
**
constant
OuterWPThickness[m]
0.1
**
constant
InnerWPThickness[m]
0.02
**
constant
MetalGrainRadius[micrometer
]
13.75
**
constant
GrainBoundaryThickness[micr
ometer]
7.0e-4
**
constant
DryOxidationConstant
0.00001
**
constant
CriticalRelativeHumidityHum
idAirCorrosion
0.55
**
constant
CriticalRelativeHumidityAqu
eousCorrosion
     0.80000000000000
**
constant
ThicknessOfWaterFilm[m]
     2.0000000000000D-03
**
constant
BoilingPointOfWater[C]
97.0
**
constant
OuterOverpackErpIntercept
-620.3
**
constant
TempCoefOfOuterPackErpInter
cept
0.47
**
constant
OuterOverpackErpSlope
-95.2
**
constant
TempCoefOfOuterPackErpSlope
0.88
**
constant
InnerOverpackErpIntercept
     1140.0000000000
**48.5, 148.5  >>> 625 <<<
**
constant
TempCoefOfInnerPackErpInter
cept
0.0
**
constant
InnerOverpackErpSlope
0.0
**-160.8   >>> 625 <<<
**
constant
TempCoefOfInnerPackErpSlope
0.0
**
constant
OuterWPBetaKineticsParamete
rforOxygen
0.75
**
constant
OuterWPBetaKineticsParamete
rforWater
0.5
**
constant
InnerWPBetaKineticsParamete
rforOxygen
0.75
**
constant
InnerWPBetaKineticsParamete
rforWater
0.5
**
constant
OuterWPRateConstantforOxyge
nReduction[coulomb-
m/mole/yr]
3.8e12
**
constant
OuterWPRateConstantforWater
Reduction[coulomb-m/m^2/yr]
1.6e-1
**
constant
OuterWPActivationEnergyforO
xygenReduction[J/mole]
37300.0
**
constant
OuterWPActivationEnergyforW
aterReduction[J/mole]
25000.0
**
constant
InnerWPRateConstantforOxyge
nReduction[coulomb-
m/mole/yr]
3.0e10
**
constant
InnerWPRateConstantforWater
Reduction[coulomb-m/m^2/yr]
3.2
**
constant
```

```
InnerWPActivationEnergyforO
xygenReduction[J/mole]
40000.0
**
constant
InnerWPActivationEnergyforW
aterReduction[J/mole]
25000.0
**
constant
AA_1_1[C/m2/yr]
3.15e5
**
constant
AA_2_1[C/m2/yr]
     41500.000000000
**
constant
MeasuredGalvanicCouplePoten
tial
-0.46
**
constant
CoefForLocCorrOfOuterOverpa
ck
     4.7630000000000D-03
**
constant
ExponetForLocCorrOfOuterOve
rpack
0.45
**
constant
HumidAirCorrosionRate[m/yr]
1.16e-5
**
constant
LocalizedCorrRateOfInnerOve
rpack[m/yr]
2.5e-4
**
constant
FractionalCouplingStrength
0.0
**
constant
FactorForDefiningChoiceOfCr
itPotential
0.0
**
constant
CritChlorideConcForFirstLay
er[moL/L]
3.0e-4
**
constant
CritChlorideConcForSecondLa
yer[moL/L]
1.0
**3.0e-2  >>> 625 <<<
**
constant
ChlorideMultFactor
     15.500000000000
**
constant
ReferencepH
9.0
**
constant
WPsurfaceScaleThickness[m]
0.0
**
constant
TortuosityOfScaleonWP
1.0
**
constant
PorosityOfScaleonWP
1.0
**
constant
YieldStrength[MPa]
205.0
**
constant
SafetyFactor
1.4
**
constant
FractureToughness[MPa-
m**0.5]
250.0
**
**          ***>>> SEISMO
<<<***
**
hazardcurve
SeismicHazardCurveforSEISMO
10
0.05 180.0
0.10 500.0
0.15 1200.0
0.20 2400.0
0.25 4400.0
0.30 7800.0
0.35 11000.0
0.40 20000.0
0.45 30000.0
0.50 44000.0
**
constant
WeightPercentageOfRockFallT
hatHitsWPforSEISMO
1.0
**
constant
WeightOfWPforSEISMO[N]
1.27D05
**
constant
WPStiffnessforSEISMO[Pa*m]
1.21D10
**
constant
WPModulusOfElasticityforSEI
SMO[Pa]
2.07D11
**
constant
RockModulusOfElasticityforS
EISMO[Pa]
     34500000000.000
**
constant
WPPoissonRatioforSEISMO[]
0.2D0
**
constant
RockPoissonRatioforSEISMO[]
     0.20000000000000
**
constant
RockFallingDistanceforSEISM
O[m]
2.0D0
**
constant
WPFallingDistanceforSEISMO[
m]
0.3D0
**
iconstant
WPNumberofSupportPairforSEI
SMO
2
**
constant
WPSupportStiffnessforSEISMO
[pa*m]
5.5D09
**
constant
DistributionJointSpacing1fo
rSEISMO
5.0D-03
**
constant
DistributionJointSpacing2fo
rSEISMO
5.0D-03
**
constant
DistributionJointSpacing3fo
rSEISMO
5.0D-03
**
constant
DistributionJointSpacing4fo
rSEISMO
0.629D0
**
constant
DistributionJointSpacing5fo
rSEISMO
0.356D0
**
constant
SEISMOJointSpacing1[m]
     0.53300000000000
**
constant
SEISMOJointSpacing2[m]
     0.39950000000000
**
constant
SEISMOJointSpacing3[m]
     0.26650000000000
**
constant
SEISMOJointSpacing4[m]
     0.13000000000000
**
constant
SEISMOJointSpacing5[m]
      4.5000000000000D-02
**
**  5/28/1998 tpa3.2 new
value (smh)
**
constant
WPUltimateStrength[N/m^2]
```

```
4.5D08
**
constant
GrainDensityforTSw2SEISMO[]
2.55
**
**  5/28/1998 tpa3.2 new
values next 60
parameters(replacing
seismo.dat)
**
constant
FractionAreaForGroundMotion
1
0.05
**
constant
FractionAreaForGroundMotion
2
0.12
**
constant
FractionAreaForGroundMotion
3
0.17
**
constant
FractionAreaForGroundMotion
4
0.23
**
constant
FractionAreaForGroundMotion
5
0.28
**
constant
FractionAreaForGroundMotion
6
0.34
**
constant
FractionAreaForGroundMotion
7
0.4
**
constant
FractionAreaForGroundMotion
8
0.46
**
constant
FractionAreaForGroundMotion
9
0.5
**
constant
FractionAreaForGroundMotion
10
0.54
**
** rwr 7/8/98 modify the
VerticalExtentOfRockFall
names by adding "_"
constant
VerticalExtentOfRockFall1_1
[m]
0.0
**
constant
VerticalExtentOfRockFall1_2
[m]
0.0
**
constant
VerticalExtentOfRockFall1_3
[m]
0.0
**
constant
VerticalExtentOfRockFall1_4
[m]
0.0
**
constant
VerticalExtentOfRockFall1_5
[m]
0.0
**
constant
VerticalExtentOfRockFall1_6
[m]
0.0
**
constant
VerticalExtentOfRockFall1_7
[m]
0.0
**
constant
VerticalExtentOfRockFall1_8
[m]
0.0
constant
VerticalExtentOfRockFall1_9
[m]
0.0
**
constant
VerticalExtentOfRockFall1_1
0[m]
0.0
**
constant
VerticalExtentOfRockFall2_1
[m]
    0.55000000000000
**
constant
VerticalExtentOfRockFall2_2
[m]
    0.75000000000000
**
constant
VerticalExtentOfRockFall2_3
[m]
    0.80000000000000
**
constant
VerticalExtentOfRockFall2_4
[m]
    0.85000000000000
**
constant
VerticalExtentOfRockFall2_5
[m]
    0.90000000000000
**
constant
VerticalExtentOfRockFall2_6
[m]
    0.95000000000000
**
constant
VerticalExtentOfRockFall2_7
[m]
    0.97500000000000
**
constant
VerticalExtentOfRockFall2_8
[m]
     1.0000000000000
**
constant
VerticalExtentOfRockFall2_9
[m]
     1.0750000000000
**
constant
VerticalExtentOfRockFall2_1
0[m]
    0.90000000000000
**
constant
VerticalExtentOfRockFall3_1
[m]
    0.75000000000000
**
constant
VerticalExtentOfRockFall3_2
[m]
     1.2500000000000
**
constant
VerticalExtentOfRockFall3_3
[m]
     1.5000000000000
**
constant
VerticalExtentOfRockFall3_4
[m]
     1.7500000000000
**
constant
VerticalExtentOfRockFall3_5
[m]
     2.0000000000000
**
constant
VerticalExtentOfRockFall3_6
[m]
     2.2500000000000
**
constant
VerticalExtentOfRockFall3_7
[m]
     2.5000000000000
**
constant
VerticalExtentOfRockFall3_8
[m]
     2.7500000000000
**
constant
VerticalExtentOfRockFall3_9
[m]
     3.1000000000000
**
constant
VerticalExtentOfRockFall3_1
0[m]
     3.5000000000000
```

```
**
constant
VerticalExtentOfRockFall4_1
[m]
     1.6000000000000
**
constant
VerticalExtentOfRockFall4_2
[m]
     3.0000000000000
**
constant
VerticalExtentOfRockFall4_3
[m]
     3.2500000000000
**
constant
VerticalExtentOfRockFall4_4
[m]
     3.5000000000000
**
constant
VerticalExtentOfRockFall4_5
[m]
     3.7500000000000
**
constant
VerticalExtentOfRockFall4_6
[m]
     4.0000000000000
**
constant
VerticalExtentOfRockFall4_7
[m]
     4.2500000000000
**
constant
VerticalExtentOfRockFall4_8
[m]
     4.5000000000000
**
constant
VerticalExtentOfRockFall4_9
[m]
     4.9000000000000
**
constant
VerticalExtentOfRockFall4_1
0[m]
     5.2500000000000
**
constant
VerticalExtentOfRockFall5_1
[m]
     2.6000000000000
**
constant
VerticalExtentOfRockFall5_2
[m]
     4.9150000000000
**
constant
VerticalExtentOfRockFall5_3
[m]
     5.1000000000000
**
constant
VerticalExtentOfRockFall5_4
[m]
     5.2500000000000
**
constant
VerticalExtentOfRockFall5_5
[m]
     5.6000000000000
**
constant
VerticalExtentOfRockFall5_6
[m]
     5.9150000000000
**
constant
VerticalExtentOfRockFall5_7
[m]
     6.2500000000000
**
constant
VerticalExtentOfRockFall5_8
[m]
     6.5800000000000
**
constant
VerticalExtentOfRockFall5_9
[m]
     6.9000000000000
**
constant
VerticalExtentOfRockFall5_1
0[m]
     7.2500000000000
**
**  5/28/1998 tpa3.2 two
new parameters introduced
**
constant
WPYieldPoint[]
0.002
**
constant
WPPlasticElongation[]
0.02
**
**
**          ***>>>  EBSREL
<<<***
**
** rwr 7/8/98 modify flow
model flag
iflag
FlowModelFlag(0=BathTub,1=F
lowThrough)
0
**
constant
FowFactor
    0.17320508075689
**
constant
FmultFactor
     4.4721359549996D-02
**
constant
SubAreaWetFraction
    0.50000000000000
**
**  5/21/98 tpa3.2: New
parameter; nonzero initial
failure times
**
constant
InitialFailureTime[yr]
0.0
**
constant
DefectiveFractionOfWPs/cell
     5.0500000000000D-03
**
**  6/2/1998 tpa3.2 5 new
parameters; number of
SEISMO inservals not to
exceed 4
**
iconstant
NumberOfSEISMOWPFailureInte
rvals
4
**
constant
BeginningOfSEISMOWPFailureI
nterval1[yr]
0.0
**
constant
BeginningOfSEISMOWPFailureI
nterval2[yr]
2000.0
**
constant
BeginningOfSEISMOWPFailureI
nterval3[yr]
5000.0
**
constant
BeginningOfSEISMOWPFailureI
nterval4[yr]
10000.0
**
constant
WPInternalVolume[m3]
4.83
**
constant
FlowOnsetTemperature[C]
999.
**
constant
SFDensity[kg/m3]
10600.
**
iconstant
SurfaceAreaModel
1
**
iconstant
IModel
2
**
constant
OxygenPartialPressure[atm]
0.21
**
constant
NegativeLog10CarbonateConce
ntration[mol/L]
3.71
**
constant
UserLeachRate[kg/yr/m2]
2.5e-6
**
constant
RD_Invert_Cm
6.00e3
```

```
**
constant
RD_Invert_Pu
3.00e3
**
constant
RD_Invert_U
6.01e2
**
constant
RD_Invert_Am
3.00e3
**
constant
RD_Invert_Np
1.20e3
**
constant
RD_Invert_Th
3.00e3
**
constant
RD_Invert_Ra
6.01e2
**
constant
RD_Invert_Pb
3.01e2
**
constant
RD_Invert_Cs
1.21e2
**
constant
RD_Invert_I
7.00e0
**
constant
RD_Invert_Tc
1.0
**
constant
RD_Invert_Ni
6.10e1
**
constant
RD_Invert_Cl
1.0
**
constant
RD_Invert_C
6.10e1
**
constant
RD_Invert_Se
1.0
**
constant
RD_Invert_Nb
6.01e2
**
constant
GapFractionForCM246
0.0
**
constant
GapFractionForU238
0.0
**
constant
GapFractionForCM245
0.0
**
constant
GapFractionForAM241
0.0
**
constant
GapFractionForNP237
0.0
**
constant
GapFractionForAM243
0.0
**
constant
GapFractionForPU239
0.0
**
constant
GapFractionForPU240
0.0
**
constant
GapFractionForU234
0.0
**
constant
GapFractionForTH230
0.0
**
constant
GapFractionForRA226
0.0
**
constant
GapFractionForPB210
0.0
**
constant
GapFractionForCS135
0.06
**
constant
GapFractionForI129
0.06
**
constant
GapFractionForTC99
0.01
**
constant
GapFractionForNI59
0.0
**
constant
GapFractionForCL36
0.12
**
constant
GapFractionForC14
0.1
**
constant
GapFractionForSE79
0.06
**
constant
GapFractionForNB94
0.0
**
constant
InitialRadiusOfSFParticle[m
]
     1.8500000000000D-03
**
constant
RadiusOfSFGrain[m]
1.25e-5
**
constant
CladdingCorrectionFactor
1.0
**
constant
SubGrainFragmentRadiusAfter
TransFrac[m]
     1.2500000000000D-06
**
constant
ThicknessOfCladding[m]
6.1e-4
**
constant
SFC-14InventoryPerKgSF[ci]
7.2e-4
**
constant
CladC-
14InventoryPerKgSF[ci]
4.89e-4
**
constant
ZyrOxideAndCrudC-
14InvPerKgSF[ci]
2.48e-5
**
constant
GapAndGrainBoundaryInventor
yPerKgSF[ci]
6.2e-6
**
constant
SolubilityAm[kg/m3]
     1.2001200000000D-04
**
constant
SolubilityNp[kg/m3]
     2.1393924964957D-02
**
constant
Solubility_I[kg/m3]
1.29e2
**
constant
SolubilityTc[kg/m3]
9.93e1
**
constant
SolubilityCl[kg/m3]
3.6e1
**
constant
Solubility_C[kg/m3]
1.4e1
**
constant
Solubility_U[kg/m3]
7.6e-3
**
constant
SolubilityCm[kg/m3]
2.4e-4
```

```
**
constant
SolubilityPu[kg/m3]
     1.21200000000000D-04
**
constant
SolubilityTh[kg/m3]
2.3e-4
**
constant
SolubilityRa[kg/m3]
2.3e-5
**
constant
SolubilityPb[kg/m3]
6.6e-5
**
constant
SolubilityCs[kg/m3]
1.35e2
**
constant
SolubilityNi[kg/m3]
1.1e-1
**
constant
SolubilitySe[kg/m3]
7.9e1
**
constant
SolubilityNb[kg/m3]
9.3e-7
**
**  6/2/1998 tpa3.2 next
parameter replaced with 44
new parameters
**
SFWettedFraction_(failureki
nd)_subarea
**
constant
SFWettedFraction_Initial_1
    0.50000000000000
**
constant
SFWettedFraction_Initial_2
    0.50000000000000
**
constant
SFWettedFraction_Initial_3
    0.50000000000000
**
constant
SFWettedFraction_Initial_4
    0.50000000000000
**
constant
SFWettedFraction_Initial_5
    0.50000000000000
**
constant
SFWettedFraction_Initial_6
    0.50000000000000
**
constant
SFWettedFraction_Initial_7
    0.50000000000000
**
constant
SFWettedFraction_FAULTO
    0.50000000000000
**
constant
SFWettedFraction_VOLCANO
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_1
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_2
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_3
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_4
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_5
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_6
    0.50000000000000
**
constant
SFWettedFraction_SEISMO1_7
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_1
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_2
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_3
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_4
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_5
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_6
    0.50000000000000
**
constant
SFWettedFraction_SEISMO2_7
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_1
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_2
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_3
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_4
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_5
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_6
    0.50000000000000
**
constant
SFWettedFraction_SEISMO3_7
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_1
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_2
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_3
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_4
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_5
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_6
    0.50000000000000
**
constant
SFWettedFraction_SEISMO4_7
    0.50000000000000
**
constant
SFWettedFraction_Corrosion_
1
    0.50000000000000
**
constant
SFWettedFraction_Corrosion_
2
    0.50000000000000
**
constant
SFWettedFraction_Corrosion_
3
    0.50000000000000
**
constant
SFWettedFraction_Corrosion_
4
    0.50000000000000
**
constant
SFWettedFraction_Corrosion_
5
    0.50000000000000
**
```

```
constant
SFWettedFraction_Corrosion_
6
    0.50000000000000
**
constant
SFWettedFraction_Corrosion_
7
    0.50000000000000
**
**  7/4/1998 tpa3.2 four
new parameters for invert
**
iflag
InvertBypass(0=ebsfilt,1=by
pass-ebsfilt)
0
**
constant
InvertRockPorosity
0.3
**
constant
InvertThickness[m]
0.75
**
constant
InvertDiffusionCoefficient[
m^2/yr]
4.4e-5
**
constant
InvertMatrixPermeability[m^
2]
     2.0000000000000D-17
**
**
**           ***>>>  UZFT
<<<***
**
constant
UnsaturatedZoneMinimumVeloc
ityChangeFactor[Fraction]
0.4
**
constant
MatrixLongitudinalDispersiv
ity[FractionOfLayer]
0.1
**
constant
FractureLongitudinalDispers
ivity[FractionOfLayer]
0.1
**
constant
MatrixKD_TSw_Am[m3/kg]
     3994.9968710876
**
constant
MatrixKD_CHnvAm[m3/kg]
     12489.995996797
**
constant
MatrixKD_CHnzAm[m3/kg]
     11489.125293076
**
constant
MatrixKD_PPw_Am[m3/kg]
     9091.2045406536
**
constant
MatrixKD_UCF_Am[m3/kg]
     9539.3920141695
**
constant
MatrixKD_BFw_Am[m3/kg]
     3894.8684188301
**
constant
MatrixKD_UFZ_Am[m3/kg]
     3694.5906403822
**
constant
MatrixKD_TSw_Np[m3/kg]
     5.9329587896765D-04
**
constant
MatrixKD_CHnvNp[m3/kg]
     1.7798876369030D-03
**
constant
MatrixKD_CHnzNp[m3/kg]
     1.6248076809272D-03
**
constant
MatrixKD_PPw_Np[m3/kg]
     1.3416407864999D-03
**
constant
MatrixKD_UCF_Np[m3/kg]
     1.4057026712644D-03
**
constant
MatrixKD_BFw_Np[m3/kg]
     5.6124860801609D-04
**
constant
MatrixKD_UFZ_Np[m3/kg]
     5.4772255750517D-04
**
constant
MatrixKD_TSw_I[m3/kg]
0.0
**
constant
MatrixKD_CHnvI[m3/kg]
0.0
**
constant
MatrixKD_CHnzI[m3/kg]
0.0
**
constant
MatrixKD_PPw_I[m3/kg]
0.0
**
constant
MatrixKD_UCF_I[m3/kg]
0.0
**
constant
MatrixKD_BFw_I[m3/kg]
0.0
**
constant
MatrixKD_UFZ_I[m3/kg]
0.0
**
constant
MatrixKD_TSw_Tc[m3/kg]
0.0
**
constant
MatrixKD_CHnvTc[m3/kg]
0.0
**
constant
MatrixKD_CHnzTc[m3/kg]
0.0
**
constant
MatrixKD_PPw_Tc[m3/kg]
0.0
**
constant
MatrixKD_UCF_Tc[m3/kg]
0.0
**
constant
MatrixKD_BFw_Tc[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Tc[m3/kg]
0.0
**
constant
MatrixKD_TSw_Cl[m3/kg]
0.0
**
constant
MatrixKD_CHnvCl[m3/kg]
0.0
**
constant
MatrixKD_CHnzCl[m3/kg]
0.0
**
constant
MatrixKD_PPw_Cl[m3/kg]
0.0
**
constant
MatrixKD_UCF_Cl[m3/kg]
0.0
**
constant
MatrixKD_BFw_Cl[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Cl[m3/kg]
0.0
**
constant
MatrixKD_TSw_Cm[m3/kg]
0.0
**
constant
MatrixKD_CHnvCm[m3/kg]
0.0
**
constant
MatrixKD_CHnzCm[m3/kg]
0.0
**
constant
MatrixKD_PPw_Cm[m3/kg]
0.0
**
constant
MatrixKD_UCF_Cm[m3/kg]
```

```
0.0
**
constant
MatrixKD_BFw_Cm[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Cm[m3/kg]
0.0
**
constant
MatrixKD_TSw_U[m3/kg]
     2.1494185260205D-05
**
constant
MatrixKD_CHnvU[m3/kg]
     6.5498091575251D-05
**
constant
MatrixKD_CHnzU[m3/kg]
     6.0000000000000D-05
**
constant
MatrixKD_PPw_U[m3/kg]
     4.8989794855664D-05
**
constant
MatrixKD_UCF_U[m3/kg]
     5.0990195135928D-05
**
constant
MatrixKD_BFw_U[m3/kg]
     2.0248456731317D-05
**
constant
MatrixKD_UFZ_U[m3/kg]
     1.9748417658131D-05
**
constant
MatrixKD_TSw_Pu[m3/kg]
    0.71133676975115
**
constant
MatrixKD_CHnvPu[m3/kg]
     2.1810547906919
**
constant
MatrixKD_CHnzPu[m3/kg]
     1.9912307751740
**
constant
MatrixKD_PPw_Pu[m3/kg]
     1.6278820596100
**
constant
MatrixKD_UCF_Pu[m3/kg]
     1.7064583206161
**
constant
MatrixKD_BFw_Pu[m3/kg]
    0.69498201415576
**
constant
MatrixKD_UFZ_Pu[m3/kg]
    0.67970581871866
**
constant
MatrixKD_TSw_Th[m3/kg]
    0.34641016151378
**
constant
MatrixKD_CHnvTh[m3/kg]
     1.0677078252031
**
constant
MatrixKD_CHnzTh[m3/kg]
     0.94710083940413
**
constant
MatrixKD_PPw_Th[m3/kg]
     0.79183331579317
**
constant
MatrixKD_UCF_Th[m3/kg]
     0.80560536244491
**
constant
MatrixKD_BFw_Th[m3/kg]
     0.33585711247493
**
constant
MatrixKD_UFZ_Th[m3/kg]
     0.32171415884291
**
constant
MatrixKD_TSw_Ra[m3/kg]
     0.22360679774998
**
constant
MatrixKD_CHnvRa[m3/kg]
     7.0710678118655D-02
**
constant
MatrixKD_CHnzRa[m3/kg]
     2.2360679774998
**
constant
MatrixKD_PPw_Ra[m3/kg]
     0.22360679774998
**
constant
MatrixKD_UCF_Ra[m3/kg]
     0.22360679774998
**
constant
MatrixKD_BFw_Ra[m3/kg]
     0.22360679774998
**
constant
MatrixKD_UFZ_Ra[m3/kg]
     0.22360679774998
**
constant
MatrixKD_TSw_Pb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_CHnvPb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_CHnzPb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_PPw_Pb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_UCF_Pb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_BFw_Pb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_UFZ_Pb[m3/kg]
     0.22360679774998
**
constant
MatrixKD_TSw_Cs[m3/kg]
     0.14142135623731
**
constant
MatrixKD_CHnvCs[m3/kg]
     3.1622776601684D-02
**
constant
MatrixKD_CHnzCs[m3/kg]
     1.5811388300842
**
constant
MatrixKD_PPw_Cs[m3/kg]
     0.14142135623731
**
constant
MatrixKD_UCF_Cs[m3/kg]
     0.14142135623731
**
constant
MatrixKD_BFw_Cs[m3/kg]
     0.14142135623731
**
constant
MatrixKD_UFZ_Cs[m3/kg]
     0.14142135623731
**
constant
MatrixKD_TSw_Ni[m3/kg]
     1.5811388300842D-03
**
constant
MatrixKD_CHnvNi[m3/kg]
     3.1622776601684D-04
**
constant
MatrixKD_CHnzNi[m3/kg]
     1.5811388300842D-03
**
constant
MatrixKD_PPw_Ni[m3/kg]
     1.5811388300842D-03
**
constant
MatrixKD_UCF_Ni[m3/kg]
     1.5811388300842D-03
**
constant
MatrixKD_BFw_Ni[m3/kg]
     1.5811388300842D-03
**
constant
MatrixKD_UFZ_Ni[m3/kg]
     1.5811388300842D-03
**
constant
MatrixKD_TSw_C[m3/kg]
0.0
**
constant
MatrixKD_CHnvC[m3/kg]
0.0
```

```
**
constant
MatrixKD_CHnzC[m3/kg]
0.0
**
constant
MatrixKD_PPw_C[m3/kg]
0.0
**
constant
MatrixKD_UCF_C[m3/kg]
0.0
**
constant
MatrixKD_BFw_C[m3/kg]
0.0
**
constant
MatrixKD_UFZ_C[m3/kg]
0.0
**
constant
MatrixKD_TSw_Se[m3/kg]
     9.4868329805051D-05
**
constant
MatrixKD_CHnvSe[m3/kg]
     6.3245553203368D-05
**
constant
MatrixKD_CHnzSe[m3/kg]
     4.7434164902526D-05
**
constant
MatrixKD_PPw_Se[m3/kg]
     9.4868329805051D-05
**
constant
MatrixKD_UCF_Se[m3/kg]
     9.4868329805051D-05
**
constant
MatrixKD_BFw_Se[m3/kg]
     9.4868329805051D-05
**
constant
MatrixKD_UFZ_Se[m3/kg]
     9.4868329805051D-05
**
constant
MatrixKD_TSw_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_CHnvNb[m3/kg]
0.10, 1.0
**
constant
MatrixKD_CHnzNb[m3/kg]
0.10, 1.0
**
constant
MatrixKD_PPw_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_UCF_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_BFw_Nb[m3/kg]
0.10, 2.0
**
constant
MatrixKD_UFZ_Nb[m3/kg]
0.10, 2.0
**
constant
FractureRD_TSw_Am
1.0
**
constant
FractureRD_CHnvAm
1.0
**
constant
FractureRD_CHnzAm
1.0
**
constant
FractureRD_PPw_Am
1.0
**
constant
FractureRD_UCF_Am
1.0
**
constant
FractureRD_BFw_Am
1.0
**
constant
FractureRD_UFZ_Am
1.0
**
constant
FractureRD_TSw_Np
1.0
**
constant
FractureRD_CHnvNp
1.0
**
constant
FractureRD_CHnzNp
1.0
**
constant
FractureRD_PPw_Np
1.0
**
constant
FractureRD_UCF_Np
1.0
**
constant
FractureRD_BFw_Np
1.0
**
constant
FractureRD_UFZ_Np
1.0
**
constant
FractureRD_TSw_I
1.0
**
constant
FractureRD_CHnvI
1.0
**
constant
FractureRD_CHnzI
1.0
**
constant
FractureRD_PPw_I
1.0
**
constant
FractureRD_UCF_I
1.0
**
constant
FractureRD_BFw_I
1.0
**
constant
FractureRD_UFZ_I
1.0
**
constant
FractureRD_TSw_Tc
1.0
**
constant
FractureRD_CHnvTc
1.0
**
constant
FractureRD_CHnzTc
1.0
**
constant
FractureRD_PPw_Tc
1.0
**
constant
FractureRD_UCF_Tc
1.0
**
constant
FractureRD_BFw_Tc
1.0
**
constant
FractureRD_UFZ_Tc
1.0
**
constant
FractureRD_TSw_Cl
1.0
**
constant
FractureRD_CHnvCl
1.0
**
constant
FractureRD_CHnzCl
1.0
**
constant
FractureRD_PPw_Cl
1.0
**
constant
FractureRD_UCF_Cl
1.0
**
constant
FractureRD_BFw_Cl
1.0
**
```

```
constant
FractureRD_UFZ_Cl
1.0
**
constant
FractureRD_TSw_Cm
1.0
**
constant
FractureRD_CHnvCm
1.0
**
constant
FractureRD_CHnzCm
1.0
**
constant
FractureRD_PPw_Cm
1.0
**
constant
FractureRD_UCF_Cm
1.0
**
constant
FractureRD_BFw_Cm
1.0
**
constant
FractureRD_UFZ_Cm
1.0
**
constant
FractureRD_TSw_U
1.0
**
constant
FractureRD_CHnvU
1.0
**
constant
FractureRD_CHnzU
1.0
**
constant
FractureRD_PPw_U
1.0
**
constant
FractureRD_UCF_U
1.0
**
constant
FractureRD_BFw_U
1.0
**
constant
FractureRD_UFZ_U
1.0
**
constant
FractureRD_TSw_Pu
1.0
**
constant
FractureRD_CHnvPu
1.0
**
constant
FractureRD_CHnzPu
1.0
**
constant
FractureRD_PPw_Pu
1.0
**
constant
FractureRD_UCF_Pu
1.0
**
constant
FractureRD_BFw_Pu
1.0
**
constant
FractureRD_UFZ_Pu
1.0
**
constant
FractureRD_TSw_Th
1.0
**
constant
FractureRD_CHnvTh
1.0
**
constant
FractureRD_CHnzTh
1.0
**
constant
FractureRD_PPw_Th
1.0
**
constant
FractureRD_UCF_Th
1.0
**
constant
FractureRD_BFw_Th
1.0
**
constant
FractureRD_UFZ_Th
1.0
**
constant
FractureRD_TSw_Ra
1.0
**
constant
FractureRD_CHnvRa
1.0
**
constant
FractureRD_CHnzRa
1.0
**
constant
FractureRD_PPw_Ra
1.0
**
constant
FractureRD_UCF_Ra
1.0
**
constant
FractureRD_BFw_Ra
1.0
**
constant
FractureRD_UFZ_Ra
1.0
**
constant
FractureRD_TSw_Pb
1.0
**
constant
FractureRD_CHnvPb
1.0
**
constant
FractureRD_CHnzPb
1.0
**
constant
FractureRD_PPw_Pb
1.0
**
constant
FractureRD_UCF_Pb
1.0
**
constant
FractureRD_BFw_Pb
1.0
**
constant
FractureRD_UFZ_Pb
1.0
**
constant
FractureRD_TSw_Cs
1.0
**
constant
FractureRD_CHnvCs
1.0
**
constant
FractureRD_CHnzCs
1.0
**
constant
FractureRD_PPw_Cs
1.0
**
constant
FractureRD_UCF_Cs
1.0
**
constant
FractureRD_BFw_Cs
1.0
**
constant
FractureRD_UFZ_Cs
1.0
**
constant
FractureRD_TSw_Ni
1.0
**
constant
FractureRD_CHnvNi
1.0
**
constant
FractureRD_CHnzNi
1.0
**
constant
```

```
FractureRD_PPw_Ni
1.0
**
constant
FractureRD_UCF_Ni
1.0
**
constant
FractureRD_BFw_Ni
1.0
**
constant
FractureRD_UFZ_Ni
1.0
**
constant
FractureRD_TSw_C
1.0
**
constant
FractureRD_CHnvC
1.0
**
constant
FractureRD_CHnzC
1.0
**
constant
FractureRD_PPw_C
1.0
**
constant
FractureRD_UCF_C
1.0
**
constant
FractureRD_BFw_C
1.0
**
constant
FractureRD_UFZ_C
1.0
**
constant
FractureRD_TSw_Se
1.0
**
constant
FractureRD_CHnvSe
1.0
**
constant
FractureRD_CHnzSe
1.0
**
constant
FractureRD_PPw_Se
1.0
**
constant
FractureRD_UCF_Se
1.0
**
constant
FractureRD_BFw_Se
1.0
**
constant
FractureRD_UFZ_Se
1.0
**
constant
FractureRD_TSw_Nb
1.0
**
constant
FractureRD_CHnvNb
1.0
**
constant
FractureRD_CHnzNb
1.0
**
constant
FractureRD_PPw_Nb
1.0
**
constant
FractureRD_UCF_Nb
1.0
**
constant
FractureRD_BFw_Nb
1.0
**
constant
FractureRD_UFZ_Nb
1.0
**
constant
MatrixPermeability_TSw_[m2]
     2.0000000000000D-19
**
constant
MatrixPermeability_CHnv[m2]
     2.0000000000000D-14
**
constant
MatrixPermeability_CHnz[m2]
     5.0000000000000D-18
**
constant
MatrixPermeability_PPw_[m2]
     1.0000000000000D-17
**
constant
MatrixPermeability_UCF_[m2]
     3.0000000000000D-18
**
constant
MatrixPermeability_BFw_[m2]
     2.0000000000000D-19
**
constant
MatrixPermeability_UFZ_[m2]
     1.9442222095224D-17
**
constant
MatrixPorosity_TSw_
0.12
**
constant
MatrixPorosity_CHnv
0.33
**
constant
MatrixPorosity_CHnz
0.32
**
constant
MatrixPorosity_PPw_
0.28
**
constant
MatrixPorosity_UCF_
0.28
**
constant
MatrixPorosity_BFw_
0.12
**
constant
MatrixPorosity_UFZ_
0.12
**
constant
MatrixBeta_TSw_
1.5
**
constant
MatrixBeta_CHnv
1.3
**
constant
MatrixBeta_CHnz
2.3
**
constant
MatrixBeta_PPw_
1.5
**
constant
MatrixBeta_UCF_
1.4
**
constant
MatrixBeta_BFw_
1.7
**
constant
MatrixBeta_UFZ_
2.3
**
constant
MatrixGrainDensity_TSw_[kg/
m3]
2460.0
**
constant
MatrixGrainDensity_CHnv[kg/
m3]
2260.0
**
constant
MatrixGrainDensity_CHnz[kg/
m3]
2400.0
**
constant
MatrixGrainDensity_PPw_[kg/
m3]
2540.0
**
constant
MatrixGrainDensity_UCF_[kg/
m3]
2420.0
**
constant
MatrixGrainDensity_BFw_[kg/
m3]
2570.0
**
```

```
constant
MatrixGrainDensity_UFZ_[kg/
m3]
2630.0
**
constant
FracturePermeability_TSw_[m
2]
     8.0000000000000D-13
**
constant
FracturePermeability_CHnv[m
2]
     8.0000000000000D-13
**
constant
FracturePermeability_CHnz[m
2]
     6.0000000000000D-13
**
constant
FracturePermeability_PPw_[m
2]
     6.0000000000000D-13
**
constant
FracturePermeability_UCF_[m
2]
     6.0000000000000D-13
**
constant
FracturePermeability_BFw_[m
2]
     3.0000000000000D-13
**
constant
FracturePermeability_UFZ_[m
2]
     1.0000000000000D-12
**
constant
FracturePorosity_TSw_
     3.1622776601684D-03
**
constant
FracturePorosity_CHnv
     3.1622776601684D-03
**
constant
FracturePorosity_CHnz
     3.1622776601684D-03
**
constant
FracturePorosity_PPw_
     3.1622776601684D-03
**
constant
FracturePorosity_UCF_
     3.1622776601684D-03
**
constant
FracturePorosity_BFw_
     3.1622776601684D-03
**
constant
FracturePorosity_UFZ_
     3.1622776601684D-03
**
constant
FractureBeta_TSw_
3.0
**
constant
FractureBeta_CHnv
3.0
**
constant
FractureBeta_CHnz
3.0
**
constant
FractureBeta_PPw_
3.0
**
constant
FractureBeta_UCF_
3.0
**
constant
FractureBeta_BFw_
3.0
**
constant
FractureBeta_UFZ_
3.0
**
constant
InletArea__1SubArea[m2]
5.4e5
**
constant
InletArea__2SubArea[m2]
5.4e5
**
constant
InletArea__3SubArea[m2]
5.4e5
**
constant
InletArea__4SubArea[m2]
5.4e5
**
constant
InletArea__5SubArea[m2]
5.4e5
**
constant
InletArea__6SubArea[m2]
5.4e5
**
constant
InletArea__7SubArea[m2]
5.4e5
**
constant
TSw_Thickness_1SubArea[m]
33.0
**
constant
CHnvThickness_1SubArea[m]
0.0
**
constant
CHnzThickness_1SubArea[m]
163.0
**
constant
PPw_Thickness_1SubArea[m]
34.0
**
constant
UCF_Thickness_1SubArea[m]
67.0
**
constant
BFw_Thickness_1SubArea[m]
0.0
**
constant
UFZ_Thickness_1SubArea[m]
0.0
**
constant
TSw_Thickness_2SubArea[m]
116.0
**
constant
CHnvThickness_2SubArea[m]
0.0
**
constant
CHnzThickness_2SubArea[m]
154.0
**
constant
PPw_Thickness_2SubArea[m]
39.0
**
constant
UCF_Thickness_2SubArea[m]
20.0
**
constant
BFw_Thickness_2SubArea[m]
0.0
**
constant
UFZ_Thickness_2SubArea[m]
0.0
**
constant
TSw_Thickness_3SubArea[m]
20.0
**
constant
CHnvThickness_3SubArea[m]
0.0
**
constant
CHnzThickness_3SubArea[m]
122.0
**
constant
PPw_Thickness_3SubArea[m]
40.0
**
constant
UCF_Thickness_3SubArea[m]
158.0
**
constant
BFw_Thickness_3SubArea[m]
0.0
**
constant
UFZ_Thickness_3SubArea[m]
0.0
**
constant
TSw_Thickness_4SubArea[m]
110.0
**
constant
```

```
CHnvThickness_4SubArea[m]
0.0
**
constant
CHnzThickness_4SubArea[m]
132.0
**
constant
PPw_Thickness_4SubArea[m]
34.0
**
constant
UCF_Thickness_4SubArea[m]
57.0
**
constant
BFw_Thickness_4SubArea[m]
0.0
**
constant
UFZ_Thickness_4SubArea[m]
0.0
**
constant
TSw_Thickness_5SubArea[m]
20.0
**
constant
CHnvThickness_5SubArea[m]
113.0
**
constant
CHnzThickness_5SubArea[m]
0.0
**
constant
PPw_Thickness_5SubArea[m]
38.0
**
constant
UCF_Thickness_5SubArea[m]
158.0
**
constant
BFw_Thickness_5SubArea[m]
32.0
**
constant
UFZ_Thickness_5SubArea[m]
0.0
**
constant
TSw_Thickness_6SubArea[m]
53.0
**
constant
CHnvThickness_6SubArea[m]
125.0
**
constant
CHnzThickness_6SubArea[m]
0.0
**
constant
PPw_Thickness_6SubArea[m]
26.0
**
constant
UCF_Thickness_6SubArea[m]
136.0
**
constant
BFw_Thickness_6SubArea[m]
0.0
**
constant
UFZ_Thickness_6SubArea[m]
0.0
**
constant
TSw_Thickness_7SubArea[m]
121.0
**
constant
CHnvThickness_7SubArea[m]
0.0
**
constant
CHnzThickness_7SubArea[m]
114.0
**
constant
PPw_Thickness_7SubArea[m]
43.0
**
constant
UCF_Thickness_7SubArea[m]
63.0
**
constant
BFw_Thickness_7SubArea[m]
0.0
**
constant
UFZ_Thickness_7SubArea[m]
0.0
**
**
**           ***>>>  SZFT
<<<***
**
constant
MixingZoneDispersionFractio
n
0.01
**
constant
DispersionFraction_STFF
0.01
**
constant
DispersionFraction_SAV
0.1
**
constant
MinimumResidenceTime_STFF[y
r]
10.0
**
constant
MinimumResidenceTime_SAV[yr
]
10.0
**
constant
FractureRD_STFF_Am
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
constant
AlluviumMatrixRD_SAV_Am
     71414284.285428
**
constant
FractureRD_STFF_Np
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
constant
AlluviumMatrixRD_SAV_Np
     62.449979983984
**
constant
FractureRD_STFF_I
1.0
**
constant
AlluviumMatrixRD_SAV_I
     2.0000000000000
**
constant
FractureRD_STFF_Tc
1.0
**
constant
AlluviumMatrixRD_SAV_Tc
     5.4772255750517
**
constant
FractureRD_STFF_Cl
1.0
**
constant
AlluviumMatrixRD_SAV_Cl
1.0
**
constant
FractureRD_STFF_Cm
1.0
**
constant
AlluviumMatrixRD_SAV_Cm
1.0
**
constant
FractureRD_STFF_U
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
constant
AlluviumMatrixRD_SAV_U
     137.84048752090
**
constant
FractureRD_STFF_Pu
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
constant
AlluviumMatrixRD_SAV_Pu
     12798.437404621
```

```
**
constant
FractureRD_STFF_Th
1.0
**
** rwr 7/8/98 use KDs from
D. Turner with
** por = 0.125 and grain
dens = 2470 kg/m3
constant
AlluviumMatrixRD_SAV_Th
     9246.6210044535
**
constant
FractureRD_STFF_Ra
1.0
**
constant
AlluviumMatrixRD_SAV_Ra
     4000.0000000000
**
constant
FractureRD_STFF_Pb
1.0
**
constant
AlluviumMatrixRD_SAV_Pb
     4000.0000000000
**
constant
FractureRD_STFF_Cs
1.0
**
constant
AlluviumMatrixRD_SAV_Cs
     94868.329805051
**
constant
FractureRD_STFF_Ni
1.0
**
constant
AlluviumMatrixRD_SAV_Ni
     89.442719099992
**
constant
FractureRD_STFF_C
1.0
**
constant
AlluviumMatrixRD_SAV_C
1.0
**
constant
FractureRD_STFF_Se
1.0
**
constant
AlluviumMatrixRD_SAV_Se
     22.360679774998
**
constant
FractureRD_STFF_Nb
1.0
**
constant
AlluviumMatrixRD_SAV_Nb
     7745.9666924148
**
constant
FracturePorosity_STFF
     3.1622776601684D-03
**
constant
AlluviumMatrixPorosity_SAV
     0.12500000000000
**
constant
ImmobileRD_STFF_Am
1.8e4
**
constant
ImmobileRD_STFF_Np
19.0
**
constant
ImmobileRD_STFF_I
1.0
**
constant
ImmobileRD_STFF_Tc
1.0
**
constant
ImmobileRD_STFF_Cl
1.0
**
constant
ImmobileRD_STFF_Cm
1.0
**
constant
ImmobileRD_STFF_U
37.0
**
constant
ImmobileRD_STFF_Pu
1.8e3
**
constant
ImmobileRD_STFF_Th
1.8e4
**
constant
ImmobileRD_STFF_Ra
5.4e3
**
constant
ImmobileRD_STFF_Pb
5.4e3
**
constant
ImmobileRD_STFF_Cs
9.0e3
**
constant
ImmobileRD_STFF_Ni
1.8e3
**
constant
ImmobileRD_STFF_C
1.0
**
constant
ImmobileRD_STFF_Se
55.0
**
constant
ImmobileRD_STFF_Nb
1.8e4
**
constant
ImmobilePorosity_STFF
0.01
**
constant
DiffusionRate_STFF
0.0
**
**
**          ***>>>   DCAGW
<<<***
**
constant
DistanceToReceptorGroup[km]
[should_be_10_or_20]
20.0
**
constant
WellPumpingRateAtReceptorGr
oup10km[gal/day]
     138750.00000000
**
constant
WellPumpingRateAtReceptorGr
oup20km[gal/day]
     8750000.0000000
**
constant
PlumeThickness5km[m]
     55.000000000000
**
constant
AquiferThickness5km[m]
     500.00000000000
**
constant
MixingZoneThickness20km[m]
     125.00000000000
**
**
**        ***>>> FAULTO
<<<***
**
constant
TimeOfNextFaultingEventinRe
gionOfInterest[yr]
     4886.7566333600
**
constant
ThresholdDisplacementforFau
ltDisruptionOfWP[m]
    0.20000000000000
**
constant
XLocationOfFaultingEventInR
egionOfInterest[m]
     548000.00000000
**
constant
YLocationOfFaultingEventInR
egionOfInterest[m]
     4077620.0000000
**
constant
ProbabilityForNWOrientation
OfFaults
0.05
**
constant
RNtoDetermineFaultOrientati
on
    0.50000000000000
```

```
**
constant
NWFaultStrikeOrientationMea
suredfromNorthClockwise[deg
rees]
-32.5
**
constant
NEFaultStrikeOrientationMea
suredfromNorthClockwise[deg
rees]
10.0
**
constant
NWFaultTraceLength[m]
4000.0
**
constant
NEFaultTraceLength[m]
4000.0
**
constant
NWFaultZoneWidth[m]
     21.615384615385
**
constant
NEFaultZoneWidth[m]
     28.538461538462
**
constant
NWAmountOfLargestCredibleDi
splacement[m]
    0.13361511890501
**
constant
NEAmountOfLargestCredibleDi
splacement[m]
    0.13361511890501
**
constant
NWCumulativeDisplacementRat
e[mm/yr]
0.00005
**
constant
NECumulativeDisplacementRat
e[mm/yr]
0.00005
**
**
**          ***>>> VOLCANO
<<<***
**
constant
TimeOfNextVolcanicEventinRe
gionOfInterest[yr]
     5049.1832499076
**
constant
XLocationInRegionOfInterest
[m]
548000.0
**
constant
YLocationInRegionOfInterest
[m]
4078000.0
**
constant
RNtoDetermineIfExtrusiveOrI
ntrusiveVolcanicEvent
     0.50000000000000
**
constant
FractionOfTimeVolcanicEvent
IsExtrusive
0.999
**
constant
AngleOfVolcanicDikeMeasured
FromNorthClockwise[degrees]
     7.5000000000000
**
constant
LengthOfVolcanicDike[m]
     6500.0000000000
**
constant
WidthOfVolcanicDike[m]
     5.5000000000000
**
constant
DiameterOfVolcanicCone[m]
     51.250000000000
**
**
**          ***>>> ASHPLUMO
<<<***
**
constant
DensityOfAirAtSTP[g/cm3]
0.00129
**
constant
ViscosityOfAirAtSTP[g/cm-s]
0.00018
**
constant
ConstantRelatingFallTimeToE
ddyDiffusivity[cm2/s5/2]
400.0
**
constant
MaximumParticleDiameterForP
articleTransport[cm]
10.d0
**
constant
MinimumFuelParticulateSize[
cm]
0.0001
**
constant
ModeFuelParticulateSize[cm]
0.001
**
constant
MaximumFuelParticulateSize[
cm]
0.01
**
constant
MinimumAshDensityForVariati
onWithSize[g/cm3]
1.2
**
constant
MaximumAshDensityForVariati
onWithSize[g/cm3]
2.0
**
constant
MinimumAshLogdiameterForDen
sityVariation
-2.0
**
constant
MaximumAshLogdiameterForDen
sityVariation
-1.0
**
constant
ParticleShapeParameter
0.5
**
constant
IncorporationRatio
0.3
**
constant
WindDirection[degrees]
-90.0
**
constant
WindSpeed[cm/s]
     1204.8192771084
**
constant
VolcanicEventDuration[s]
     666192.16446908
**
constant
VolcanicEventPower[W]
     30205132014.279
**
constant
VolcanicColumnConstantBeta
10.0
**
constant
AshMeanParticleLogDiameter[
d_in_cm]
     1.0000000000000D-01
**
constant
AshParticleSizeDistribution
StandardDeviation
1.0
**
**
**          ***>>> ASHRMOVO
<<<***
**
constant
RelativeRateOfBlanketRemova
l[1/yr]
0.0001
**
constant
FractionOfPrecipitationLost
ToEvapotranspiration
0.68
**
constant
FractionOfIrrigationLostToE
vapotranspiration
0.5
**
constant
AnnualPrecipitation[m/yr]
0.085
**
constant
```

```
AnnualIrrigation[m/yr]
1.52
**
constant
FractionOfYearSoilIsSaturat
edDueToPrecipitation
0.0054
**
constant
FractionOfYearSoilIsSaturat
edDueToIrrigation
0.2
**
constant
AshBulkDensity[g/cm3]
1.4
**
constant
AshVolumetricMoistureFracti
onAtSaturation
0.4
**
constant
DepthOfTheRootingZone[m]
0.15
**
constant
KdOfUraniumInVolcanicAsh[cm
3/g]
35.0
**
constant
KdOfCuriumInVolcanicAsh[cm3
/g]
4000.0
**
constant
KdOfPlutoniumInVolcanicAsh[
cm3/g]
550.0
**
constant
KdOfAmericiumInVolcanicAsh[
cm3/g]
1900.0
**
constant
KdOfThoriumInVolcanicAsh[cm
3/g]
3200.0
**
constant
KdOfRadiumInVolcanicAsh[cm3
/g]
500.0
**
constant
KdOfLeadInVolcanicAsh[cm3/g
]
270.0
**
constant
KdOfProtactiniumInVolcanicA
sh[cm3/g]
550.0
**
constant
KdOfActiniumInVolcanicAsh[c
m3/g]
450.0
**
constant
KdOfNeptuniumInVolcanicAsh[
cm3/g]
5.0
**
constant
KdOfSamariumInVolcanicAsh[c
m3/g]
245.0
**
constant
KdOfCesiumInVolcanicAsh[cm3
/g]
280.0
**
constant
KdOfIodineInVolcanicAsh[cm3
/g]
1.0
**
constant
KdOfTinInVolcanicAsh[cm3/g]
130.0
**
constant
KdOfSilverInVolcanicAsh[cm3
/g]
55.0
**
constant
KdOfPaladiumInVolcanicAsh[c
m3/g]
55.0
**
constant
KdOfTechnetiumInVolcanicAsh
[cm3/g]
0.1
**
constant
KdOfMolybdenumInVolcanicAsh
[cm3/g]
10.0
**
constant
KdOfNiobiumInVolcanicAsh[cm
3/g]
160.0
**
constant
KdOfZirconiumInVolcanicAsh[
cm3/g]
600.0
**
constant
KdOfStrontiumInVolcanicAsh[
cm3/g]
15.0
**
constant
KdOfSeleniumInVolcanicAsh[c
m3/g]
150.0
**
constant
KdOfNickelInVolcanicAsh[cm3
/g]
400.0
**
constant
KdOfChlorineInVolcanicAsh[c
m3/g]
0.0
**
constant
KdOfCarbonInVolcanicAsh[cm3
/g]
5.0
**
constant
SolubilityOfUraniumInVolcan
icAsh[moles/liter]
4.5e-5
**
constant
SolubilityOfCuriumInVolcani
cAsh[moles/liter]
1.0e-6
**
constant
SolubilityOfPlutoniumInVolc
anicAsh[moles/liter]
5.0e-6
**
constant
SolubilityOfAmericiumInVolc
anicAsh[moles/liter]
1.0e-6
**
constant
SolubilityOfThoriumInVolcan
icAsh[moles/liter]
3.2e-9
**
constant
SolubilityOfRadiumInVolcani
cAsh[moles/liter]
1.0e-7
**
constant
SolubilityOfLeadInVolcanicA
sh[moles/liter]
3.2e-7
**
constant
SolubilityOfProtactiniumInV
olcanicAsh[moles/liter]
3.2e-8
**
constant
SolubilityOfActiniumInVolca
nicAsh[moles/liter]
1.0e-6
**
constant
SolubilityOfNeptuniumInVolc
anicAsh[moles/liter]
1.0e-4
**
constant
SolubilityOfSamariumInVolca
nicAsh[moles/liter]
5.0e-6
**
constant
SolubilityOfCesiumInVolcani
cAsh[moles/liter]
1.0
**
constant
```

```
SolubilityOfIodineInVolcani
cAsh[moles/liter]
1.0
**
constant
SolubilityOfTinInVolcanicAs
h[moles/liter]
5.0e-8
**
constant
SolubilityOfSilverInVolcani
cAsh[moles/liter]
1.0
**
constant
SolubilityOfPaladiumInVolca
nicAsh[moles/liter]
9.5e-4
**
constant
SolubilityOfTechnetiumInVol
canicAsh[moles/liter]
1.0
**
constant
SolubilityOfMolybdenumInVol
canicAsh[moles/liter]
1.0
**
constant
SolubilityOfNiobiumInVolcan
icAsh[moles/liter]
1.0e-8
**
constant
SolubilityOfZirconiumInVolc
anicAsh[moles/liter]
3.2e-10
**
constant
SolubilityOfStrontiumInVolc
anicAsh[moles/liter]
1.3e-4
**
constant
SolubilityOfSeleniumInVolca
nicAsh[moles/liter]
1.0
**
constant
SolubilityOfNickelInVolcani
cAsh[moles/liter]
2.0e-3
**
constant
SolubilityOfChlorineInVolca
nicAsh[moles/liter]
1.0
**
constant
SolubilityOfCarbonInVolcani
cAsh[moles/liter]
1.0
**
**
**          ***>>>   DCAGS
<<<***
**
constant
DistanceCutoffForDoseConver
sionDualityInDCAGS[km]
19.99
**
constant
AirborneMassLoadForVolcanis
mDoseCalculation[g/m3]
     1.0000000000000D-03
**
constant
OccupancyFactorForVolcanism
DoseCalculation[-]
0.24
**
constant
DepthOfResuspendableLayer[c
m]
0.3
**
endoffile
```

The following are the parameters values for the invert taken from the mean values file provided by R. Janetzke:

```
iflag
InvertBypass(0=ebsfilt,1=bypass-ebsfilt)
0
**
constant
InvertRockPorosity
0.3
**
constant
InvertThickness[m]
0.75
**
constant
InvertDiffusionCoefficient[m^2/yr]
4.4e-5
**
constant
InvertMatrixPermeability[m^2]
     2.0000000000000D-17
**
```

The above values are the same as those used by R. Rice, except that the invert permeability is set to a constant value of 2E-17, compared to the range of 2E-16 to 2E-18 used by R. Rice. Also, the file provided by Janetzke has a value of 1000 for the number of realizations. For the present purpose, only 250 realizations will be run. Thus, the mean values file will be modified accordingly prior to running the TPA 3.2 code.

TPA 3.2 was run using the means value dataset provided by R. Janetzke. According to Janetzke, the number of realizations can be set to one because none of the parameters in the file are sampled, thus all realizations will produce the same result. This run will be referred to as case TPAMEAN-1.

The following is a copy of the relgwgs.res file:

```
Input file tpa.inp as supplied with TPA Version 3.2 Code.
Base case data set Rev 3.2   7/16/98
TPA 3.2, Job started: Tue Dec 15 13:12:35 1998
EPA Groundwater, Ground Surface, and Total Release
Normalized - Values for Each Vector

    vector          gwepasum         gsepasum          epasum
   unitless         unitless         unitless         unitless
         1       2.1383E-02       0.0000E+00       2.1383E-02
```

In the TPA 3.2 input file, there are four parameters used in the EBSFILT module. These are InvertRockPorosity, InvertThickness[m], InvertDiffusionCoefficient[m^2/yr], and InvertMatrixPermeability[m^2], plus the Rd values for the 16 radionuclides for sorption on the invert. For the sensitivity analyses, all parameters except one will be kept constant. The parameters of interest be will varied individually over some range, and the sensitivity of the TPA results will be determined by plotting total EPA (normalized) release versus the values of the sampled parameter.

**12/17/98**

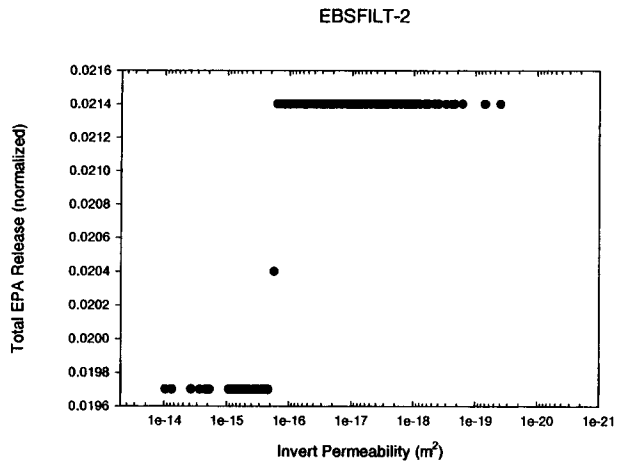
A TPA 3.2 run, to be referred to as case EBSFILT-2, was initiated on 12/15/98. All parameters were set to mean values except for the invert matrix permeability, which was given a range of 2E-14 to 2E-20 and a lognormal distribution. The program ran for about two days. The relgwgs.res file is copied below:

```
Input file tpa.inp as supplied with TPA Version 3.2 Code.
Base case data set Rev 3.2   7/16/98
TPA 3.2, Job started: Tue Dec 15 15:10:19 1998
EPA Groundwater, Ground Surface, and Total Release
Normalized - Values for Each Vector
```

| vector unitless | gwepasum unitless | gsepasum unitless | epasum unitless |
|---|---|---|---|
| 1 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 2 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 3 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 4 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 5 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 6 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 7 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 8 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 9 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 10 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 11 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 12 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 13 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 14 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 15 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 16 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 17 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 18 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 19 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 20 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 21 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 22 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 23 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 24 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 25 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 26 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 27 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 28 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 29 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 30 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 31 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 32 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 33 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 34 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 35 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 36 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 37 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 38 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 39 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 40 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 41 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 42 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 43 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 44 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 45 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 46 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 47 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 48 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 49 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 50 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 51 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 52 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 53 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 54 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 55 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 56 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 57 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 58 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 59 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 60 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 61 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 62 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 63 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 64 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 65 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 66 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 67 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 68 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 69 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 70 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 71 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 72 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 73 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 74 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 75 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 76 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 77 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 78 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 79 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 80 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 81 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 82 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 83 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 84 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 85 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 86 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 87 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 88 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 89 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 90 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 91 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 92 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 93 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 94 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 95 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 96 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 97 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 98 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 99 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 100 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 101 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 102 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 103 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 104 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 105 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 106 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 107 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 108 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 109 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 110 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 111 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 112 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 113 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 114 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 115 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 116 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 117 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 118 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 119 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 120 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 121 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 122 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 123 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 124 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |

| | | | |
|---|---|---|---|
| 125 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 126 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 127 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 128 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 129 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 130 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 131 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 132 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 133 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 134 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 135 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 136 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 137 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 138 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 139 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 140 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 141 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 142 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 143 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 144 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 145 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 146 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 147 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 148 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 149 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 150 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 151 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 152 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 153 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 154 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 155 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 156 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 157 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 158 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 159 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 160 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 161 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 162 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 163 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 164 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 165 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 166 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 167 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 168 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 169 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 170 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 171 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 172 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 173 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 174 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 175 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 176 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 177 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 178 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 179 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 180 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 181 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 182 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 183 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 184 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 185 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 186 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 187 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 188 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 189 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 190 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 191 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 192 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 193 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 194 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 195 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 196 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 197 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 198 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 199 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 200 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 201 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 202 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 203 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 204 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 205 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 206 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 207 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 208 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 209 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 210 | 2.0379E-02 | 0.0000E+00 | 2.0379E-02 |
| 211 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 212 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 213 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 214 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 215 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 216 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 217 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 218 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 219 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 220 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 221 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 222 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 223 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 224 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 225 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 226 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 227 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 228 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 229 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 230 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 231 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 232 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 233 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 234 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 235 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 236 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 237 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 238 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 239 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 240 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 241 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 242 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 243 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 244 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 245 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 246 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 247 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 248 | 1.9656E-02 | 0.0000E+00 | 1.9656E-02 |
| 249 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |
| 250 | 2.1383E-02 | 0.0000E+00 | 2.1383E-02 |

Below is a plot of total EPA (normalized) release versus invert matrix permeability:




Note the step function as an invert permeability ~1.8E-16 $m^2$. Below this value, the average groundwater flow rate for 50,000 yrs is low enough that matrix flow through the invert occurs, resulting in enhanced retardation of radionuclides and lower total release. Above that value, the average flow rate is high enough that EBSFILT is not invoked by the TPA 3.2 code, i.e., the presence of the invert is ignored.

1645 hours - A TPA 3.2 run was initiated in which the invert permeability was given a range 2e-14 to 2e-20 and lognormal distribution, as in case EBSFILT-2, and the invert thickness was given a range of 0.1 to 10.0 m and lognormal distribution. This run will be referred to as case EBSFILT-3.

**[The rest of this page is left blank.]**

**12/18/98**

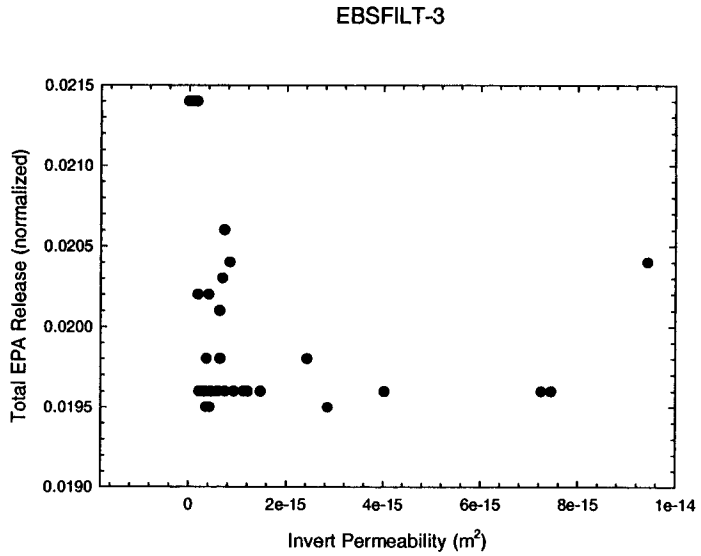
The program to extract sampled parameter values from the samplpar.res file was modified because it was incorrectly reading input files with less than 5 values per line. A copy of the modified program follows:

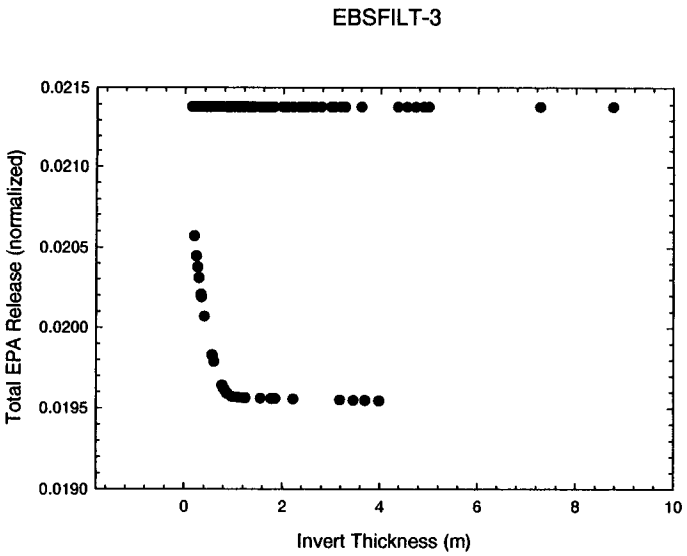
```
      PROGRAM READSAMPPAR
      IMPLICIT REAL (A-H,O-Z)
      DIMENSION PARVAL(1000)
C
      OPEN(UNIT=5,FILE='SAMPPAR.INP')
      OPEN(UNIT=6,FILE='SAMPPAR.OUT')
C
C     READ FROM INPUT FILE # OF REALIZATIONS, # OF SAMPLED PARAMETERS,
C     # OF VALUES PER LINE IN INPUT.FILE
      READ(5,*) NVECTOR, NSAMPPAR
C     WRITE TO OUTPUT FILE # OF REALIZATIONS, # OF SAMPLED PARAMETERS
      WRITE(6,*)'# OF REALIZATIONS: ',NVECTOR, '; # OF SAMPLED PARS.: '
     1 , NSAMPPAR
C
C     READ FROM INPUT FILE THE SAMPLE PARAMETER # OF INTEREST'
      READ(5,*) IPAR
C
C--READ VALUES OF SAMPLED PARAMETERS FOR EACH REALIZATION.
C  READ THE FIRST (HEADER) LINE BUT IGNORE VALUES.
C
      WRITE(6,*)'SAMPLED PAR# = ',IPAR
      WRITE(6,*)'REALIZ# ; PAR. VALUE'
      DO 20 K=1,NVECTOR
      READ(5,*)
      READ(5,*,END=25)(PARVAL(J),J=1,NSAMPPAR)
25    CONTINUE
      WRITE(6,*)K,PARVAL(IPAR)
20    CONTINUE
      CLOSE(5)
      CLOSE(6)
      STOP
      END
```

The above program was tested with the EBSFILT-1 samppar.inp file, and with new samppar.inp files with one to five values per line, and the results are correct.

**12/21/98**

The TPA 3.2 run for case EBSFILT-3 is completed. The values of the sampled parameters (invert permeability and invert thickness) were extracted from the samplpar.res file, and values of total EPA release were taken from the relgwgs.file. For some unknown reason, only 229 realizations were completed, instead of the 250 realizations specified in the tpa.inp file. Plots of total release vs permeability and total release vs thickness are shown below:



**Entries into Scientific Notebook No. 185, Volume 7, for the period October 1, 1998, to December 31, 1998, have been made by**

**Roberto T. Pabalan / Date**

**No original entry into this Scientific Notebook has been removed.**

The entries in this electronic scientific notebook #185, Volume 8, document activities conducted during the Period October 1, 1999, through December 31, 1999, under the Evolution of the Near-field Environment Key Technical Issue (Project Number 20-1402-561). **Note that no entries were made during the periods January 1, 1999 through March 31, 1999; April 1, 1999 through June 30, 1999; and July 1, 1999 through September 30, 1999. This lack of entry for those periods was communicated to Bruce Mabrito via email.**

10

**11/18/99**

**Below is a copy of an email, including attachments, from Bret Leslie (NRC) regarding the composition of cementitious grout that maybe used at Yucca Mountain:**

Bobby et al.,

The attached note contains information on grout that may be used. This is the information that Fred Glasser could use that I promised to track down. Let me know if you need anything else.

Bret


FileItem.txt


RFC822.TXT

```
Received: from igate.nrc.gov ([148.184.176.31])
      by smtp (GroupWise SMTP/MIME daemon 4.1 v3)
      ; Mon, 18 Oct 99 15:05:24 EDT
Received: from nrc.gov
           by smtp-gateway ESMTPœ id PAA11156
           for <bwl@nrc.gov>; Mon, 18 Oct 1999 15:05:36 -0400 (EDT)
From: Gerald_Thiers@notes.ymp.gov
Received: from ymln11.ymp.gov (ymln11.ymp.gov [192.12.95.129])
 by ymps5.ymp.gov (PMDF V5.2-29 #32802)
 with SMTP id <0FJT00A0IBUMWQ@ymps5.ymp.gov> for bwl@nrc.gov; Mon,
 18 Oct 1999 12:08:46 -0700 (PDT)
Received: by ymln11.ymp.gov(Lotus SMTP MTA v4.6.3 (778.2 1-4-1999))
  id 8825680E.0068D28B ; Mon, 18 Oct 1999 12:04:56 -0700
Date: Mon, 18 Oct 1999 12:04:31 -0700
Subject: Grout Information for Bret Leslie
To: bwl@nrc.gov
Cc: Richard_Nolting@notes.ymp.gov, Daniel_McKenzie@notes.ymp.gov,
       Kalyan_Bhattacharyya@notes.ymp.gov, David_Tang@notes.ymp.gov
Message-id: <8825680E.0068D25D.00@ymln11.ymp.gov>
X-Lotus-FromDomain: CRWMS
Mime-Version: 1.0
Content-Type: multipart/mixed; boundary="=_4A137463.60016D55"

--=_4A137463.60016D55
Content-Type: text/plain; charset=US-ASCII
Content-Transfer-Encoding: quoted-printable
```

Content-Disposition: inline

Bret, The information requested is included below. Please let me know =
if
you need more. Jerry Thiers

---------- Forwarded by Gerald Thiers/YM/RWDOE on 10/18/99 =
11:57 AM
---

David Tang
10/15/99 02:22 PM

To: Daniel McKenzie/YM/RWDOE@CRWMS
cc: Richard Nolting/YM/RWDOE@CRWMS, Gerald Thiers/YM/RWDOE@CRWMS, Kalyan
Bhattacharyya/YM/RWDOE@CRWMS

Subject: Call from Bret Leslie

For your information, the Longevity of Emplacement Drift Ground Support Materials report is being checked at the moment, which is expected to be
approved around the end of this month or early November. Although the =
mix
design of the cement grout for rock bolts is not within the scope of the =
study,
a preliminary mixture proportioning of the ingredients for cement grout =
for rock
bolts was discussed, which is summarized as follows:

Cement type - Type E-1 (K) cement, about 90 percent by weight of solid =
mass
Water/cementitious material ratio: 0.4 to 0.6
No fine aggregate will be used
Silica fume: 5 to 10 percent by weight of cement
Superplasticizer: 1 percent of cement plus silica fume by weight.

The typical chemical analysis of Type E-1 (K) cement is shown in the = attached
table.

Please note that this mix design for the cement grout is preliminary. =
The
final cement type, admixture and the actual proportioning must be = developed by

further investigation, detailed calculation, and testing on trial =
mixtures.

Please let me know if you have any comments.

Thanks,

David

(See attached file: Type E-1 (K) Cement.doc)

---------- Forwarded by David Tang/YM/RWDOE on 10/15/99
01:31 =
PM
---

Richard Nolting
10/14/99 02:41 PM

To: David Tang/YM/RWDOE@CRWMS
cc:

Subject: Call from Bret Leslie

David,

Can you put something together on this and give it to McKenzie?

Thanks, Rick
---------- Forwarded by Richard Nolting/YM/RWDOE on
10/14/99 =
02:41
PM ---

Daniel McKenzie
10/14/99 07:47 AM

To: Richard Nolting/YM/RWDOE@CRWMS
cc: Gerald Thiers/YM/RWDOE@CRWMS, Kalyan Bhattacharyya/YM/RWDOE@CRWMS

Subject: Call from Bret Leslie

Typical Chemical Analysis for Type E-1 (K) Cement

| Chemical Component | Composition, % |
|---|---|
| $SiO_2$ | 19.4 |
| $Al_2O_3$ | 5.2 |
| $Fe_2O_3$ | 2.8 |
| CaO | 61.9 |
| MgO | 1.4 |
| $SO_3$ | 6.9 |
| Loss on Ignition at 950 °C | 1.1 |
| $Na_2O$ | 0.10 |
| $K_2O$ | 0.59 |
| SrO | 0.05 |
| ZnO | 0.02 |
| $TiO_2$ | 0.28 |
| $P_2O_5$ | 0.10 |
| $MnO_3$ | 0.04 |

**The rest of this page is left blank.**

**November 16, 1999**

**REACTION PATH MODELING OF THE CHEMICAL EVOLUTION OF WATER INSIDE WASTE PACKAGES**

**Objective: The determine the chemistry of water inside the waste package as a function of time and its evolution as it interacts with the waste package components.**

**Rationale: The solubility of the waste form is highly dependent on the chemistry of water inside the waste package. The corrosion of the waste container, hence the release of radionuclides from the waste package, is also dependent on the water chemistry. Interactions between the water and the waste package components will affect water chemistry.**

**Technical Approach: Reaction path modeling using geochemical codes, such as EQ3/6 and Geochemist's Workbench will be used to model the water/gas/waste component interactions. The approach will be similar to that used by Zhang and Stockman (1999).**

**Reference: Title: Zhang, Peng-Chu and Harlan W. Stockman. 1999. EQ6 Calculation for Chemical Degradation of Pu-Ceramic Waste Packages: Effects of Updated Materials, Composition and Rates. Document Identifier: CAL-EDC-MD-000003. Albuqueque, NM: Sandia National Laboratories.**

**The following is a copy of email communications with H. Stockman (Sandia) regarding their work on EQ6 reaction path calculations:**

Hi –

I placed the CD contents on the following location: http://garnet.energylan.sandia.gov/~ymp/ This address points to a public Outbox on a secure system. The best way to access the site is probably through your browser; just click on the link above, then select directory Pu-ceram_CD. The directories correspond to those in the Pu-ceram report attachment. I tried to transfer most files as binary, but some of the text files may have been futzed with by the ftp client. The best way to view the *.elem_???.txt files is to drop them onto Excel. With the *.6i and *.6o files, you should have a pretty complete set of results. That FTP server will soon run out of room, so if you really want to see the files, yor should check them out in the next week, before I clean the system. The binaries (*.bin files) are large; however, they provide the best way to explore the chemistry of the test cases. To view them, you will need to download pp.exe, prefer.pp, help_pp, external.fnt and the associated files into a directory on a Win95, Win98 or Win3.1x machine. Load the binary you wish to see into that directory, open a DOS box into that directory, and invoke the program: pp /4 myfile.bin where myfile.bin is the name of the particular binary. If the screen gets garbage, use the command line

pp 6 /4 myfile.bin

to enforce low-res VGA mode. There is an old manual for the PP program in http://garnet.energylan.sandia.gov/~ymp/eq/PP.doc . Since you won't have the proper environment variables set, the only way to use the "What is this?" capability would be to

copy the data0 file of choice to data0.com, within the same directory. On multiflo: we wanted to use that code. Bob MacKinnon did the legwork, but the paperwork inertia was far too great, and qualification looked really complicated, since there were few tests cases available, and the range of capabilities is so large. Since TOUGHREACT is already qualified, it would be very hard to push for qualification of a similar code.

Roberto Pabalan <rpabalan@swri.edu> said:

> Harlan:
>
Thank you for your quick reply to David's questions. I find your work presented in the Pu-ceramic report very interesting. We have initiated new activities--modeling and experimental--designed to provide a better understanding of the chemistry of water inside corroding waste packages. We may take a similar approach of using EQ3/6 in the calculations, perhaps supplemented by reactive transport calculations with MULTIFLO and coupled corrosion/transport calculations with TECTRAN (currently proprietary, funded by GRI). I would appreciate receiving a copy of the electronic data for EQ6 calculations, mainly for benchmarking our calculations. At some point, we would also be interested in getting a copy of the YMP-qualified EQ3/6 database, either through you or from Tom/Jim or Dave Sassani.

You can try sending a copy of the electronic data via ftp to ftp.swri.edu/pub. Please advise me if you were able to do so--I'll retrieve the file right away to free up the disk space. However, I'm not sure if there is enough room for 600 MB.
>
> Thanks.
>
> bobby pabalan
> _____Reply Separator_____
> Subject: Fwd:Re: geochemistry calculations
> Author: David Pickett
> Date: 11/8/99 5:38 PM
>
> Bobby - Reply from Stockman.
>
> David
>
> _____Forward Header_____
> Subject: Re: geochemistry calculations
> Author: "H.W. Stockman" <hwstock@wizard.com>
> Date: 11/8/99 3:39 PM
>
>
> ----- Original Message -----
> From: David Pickett <dpickett@swri.edu>
> To: <hwstock@wizard.com>

> Sent: Monday, November 08, 1999 1:44 PM
> Subject: geochemistry calculations
>
>
> >
> > Harlan,
> >
Thanks again for the report you sent several weeks ago. Bobby Pabalan is the lead here on near field issues, and he was wondering if there are similar reports available for related calculations having to do with in-package or in-drift chemistry (more generally than just related to criticality). I realize that is a rather open-ended question, but I would appreciate any suggestions you might have. We're not so much interested in the results and conclusions as we are in getting a better idea of how DOE plans to do this type of work in the future.

Actually, we should have some pretty good examples soon. JP Nicot qualified PHREEQC, and is completing a set of calculations on U-silicate precipitation in fractures He sent up some rather interesting plots this morning, with calculatons of soddyite precipitation over a 250 meter path, and I believe he is writing up the discussion now. We will have the draft of our Pu-ceramic extermal criticality report out in early January, and assuming it is "legal" and my bosses agree, I can send reults of intermediate work by the end of November. >

We have broadened our work to include more realistic models, and more sensitivity studies. There are still substantial uncertainties in the effective surface area for the near field calculations We are going to rerun many of our calculations with a new thermo database soon, and it might be appropriate to wait for the comparison between old and new.

We are in the process of getting a single EQ6 database qualified for use at YMP. Paul Cloke arranged meetings with Dave Sassani, the DOE reps, Tom Wolery and Jim Johnson of LLNL, Wolfgang Runde of LANL, and various M&O folks to hammer out a sensible and defensible data set. Johnson and Sassani are plugged into the Helgeson-derived datasets, so we have some academic credibility. Sensitive issues that we wish to resolve include: the stability of Pu carbonate complexes; methods of calculating activity coefficients for the Pu carbonate species; and the current uncertainty in U-silicate data.

He also asked about a set of data cited in your Pu ceramic report as CRWMS M&O 1999: "Electronic data for EQ6 calculations...." Is that available?

It is. As a CD, it is about 600 MB, but most of that is in the binary files, which we use only for graphing data (the graphing software is included on the CD). I can either cut a copy of the CD, or I can put the files on an FTP server (I think the latter makes more sense; do you have an FTP site not within a firewall?). I'll forward this note to myself at work; but if you don't hear from me in a day, send a gentle reminder.

**NOTE:** The files referred to by H. Stockman in his email was downloaded from the website,except for the *.exe files. Problems with the Sandia server prevented getting these *.exe files. H. Stockman subsequently sent a copy of the PP code files via email. The PP code is used to graphically illustrate the results of the EQ6 runs.

Test calculations were done to determine if EQ3/6 results will be the same as those of Stockman. The file j13noc30.3I was used in the calculations. **Error messages were encountered when running EQ3 using the Stockman files downloaded from the website. It was found that one needs to open the input file in an MS-DOS window and resaved (with no changes required) before the input file will be read successfully by EQ3.**

The following is the resulting output file from the test run. A careful comparison with the Stockman j13noc30.3o file indicates that the results are identical. **The calculations used the data0.com.R2 version of the thermodynamic database.** A recalculation will need to be done using the V8.R6 version of the database.

```
 EQ3/6, Version 7.2b (EQ3/6-V7-REL-V7.2b-PC)
 EQ3NR Speciation-Solubility Code (EQ3/6-V7-EQ3NR-EXE-R139-P5)
 Supported by the EQLIB library (EQ3/6-V7-EQLIB-LIB-R168-P5)

 Copyright (c) 1987, 1990-1993, 1995 The Regents of the University of
 California, Lawrence Livermore National Laboratory. All rights
 reserved.

 This work is subject to additional statements and
 disclaimers which may be found in the README.txt file
 included in the EQ3/6 software transmittal package.


 Run  16:41:37  11/16/99


 --- Reading the input file ---
|---------------------------------------------------------------------|
|EQ3NR input file name= j13noc30.3i                                   |
|  Ca++ not fixed by CALcite, Log10fCO2 fixed -3.0 (hence the "30").  |
|==== j13[cal,noc][25,30,35].3i General Series Notes: ================|
|2-10-99 HWStockman xcif3 Wolery's J13wsf.3i to Davelar format, then  |
|  determine sensitivity to CO2, O2 constraints as cross-check on the |
|  variants used by PLCloke. HPO4-- corrected for H; 120 PO4--- from  |
|  Harrar et al. mul by 95.979/94.971 MolWts from EQ6 DB.             |
|==== j13hws??.3i specific comments for versions ======================|
|  2-10-99 j13hws03: Like 02, but set log fCO2 = -3.5, pH init=8.5, and |
|  balance on H+.                                                     |
|  2-10-99 j13hws02: Like 01, but raise init pH from 7.5 to 7.6.      |
|  2-10-99 j13hws01: Like 00, but raise pH slightly.                  |
|==== TJWolery original comments on J13wsf.3i below ==================|
|Description= "J-13 well water, with traces of spent fuel components" |
|Version level= 7.2                                                   |
|Revised 08/08/95    Revisor= T. J. Wolery                            |
|This is part of the EQ3NR Test Case Library (EQ3/6-V7-EQ3NR-TST-R04) |
|                                                                     |
|  Water from well J-13 at the Nevada Test Site, spiked with          |
|trace amounts of spent nuclear fuel components. The composition      |
|is otherwise identical to that in the EQ3NR test case input file     |
|J13W.3I, which is based on data reported by Harrar et al. (1990).    |
|Water from this well is commonly used to represent the groundwater   |
|at the proposed high-level nuclear waste repository at Yucca         |
|Mountain, Nevada.                                                    |
|                                                                     |
|  Purpose: to initialize the EQ6 test case input file J13WSF.6I,     |
|which simulates the interaction of J-13 well water with spent        |
|nuclear fuel. This test case also tests the ability of EQ3NR to      |
|handle a system containing many components.                          |
|                                                                     |
|                                                                     |
|                            References                               |
|                                                                     |
|Harrar, J. E., Carley, J. F., Isherwood, W. F., and Raber, E., 1990, |
|  Report of the Committee to Review the Use of J-13 Well Water in    |
|  Nevada Nuclear Waste Storage Investigations: UCID-21867, Lawrence  |
```

| Livermore National Laboratory, Livermore, California. TIC# 209096. |
|---|
| (HWStockman adds TIC # 2-10-99 above) |

| Temperature (C) | 25.00 | Density(gm/cm3) | 1.00000 |
|---|---|---|---|

| Total Dissolved Salts | | mg/kg | mg/l | *not used |
|---|---|---|---|---|

| Electrical Balancing on | H+ | code selects | not performed |
|---|---|---|---|

| SPECIES | BASIS SWITCH/CONSTRAINT | CONC/ETC | UNITS OR TYPE |
|---|---|---|---|
| redox | | -0.7000 | LogfO2 |
| Na+ | | 45.800 | mg/L |
| SiO2(aq) | | 60.970 | mg/L |
| Ca++ | | 13.000 | mg/L |
| K+ | | 5.0400 | mg/L |
| Mg++ | | 2.0100 | mg/L |
| Li+ | | 0.48000E-01 | mg/L |
| H+ | | 8.1000 | pH |
| HCO3- | CO2(g) | -3.0000 | Log fugacity |
| O2(aq) | | 5.6000 | mg/L |
| F- | | 2.1800 | mg/L |
| Cl- | | 7.1400 | mg/L |
| NO3- | NH3(aq) | 8.7800 | mg/L |
| SO4-- | | 18.400 | mg/L |
| B(OH)3(aq) | | 0.76600 | mg/L |
| Al+++ | Diaspore | 0.000000 | Mineral |
| Mn++ | Pyrolusite | 0.000000 | Mineral |
| Fe++ | Goethite | 0.000000 | Mineral |
| HPO4-- | | 0.121 | mg/L |
| Ba++ | | 0.10000E-15 | Molality |
| CrO4-- | | 0.10000E-15 | Molality |
| Cu++ | | 0.10000E-15 | Molality |
| Gd+++ | | 0.10000E-15 | Molality |
| MoO4-- | | 0.10000E-15 | Molality |
| Ni++ | | 0.10000E-15 | Molality |
| Np++++ | | 0.10000E-15 | Molality |
| Pb++ | | 0.10000E-15 | Molality |
| Pu++++ | | 0.10000E-15 | Molality |
| TcO4- | | 0.10000E-15 | Molality |
| Ti(OH)4(aq) | | 0.10000E-15 | Molality |
| UO2++ | | 0.10000E-15 | Molality |
| Zr(OH)2++ | | 0.10000E-15 | Molality |

| Input Solid Solutions | | | |
|---|---|---|---|
| none | | | |

| SUPPRESSED SPECIES (suppress,replace,augmentk,augmentg) | value |
|---|---|
| none | |

OPTIONS

- SOLID SOLUTIONS -
  - * ignore solid solutions
    process hypothetical solid solutions
    process input and hypothetical solid solutions
- LOADING OF SPECIES INTO MEMORY -
  - * does nothing
    lists species loaded into memory
- ECHO DATABASE INFORMATION -
  - * does nothing
    lists all reactions
    lists reactions and log K values
    lists reactions, log K values and polynomial coef.
- LIST OF AQUEOUS SPECIES (ordering) -
  - * in order of decreasing concentration
    in same order as input file
- LIST OF AQUEOUS SPECIES (concentration limit) -
  - * all species
    only species > 10**-20 molal
    only species > 10**-12 molal
    not printed
- LIST OF AQUEOUS SPECIES (by element) -
  - * print major species
    print all species
    don't print
- MINERAL SATURATION STATES -
  - * print if affinity > -10 kcals
    print all
    don't print
- pH SCALE CONVENTION -
  - * modified NBS
    internal
    rational
- ACTIVITY COEFFICIENT OPTIONS -
  - * use B-dot equation
    Davies' equation
    Pitzer's equations
- AUTO BASIS SWITCHING -
  - * off
    on

```
| - PITZER DATABASE INFORMATION -                                          |
|    * print only warnings                                                 |
|      print species in model and number of Pitzer coefficients           |
|      print species in model and names of Pitzer coefficients            |
| - PICKUP FILE -                                                          |
|    * write pickup file                                                   |
|      don't write pickup file                                             |
| - LIST MEAN IONIC PROPERTIES -                                           |
|    * don't print                                                         |
|      print                                                               |
| - LIST AQUEOUS SPECIES, ION SIZES, AND HYDRATION NUMBERS -               |
|    * print                                                               |
|      don't print                                                         |
| - CONVERGENCE CRITERIA -                                                 |
|    * test both residual functions and correction terms                   |
|      test only residual functions                                        |
|--------------------------------------------------------------------------|
|DEBUGGING SWITCHES (0 = off, 1,2 = on                                     |
|--------------------------------------------------------------------------|
|0  generic debugging information                                          |2
|0  print details of pre-Newton-Raphson iteration                          |2
|0  print details of Newton-Raphson iteration                              |
|0  print details of stoichiometric factors                                |2
|0  print details of stoichiometric factors calculation                    |
|0  write reactions on RLIST                                               |
|0  list stoichiometric concentrations of master species                   |
|0  request iteration variables to be killed                               |
|--------------------------------------------------------------------------|
|DEVELOPMENT OPTIONS  (used for code development)                           |
|--------------------------------------------------------------------------|
| none                                                                     |
|--------------------------------------------------------------------------|
|TOLERANCES                  (desired values)        (defaults)            |
|--------------------------------------------------------------------------|
|      residual functions  |                     |1.0e-10  tolbt          |
|        correction terms  |                     |1.0e-10  toldl          |
|        saturation state  |                     |0.5      tolsat         |
|number of N-R iterations  |                     |30       itermx         |
|--------------------------------------------------------------------------|

 --- The input file has been successfully read ---

 --- Reading the datal file ---

 --- The datal file has been successfully read ---

 * note - (eqlib/inbdot) The following aqueous species
       have been assigned a default hard core diameter of
         4.000 Angstroms-
         Ba(CH3COO)2(aq)
         BaCO3(aq)
         CO(aq)
         Ca(CH3COO)2(aq)
         CaCO3(aq)
         CaCl2(aq)
         CaSO4(aq)
         Cu(CH3COO)2(aq)
         CuCH3COO(aq)
         Fe(CH3COO)2(aq)
         FeCl2(aq)
         Gd(CH3COO)3(aq)
         HCN(aq)
         KCH3COO(aq)
         KCl(aq)
         KHSO4(aq)
         KOH(aq)
         LiCH3COO(aq)
         LiCl(aq)
         Mg(CH3COO)2(aq)
         MgCO3(aq)
         Mn(CH3COO)2(aq)
         MnSO4(aq)
         NH4CH3COO(aq)
         NaCH3COO(aq)
         NaF(aq)
         NaHSiO3(aq)
         Ni(CH3COO)2(aq)
         Pb(CH3COO)2(aq)
         PbCl2(aq)
```

```
eeee   qqq   33333  n   n  rrrr
e     q   q      3  nn  n  r   r
eeee  q   q    33   n n n  rrrr
e     q q q      3  n  nn  r  r
eeee   qqq   3333   n   n  r   r
          q
```

```
EQ3NR, version 7.2b (R139    )
 supported by EQLIB, version 7.2b (R168    )


|EQ3NR input file name= j13noc30.3i                                      |
| Ca++ not fixed by CALcite, Log10fCO2 fixed -3.0 (hence the "30").      |
|==== j13[cal,noc][25,30,35].3i General Series Notes: ================|
|2-10-99 HWStockman xcif3 Wolery's J13wsf.3i to Davelar format, then     |
|  determine sensitivity to CO2, O2 constraints as cross-check on the    |
|  variants used by PLCloke. HPO4-- corrected for H; 120 PO4--- from     |
|  Harrar et al. mul by 95.979/94.971 MolWts from EQ6 DB.                |
|==== j13hws??.3i specific comments for versions ======================|
| 2-10-99 j13hws03: Like 02, but set log fCO2 = -3.5, pH init=8.5, and   |
|  balance on H+.                                                        |
| 2-10-99 j13hws02: Like 01, but raise init pH from 7.5 to 7.6.          |
| 2-10-99 j13hws01: Like 00, but raise pH slightly.                      |
|==== TJWolery original comments on J13wsf.3i below ===================|
|Description= "J-13 well water, with traces of spent fuel components"    |
|Version level= 7.2                                                      |
|Revised 08/08/95    Revisor= T. J. Wolery                               |
|This is part of the EQ3NR Test Case Library (EQ3/6-V7-EQ3NR-TST-R04)    |
|                                                                        |
|  Water from well J-13 at the Nevada Test Site, spiked with             |
|trace amounts of spent nuclear fuel components. The composition         |
|is otherwise identical to that in the EQ3NR test case input file        |
|J13W.3I, which is based on data reported by Harrar et al. (1990).       |
|Water from this well is commonly used to represent the groundwater      |
|at the proposed high-level nuclear waste repository at Yucca            |
|Mountain, Nevada.                                                       |
|                                                                        |
|  Purpose: to initialize the EQ6 test case input file J13WSF.6I,        |
|which simulates the interaction of J-13 well water with spent           |
|nuclear fuel. This test case also tests the ability of EQ3NR to         |
|handle a system containing many components.                             |
|                                                                        |
|                                                                        |
|                              References                                |
|                                                                        |
|Harrar, J. E., Carley, J. F., Isherwood, W. F., and Raber, E., 1990,    |
|  Report of the Committee to Review the Use of J-13 Well Water in       |
|  Nevada Nuclear Waste Storage Investigations: UCID-21867, Lawrence     |
|  Livermore National Laboratory, Livermore, California. TIC# 209096.    |
|(HWStockman adds TIC # 2-10-99 above)                                   |

data0.com.R2
CII: GEMBOCHS.V2-EQ8-DATA0.COM.R2
THERMODYNAMIC DATABASE
generated by GEMBOCHS.V2-JEWEL.SRC.R3 02-aug-1995 16:45:06
Output package:  eq3
Data set:        com
+---------------------------------------------------------------------

  The activity coefficients of aqueous solute species
and the activity of water are calculated according to the
B-dot equation plus others


Temperature=  25.00 degrees Celsius
pressure=    1.0132 bars


        79 elements are in the data base
       100 elements can be loaded into memory
        31 elements are active in this problem


       972 aqueous species are in the data base
       673 aqueous species were loaded into memory
       800 aqueous species can be loaded into memory
       591 aqueous species are active in this problem

       892 aqueous reactions are in the data base
       593 aqueous reactions were loaded into memory
       699 aqueous reactions can be loaded into memory


           942 minerals are in the data base
           600 minerals were loaded into memory
           850 minerals can be loaded into memory
           598 minerals are active in this problem

            12 solid solutions are in the data base
            50 solid solutions can be loaded into memory

            88 gases are in the data base
            56 gases were loaded into memory
            80 gases can be loaded into memory
            56 gases are active in this problem
```

```
iopt1  =  0 (redox option switch)
iopt2  =  0 (automatic basis switching switch)
iopt3  =  0 (interfacing output control switch)
iopt4  =  0 (turn-on solid solutions switch)
iopt5  =  0 (not used)
iopt6  =  0 (conv. test criteria switch)
iopt7  =  0 (0/1 version 7/post-version 7 pickup file)
iopt8  =  0 (not used)
iopt9  =  0 (not used)
iopt10 =  0 (not used)


iopg1  =  0 (act. coeff. choice)
iopg2  =  0 (pH scale convention switch)
iopg3  =  0 (not used)
iopg4  =  0 (not used)
iopg5  =  0 (not used)
iopg6  =  0 (not used)
iopg7  =  0 (not used)
iopg8  =  0 (not used)
iopg9  =  0 (not used)
iopg10 =  0 (not used)


iopr1  =  0 (list loading of species)
iopr2  =  0 (list reactions and log K values)
iopr3  =  0 (aqueous species print order control)
iopr4  =  0 (aqueous species print cut-off control)
iopr5  =  0 (mass balance percentages print control)
iopr6  =  0 (mean ionic act coeff print control)
iopr7  =  0 (mineral affinity print control)
iopr8  =  0 (ion size and hydr. no. print control)
iopr9  =  0 (Pitzer coefficients tabulation)
iopr10 =  0 (print concbs array)
iopr11 =  0 (not used)
iopr12 =  0 (not used)
iopr13 =  0 (not used)
iopr14 =  0 (not used)
iopr15 =  0 (not used)
iopr16 =  0 (not used)
iopr17 =  0 (not used)
iopr18 =  0 (not used)
iopr19 =  0 (not used)
iopr20 =  0 (not used)


iodb1  =  0 (print info. messages switch)
iodb2  =  0 (print pre-Newton-Raphson optimizations switch)
iodb3  =  0 (request iteration variables to kill)
iodb4  =  0 (print Newton-Raphson iterations switch)
iodb5  =  0 (list stoichiometric equivalences)
iodb6  =  0 (controls iodb5 level of detail)
iodb7  =  0 (write reactions on file rlist switch)
iodb8  =  0 (not used)
iodb9  =  0 (not used)
iodb10 =  0 (not used)

The default redox state is constrained by log fO2 =   -0.7000 (log bars)

Solution density =  1.00000 g/mL

Total dissolved salts =       0.00 mg/kg solution
Total dissolved salts =       0.00 mg/L


Tolbt  =  0.10000E-05 (convergence tolerance on residual functions)
Told1  =  0.10000E-05 (convergence tolerance on correction terms)
Tolsat =  0.50000E+00 (phase saturation tolerance, does not affect
                       convergence)


                    --- Input Constraints ---

   Species                  Csp      Jflag   Input Type/Co-species

Na+                      4.5800E+01    2    Total conc, mg/L
SiO2(aq)                 6.0970E+01    2    Total conc, mg/L
Ca++                     1.3000E+01    2    Total conc, mg/L
K+                       5.0400E+00    2    Total conc, mg/L
Mg++                     2.0100E+00    2    Total conc, mg/L
Li+                      4.8000E-02    2    Total conc, mg/L
H+                      -8.1000E+00   16    Log activity
HCO3-                   -3.0000E+00   21    Gas equilibrium
                                              CO2(g)

                  1.000  CO2(g)
                +  1.000  H2O
                    ==
```

```
                    1.000  H+
                  + 1.000  HCO3-
O2(aq)                    5.6000E+00    2    Total conc, mg/L
F-                        2.1800E+00    2    Total conc, mg/L
Cl-                       7.1400E+00    2    Total conc, mg/L
NO3-                      8.7800E+00    2    Total conc, mg/L
    switch with NH3(aq)
SO4--                     1.8400E+01    2    Total conc, mg/L
B(OH)3(aq)                7.6600E-01    2    Total conc, mg/L
Al+++                     0.0000E+00   19    Mineral equilibrium
                                               Diaspore

                    1.000  Diaspore
                  + 3.000  H+
                       ==
                    2.000  H2O
                  + 1.000  Al+++
Mn++                      0.0000E+00   19    Mineral equilibrium
                                               Pyrolusite

                    1.000  Pyrolusite
                  + 2.000  H+
                       ==
                    1.000  H2O
                  + 1.000  Mn++
                  + 0.500  O2(g)
Fe++                      0.0000E+00   19    Mineral equilibrium
                                               Goethite

                    1.000  Goethite
                  + 3.000  H+
                       ==
                    2.000  H2O
                  + 1.000  Fe+++
HPO4--                    1.2100E-01    2    Total conc, mg/L
Ba++                      1.0000E-16    0    Total conc, molal
CrO4--                    1.0000E-16    0    Total conc, molal
Cu++                      1.0000E-16    0    Total conc, molal
Gd+++                     1.0000E-16    0    Total conc, molal
MoO4--                    1.0000E-16    0    Total conc, molal
Ni++                      1.0000E-16    0    Total conc, molal
Np++++                    1.0000E-16    0    Total conc, molal
Pb++                      1.0000E-16    0    Total conc, molal
Pu++++                    1.0000E-16    0    Total conc, molal
TcO4-                     1.0000E-16    0    Total conc, molal
Ti(OH)4(aq)               1.0000E-16    0    Total conc, molal
UO2++                     1.0000E-16    0    Total conc, molal
Zr(OH)2++                 1.0000E-16    0    Total conc, molal


Electrical balance will be achieved by adjusting
  the concentration of "H+                    ". Any other specified
  constraint will be overridden.


    Switching NO3- into the basis set for NH3(aq)


                    1.000  NO3-
                  + 1.000  H2O
                  + 1.000  H+
                       ==
                    1.000  NH3(aq)
                  + 2.000  O2(g)

                    1.000  NH3(aq)
                  + 2.000  O2(g)
                       ==
                    1.000  H2O
                  + 1.000  H+
                  + 1.000  NO3-

        --- Inactive Aqueous Species ---



                     --- Modified Input Constraints ---

   Species                   Csp      Jflag   Input Type/Co-species

Al+++                     0.0000E+00   19    Mineral equilibrium
                                               Diaspore

                    1.000  Diaspore
                  + 3.000  H+
                       ==
                    2.000  H2O
                  + 1.000  Al+++
B(OH)3(aq)                1.2388E-05    0    Total conc, molal
Ba++                      1.0000E-16    0    Total conc, molal
Ca++                      3.2437E-04    0    Total conc, molal
Cl-                       2.0140E-04    0    Total conc, molal
```

```
CrO4--                    1.0000E-16    0    Total conc, molal
Cu++                      1.0000E-16    0    Total conc, molal
F-                        1.1475E-04    0    Total conc, molal
Fe++                      0.0000E+00   19    Mineral equilibrium
                                                 Goethite

                        1.000  Goethite
                      +  2.000  H+
                           ==
                        1.500  H2O
                      +  1.000  Fe++
                      +  0.250  O2(g)
Gd+++                     1.0000E-16    0    Total conc, molal
H+                       -8.1000E+00   16    Log activity
HCO3-                    -3.0000E+00   21    Gas equilibrium
                                                 CO2(g)

                        1.000  CO2(g)
                      +  1.000  H2O
                           ==
                        1.000  H+
                      +  1.000  HCO3-
HCO3-                    -3.0000E+00   21    Gas equilibrium
HPO4--                    1.2607E-06    0    Total conc, molal
K+                        1.2891E-04    0    Total conc, molal
Li+                       6.9154E-06    0    Total conc, molal
Mg++                      8.2699E-05    0    Total conc, molal
Mn++                      0.0000E+00   19    Mineral equilibrium
                                                 Pyrolusite

                        1.000  Pyrolusite
                      +  2.000  H+
                           ==
                        1.000  H2O
                      +  1.000  Mn++
                      +  0.500  O2(g)
MoO4--                    1.0000E-16    0    Total conc, molal
NO3-                      1.4160E-04    0    Total conc, molal
Na+                       1.9922E-03    0    Total conc, molal
Ni++                      1.0000E-16    0    Total conc, molal
Np++++                    1.0000E-16    0    Total conc, molal
Pb++                      1.0000E-16    0    Total conc, molal
Pu++++                    1.0000E-16    0    Total conc, molal
SO4--                     1.9154E-04    0    Total conc, molal
SiO2(aq)                  1.0147E-03    0    Total conc, molal
TcO4-                     1.0000E-16    0    Total conc, molal
Ti(OH)4(aq)               1.0000E-16    0    Total conc, molal
UO2++                     1.0000E-16    0    Total conc, molal
Zr(OH)2++                 1.0000E-16    0    Total conc, molal
HS-                       0.0000E+00   30    Eliminated species
Acetic acid(aq)           0.0000E+00   30    Eliminated species
S2--                      0.0000E+00   30    Eliminated species
S2O3--                    0.0000E+00   30    Eliminated species
Acetone(aq)               0.0000E+00   30    Eliminated species
Benzene(aq)               0.0000E+00   30    Eliminated species
Butanoic acid(aq)         0.0000E+00   30    Eliminated species
CN-                       0.0000E+00   30    Eliminated species
ClO-                      0.0000E+00   30    Eliminated species
ClO2-                     0.0000E+00   30    Eliminated species
ClO3-                     0.0000E+00   30    Eliminated species
ClO4-                     0.0000E+00   30    Eliminated species
Cr++                      0.0000E+00   30    Eliminated species
Cr+++                     0.0000E+00   30    Eliminated species
CrO4---                   0.0000E+00   30    Eliminated species
Cu+                       0.0000E+00   30    Eliminated species
Ethanamine(aq)            0.0000E+00   30    Eliminated species
Ethane(aq)                0.0000E+00   30    Eliminated species
Ethanol(aq)               0.0000E+00   30    Eliminated species
Ethylene(aq)              0.0000E+00   30    Eliminated species
Ethyne(aq)                0.0000E+00   30    Eliminated species
Fe+++                     0.0000E+00   30    Eliminated species
Formic acid(aq)           0.0000E+00   30    Eliminated species
Glycine(aq)               0.0000E+00   30    Eliminated species
H2(aq)                    0.0000E+00   27    Dependent species
HSO5-                     0.0000E+00   30    Eliminated species
Methane(aq)               0.0000E+00   30    Eliminated species
Mn+++                     0.0000E+00   30    Eliminated species
MnO4--                    0.0000E+00   30    Eliminated species
N2(aq)                    0.0000E+00   30    Eliminated species
N3-                       0.0000E+00   30    Eliminated species
NO2-                      0.0000E+00   30    Eliminated species
NH3(aq)                   0.0000E+00   30    Eliminated species
Np+++                     0.0000E+00   30    Eliminated species
NpO2+                     0.0000E+00   30    Eliminated species
NpO2++                    0.0000E+00   30    Eliminated species
O2(aq)                    1.7501E-04    0    Total conc, molal
Pb++++                    0.0000E+00   30    Eliminated species
Pentanoic acid(aq)        0.0000E+00   30    Eliminated species
Phenol(aq)                0.0000E+00   30    Eliminated species
Propanoic acid(aq)        0.0000E+00   30    Eliminated species
Pu+++                     0.0000E+00   30    Eliminated species
PuO2+                     0.0000E+00   30    Eliminated species
PuO2++                    0.0000E+00   30    Eliminated species
```

```
S2O4--                    0.0000E+00   30    Eliminated species
S2O6--                    0.0000E+00   30    Eliminated species
S2O8--                    0.0000E+00   30    Eliminated species
S3--                      0.0000E+00   30    Eliminated species
S3O6--                    0.0000E+00   30    Eliminated species
S4--                      0.0000E+00   30    Eliminated species
S4O6--                    0.0000E+00   30    Eliminated species
S5--                      0.0000E+00   30    Eliminated species
S5O6--                    0.0000E+00   30    Eliminated species
SCN-                      0.0000E+00   30    Eliminated species
SO3--                     0.0000E+00   30    Eliminated species
Tc+++                     0.0000E+00   30    Eliminated species
TcO++                     0.0000E+00   30    Eliminated species
TcO4--                    0.0000E+00   30    Eliminated species
TcO4---                   0.0000E+00   30    Eliminated species
Toluene(aq)               0.0000E+00   30    Eliminated species
U+++                      0.0000E+00   30    Eliminated species
U++++                     0.0000E+00   30    Eliminated species
UO2+                      0.0000E+00   30    Eliminated species
Zr++++                    0.0000E+00   30    Eliminated species
o-Phthalate               0.0000E+00   30    Eliminated species


--- Optimization ended within requested limits ---


iter=   0
       del(                )=  0.00000E+00, delfnc=  0.00000E+00
      beta(conc    Pu++++  )=  9.15716E-02, betfnc=  0.00000E+00
        bbig=  9.15716E-02, ubbig= Pu++++
        bneg= -1.78863E-02, ubneg= HPO4--
        bgamx=  4.56553E-03, ubgamx= Al13O4(OH)24(7+)
        bsigmm=  1.34750E-03
        bxi= -7.57433E-03
        btfcnr=  0.00000E+00

iter=   1
       del(conc    UO2++   )=  3.32143E-02, delfnc=  0.00000E+00
      beta(conc    Pu++++  )=  6.65692E-03, betfnc=  9.27304E-01
        bbig=  6.65692E-03, ubbig= Pu++++
        bneg= -1.32894E-03, ubneg= UO2++
        bgamx=  5.28518E-03, ubgamx= Al13O4(OH)24(7+)
        bsigmm= -6.39222E-03
        bxi= -8.79162E-03
        btfcnr=  9.57497E-01

iter=   2
       del(conc    Pu++++  )= -3.33853E-03, delfnc=  8.99485E-01
      beta(conc    Pu++++  )=  5.61820E-05, betfnc=  9.91560E-01
        bbig=  5.61820E-05, ubbig= Pu++++
        bneg= -1.74583E-05, ubneg= UO2++
        bgamx=  6.57431E-05, ubgamx= Al13O4(OH)24(7+)
        bsigmm= -5.90316E-05
        bxi= -1.10034E-04
        btfcnr=  9.96700E-01

iter=   3
       del(conc    Pu++++  )= -3.40383E-05, delfnc=  9.89804E-01
      beta(conc    Np++++  )=  1.36455E-07, betfnc=  9.97571E-01
        bbig=  1.36455E-07, ubbig= Np++++
        bneg= -6.43568E-08, ubneg= UO2++
        bgamx=  2.31143E-07, ubgamx= Al13O4(OH)24(7+)
        bsigmm= -7.40745E-08
        bxi= -3.86891E-07
        btfcnr=  9.99821E-01

iter=   4
       del(conc    Np++++  )= -8.96378E-08, delfnc=  9.97367E-01
      beta(conc    Np++++  )=  4.60840E-10, betfnc=  9.96623E-01
        bbig=  4.60840E-10, ubbig= Np++++
        bneg= -2.19400E-10, ubneg= UO2++
        bgamx=  7.86105E-10, ubgamx= Al13O4(OH)24(7+)
        bsigmm= -2.39265E-10
        bxi= -1.31580E-09
        btfcnr=  9.99835E-01


Hybrid Newton-Raphson iteration converged in   4 steps.


                --- Summary of the Aqueous Solution ---

          --- Elemental Composition of the Aqueous Solution ---

  Element          mg/L          mg/kg          Moles/kg

     O         0.88826E+06    0.88826E+06    0.5551831255E+02
     Al        0.68884E-03    0.68884E-03    0.2552998884E-07
```

| | | | |
|---|---|---|---|
| B | 0.13393 | 0.13393 | 0.1238820353E-04 |
| Ba | 0.13733E-10 | 0.13733E-10 | 0.1000000000E-15 |
| Ca | 13.000 | 13.000 | 0.3243674988E-03 |
| Cl | 7.1400 | 7.1400 | 0.2013951078E-03 |
| Cr | 0.51996E-11 | 0.51996E-11 | 0.1000000000E-15 |
| Cu | 0.63546E-11 | 0.63546E-11 | 0.1000000000E-15 |
| F | 2.1800 | 2.1800 | 0.1147465104E-03 |
| Fe | 0.20104E-06 | 0.20104E-06 | 0.3599899806E-11 |
| Gd | 0.15725E-10 | 0.15725E-10 | 0.1000000000E-15 |
| H | 0.11190E+06 | 0.11190E+06 | 0.1110189628E+03 |
| C | 25.152 | 25.152 | 0.2094119146E-02 |
| P | 0.39048E-01 | 0.39048E-01 | 0.1260688563E-05 |
| K | 5.0400 | 5.0400 | 0.1289058665E-03 |
| Li | 0.48000E-01 | 0.48000E-01 | 0.6915430382E-05 |
| Mg | 2.0100 | 2.0100 | 0.8269903705E-04 |
| Mn | 0.16774E-10 | 0.16774E-10 | 0.3053263331E-15 |
| Mo | 0.95940E-11 | 0.95940E-11 | 0.1000000000E-15 |
| N | 1.9834 | 1.9834 | 0.1416016275E-03 |
| Na | 45.800 | 45.800 | 0.1992190534E-02 |
| Ni | 0.58690E-11 | 0.58690E-11 | 0.1000000000E-15 |
| Np | 0.23705E-10 | 0.23705E-10 | 0.1000000000E-15 |
| Pb | 0.20720E-10 | 0.20720E-10 | 0.1000000000E-15 |
| Pu | 0.24400E-10 | 0.24400E-10 | 0.1000000000E-15 |
| S | 6.1419 | 6.1419 | 0.1915397807E-03 |
| Si | 28.500 | 28.500 | 0.1014741004E-02 |
| Tc | 0.98000E-11 | 0.98000E-11 | 0.1000000000E-15 |
| Ti | 0.47880E-11 | 0.47880E-11 | 0.1000000000E-15 |
| U | 0.23803E-10 | 0.23803E-10 | 0.9999999998E-16 |
| Zr | 0.91224E-11 | 0.91224E-11 | 0.1000000000E-15 |

--- Elemental Composition as Strict Basis Species ---

| Species | mg/L | mg/kg | Moles/kg |
|---|---|---|---|
| H2O | 0.10002E+07 | 0.10002E+07 | 0.5551831255E+02 |
| Al+++ | 0.68884E-03 | 0.68884E-03 | 0.2552998884E-07 |
| B(OH)3(aq) | 0.76600 | 0.76600 | 0.1238820353E-04 |
| Ba++ | 0.13733E-10 | 0.13733E-10 | 0.1000000000E-15 |
| Ca++ | 13.000 | 13.000 | 0.3243674988E-03 |
| Cl- | 7.1400 | 7.1400 | 0.2013951078E-03 |
| CrO4-- | 0.11599E-10 | 0.11599E-10 | 0.1000000000E-15 |
| Cu++ | 0.63546E-11 | 0.63546E-11 | 0.1000000000E-15 |
| F- | 2.1800 | 2.1800 | 0.1147465104E-03 |
| Fe++ | 0.20104E-06 | 0.20104E-06 | 0.3599899806E-11 |
| Gd+++ | 0.15725E-10 | 0.15725E-10 | 0.1000000000E-15 |
| H+ | 0.11190E+06 | 0.11190E+06 | 0.1110189628E+03 |
| HCO3- | 127.78 | 127.78 | 0.2094119146E-02 |
| HPO4-- | 0.12100 | 0.12100 | 0.1260688563E-05 |
| K+ | 5.0400 | 5.0400 | 0.1289058665E-03 |
| Li+ | 0.48000E-01 | 0.48000E-01 | 0.6915430382E-05 |
| Mg++ | 2.0100 | 2.0100 | 0.8269903705E-04 |
| Mn++ | 0.16774E-10 | 0.16774E-10 | 0.3053263331E-15 |
| MoO4-- | 0.15994E-10 | 0.15994E-10 | 0.1000000000E-15 |
| NO3- | 8.7800 | 8.7800 | 0.1416016275E-03 |
| Na+ | 45.800 | 45.800 | 0.1992190534E-02 |
| Ni++ | 0.58690E-11 | 0.58690E-11 | 0.1000000000E-15 |
| Np++++ | 0.23705E-10 | 0.23705E-10 | 0.1000000000E-15 |
| Pb++ | 0.20720E-10 | 0.20720E-10 | 0.1000000000E-15 |
| Pu++++ | 0.24400E-10 | 0.24400E-10 | 0.1000000000E-15 |
| SO4-- | 18.400 | 18.400 | 0.1915397807E-03 |
| SiO2(aq) | 60.970 | 60.970 | 0.1014741004E-02 |
| TcO4- | 0.16200E-10 | 0.16200E-10 | 0.1000000000E-15 |
| Ti(OH)4(aq) | 0.11591E-10 | 0.11591E-10 | 0.1000000000E-15 |
| UO2++ | 0.27003E-10 | 0.27003E-10 | 0.9999999998E-16 |
| Zr(OH)2++ | 0.12524E-10 | 0.12524E-10 | 0.1000000000E-15 |

--- Equivalent Composition of the Aqueous Solution ---

--- Original Basis ---

| Species | Moles/kg H2O |
|---|---|
| H2O | 0.5551753773E+02 |
| Al+++ | 0.2552998884E-07 |
| B(OH)3(aq) | 0.1238820353E-04 |
| Ba++ | 0.1000000000E-15 |
| Ca++ | 0.3243674988E-03 |
| Cl- | 0.2013951078E-03 |
| CrO4-- | 0.1000000000E-15 |
| Cu++ | 0.1000000000E-15 |
| F- | 0.1147465104E-03 |
| Fe++ | 0.3599899806E-11 |
| Gd+++ | 0.1000000000E-15 |
| H+ | 0.1110189628E+03 |
| HCO3- | 0.2094119146E-02 |
| HPO4-- | 0.1260688563E-05 |
| K+ | 0.1289058665E-03 |
| Li+ | 0.6915430382E-05 |
| Mg++ | 0.8269903705E-04 |
| Mn++ | 0.3053263331E-15 |

| | |
|---|---|
| MoO4-- | 0.1000000000E-15 |
| NO3- | 0.1416016275E-03 |
| Na+ | 0.1992190534E-02 |
| Ni++ | 0.1000000000E-15 |
| Np++++ | 0.1000000000E-15 |
| Pb++ | 0.1000000000E-15 |
| Pu++++ | 0.1000000000E-15 |
| SO4-- | 0.1915397807E-03 |
| SiO2(aq) | 0.1014741004E-02 |
| TcO4- | 0.1000000000E-15 |
| Ti(OH)4(aq) | 0.1000000000E-15 |
| UO2++ | 0.9999999998E-16 |
| Zr(OH)2++ | 0.1000000000E-15 |
| O2(aq) | 0.1750065711E-03 |

--- Current Basis (cte) ---

| Species | Moles/kg H2O |
|---|---|
| H2O | 0.5551753773E+02 |
| Al+++ | 0.2552998884E-07 |
| B(OH)3(aq) | 0.1238820353E-04 |
| Ba++ | 0.1000000000E-15 |
| Ca++ | 0.3243674988E-03 |
| Cl- | 0.2013951078E-03 |
| CrO4-- | 0.1000000000E-15 |
| Cu++ | 0.1000000000E-15 |
| F- | 0.1147465104E-03 |
| Fe++ | 0.3599899806E-11 |
| Gd+++ | 0.1000000000E-15 |
| H+ | 0.1110189628E+03 |
| HCO3- | 0.2094119146E-02 |
| HPO4-- | 0.1260688563E-05 |
| K+ | 0.1289058665E-03 |
| Li+ | 0.6915430382E-05 |
| Mg++ | 0.8269903705E-04 |
| Mn++ | 0.3053263331E-15 |
| MoO4-- | 0.1000000000E-15 |
| NO3- | 0.1416016275E-03 |
| Na+ | 0.1992190534E-02 |
| Ni++ | 0.1000000000E-15 |
| Np++++ | 0.1000000000E-15 |
| Pb++ | 0.1000000000E-15 |
| Pu++++ | 0.1000000000E-15 |
| SO4-- | 0.1915397807E-03 |
| SiO2(aq) | 0.1014741004E-02 |
| TcO4- | 0.1000000000E-15 |
| Ti(OH)4(aq) | 0.1000000000E-15 |
| UO2++ | 0.9999999998E-16 |
| Zr(OH)2++ | 0.1000000000E-15 |
| O2(aq) | 0.1750065711E-03 |

Single ion activities and activity coefficients are here defined
with respect to the modified NBS pH scale

| | pH | Eh | pe |
|---|---|---|---|
| modified NBS pH scale | 8.0934 | 0.7399 | 1.2508E+01 |
| rational pH scale | 8.0672 | 0.7415 | 1.2534E+01 |

pHCl = 11.8173

Activity of water = 0.99989
Log activity of water = -0.00005

True osmotic coefficient= 0.97782
Stoichiometric osmotic coefficient= 0.96860

Sum of true molalities= 0.0064545085230
Sum of stoichiometric molalities= 0.0065159571521

True ionic strength= 0.0034850827817
Stoichiometric ionic strength= 0.0035568133199

--- Electrical Balance Totals ---

| | equiv/kg H2O |
|---|---|
| Sigma(mz) cations = | 0.2900307311E-02 |
| Sigma(mz) anions = | -0.2900307311E-02 |
| Total charge = | 0.5800614623E-02 |
| Mean charge = | 0.2900307311E-02 |
| Charge imbalance = | 0.6054184931E-14 |

Total charge = sigma(mz) cations + abs ( sigma(mz) anions )
Mean charge = 1/2 total charge

The electrical imbalance is

0.104E-09 per cent of the total charge
0.209E-09 per cent of the mean charge
0.209E-09 per cent of sigma(mz) cations
0.209E-09 per cent of abs ( sigma(mz) anions )

--- Electrical Balancing on H+ ---

Log activity

| | |
|---|---|
| input | -8.1000 |
| final | -8.0934 |
| adj | 0.65544E-02 |

--- Activity Ratios of Ions -----

| | | | |
|---|---|---|---|
| Log ( act(Al+++ | ) / act(H+)xx 3 ) = | 7.1604 |
| Log ( act(B(OH)3(aq) | ) = | -4.9392 |
| Log ( act(Ba++ | ) / act(H+)xx 2 ) = | 0.0736 |
| Log ( act(Ca++ | ) / act(H+)xx 2 ) = | 12.5667 |
| Log ( act(Cl- | ) x act(H+)xx 1 ) = | -11.8173 |
| Log ( act(CrO4-- | ) x act(H+)xx 2 ) = | -32.3064 |
| Log ( act(Cu++ | ) / act(H+)xx 2 ) = | -1.8577 |
| Log ( act(F- | ) x act(H+)xx 1 ) = | -12.0621 |
| Log ( act(Fe++ | ) / act(H+)xx 2 ) = | -7.0558 |
| Log ( act(Gd+++ | ) / act(H+)xx 3 ) = | 8.0308 |
| Log ( act(HCO3- | ) x act(H+)xx 1 ) = | -10.8136 |
| Log ( act(HPO4-- | ) x act(H+)xx 2 ) = | -22.3130 |
| Log ( act(K+ | ) / act(H+)xx 1 ) = | 4.1742 |
| Log ( act(Li+ | ) / act(H+)xx 1 ) = | 2.9044 |
| Log ( act(Mg++ | ) / act(H+)xx 2 ) = | 11.9746 |
| Log ( act(Mn++ | ) / act(H+)xx 2 ) = | 0.3625 |
| Log ( act(MoO4-- | ) x act(H+)xx 2 ) = | -32.2975 |
| Log ( act(NO3- | ) x act(H+)xx 1 ) = | -11.9706 |
| Log ( act(Na+ | ) / act(H+)xx 1 ) = | 5.3625 |
| Log ( act(Ni++ | ) / act(H+)xx 2 ) = | 0.0682 |
| Log ( act(Np++++ | ) / act(H+)xx 4 ) = | -17.8312 |
| Log ( act(Pb++ | ) / act(H+)xx 2 ) = | 0.0732 |
| Log ( act(Pu++++ | ) / act(H+)xx 4 ) = | -11.3212 |
| Log ( act(SO4-- | ) x act(H+)xx 2 ) = | -20.0353 |
| Log ( act(SiO2(aq) | ) = | -3.0005 |
| Log ( act(TcO4- | ) x act(H+)xx 1 ) = | -24.1207 |
| Log ( act(Ti(OH)4(aq) | ) = | -16.0000 |
| Log ( act(UO2++ | ) / act(H+)xx 2 ) = | -7.2520 |
| Log ( act(Zr(OH)2++ | ) / act(H+)xx 2 ) = | -14.7718 |
| Log ( act(HS- | ) x act(H+)xx 1 ) = | -151.1556 |
| Log ( act(Acetic acid(aq) | ) = | -156.4229 |
| Log ( act(S2-- | ) x act(H+)xx 2 ) = | -270.8430 |
| Log ( act(S2O3-- | ) x act(H+)xx 2 ) = | -166.4133 |
| Log ( act(Acetone(aq) | ) = | -309.9031 |
| Log ( act(Benzene(aq) | ) = | -575.3964 |
| Log ( act(Butanoic acid(aq) | ) = | -384.2223 |
| Log ( act(CN- | ) x act(H+)xx 1 ) = | -131.9391 |
| Log ( act(ClO- | ) x act(H+)xx 1 ) = | -28.7179 |
| Log ( act(ClO2- | ) x act(H+)xx 1 ) = | -38.5236 |
| Log ( act(ClO3- | ) x act(H+)xx 1 ) = | -34.4756 |
| Log ( act(ClO4- | ) x act(H+)xx 1 ) = | -34.7230 |
| Log ( act(Cr++ | ) / act(H+)xx 2 ) = | -50.3453 |
| Log ( act(Cr+++ | ) / act(H+)xx 3 ) = | -21.2234 |
| Log ( act(CrO4--- | ) x act(H+)xx 3 ) = | -51.1779 |
| Log ( act(Cu+ | ) / act(H+)xx 1 ) = | -19.7286 |
| Log ( act(Ethanamine(aq) | ) = | -301.3535 |
| Log ( act(Ethane(aq) | ) = | -263.5366 |
| Log ( act(Ethanol(aq) | ) = | -234.9739 |
| Log ( act(Ethylene(aq) | ) = | -239.4396 |
| Log ( act(Ethyne(aq) | ) = | -222.0158 |
| Log ( act(Fe+++ | ) / act(H+)xx 3 ) = | 0.5346 |
| Log ( act(Formic acid(aq) | ) = | -48.0669 |
| Log ( act(Glycine(aq) | ) = | -191.2754 |
| Log ( act(H2(aq) | ) = | -44.3075 |
| Log ( act(HSO5- | ) x act(H+)xx 1 ) = | -39.1210 |
| Log ( act(Methane(aq) | ) = | -147.7582 |
| Log ( act(Mn+++ | ) / act(H+)xx 3 ) = | -4.6181 |
| Log ( act(MnO4-- | ) x act(H+)xx 2 ) = | -35.6504 |
| Log ( act(N2(aq) | ) = | -22.6847 |
| Log ( act(N3- | ) x act(H+)xx 1 ) = | -110.8510 |
| Log ( act(NO2- | ) x act(H+)xx 1 ) = | -25.4063 |
| Log ( act(NH3(aq) | ) = | -66.8742 |
| Log ( act(Np+++ | ) / act(H+)xx 3 ) = | -35.9447 |
| Log ( act(NpO2+ | ) / act(H+)xx 1 ) = | -8.1380 |
| Log ( act(NpO2++ | ) / act(H+)xx 2 ) = | -8.4198 |
| Log ( act(O2(aq) | ) = | -3.7566 |
| Log ( act(Pb++++ | ) / act(H+)xx 4 ) = | -15.9061 |
| Log ( act(Pentanoic acid(aq) | ) = | -498.2650 |
| Log ( act(Phenol(aq) | ) = | -543.0653 |
| Log ( act(Propanoic acid(aq) | ) = | -269.9891 |
| Log ( act(Pu+++ | ) / act(H+)xx 3 ) = | -14.9287 |
| Log ( act(PuO2+ | ) / act(H+)xx 1 ) = | -9.2840 |

| | | | |
|---|---|---|---|
| Log ( act(PuO2++ | ) / act(H+)xx 2 ) = | -4.9932 |
| Log ( act(S2O4-- | ) x act(H+)xx 2 ) = | -153.1294 |
| Log ( act(S2O6-- | ) x act(H+)xx 2 ) = | -89.6913 |
| Log ( act(S2O8-- | ) x act(H+)xx 2 ) = | -64.3696 |
| Log ( act(S3-- | ) x act(H+)xx 2 ) = | -377.6734 |
| Log ( act(S3O6-- | ) x act(H+)xx 2 ) = | -199.0139 |
| Log ( act(S4-- | ) x act(H+)xx 2 ) = | -484.7238 |
| Log ( act(S4O6-- | ) x act(H+)xx 2 ) = | -292.4303 |
| Log ( act(S5-- | ) x act(H+)xx 2 ) = | -591.9941 |
| Log ( act(S5O6-- | ) x act(H+)xx 2 ) = | -414.7273 |
| Log ( act(SCN- | ) x act(H+)xx 1 ) = | -225.8363 |
| Log ( act(SO3-- | ) x act(H+)xx 2 ) = | -64.8605 |
| Log ( act(Tc+++ | ) / act(H+)xx 3 ) = | -68.1363 |
| Log ( act(TcO++ | ) / act(H+)xx 2 ) = | -52.9278 |
| Log ( act(TcO4-- | ) x act(H+)xx 2 ) = | -55.0408 |
| Log ( act(TcO4--- | ) x act(H+)xx 3 ) = | -85.6105 |
| Log ( act(Toluene(aq) | ) | ) = | -686.7123 |
| Log ( act(U+++ | ) / act(H+)xx 3 ) = | -69.3561 |
| Log ( act(U++++ | ) / act(H+)xx 4 ) = | -39.4018 |
| Log ( act(UO2+ | ) / act(H+)xx 1 ) = | -26.3693 |
| Log ( act(Zr++++ | ) / act(H+)xx 4 ) = | -14.5332 |
| Log ( act(o-Phthalate | ) x act(H+)xx 2 ) = | -602.3552 |

--- Distribution of Aqueous Species ---

| Species | Molality | Log molality | Log gamma | Log activity |
|---|---|---|---|---|
| HCO3- | 2.0278E-03 | -2.6930 | -0.0272 | -2.7202 |
| Na+ | 1.9840E-03 | -2.7025 | -0.0285 | -2.7310 |
| SiO2(aq) | 9.9889E-04 | -3.0005 | 0.0000 | -3.0005 |
| Ca++ | 3.0844E-04 | -3.5108 | -0.1093 | -3.6202 |
| Cl- | 2.0132E-04 | -3.6961 | -0.0277 | -3.7239 |
| SO4-- | 1.8291E-04 | -3.7378 | -0.1106 | -3.8484 |
| O2(aq) | 1.7501E-04 | -3.7569 | 0.0004 | -3.7566 |
| NO3- | 1.4143E-04 | -3.8495 | -0.0277 | -3.8772 |
| K+ | 1.2877E-04 | -3.8902 | -0.0290 | -3.9192 |
| F- | 1.1443E-04 | -3.9414 | -0.0272 | -3.9687 |
| Mg++ | 7.8233E-05 | -4.1066 | -0.1057 | -4.2123 |
| CO2(aq) | 3.3942E-05 | -4.4693 | 0.0004 | -4.4689 |
| HSiO3- | 1.4711E-05 | -4.8324 | -0.0272 | -4.8596 |
| CO3-- | 1.4226E-05 | -4.8469 | -0.1086 | -4.9556 |
| B(OH)3(aq) | 1.1503E-05 | -4.9392 | 0.0000 | -4.9392 |
| Li+ | 6.9096E-06 | -5.1605 | -0.0285 | -5.1891 |
| CaCO3(aq) | 5.6415E-06 | -5.2486 | 0.0000 | -5.2486 |
| CaHCO3+ | 5.4309E-06 | -5.2651 | -0.0285 | -5.2937 |
| NaHCO3(aq) | 5.0456E-06 | -5.2971 | 0.0000 | -5.2971 |
| CaSO4(aq) | 4.3911E-06 | -5.3574 | 0.0000 | -5.3574 |
| MgSO4(aq) | 2.2440E-06 | -5.6490 | 0.0000 | -5.6490 |
| NaSO4- | 1.8529E-06 | -5.7321 | -0.0272 | -5.7594 |
| MgHCO3+ | 1.3543E-06 | -5.8683 | -0.0285 | -5.8968 |
| OH- | 1.3367E-06 | -5.8740 | -0.0277 | -5.9017 |
| NaHSiO3(aq) | 1.1427E-06 | -5.9421 | 0.0000 | -5.9421 |
| HPO4-- | 9.6502E-07 | -6.0155 | -0.1106 | -6.1261 |
| BO2- | 8.6423E-07 | -6.0634 | -0.0272 | -6.0906 |
| MgCO3(aq) | 6.4721E-07 | -6.1890 | 0.0000 | -6.1890 |
| CaNO3+ | 1.7029E-07 | -6.7688 | -0.0285 | -6.7973 |
| MgF+ | 1.5848E-07 | -6.8000 | -0.0285 | -6.8286 |
| KSO4- | 1.3779E-07 | -6.8608 | -0.0272 | -6.8880 |
| CaF+ | 1.3225E-07 | -6.8786 | -0.0285 | -6.9071 |
| H2PO4- | 1.0306E-07 | -6.9869 | -0.0272 | -7.0141 |
| CaHPO4(aq) | 9.8576E-08 | -7.0062 | 0.0000 | -7.0062 |
| NaCO3- | 7.1627E-08 | -7.1449 | -0.0272 | -7.1721 |
| NaCl(aq) | 5.8635E-08 | -7.2318 | 0.0000 | -7.2318 |
| MgHPO4(aq) | 3.7293E-08 | -7.4284 | 0.0000 | -7.4284 |
| CaPO4- | 3.2556E-08 | -7.4874 | -0.0272 | -7.5146 |
| AlO2- | 2.4984E-08 | -7.6023 | -0.0272 | -7.6296 |
| NaF(aq) | 2.0079E-08 | -7.6972 | 0.0000 | -7.6972 |
| CaB(OH)4+ | 1.3816E-08 | -7.8596 | -0.0285 | -7.8881 |
| NaHPO4- | 1.2307E-08 | -7.9098 | -0.0272 | -7.9371 |
| MgPO4- | 1.1207E-08 | -7.9505 | -0.0272 | -7.9777 |
| CaCl+ | 9.7481E-09 | -8.0111 | -0.0285 | -8.0396 |
| MgCl+ | 9.0672E-09 | -8.0425 | -0.0285 | -8.0711 |
| H+ | 8.5657E-09 | -8.0672 | -0.0262 | -8.0934 |
| LiSO4- | 5.7514E-09 | -8.2402 | -0.0272 | -8.2675 |
| CaOH+ | 4.4851E-09 | -8.3482 | -0.0285 | -8.3768 |
| MgB(OH)4+ | 4.2047E-09 | -8.3763 | -0.0285 | -8.4048 |
| NaB(OH)4(aq) | 2.8134E-09 | -8.5508 | 0.0000 | -8.5508 |
| HF(aq) | 1.2764E-09 | -8.8940 | 0.0000 | -8.8940 |
| KCl(aq) | 7.2830E-10 | -9.1377 | 0.0000 | -9.1377 |
| KHPO4- | 5.7797E-10 | -9.2381 | -0.0272 | -9.2653 |
| HAlO2(aq) | 5.3383E-10 | -9.2726 | 0.0000 | -9.2726 |
| H6(H2SiO4)4-- | 4.5204E-10 | -9.3448 | -0.1106 | -9.4554 |
| NaOH(aq) | 3.6950E-10 | -9.4324 | 0.0000 | -9.4324 |
| H2SiO4-- | 2.1723E-10 | -9.6631 | -0.1106 | -9.7737 |
| HSO4- | 1.1601E-10 | -9.9355 | -0.0272 | -9.9627 |
| PO4--- | 7.8633E-11 | -10.1044 | -0.2500 | -10.3544 |
| KOH(aq) | 5.1780E-11 | -10.2858 | 0.0000 | -10.2858 |
| LiCl(aq) | 3.7634E-11 | -10.4244 | 0.0000 | -10.4244 |
| LiOH(aq) | 1.8379E-11 | -10.7357 | 0.0000 | -10.7357 |
| PO3F-- | 1.3237E-11 | -10.8782 | -0.1106 | -10.9888 |
| NaAlO2(aq) | 7.8734E-12 | -11.1038 | 0.0000 | -11.1038 |
| Fe(OH)3(aq) | 3.4233E-12 | -11.4655 | 0.0000 | -11.4655 |

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|---|---|---|---|---|
| Al(OH)2+ | 3.1687E-12 | -11.4991 | -0.0285 | -11.5276 |
| CaCl2(aq) | 1.9433E-12 | -11.7115 | 0.0000 | -11.7115 |
| AlF3(aq) | 4.7214E-13 | -12.3259 | 0.0000 | -12.3259 |
| AlF2+ | 3.7261E-13 | -12.4287 | -0.0285 | -12.4573 |
| HCl(aq) | 3.2561E-13 | -12.4873 | 0.0000 | -12.4873 |
| CaP2O7-- | 1.9591E-13 | -12.7079 | -0.1106 | -12.8186 |
| MgP2O7-- | 1.3149E-13 | -12.8811 | -0.1106 | -12.9917 |
| H3PO4(aq) | 1.1538E-13 | -12.9379 | 0.0000 | -12.9379 |
| Fe(OH)4- | 1.1352E-13 | -12.9449 | -0.0272 | -12.9722 |
| Fe(OH)2+ | 6.3035E-14 | -13.2004 | -0.0285 | -13.2289 |
| HNO3(aq) | 5.3317E-14 | -13.2731 | 0.0000 | -13.2731 |
| HF2- | 3.5265E-14 | -13.4527 | -0.0272 | -13.4799 |
| AlF4- | 1.3571E-14 | -13.8674 | -0.0272 | -13.8946 |
| AlOH++ | 1.3446E-14 | -13.8714 | -0.1122 | -13.9836 |
| AlF++ | 1.0559E-14 | -13.9764 | -0.1122 | -14.0886 |
| BF2(OH)2- | 4.7284E-15 | -14.3253 | -0.0272 | -14.3525 |
| HP2O7--- | 2.2609E-15 | -14.6457 | -0.2500 | -14.8958 |
| HPO3F- | 1.1077E-15 | -14.9556 | -0.0272 | -14.9828 |
| KHSO4(aq) | 8.9648E-16 | -15.0475 | 0.0000 | -15.0475 |
| H4(H2SiO4)4---- | 7.5326E-16 | -15.1231 | -0.4455 | -15.5685 |
| P2O7---- | 2.7995E-16 | -15.5529 | -0.4455 | -15.9984 |
| Mn++ | 1.9274E-16 | -15.7150 | -0.1093 | -15.8243 |
| AlHPO4+ | 1.5223E-16 | -15.8175 | -0.0285 | -15.8460 |
| Gd+++ | 1.0000E-16 | -16.0000 | -0.2495 | -16.2495 |
| Ti(OH)4(aq) | 1.0000E-16 | -16.0000 | 0.0000 | -16.0000 |
| TcO4- | 1.0000E-16 | -16.0000 | -0.0272 | -16.0272 |
| MoO4-- | 1.0000E-16 | -16.0000 | -0.1106 | -16.1106 |
| Zr(OH)4(aq) | 1.0000E-16 | -16.0000 | 0.0000 | -16.0000 |
| Ba++ | 9.9523E-17 | -16.0021 | -0.1112 | -16.1133 |
| Pb++ | 9.9443E-17 | -16.0024 | -0.1112 | -16.1137 |
| Ni++ | 9.8519E-17 | -16.0065 | -0.1122 | -16.1187 |
| CrO4-- | 9.7965E-17 | -16.0089 | -0.1106 | -16.1195 |
| CuCO3(aq) | 9.0179E-17 | -16.0449 | 0.0000 | -16.0449 |
| PuO2(CO3)2-- | 8.5949E-17 | -16.0658 | -0.1106 | -16.1764 |
| NaHP2O7-- | 7.6537E-17 | -16.1161 | -0.1106 | -16.2267 |
| NaP2O7--- | 6.4661E-17 | -16.1894 | -0.2500 | -16.4394 |
| NpO2+ | 6.2676E-17 | -16.2029 | -0.0285 | -16.2314 |
| H2P2O7-- | 5.5273E-17 | -16.2575 | -0.1106 | -16.3681 |
| MnCO3(aq) | 5.4967E-17 | -16.2599 | 0.0000 | -16.2599 |
| UO2(CO3)3---- | 4.9674E-17 | -16.3039 | -0.4455 | -16.7494 |
| MnO4- | 4.8859E-17 | -16.3111 | -0.0272 | -16.3383 |
| UO2(CO3)2-- | 4.6937E-17 | -16.3285 | -0.1106 | -16.4391 |
| CaH2PO4+ | 3.8802E-17 | -16.4112 | -0.0285 | -16.4397 |
| NpO2CO3- | 2.7557E-17 | -16.5598 | -0.0272 | -16.5870 |
| MgH2PO4+ | 1.8059E-17 | -16.7433 | -0.0285 | -16.7718 |
| Al+++ | 1.2977E-17 | -16.8868 | -0.2331 | -17.1199 |
| NpO2OH(aq) | 9.1616E-18 | -17.0380 | 0.0000 | -17.0380 |
| PuO2F3- | 7.1973E-18 | -17.1428 | -0.0272 | -17.1701 |
| Na2P2O7-- | 6.9220E-18 | -17.1598 | -0.1106 | -17.2704 |
| CuOH+ | 6.1629E-18 | -17.2102 | -0.0285 | -17.2387 |
| NO2- | 5.1800E-18 | -17.2857 | -0.0272 | -17.3129 |
| MnSO4(aq) | 4.7883E-18 | -17.3198 | 0.0000 | -17.3198 |
| PuO2+ | 4.4780E-18 | -17.3489 | -0.0285 | -17.3774 |
| KP2O7--- | 4.4678E-18 | -17.3499 | -0.2500 | -17.5999 |
| H2F2(aq) | 4.4033E-18 | -17.3562 | 0.0000 | -17.3562 |
| UO2(OH)2(aq) | 2.7121E-18 | -17.5667 | 0.0000 | -17.5667 |
| MnHCO3+ | 2.3205E-18 | -17.6344 | -0.0285 | -17.6629 |
| Cu(CO3)2-- | 2.1715E-18 | -17.6632 | -0.1106 | -17.7739 |
| HCrO4- | 2.0353E-18 | -17.6914 | -0.0272 | -17.7186 |
| FeOH++ | 1.8616E-18 | -17.7301 | -0.1122 | -17.8423 |
| NiSO4(aq) | 1.4408E-18 | -17.8414 | 0.0000 | -17.8414 |
| AlSO4+ | 1.1755E-18 | -17.9298 | -0.0285 | -17.9583 |
| Cu++ | 1.1606E-18 | -17.9353 | -0.1093 | -18.0446 |
| PuO2F2(aq) | 7.0715E-19 | -18.1505 | 0.0000 | -18.1505 |
| Pu(OH)5- | 6.5918E-19 | -18.1810 | -0.0272 | -18.2082 |
| PuO2F4-- | 6.5872E-19 | -18.1813 | -0.1106 | -18.2919 |
| MnOH+ | 5.1001E-19 | -18.2924 | -0.0285 | -18.3209 |
| MnF+ | 4.6293E-19 | -18.3345 | -0.0285 | -18.3630 |
| UO2(OH)3- | 4.4333E-19 | -18.3533 | -0.0272 | -18.3805 |
| MnHPO4(aq) | 4.2617E-19 | -18.3704 | 0.0000 | -18.3704 |
| PbCl+ | 4.2501E-19 | -18.3716 | -0.0285 | -18.4001 |
| BaCO3(aq) | 3.7716E-19 | -18.4235 | 0.0000 | -18.4235 |
| CuPO4- | 3.0071E-19 | -18.5218 | -0.0272 | -18.5491 |
| NpO2(CO3)3---- | 2.3560E-19 | -18.6278 | -0.4455 | -19.0733 |
| PuO2OH+ | 2.0135E-19 | -18.6960 | -0.0285 | -18.7246 |
| UO2CO3(aq) | 1.8662E-19 | -18.7290 | 0.0000 | -18.7290 |
| NpO2HPO4- | 1.4781E-19 | -18.8303 | -0.0272 | -18.8575 |
| NpO2(CO3)2--- | 1.2808E-19 | -18.8925 | -0.2500 | -19.1425 |
| PuO2OH(aq) | 1.1183E-19 | -18.9514 | 0.0000 | -18.9514 |
| FeCO3+ | 1.1149E-19 | -18.9528 | -0.0285 | -18.9813 |
| MnPO4- | 1.0926E-19 | -18.9616 | -0.0272 | -18.9888 |
| BaNO3+ | 8.6700E-20 | -19.0620 | -0.0285 | -19.0905 |
| PbHPO4(aq) | 7.2486E-20 | -19.1397 | 0.0000 | -19.1397 |
| NpO2F(aq) | 6.3083E-20 | -19.2001 | 0.0000 | -19.2001 |
| MnCl+ | 6.0482E-20 | -19.2184 | -0.0285 | -19.2469 |
| PbF+ | 5.9511E-20 | -19.2254 | -0.0285 | -19.2539 |
| MnO4-- | 4.4367E-20 | -19.3529 | -0.1106 | -19.4636 |
| UO2PO4- | 4.3202E-20 | -19.3645 | -0.0272 | -19.3917 |
| PuO2F+ | 3.5253E-20 | -19.4528 | -0.0285 | -19.4813 |
| MnNO3+ | 3.3651E-20 | -19.4730 | -0.0285 | -19.5015 |
| NiNO3+ | 2.7079E-20 | -19.5674 | -0.0285 | -19.5959 |
| NpO2SO4- | 2.2254E-20 | -19.6526 | -0.0272 | -19.6798 |
| FeHPO4+ | 2.1712E-20 | -19.6633 | -0.0285 | -19.6918 |

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| BF3OH- | 1.5348E-20 | -19.8139 | -0.0272 | -19.8412 |
| CuCO3(OH)2-- | 1.5206E-20 | -19.8180 | -0.1106 | -19.9286 |
| Al(SO4)2- | 1.2898E-20 | -19.8895 | -0.0272 | -19.9167 |
| Ni(OH)2(aq) | 1.1964E-20 | -19.9221 | 0.0000 | -19.9221 |
| CuHPO4(aq) | 7.7497E-21 | -20.1107 | 0.0000 | -20.1107 |
| BaF+ | 5.7976E-21 | -20.2368 | -0.0285 | -20.2653 |
| BaCl+ | 4.9392E-21 | -20.3063 | -0.0285 | -20.3349 |
| NpO2Cl(aq) | 4.4129E-21 | -20.3553 | 0.0000 | -20.3553 |
| NpO2(CO3)2-- | 3.9161E-21 | -20.4071 | -0.1106 | -20.5178 |
| B2O(OH)5- | 3.6074E-21 | -20.4428 | -0.0272 | -20.4700 |
| UO2OH+ | 2.9904E-21 | -20.5243 | -0.0285 | -20.5528 |
| ClO- | 2.5279E-21 | -20.5972 | -0.0272 | -20.6245 |
| BaB(OH)4+ | 1.8545E-21 | -20.7318 | -0.0285 | -20.7603 |
| CuF+ | 1.6414E-21 | -20.7848 | -0.0285 | -20.8133 |
| NiCl+ | 1.5480E-21 | -20.8102 | -0.0285 | -20.8388 |
| Pu(OH)4(aq) | 1.4494E-21 | -20.8388 | 0.0000 | -20.8388 |
| H2SO4(aq) | 8.7867E-22 | -21.0562 | 0.0000 | -21.0562 |
| PuO2++ | 8.5539E-22 | -21.0678 | -0.1122 | -21.1801 |
| UO2HPO4(aq) | 7.4961E-22 | -21.1252 | 0.0000 | -21.1252 |
| HClO(aq) | 7.1007E-22 | -21.1487 | 0.0000 | -21.1487 |
| CuCl+ | 4.9778E-22 | -21.3030 | -0.0285 | -21.3315 |
| MnH2PO4+ | 3.4678E-22 | -21.4599 | -0.0285 | -21.4885 |
| BaOH+ | 3.4563E-22 | -21.4614 | -0.0285 | -21.4899 |
| PbCl2(aq) | 2.7620E-22 | -21.5588 | 0.0000 | -21.5588 |
| NpO2OH+ | 2.0667E-22 | -21.6847 | -0.0285 | -21.7133 |
| PuO2SO4(aq) | 1.7273E-22 | -21.7626 | 0.0000 | -21.7626 |
| Mn(OH)2(aq) | 1.4536E-22 | -21.8375 | 0.0000 | -21.8375 |
| NpO2(CO3)3(5-) | 1.2557E-22 | -21.9011 | -0.6970 | -22.5981 |
| HO2- | 1.0460E-22 | -21.9805 | -0.0272 | -22.0077 |
| H3P2O7- | 8.1522E-23 | -22.0887 | -0.0272 | -22.1159 |
| HNO2(aq) | 6.5203E-23 | -22.1857 | 0.0000 | -22.1857 |
| H2PO3F(aq) | 5.3662E-23 | -22.2703 | 0.0000 | -22.2703 |
| UO2F+ | 4.6900E-23 | -22.3288 | -0.0285 | -22.3573 |
| PbF2(aq) | 3.6493E-23 | -22.4378 | 0.0000 | -22.4378 |
| NpO2HPO4(aq) | 2.9327E-23 | -22.5327 | 0.0000 | -22.5327 |
| N2(aq) | 2.0667E-23 | -22.6847 | 0.0000 | -22.6847 |
| Ni(OH)3- | 1.5977E-23 | -22.7965 | -0.0272 | -22.8237 |
| UO2F2(aq) | 1.4591E-23 | -22.8359 | 0.0000 | -22.8359 |
| Mn(NO3)2(aq) | 1.0502E-23 | -22.9787 | 0.0000 | -22.9787 |
| Fe++ | 7.3554E-24 | -23.1334 | -0.1093 | -23.2427 |
| FeHCO3+ | 6.1038E-24 | -23.2144 | -0.0285 | -23.2429 |
| Zr(OH)3+ | 5.4004E-24 | -23.2676 | -0.0285 | -23.2961 |
| CuH2PO4+ | 5.3674E-24 | -23.2702 | -0.0285 | -23.2988 |
| FeF2+ | 4.9574E-24 | -23.3047 | -0.0285 | -23.3333 |
| UO2++ | 4.7134E-24 | -23.3267 | -0.1122 | -23.4389 |
| FeF++ | 3.4223E-24 | -23.4657 | -0.1122 | -23.5779 |
| FeCO3(aq) | 3.4019E-24 | -23.4683 | 0.0000 | -23.4683 |
| Fe+++ | 3.0717E-24 | -23.5126 | -0.2331 | -23.7457 |
| Ni(NO3)2(aq) | 2.0741E-24 | -23.6832 | 0.0000 | -23.6832 |
| Mg4(OH)4++++ | 1.6342E-24 | -23.7867 | -0.4389 | -24.2256 |
| NpO2F+ | 1.1304E-24 | -23.9468 | -0.0285 | -23.9753 |
| UO2(OH)4-- | 1.0380E-24 | -23.9838 | -0.1106 | -24.0944 |
| Np(OH)5- | 9.7547E-25 | -24.0108 | -0.0272 | -24.0380 |
| PuO2H2PO4+ | 6.8366E-25 | -24.1652 | -0.0285 | -24.1937 |
| UO2SO4(aq) | 6.0678E-25 | -24.2170 | 0.0000 | -24.2170 |
| NpO2++ | 3.2031E-25 | -24.4944 | -0.1122 | -24.6066 |
| Pu(HPO4)4---- | 3.1108E-25 | -24.5071 | -0.4455 | -24.9526 |
| UO2F3- | 2.9036E-25 | -24.5371 | -0.0272 | -24.5643 |
| FeOH+ | 2.3944E-25 | -24.6208 | -0.0285 | -24.6493 |
| Pu(OH)3+ | 2.1514E-25 | -24.6673 | -0.0285 | -24.6958 |
| NpO2F2(aq) | 1.8031E-25 | -24.7440 | 0.0000 | -24.7440 |
| FeSO4(aq) | 1.2850E-25 | -24.8911 | 0.0000 | -24.8911 |
| CuO2-- | 9.7715E-26 | -25.0100 | -0.1106 | -25.1207 |
| PuO2Cl+ | 8.2454E-26 | -25.0838 | -0.0285 | -25.1123 |
| NpO2SO4(aq) | 6.9980E-26 | -25.1550 | 0.0000 | -25.1550 |
| NiP2O7-- | 6.9343E-26 | -25.1590 | -0.1106 | -25.2696 |
| Al2(OH)2++++ | 4.9617E-26 | -25.3044 | -0.4389 | -25.7433 |
| CuCl2(aq) | 4.6361E-26 | -25.3338 | 0.0000 | -25.3338 |
| PbCl3- | 2.6921E-26 | -25.5699 | -0.0272 | -25.5971 |
| FeSO4+ | 2.3015E-26 | -25.6380 | -0.0285 | -25.6665 |
| FePO4- | 2.2912E-26 | -25.6399 | -0.0272 | -25.6672 |
| Mn(OH)3- | 1.8000E-26 | -25.7447 | -0.0272 | -25.7720 |
| FeHPO4(aq) | 1.7030E-26 | -25.7688 | 0.0000 | -25.7688 |
| FeF+ | 1.5036E-26 | -25.8229 | -0.0285 | -25.8514 |
| UO2H2PO4+ | 1.1016E-26 | -25.9580 | -0.0285 | -25.9865 |
| ClO3- | 4.4164E-27 | -26.3549 | -0.0272 | -26.3822 |
| FeNO3++ | 3.0853E-27 | -26.5107 | -0.1122 | -26.6229 |
| ClO4- | 2.5014E-27 | -26.6018 | -0.0277 | -26.6296 |
| CrO4--- | 2.2517E-27 | -26.6475 | -0.2500 | -26.8975 |
| UO2Cl+ | 1.0543E-27 | -26.9770 | -0.0285 | -27.0055 |
| UO2NO3+ | 9.8390E-28 | -27.0071 | -0.0285 | -27.0356 |
| UO2(SO4)2-- | 9.0275E-28 | -27.0444 | -0.1106 | -27.1550 |
| BF4- | 8.6715E-28 | -27.0619 | -0.0272 | -27.0891 |
| FeCl+ | 7.9699E-28 | -27.0985 | -0.0285 | -27.1271 |
| H2CrO4(aq) | 7.3886E-28 | -27.1314 | 0.0000 | -27.1314 |
| NiHP2O7- | 6.7758E-28 | -27.1690 | -0.0272 | -27.1963 |
| MnCl3- | 4.9994E-28 | -27.3011 | -0.0272 | -27.3283 |
| Np(OH)4(aq) | 3.7034E-28 | -27.4314 | 0.0000 | -27.4314 |
| Fe(OH)2(aq) | 2.2084E-28 | -27.6559 | 0.0000 | -27.6559 |
| UO2F4-- | 2.1766E-28 | -27.6622 | -0.1106 | -27.7728 |
| Cu+ | 1.6088E-28 | -27.7935 | -0.0285 | -27.8220 |
| Np(HPO4)5(6-) | 1.4761E-28 | -27.8309 | -1.0045 | -28.8354 |
| AlH2PO4++ | 7.4603E-29 | -28.1272 | -0.1122 | -28.2395 |

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| FeCl++ | 6.7894E-29 | -28.1682 | -0.1122 | -28.2804 |
| Fe(SO4)2- | 6.2867E-29 | -28.2016 | -0.0272 | -28.2288 |
| (UO2)2CO3(OH)3- | 3.8017E-29 | -28.4200 | -0.0272 | -28.4472 |
| CrO3Cl- | 3.3418E-29 | -28.4760 | -0.0272 | -28.5032 |
| NpO2Cl+ | 3.1479E-29 | -28.5020 | -0.0285 | -28.5305 |
| Pu(HPO4)3-- | 3.1425E-29 | -28.5027 | -0.1106 | -28.6133 |
| Mn+++ | 2.2440E-29 | -28.6490 | -0.2495 | -28.8985 |
| H4P2O7(aq) | 1.9971E-29 | -28.6996 | 0.0000 | -28.6996 |
| PbH2PO4+ | 1.5680E-29 | -28.8047 | -0.0285 | -28.8332 |
| FeCl2+ | 9.2274E-30 | -29.0349 | -0.0285 | -29.0634 |
| PbCl4-- | 3.9123E-30 | -29.4076 | -0.1106 | -29.5182 |
| Pu(OH)2++ | 1.9077E-30 | -29.7195 | -0.1122 | -29.8317 |
| NpO2H2PO4(aq) | 1.4095E-30 | -29.8510 | 0.0000 | -29.8510 |
| Fe(OH)3- | 1.1606E-30 | -29.9353 | -0.0272 | -29.9625 |
| UO2(H2PO4)2(aq) | 7.3412E-31 | -30.1342 | 0.0000 | -30.1342 |
| ClO2- | 3.9543E-31 | -30.4029 | -0.0272 | -30.4302 |
| CuCl2- | 3.7905E-31 | -30.4213 | -0.0272 | -30.4485 |
| Zr(OH)2++ | 1.4241E-31 | -30.8465 | -0.1122 | -30.9587 |
| HSO5- | 9.9930E-32 | -31.0003 | -0.0272 | -31.0275 |
| Np(HPO4)4---- | 8.6335E-32 | -31.0638 | -0.4455 | -31.5093 |
| Mn2(OH)3+ | 5.7548E-32 | -31.2400 | -0.0285 | -31.2685 |
| Mn(OH)4-- | 2.2901E-32 | -31.6401 | -0.1106 | -31.7508 |
| Np(OH)3+ | 2.0124E-32 | -31.6963 | -0.0285 | -31.7248 |
| UO2Cl2(aq) | 9.7298E-33 | -32.0119 | 0.0000 | -32.0119 |
| Pu(HPO4)2(aq) | 7.9642E-33 | -32.0989 | 0.0000 | -32.0989 |
| Al3(OH)4(5+) | 6.4955E-33 | -32.1874 | -0.6791 | -32.8665 |
| SiF6-- | 1.5826E-33 | -32.8006 | -0.1106 | -32.9113 |
| FeCl2(aq) | 7.1693E-34 | -33.1445 | 0.0000 | -33.1445 |
| CuCl3-- | 5.5710E-34 | -33.2541 | -0.1106 | -33.3647 |
| CuNO2+ | 4.9091E-34 | -33.3090 | -0.0285 | -33.3375 |
| FeH2PO4++ | 2.0747E-34 | -33.6830 | -0.1122 | -33.7953 |
| Cr2O7-- | 1.5991E-34 | -33.7961 | -0.1106 | -33.9067 |
| Fe2(OH)2++++ | 1.5284E-34 | -33.8158 | -0.4389 | -34.2547 |
| Mn2OH+++ | 1.3621E-34 | -33.8658 | -0.2495 | -34.1153 |
| (PuO2)2(OH)2++ | 4.7457E-35 | -34.3237 | -0.1122 | -34.4359 |
| UO2H3PO4++ | 4.7018E-35 | -34.3277 | -0.1122 | -34.4400 |
| UO2+ | 3.6792E-35 | -34.4342 | -0.0285 | -34.4628 |
| Ni2OH+++ | 2.5438E-35 | -34.5945 | -0.2495 | -34.8440 |
| FeH2PO4+ | 1.8462E-35 | -34.7337 | -0.0285 | -34.7622 |
| Np(HPO4)3-- | 8.4604E-36 | -35.0726 | -0.1106 | -35.1832 |
| HClO2(aq) | 4.4279E-36 | -35.3538 | 0.0000 | -35.3538 |
| Np(CO3)5(6-) | 2.0975E-36 | -35.6783 | -1.0045 | -36.6828 |
| PuOH+++ | 1.3902E-36 | -35.8569 | -0.2495 | -36.1064 |
| PuF2++ | 7.5839E-37 | -36.1201 | -0.1122 | -36.2323 |
| (UO2)2(OH)2++ | 6.1185E-37 | -36.2134 | -0.1122 | -36.3256 |
| ZrF5- | 3.8611E-37 | -36.4133 | -0.0272 | -36.4405 |
| NpO2H2PO4+ | 3.1795E-37 | -36.4976 | -0.0285 | -36.5262 |
| ZrF6-- | 2.5730E-37 | -36.5896 | -0.1106 | -36.7002 |
| PuHPO4++ | 2.0019E-37 | -36.6986 | -0.1122 | -36.8108 |
| Np(OH)2++ | 1.9680E-37 | -36.7060 | -0.1122 | -36.8182 |
| Fe(OH)4-- | 1.7437E-37 | -36.7585 | -0.1106 | -36.8691 |
| ZrF4(aq) | 1.4436E-37 | -36.8405 | 0.0000 | -36.8405 |
| UO2(H2PO4)(H3PO4)+ | 6.4691E-38 | -37.1892 | -0.0285 | -37.2177 |
| CuCl4-- | 4.0037E-38 | -37.3975 | -0.1106 | -37.5082 |
| ZrF3+ | 3.1243E-38 | -37.5053 | -0.0285 | -37.5338 |
| FeNO2++ | 1.5981E-38 | -37.7964 | -0.1122 | -37.9086 |
| HTcO4- | 6.1232E-39 | -38.2130 | -0.0272 | -38.2402 |
| ZrOH+++ | 3.0311E-39 | -38.5184 | -0.2495 | -38.7679 |
| TcO4-- | 1.8060E-39 | -38.7433 | -0.1106 | -38.8539 |
| Np(HPO4)2(aq) | 1.7493E-39 | -38.7571 | 0.0000 | -38.7571 |
| PuF+++ | 1.1113E-39 | -38.9542 | -0.2495 | -39.2037 |
| Pu+++ | 1.0975E-39 | -38.9596 | -0.2495 | -39.2091 |
| PuOH++ | 1.0679E-39 | -38.9715 | -0.1122 | -39.0837 |
| Cr(OH)2+ | 1.0270E-39 | -38.9884 | -0.0285 | -39.0170 |
| ZrF2++ | 1.0130E-39 | -38.9944 | -0.1122 | -39.1066 |
| Cr(OH)3(aq) | 5.9764E-40 | -39.2236 | 0.0000 | -39.2236 |
| (NpO2)2(OH)2++ | 4.8498E-40 | -39.3143 | -0.1122 | -39.4265 |
| FeCl4- | 3.9452E-40 | -39.4039 | -0.0272 | -39.4312 |
| PuSO4+ | 2.9145E-40 | -39.5354 | -0.0285 | -39.5640 |
| FeCl4-- | 1.1816E-40 | -39.9275 | -0.1106 | -40.0381 |
| Cr(OH)4- | 3.1409E-41 | -40.5029 | -0.0272 | -40.5302 |
| Pu(SO4)2- | 2.7630E-41 | -40.5586 | -0.0272 | -40.5858 |
| Pu(SO4)2(aq) | 7.1423E-42 | -41.1462 | 0.0000 | -41.1462 |
| (UO2)2OH+++ | 5.7268E-42 | -41.2421 | -0.2495 | -41.4916 |
| UO2(CO3)3(5-) | 5.3683E-42 | -41.2702 | -0.6970 | -41.9671 |
| CrOH++ | 5.0335E-42 | -41.2981 | -0.1122 | -41.4104 |
| PuSO4++ | 2.1870E-42 | -41.6602 | -0.1122 | -41.7724 |
| ZrF+++ | 9.0644E-43 | -42.0427 | -0.2495 | -42.2921 |
| NpF2++ | 2.3437E-43 | -42.6301 | -0.1122 | -42.7423 |
| NpOH+++ | 1.3737E-43 | -42.8621 | -0.2495 | -43.1116 |
| Pu++++ | 5.5452E-44 | -43.2561 | -0.4389 | -43.6950 |
| NpHPO4++ | 4.7990E-44 | -43.3188 | -0.1122 | -43.4311 |
| PuH2PO4++ | 2.3191E-44 | -43.6347 | -0.1122 | -43.7469 |
| Formate | 1.9986E-44 | -43.6993 | -0.0272 | -43.7265 |
| U(OH)4(aq) | 1.0665E-44 | -43.9720 | 0.0000 | -43.9720 |
| H2(aq) | 4.9213E-45 | -44.3079 | 0.0004 | -44.3075 |
| Fe3(OH)4(5+) | 3.2773E-45 | -44.4845 | -0.6791 | -45.1636 |
| (UO2)3(OH)7- | 2.0584E-45 | -44.6865 | -0.0272 | -44.7137 |
| (PuO2)3(OH)5+ | 1.9968E-45 | -44.6997 | -0.0285 | -44.7282 |
| (UO2)3(CO3)6(6-) | 7.3652E-46 | -45.1328 | -1.0045 | -46.1373 |
| NpF+++ | 5.9681E-46 | -45.2242 | -0.2495 | -45.4737 |
| Cr+++ | 5.5685E-46 | -45.2543 | -0.2495 | -45.5037 |
| (UO2)3(OH)5+ | 3.9142E-46 | -45.4074 | -0.0285 | -45.4359 |

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|---|---|---|---|---|
| H2TcO4(aq) | 9.2068E-47 | -46.0359 | 0.0000 | -46.0359 |
| Zr++++ | 3.4035E-47 | -46.4681 | -0.4389 | -46.9070 |
| ZrSO4++ | 9.1887E-48 | -47.0367 | -0.1122 | -47.1490 |
| Pb++++ | 1.4421E-48 | -47.8410 | -0.4389 | -48.2799 |
| Np(SO4)2(aq) | 9.9598E-49 | -48.0018 | 0.0000 | -48.0018 |
| Formic acid(aq) | 8.5714E-49 | -48.0669 | 0.0000 | -48.0669 |
| S2O8-- | 8.4705E-49 | -48.0721 | -0.1106 | -48.1827 |
| Zr(SO4)2(aq) | 4.9289E-49 | -48.3072 | 0.0000 | -48.3072 |
| NpSO4++ | 3.6212E-49 | -48.4411 | -0.1122 | -48.5534 |
| SO3-- | 2.7355E-49 | -48.5630 | -0.1106 | -48.6736 |
| CrCl++ | 5.4402E-50 | -49.2644 | -0.1122 | -49.3766 |
| UO2ClO3+ | 5.0048E-50 | -49.3006 | -0.0285 | -49.3291 |
| HSO3- | 2.9214E-50 | -49.5344 | -0.0272 | -49.5616 |
| Cu(NO2)2(aq) | 2.2887E-50 | -49.6404 | 0.0000 | -49.6404 |
| (UO2)3(OH)4++ | 1.7384E-50 | -49.7599 | -0.1122 | -49.8721 |
| Np++++ | 1.7137E-50 | -49.7661 | -0.4389 | -50.2050 |
| (UO2)3(OH)5CO2+ | 5.5699E-51 | -50.2542 | -0.0285 | -50.2827 |
| PuF3+ | 5.3399E-51 | -50.2725 | -0.0285 | -50.3010 |
| (UO2)3O(OH)2(HCO3)+ | 4.4916E-51 | -50.3476 | -0.0285 | -50.3761 |
| CO(aq) | 1.9289E-51 | -50.7147 | 0.0000 | -50.7147 |
| (NpO2)3(OH)5+ | 1.4982E-51 | -50.8244 | -0.0285 | -50.8530 |
| Zr(SO4)3-- | 9.1030E-52 | -51.0408 | -0.1106 | -51.1514 |
| CrCl2+ | 1.7245E-53 | -52.7633 | -0.0285 | -52.7919 |
| NpCl+++ | 3.3162E-54 | -53.4794 | -0.2495 | -53.7288 |
| PuF4(aq) | 4.2692E-56 | -55.3697 | 0.0000 | -55.3697 |
| H2SO3(aq) | 2.2528E-56 | -55.6473 | 0.0000 | -55.6473 |
| SO2(aq) | 1.6039E-56 | -55.7948 | 0.0000 | -55.7948 |
| U(CO3)4---- | 8.1177E-57 | -56.0906 | -0.4455 | -56.5361 |
| TcO(OH)2(aq) | 5.6235E-57 | -56.2500 | 0.0000 | -56.2500 |
| NpCl2++ | 2.2884E-58 | -57.6405 | -0.1122 | -57.7527 |
| NpOH++ | 9.5620E-60 | -59.0195 | -0.1122 | -59.1317 |
| (UO2)4(OH)7+ | 9.4614E-60 | -59.0240 | -0.0285 | -59.0526 |
| Ni4(OH)4++++ | 4.5435E-60 | -59.3426 | -0.4389 | -59.7815 |
| Np+++ | 1.0578E-60 | -59.9756 | -0.2495 | -60.2251 |
| Al13O4(OH)24(7+) | 1.0693E-61 | -60.9709 | -1.3294 | -62.3003 |
| TcO4--- | 8.3149E-62 | -61.0801 | -0.2500 | -61.3302 |
| U(CO3)5(6-) | 2.3888E-62 | -61.6218 | -1.0045 | -62.6263 |
| TcOOH+ | 7.4428E-63 | -62.1283 | -0.0285 | -62.1568 |
| UF3+ | 6.7221E-63 | -62.1725 | -0.0285 | -62.2010 |
| UF4(aq) | 6.1733E-63 | -62.2095 | 0.0000 | -62.2095 |
| UF2++ | 3.5462E-64 | -63.4502 | -0.1122 | -63.5625 |
| UOH+++ | 1.0473E-64 | -63.9799 | -0.2495 | -64.2294 |
| UF5- | 1.6568E-65 | -64.7807 | -0.0272 | -64.8079 |
| UO2SO3(aq) | 4.3725E-66 | -65.3593 | 0.0000 | -65.3593 |
| NH4+ | 2.0064E-66 | -65.6976 | -0.0290 | -65.7266 |
| UF+++ | 5.5654E-67 | -66.2545 | -0.2495 | -66.5040 |
| Cr++ | 3.8018E-67 | -66.4200 | -0.1122 | -66.5322 |
| UF6-- | 2.3131E-67 | -66.6358 | -0.1106 | -66.7464 |
| NH3(aq) | 1.3360E-67 | -66.8742 | 0.0000 | -66.8742 |
| TcO++ | 9.9435E-70 | -69.0025 | -0.1122 | -69.1147 |
| USO4++ | 9.7390E-70 | -69.0115 | -0.1122 | -69.1237 |
| U(SO4)2(aq) | 7.5563E-70 | -69.1217 | 0.0000 | -69.1217 |
| U++++ | 4.6056E-72 | -71.3367 | -0.4389 | -71.7756 |
| NpH2PO4++ | 1.1685E-72 | -71.9324 | -0.1122 | -72.0446 |
| S2O6-- | 4.0384E-74 | -73.3938 | -0.1106 | -73.5044 |
| UCl+++ | 2.8662E-74 | -73.5427 | -0.2495 | -73.7922 |
| UNO3+++ | 1.1150E-74 | -73.9527 | -0.2495 | -74.2022 |
| U(NO3)2++ | 6.9697E-78 | -77.1568 | -0.1122 | -77.2690 |
| NH4SO4- | 1.4165E-78 | -77.8488 | -0.0272 | -77.8760 |
| Cr2(OH)2++++ | 3.6158E-80 | -79.4418 | -0.4389 | -79.8807 |
| CuNH3++ | 1.7116E-81 | -80.7666 | -0.1122 | -80.8788 |
| Np(H2PO4)2+ | 1.1599E-85 | -84.9356 | -0.0285 | -84.9641 |
| Tc+++ | 6.8059E-93 | -92.1671 | -0.2495 | -92.4166 |
| U+++ | 4.1028E-94 | -93.3869 | -0.2495 | -93.6364 |
| Formaldehyde(aq) | 1.6300E-94 | -93.7878 | 0.0000 | -93.7878 |
| Np(H2PO4)3(aq) | 5.2043E-98 | -97.2836 | 0.0000 | -97.2836 |
| N3- | 1.8609-103 | -102.7303 | -0.0272 | -102.7575 |
| S2O5-- | 1.4788-104 | -103.8301 | -0.1106 | -103.9407 |
| (TcO(OH)2)2(aq) | 1.0402-106 | -105.9829 | 0.0000 | -105.9829 |
| HN3(aq) | 7.0656-107 | -106.1509 | 0.0000 | -106.1509 |
| Cr3(OH)4(5+) | 2.4631-112 | -111.6085 | -0.6791 | -112.2877 |
| UO2(SO3)2-- | 1.7166-113 | -112.7653 | -0.1106 | -112.8759 |
| HCN(aq) | 1.9805-123 | -122.7032 | 0.0000 | -122.7032 |
| Methanol(aq) | 4.7764-124 | -123.3209 | 0.0000 | -123.3209 |
| UO2N3+ | 2.5824-124 | -123.5880 | -0.0285 | -123.6165 |
| CN- | 1.5189-124 | -123.8185 | -0.0272 | -123.8457 |
| S2O4-- | 1.4727-137 | -136.8319 | -0.1106 | -136.9425 |
| Urea(aq) | 1.1746-138 | -137.9301 | 0.0000 | -137.9301 |
| HS- | 9.2386-144 | -143.0344 | -0.0277 | -143.0621 |
| H2S(aq) | 6.7940-145 | -144.1679 | 0.0000 | -144.1679 |
| Cu(NH3)2++ | 5.8941-145 | -144.2296 | -0.1122 | -144.3418 |
| Ni(NH3)2++ | 2.0181-145 | -144.6950 | -0.1122 | -144.8073 |
| Methane(aq) | 1.7448-148 | -147.7582 | 0.0000 | -147.7582 |
| S-- | 1.6100-148 | -147.7932 | -0.1106 | -147.9038 |
| S2O3-- | 7.6597-151 | -150.1158 | -0.1106 | -150.2264 |
| Acetate | 8.7210-154 | -153.0594 | -0.0272 | -153.0867 |
| (UO2)11(CO3)6(OH)12-- | 8.0979-155 | -154.0916 | -0.1106 | -154.2022 |
| CaCH3COO+ | 1.7890-156 | -155.7474 | -0.0285 | -155.7759 |
| NaCH3COO(aq) | 1.1994-156 | -155.9210 | 0.0000 | -155.9210 |
| MgCH3COO+ | 1.0202-156 | -155.9913 | -0.0285 | -156.0199 |
| Acetic acid(aq) | 3.7766-157 | -156.4229 | 0.0000 | -156.4229 |
| KCH3COO(aq) | 5.3729-158 | -157.2698 | 0.0000 | -157.2698 |
| HS2O3- | 5.2647-158 | -157.2786 | -0.0272 | -157.3058 |

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| LiCH3COO(aq) | 1.0534-158 | -157.9774 | 0.0000 | -157.9774 |
| GdCH3COO++ | 2.6889-167 | -166.5704 | -0.1122 | -166.6826 |
| PbCH3COO+ | 1.6792-167 | -166.7749 | -0.0285 | -166.8034 |
| MnCH3COO+ | 2.1594-168 | -167.6657 | -0.0285 | -167.6942 |
| NiCH3COO+ | 1.7888-168 | -167.7474 | -0.0285 | -167.7760 |
| AlCH3COO++ | 9.3439-169 | -168.0295 | -0.1122 | -168.1417 |
| BaCH3COO+ | 6.5774-169 | -168.1819 | -0.0285 | -168.2105 |
| CuCH3COO+ | 1.3466-169 | -168.8708 | -0.0285 | -168.8993 |
| UO2S2O3(aq) | 3.6208-172 | -171.4412 | 0.0000 | -171.4412 |
| FeCH3COO+ | 9.7556-176 | -175.0107 | -0.0285 | -175.0393 |
| CuCH3COO(aq) | 2.6371-181 | -180.5789 | 0.0000 | -180.5789 |
| S3O6-- | 1.9213-183 | -182.7164 | -0.1106 | -182.8270 |
| Methanamine(aq) | 1.4500-188 | -187.8386 | 0.0000 | -187.8386 |
| Glycine(aq) | 5.3036-192 | -191.2754 | 0.0000 | -191.2754 |
| Acetaldehyde(aq) | 1.0025-201 | -200.9989 | 0.0000 | -200.9989 |
| Cu(NH3)3++ | 5.2112-209 | -208.2831 | -0.1122 | -208.3953 |
| SCN- | 1.9249-218 | -217.7156 | -0.0272 | -217.7428 |
| NH4CH3COO(aq) | 2.5079-219 | -218.6007 | 0.0000 | -218.6007 |
| Acetamide(aq) | 2.4984-219 | -218.6023 | 0.0000 | -218.6023 |
| Ethyne(aq) | 9.6416-223 | -222.0158 | 0.0000 | -222.0158 |
| UO2(N3)2(aq) | 2.3779-225 | -224.6238 | 0.0000 | -224.6238 |
| BH4- | 1.8851-227 | -226.7247 | -0.0272 | -226.7519 |
| Ethanol(aq) | 1.0618-235 | -234.9739 | 0.0000 | -234.9739 |
| PH4+ | 1.1965-236 | -235.9221 | -0.0285 | -235.9506 |
| Ethylene(aq) | 3.6341-240 | -239.4396 | 0.0000 | -239.4396 |
| UO2SCN+ | 1.7653-240 | -239.7532 | -0.0285 | -239.7817 |
| S2-- | 2.8478-255 | -254.5455 | -0.1106 | -254.6561 |
| Ethane(aq) | 2.9064-264 | -263.5366 | 0.0000 | -263.5366 |
| Propanoate | 1.7771-267 | -266.7503 | -0.0272 | -266.7775 |
| Propanoic acid(aq) | 1.0253-270 | -269.9891 | 0.0000 | -269.9891 |
| S4O6-- | 7.3649-277 | -276.1328 | -0.1106 | -276.2434 |
| Serine(aq) | 2.1175-280 | -279.6742 | 0.0000 | -279.6742 |
| USCN+++ | 5.0240-287 | -286.2990 | -0.2495 | -286.5484 |
| Ethanamine(aq) | 4.4312-302 | -301.3535 | 0.0000 | -301.3535 |
| Alanine(aq) | 1.8481-304 | -303.7333 | 0.0000 | -303.7333 |
| Ca(CH3COO)2(aq) | 2.1855-308 | -307.6605 | 0.0000 | -307.6605 |
| Mg(CH3COO)2(aq) | 4.5268-309 | -308.3442 | 0.0000 | -308.3442 |
| Na(CH3COO)2- | 4.3494-310 | -309.3616 | -0.0272 | -309.3888 |
| Acetone(aq) | 1.2498-310 | -309.9031 | 0.0000 | -309.9031 |
| K(CH3COO)2- | 1.4377-311 | -310.8423 | -0.0272 | -310.8695 |
| Li(CH3COO)2- | 8.1629-312 | -311.0882 | -0.0272 | -311.1154 |
| Propanal(aq) | 0.0000E+00 | -314.1326 | 0.0000 | -314.1326 |
| Aspartic acid(aq) | 0.0000E+00 | -314.5427 | 0.0000 | -314.5427 |
| Gd(CH3COO)2+ | 0.0000E+00 | -317.8424 | -0.0285 | -317.8709 |
| Pb(CH3COO)2(aq) | 0.0000E+00 | -318.8859 | 0.0000 | -318.8859 |
| Al(CH3COO)2+ | 0.0000E+00 | -319.3453 | -0.0285 | -319.3738 |
| Mn(CH3COO)2(aq) | 0.0000E+00 | -319.9379 | 0.0000 | -319.9379 |
| Ni(CH3COO)2(aq) | 0.0000E+00 | -319.9684 | 0.0000 | -319.9684 |
| Cu(CH3COO)2(aq) | 0.0000E+00 | -320.5859 | 0.0000 | -320.5859 |
| Ba(CH3COO)2(aq) | 0.0000E+00 | -320.7840 | 0.0000 | -320.7840 |
| UO2(N3)3- | 0.0000E+00 | -325.9441 | -0.0272 | -325.9713 |
| Fe(CH3COO)2(aq) | 0.0000E+00 | -326.9311 | 0.0000 | -326.9311 |
| 1-Propyne(aq) | 0.0000E+00 | -331.6678 | 0.0000 | -331.6678 |
| Cu(CH3COO)2- | 0.0000E+00 | -333.6676 | -0.0272 | -333.6948 |
| 1-Propanol(aq) | 0.0000E+00 | -348.6061 | 0.0000 | -348.6061 |
| 1-Propene(aq) | 0.0000E+00 | -350.9021 | 0.0000 | -350.9021 |
| S3-- | 0.0000E+00 | -361.3759 | -0.1106 | -361.4865 |
| NH4(CH3COO)2- | 0.0000E+00 | -371.7921 | -0.0272 | -371.8193 |
| Asparagine(aq) | 0.0000E+00 | -376.6122 | 0.0000 | -376.6122 |
| Propane(aq) | 0.0000E+00 | -377.5375 | 0.0000 | -377.5375 |
| Butanoate | 0.0000E+00 | -380.9248 | -0.0272 | -380.9521 |
| Butanoic acid(aq) | 0.0000E+00 | -384.2223 | 0.0000 | -384.2223 |
| Diglycine(aq) | 0.0000E+00 | -385.1371 | 0.0000 | -385.1371 |
| Diketopiperazine(aq) | 0.0000E+00 | -387.2571 | 0.0000 | -387.2571 |
| Ethylacetate(aq) | 0.0000E+00 | -392.9378 | 0.0000 | -392.9378 |
| Threonine(aq) | 0.0000E+00 | -393.8048 | 0.0000 | -393.8048 |
| S5O6-- | 0.0000E+00 | -398.4298 | -0.1106 | -398.5404 |
| Ni(NH3)6++ | 0.0000E+00 | -408.5172 | -0.1122 | -408.6294 |
| 1-Propanamine(aq) | 0.0000E+00 | -414.4652 | 0.0000 | -414.4652 |
| a-Aminobutyric acid(aq) | 0.0000E+00 | -417.5560 | 0.0000 | -417.5560 |
| 2-Butanone(aq) | 0.0000E+00 | -423.7919 | 0.0000 | -423.7919 |
| Glutamic acid(aq) | 0.0000E+00 | -426.6942 | 0.0000 | -426.6942 |
| UO2(N3)4-- | 0.0000E+00 | -429.4383 | -0.1106 | -429.5489 |
| Butanal(aq) | 0.0000E+00 | -429.6633 | 0.0000 | -429.6633 |
| 1-Butyne(aq) | 0.0000E+00 | -445.8351 | 0.0000 | -445.8351 |
| UO2(SCN)2(aq) | 0.0000E+00 | -457.6844 | 0.0000 | -457.6844 |
| 1-Butanol(aq) | 0.0000E+00 | -463.4477 | 0.0000 | -463.4477 |
| 1-Butene(aq) | 0.0000E+00 | -465.2526 | 0.0000 | -465.2526 |
| S4-- | 0.0000E+00 | -468.4263 | -0.1106 | -468.5369 |
| Gd(CH3COO)3(aq) | 0.0000E+00 | -469.5867 | 0.0000 | -469.5867 |
| Pb(CH3COO)3- | 0.0000E+00 | -470.0468 | -0.0272 | -470.0740 |
| Cu(CH3COO)3- | 0.0000E+00 | -472.3846 | -0.0272 | -472.4118 |
| Ni(CH3COO)3- | 0.0000E+00 | -472.4341 | -0.0272 | -472.4614 |
| Mn(CH3COO)3- | 0.0000E+00 | -472.6602 | -0.0272 | -472.6874 |
| Glutamine(aq) | 0.0000E+00 | -490.7062 | 0.0000 | -490.7062 |
| n-Butane(aq) | 0.0000E+00 | -491.5940 | 0.0000 | -491.5940 |
| Pentanoate | 0.0000E+00 | -494.9896 | -0.0272 | -495.0168 |
| Alanylglycine(aq) | 0.0000E+00 | -497.9410 | 0.0000 | -497.9410 |
| Pentanoic acid(aq) | 0.0000E+00 | -498.2650 | 0.0000 | -498.2650 |
| U(SCN)2++ | 0.0000E+00 | -502.8890 | -0.1122 | -503.0013 |
| 1-Butanamine(aq) | 0.0000E+00 | -528.8157 | 0.0000 | -528.8157 |
| Valine(aq) | 0.0000E+00 | -531.4814 | 0.0000 | -531.4814 |
| 2-Pentanone(aq) | 0.0000E+00 | -538.0984 | 0.0000 | -538.0984 |

| | | | | |
|---|---|---|---|---|
| Phenol(aq) | 0.0000E+00 | -543.0653 | 0.0000 | -543.0653 |
| Pentanal(aq) | 0.0000E+00 | -543.5007 | 0.0000 | -543.5007 |
| Methionine(aq) | 0.0000E+00 | -557.4526 | 0.0000 | -557.4526 |
| 1-Pentyne(aq) | 0.0000E+00 | -559.9877 | 0.0000 | -559.9877 |
| Benzene(aq) | 0.0000E+00 | -575.3964 | 0.0000 | -575.3964 |
| S5-- | 0.0000E+00 | -575.6966 | -0.1106 | -575.8072 |
| 1-Pentanol(aq) | 0.0000E+00 | -576.3103 | 0.0000 | -576.3103 |
| 1-Pentene(aq) | 0.0000E+00 | -579.4272 | 0.0000 | -579.4272 |
| o-Phthalate | 0.0000E+00 | -586.0577 | -0.1106 | -586.1684 |
| Ca(o-Phthalate)(aq) | 0.0000E+00 | -587.3685 | 0.0000 | -587.3685 |
| 1-Pentanamine(aq) | 0.0000E+00 | -587.5884 | 0.0000 | -587.5884 |
| Na(o-Phthalate)- | 0.0000E+00 | -588.1721 | -0.0272 | -588.1993 |
| H(o-Phthalate)- | 0.0000E+00 | -588.8266 | -0.0272 | -588.8538 |
| Isoleucine(aq) | 0.0000E+00 | -590.0415 | 0.0000 | -590.0415 |
| Leucine(aq) | 0.0000E+00 | -590.1881 | 0.0000 | -590.1881 |
| o-Phthalic acid(aq) | 0.0000E+00 | -593.9972 | 0.0000 | -593.9972 |
| Ba(o-Phthalate)(aq) | 0.0000E+00 | -599.9517 | 0.0000 | -599.9517 |
| n-Pentane(aq) | 0.0000E+00 | -605.7203 | 0.0000 | -605.7203 |
| Hexanoate | 0.0000E+00 | -609.1567 | -0.0272 | -609.1840 |
| Hexanoic acid(aq) | 0.0000E+00 | -612.4176 | 0.0000 | -612.4176 |
| 2-Hexanone(aq) | 0.0000E+00 | -652.0898 | 0.0000 | -652.0898 |
| Hexanal(aq) | 0.0000E+00 | -657.6826 | 0.0000 | -657.6826 |
| 1-Hexyne(aq) | 0.0000E+00 | -674.2356 | 0.0000 | -674.2356 |
| UO2(SCN)3- | 0.0000E+00 | -674.5400 | -0.0272 | -674.5672 |
| Toluene(aq) | 0.0000E+00 | -686.7123 | 0.0000 | -686.7123 |
| 1-Hexanol(aq) | 0.0000E+00 | -691.0859 | 0.0000 | -691.0859 |
| 1-Hexene(aq) | 0.0000E+00 | -693.4112 | 0.0000 | -693.4112 |
| 1-Hexanamine(aq) | 0.0000E+00 | -701.6897 | 0.0000 | -701.6897 |
| n-Hexane(aq) | 0.0000E+00 | -719.9901 | 0.0000 | -719.9901 |
| Heptanoate | 0.0000E+00 | -723.2581 | -0.0272 | -723.2853 |
| Heptanoic acid(aq) | 0.0000E+00 | -726.4236 | 0.0000 | -726.4236 |
| Leucylglycine(aq) | 0.0000E+00 | -727.5865 | 0.0000 | -727.5865 |
| Tyrosine(aq) | 0.0000E+00 | -759.6170 | 0.0000 | -759.6170 |
| 2-Heptanone(aq) | 0.0000E+00 | -766.1837 | 0.0000 | -766.1837 |
| Heptanal(aq) | 0.0000E+00 | -772.7368 | 0.0000 | -772.7368 |
| Phenylalanine(aq) | 0.0000E+00 | -786.9746 | 0.0000 | -786.9746 |
| 1-Heptyne(aq) | 0.0000E+00 | -788.5202 | 0.0000 | -788.5202 |
| Ethylbenzene(aq) | 0.0000E+00 | -800.9016 | 0.0000 | -800.9016 |
| 1-Heptanol(aq) | 0.0000E+00 | -806.2354 | 0.0000 | -806.2354 |
| 1-Heptene(aq) | 0.0000E+00 | -807.5272 | 0.0000 | -807.5272 |
| 1-Heptanamine(aq) | 0.0000E+00 | -815.7836 | 0.0000 | -815.7836 |
| n-Heptane(aq) | 0.0000E+00 | -834.0841 | 0.0000 | -834.0841 |
| Octanoate | 0.0000E+00 | -837.3520 | -0.0272 | -837.3792 |
| Octanoic acid(aq) | 0.0000E+00 | -840.2977 | 0.0000 | -840.2977 |
| 2-Octanone(aq) | 0.0000E+00 | -880.2777 | 0.0000 | -880.2777 |
| Octanal(aq) | 0.0000E+00 | -886.1931 | 0.0000 | -886.1931 |
| 1-Octyne(aq) | 0.0000E+00 | -902.6728 | 0.0000 | -902.6728 |
| n-Propylbenzene(aq) | 0.0000E+00 | -914.7609 | 0.0000 | -914.7609 |
| 1-Octanol(aq) | 0.0000E+00 | -920.1094 | 0.0000 | -920.1094 |
| Tryptophan(aq) | 0.0000E+00 | -920.3650 | 0.0000 | -920.3650 |
| 1-Octene(aq) | 0.0000E+00 | -921.7824 | 0.0000 | -921.7824 |
| 1-Octanamine(aq) | 0.0000E+00 | -929.8776 | 0.0000 | -929.8776 |
| n-Octane(aq) | 0.0000E+00 | -948.2220 | 0.0000 | -948.2220 |

--- Major Aqueous Species Contributing to Mass Balances ---

Aqueous species accounting for 99% or more of Al+++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| AlO2- | 1.00 | 2.4984E-08 | 97.86 |
| HAlO2(aq) | 1.00 | 5.3383E-10 | 2.09 |
| Total | | 2.5530E-08 | 99.95 |

Aqueous species accounting for 99% or more of B(OH)3(aq)

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| B(OH)3(aq) | 1.00 | 1.1503E-05 | 92.86 |
| BO2- | 1.00 | 8.6423E-07 | 6.98 |
| Total | | 1.2388E-05 | 99.83 |

Aqueous species accounting for 99% or more of Ba++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Ba++ | 1.00 | 9.9523E-17 | 99.52 |
| Total | | 1.0000E-16 | 99.52 |

Aqueous species accounting for 99% or more of Ca++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Ca++ | 1.00 | 3.0844E-04 | 95.09 |
| CaCO3(aq) | 1.00 | 5.6415E-06 | 1.74 |

| | | | |
|---|---|---|---|
| CaHCO3+ | 1.00 | 5.4309E-06 | 1.67 |
| CaSO4(aq) | 1.00 | 4.3911E-06 | 1.35 |
| Total | | 3.2437E-04 | 99.86 |

Aqueous species accounting for 99% or more of Cl-

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Cl- | 1.00 | 2.0132E-04 | 99.96 |
| Total | | 2.0140E-04 | 99.96 |

Aqueous species accounting for 99% or more of CrO4--

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| CrO4-- | 1.00 | 9.7965E-17 | 97.96 |
| HCrO4- | 1.00 | 2.0353E-18 | 2.04 |
| Total | | 1.0000E-16 | 100.00 |

Aqueous species accounting for 99% or more of Cu++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| CuCO3(aq) | 1.00 | 9.0179E-17 | 90.18 |
| CuOH+ | 1.00 | 6.1629E-18 | 6.16 |
| Cu(CO3)2-- | 1.00 | 2.1715E-18 | 2.17 |
| Cu++ | 1.00 | 1.1606E-18 | 1.16 |
| Total | | 1.0000E-16 | 99.67 |

Aqueous species accounting for 99% or more of F-

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| F- | 1.00 | 1.1443E-04 | 99.73 |
| Total | | 1.1475E-04 | 99.73 |

Aqueous species accounting for 99% or more of Fe++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Fe(OH)3(aq) | 1.00 | 3.4233E-12 | 95.10 |
| Fe(OH)4- | 1.00 | 1.1352E-13 | 3.15 |
| Fe(OH)2+ | 1.00 | 6.3035E-14 | 1.75 |
| Total | | 3.5999E-12 | 100.00 |

Aqueous species accounting for 99% or more of Gd+++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Gd+++ | 1.00 | 1.0000E-16 | 100.00 |
| Total | | 1.0000E-16 | 100.00 |

Aqueous species accounting for 99% or more of HCO3-

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| HCO3- | 1.00 | 2.0278E-03 | 96.83 |
| CO2(aq) | 1.00 | 3.3942E-05 | 1.62 |
| CO3-- | 1.00 | 1.4226E-05 | 6.793E-01 |
| Total | | 2.0941E-03 | 99.13 |

Aqueous species accounting for 99% or more of HPO4--

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| HPO4-- | 1.00 | 9.6502E-07 | 76.55 |
| H2PO4- | 1.00 | 1.0306E-07 | 8.18 |
| CaHPO4(aq) | 1.00 | 9.8576E-08 | 7.82 |
| MgHPO4(aq) | 1.00 | 3.7293E-08 | 2.96 |
| CaPO4- | 1.00 | 3.2556E-08 | 2.58 |
| NaHPO4- | 1.00 | 1.2307E-08 | 9.762E-01 |
| Total | | 1.2607E-06 | 99.06 |

Aqueous species accounting for 99% or more of K+

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| K+ | 1.00 | 1.2877E-04 | 99.89 |
| Total | | 1.2891E-04 | 99.89 |

Aqueous species accounting for 99% or more of Li+

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Li+ | 1.00 | 6.9096E-06 | 99.92 |
| Total | | 6.9154E-06 | 99.92 |

Aqueous species accounting for 99% or more of Mg++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Mg++ | 1.00 | 7.8233E-05 | 94.60 |
| MgSO4(aq) | 1.00 | 2.2440E-06 | 2.71 |
| MgHCO3+ | 1.00 | 1.3543E-06 | 1.64 |
| MgCO3(aq) | 1.00 | 6.4721E-07 | 7.826E-01 |
| Total | | 8.2699E-05 | 99.73 |

Aqueous species accounting for 99% or more of Mn++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Mn++ | 1.00 | 1.9274E-16 | 63.13 |
| MnCO3(aq) | 1.00 | 5.4967E-17 | 18.00 |
| MnO4- | 1.00 | 4.8859E-17 | 16.00 |
| MnSO4(aq) | 1.00 | 4.7883E-18 | 1.57 |
| MnHCO3+ | 1.00 | 2.3205E-18 | 7.600E-01 |
| Total | | 3.0533E-16 | 99.46 |

Aqueous species accounting for 99% or more of MoO4--

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| MoO4-- | 1.00 | 1.0000E-16 | 100.00 |
| Total | | 1.0000E-16 | 100.00 |

Aqueous species accounting for 99% or more of NO3-

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| NO3- | 1.00 | 1.4143E-04 | 99.88 |
| Total | | 1.4160E-04 | 99.88 |

Aqueous species accounting for 99% or more of Na+

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Na+ | 1.00 | 1.9840E-03 | 99.59 |
| Total | | 1.9922E-03 | 99.59 |

Aqueous species accounting for 99% or more of Ni++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Ni++ | 1.00 | 9.8519E-17 | 98.52 |
| NiSO4(aq) | 1.00 | 1.4408E-18 | 1.44 |
| Total | | 1.0000E-16 | 99.96 |

Aqueous species accounting for 99% or more of Np++++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| NpO2+ | 1.00 | 6.2676E-17 | 62.68 |
| NpO2CO3- | 1.00 | 2.7557E-17 | 27.56 |
| NpO2OH(aq) | 1.00 | 9.1616E-18 | 9.16 |
| Total | | 1.0000E-16 | 99.39 |

Aqueous species accounting for 99% or more of Pb++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|

| | | | |
|---|---|---|---|
| Pb++ | 1.00 | 9.9443E-17 | 99.44 |
| Total | | 1.0000E-16 | 99.44 |

Aqueous species accounting for 99% or more of Pu++++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| PuO2(CO3)2-- | 1.00 | 8.5949E-17 | 85.95 |
| PuO2F3- | 1.00 | 7.1973E-18 | 7.20 |
| PuO2+ | 1.00 | 4.4780E-18 | 4.48 |
| PuO2F2(aq) | 1.00 | 7.0715E-19 | 7.072E-01 |
| Pu(OH)5- | 1.00 | 6.5918E-19 | 6.592E-01 |
| PuO2F4-- | 1.00 | 6.5872E-19 | 6.587E-01 |
| Total | | 1.0000E-16 | 99.65 |

Aqueous species accounting for 99% or more of SO4--

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| SO4-- | 1.00 | 1.8291E-04 | 95.49 |
| CaSO4(aq) | 1.00 | 4.3911E-06 | 2.29 |
| MgSO4(aq) | 1.00 | 2.2440E-06 | 1.17 |
| NaSO4- | 1.00 | 1.8529E-06 | 9.674E-01 |
| Total | | 1.9154E-04 | 99.93 |

Aqueous species accounting for 99% or more of SiO2(aq)

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| SiO2(aq) | 1.00 | 9.9889E-04 | 98.44 |
| HSiO3- | 1.00 | 1.4711E-05 | 1.45 |
| Total | | 1.0147E-03 | 99.89 |

Aqueous species accounting for 99% or more of TcO4-

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| TcO4- | 1.00 | 1.0000E-16 | 100.00 |
| Total | | 1.0000E-16 | 100.00 |

Aqueous species accounting for 99% or more of Ti(OH)4(aq)

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Ti(OH)4(aq) | 1.00 | 1.0000E-16 | 100.00 |
| Total | | 1.0000E-16 | 100.00 |

Aqueous species accounting for 99% or more of UO2++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| UO2(CO3)3---- | 1.00 | 4.9674E-17 | 49.67 |
| UO2(CO3)2-- | 1.00 | 4.6937E-17 | 46.94 |
| UO2(OH)2(aq) | 1.00 | 2.7121E-18 | 2.71 |
| Total | | 1.0000E-16 | 99.32 |

Aqueous species accounting for 99% or more of Zr(OH)2++

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| Zr(OH)4(aq) | 1.00 | 1.0000E-16 | 100.00 |
| Total | | 1.0000E-16 | 100.00 |

Aqueous species accounting for 99% or more of O2(aq)

| Species | Factor | Molality | Per Cent |
|---|---|---|---|
| O2(aq) | 1.00 | 1.7501E-04 | 100.00 |
| Total | | 1.7501E-04 | 100.00 |

--- Summary of Aqueous Redox Reactions ---

| Couple | Eh, volts | pe- | Log fO2 | Ah, kcal |
|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| DEFAULT | | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| HS- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Acetic acid( | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S2-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S2O3-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Acetone(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Benzene(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Butanoic aci | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| CN- | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| ClO- | /Cl- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| ClO2- | /Cl- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| ClO3- | /Cl- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| ClO4- | /Cl- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Cr++ | /CrO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Cr+++ | /CrO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| CrO4--- | /CrO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Cu+ | /Cu++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Ethanamine(a | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Ethane(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Ethanol(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Ethylene(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Ethyne(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Fe+++ | /Fe++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Formic acid( | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Glycine(aq) | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| H2(aq) | /H2O | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| HSO5- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Methane(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Mn+++ | /Mn++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| MnO4-- | /Mn++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| N2(aq) | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| N3- | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| NO2- | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| NH3(aq) | /NO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Np+++ | /Np++++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| NpO2+ | /Np++++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| NpO2++ | /Np++++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| O2(aq) | /H2O | 0.738 | 0.1247E+02 | -0.858 | 17.010 |
| Pb++++ | /Pb++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Pentanoic ac | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Phenol(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Propanoic ac | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Pu+++ | /Pu++++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| PuO2+ | /Pu++++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| PuO2++ | /Pu++++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S2O4-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S2O6-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S2O8-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S3-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S3O6-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S4-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S4O6-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S5-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| S5O6-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| SCN- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| SO3-- | /SO4-- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Tc+++ | /TcO4- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| TcO++ | /TcO4- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| TcO4-- | /TcO4- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| TcO4--- | /TcO4- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| Toluene(aq) | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| U+++ | /UO2++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| U++++ | /UO2++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| UO2+ | /UO2++ | 0.740 | 0.1251E+02 | -0.700 | 17.064 |
| o-Phthalate | /HCO3- | 0.740 | 0.1251E+02 | -0.700 | 17.064 |

--- Summary of Aqueous Non-equilibrium Non-redox Neactions ---

| Reaction | Log Q/K | Aff, kcal | State |
|---|---|---|---|

None

--- Summary of Pure Mineral Saturation States ---

(Minerals with affinities .lt. -10 kcal are not listed)

| Mineral | Log Q/K | Aff, kcal | State |
|---|---|---|---|
| Albite | 0.757 | 1.033 | ssatd |
| Albite high | -0.562 | -0.767 | |
| Albite low | 0.757 | 1.033 | ssatd |
| Amesite-14A | -4.919 | -6.711 | |
| Analcime | -0.239 | -0.326 | satd |
| Analcime-dehy | -6.601 | -9.006 | |
| Andalusite | -4.624 | -6.309 | |
| Andradite | -3.568 | -4.867 | |
| Anhydrite | -3.162 | -4.314 | |
| Anorthite | -5.692 | -7.765 | |
| Anthophyllite | -6.979 | -9.521 | |
| Antigorite | -4.434 | -6.050 | |

| | | | |
|---|---|---|---|
| Aragonite | -0.240 | -0.327 | satd |
| Artinite | -6.521 | -8.896 | |
| BaZrO3 | 79.773 | 108.834 | ssatd |
| Baddeleyite | -6.831 | -9.320 | |
| Bassanite | -3.807 | -5.194 | |
| Beidellite-Ca | 2.154 | 2.938 | ssatd |
| Beidellite-H | 1.038 | 1.416 | ssatd |
| Beidellite-K | 1.740 | 2.374 | ssatd |
| Beidellite-Mg | 2.094 | 2.857 | ssatd |
| Beidellite-Na | 1.794 | 2.448 | ssatd |
| Boehmite | -0.404 | -0.551 | |
| Boric acid | -4.781 | -6.522 | |
| Brucite | -4.324 | -5.898 | |
| CaSO4:0.5H2O(beta) | -3.975 | -5.423 | |
| CaZrO3 | 146.296 | 199.590 | ssatd |
| Calcite | -0.096 | -0.130 | satd |
| Celadonite | 3.850 | 5.252 | ssatd |
| Chalcedony | 0.728 | 0.993 | ssatd |
| Chrysotile | -1.203 | -1.641 | |
| Clinochlore-14A | -2.047 | -2.793 | |
| Clinochlore-7A | -5.421 | -7.395 | |
| Clinoptilolite-Ca | 9.899 | 13.506 | ssatd |
| Clinoptilolite-K | 6.526 | 8.903 | ssatd |
| Clinoptilolite-Na | 6.833 | 9.323 | ssatd |
| Clinoptilolite-hy-Ca | 9.901 | 13.507 | ssatd |
| Clinoptilolite-hy-K | 6.530 | 8.909 | ssatd |
| Clinoptilolite-hy-Na | 6.836 | 9.326 | ssatd |
| Clinozoisite | -5.644 | -7.700 | |
| Coesite | 0.189 | 0.258 | satd |
| Corundum | -3.991 | -5.445 | |
| Cristobalite(alpha) | 0.448 | 0.612 | ssatd |
| Cristobalite(beta) | 0.005 | 0.007 | satd |
| Dawsonite | -2.637 | -3.598 | |
| Diaspore | 0.000 | 0.000 | satd |
| Diopside | -2.424 | -3.307 | |
| Dolomite | 0.401 | 0.546 | ssatd |
| Dolomite-dis | -1.144 | -1.561 | |
| Dolomite-ord | 0.401 | 0.546 | ssatd |
| Enstatite | -2.353 | -3.210 | |
| Epidote | -1.943 | -2.650 | |
| Epidote-ord | -1.943 | -2.650 | |
| Epsomite | -6.099 | -8.320 | |
| Eucryptite | -6.546 | -8.931 | |
| Fe(OH)3 | -5.121 | -6.987 | |
| Fluorapatite | 8.827 | 12.042 | ssatd |
| Fluorite | -1.520 | -2.074 | |
| Forsterite | -6.914 | -9.433 | |
| Gibbsite | -0.596 | -0.813 | |
| Gismondine | 0.055 | 0.075 | satd |
| Goethite | 0.000 | 0.000 | satd |
| Gypsum | -2.986 | -4.074 | |
| Gyrolite | -6.778 | -9.247 | |
| Hematite | 0.960 | 1.310 | ssatd |
| Hexahydrite | -6.334 | -8.642 | |
| Huntite | -5.065 | -6.910 | |
| Hydroxylapatite | -1.031 | -1.406 | |
| Ice | -0.139 | -0.189 | satd |
| Illite | 2.439 | 3.328 | ssatd |
| Jadeite | -1.867 | -2.547 | |
| K-Feldspar | 2.608 | 3.559 | ssatd |
| Kalicinite | -6.923 | -9.445 | |
| Kalsilite | -2.565 | -3.499 | |
| Kaolinite | 1.509 | 2.059 | ssatd |
| Kyanite | -4.354 | -5.940 | |
| Lansfordite | -3.680 | -5.021 | |
| Laumontite | 1.219 | 1.662 | ssatd |
| Lawsonite | -1.327 | -1.810 | |
| Magnesite | -1.133 | -1.545 | |
| Manganite | -4.454 | -6.076 | |
| Margarite | -5.859 | -7.993 | |
| Maximum Microcline | 2.608 | 3.559 | ssatd |
| Mesolite | 3.480 | 4.747 | ssatd |
| MnO2(gamma) | -1.518 | -2.071 | |
| Monohydrocalcite | -0.929 | -1.268 | |
| Montmor-Ca | 3.486 | 4.755 | ssatd |
| Montmor-K | 3.143 | 4.287 | ssatd |
| Montmor-Mg | 3.495 | 4.769 | ssatd |
| Montmor-Na | 3.193 | 4.356 | ssatd |
| Mordenite | 2.319 | 3.164 | ssatd |
| Muscovite | 3.068 | 4.185 | ssatd |
| Nahcolite | -5.339 | -7.284 | |
| Natrolite | -2.476 | -3.379 | |
| Nepheline | -4.278 | -5.837 | |
| Nesquehonite | -3.835 | -5.232 | |
| Nontronite-Ca | 6.076 | 8.289 | ssatd |
| Nontronite-H | 4.960 | 6.767 | ssatd |
| Nontronite-K | 5.662 | 7.725 | ssatd |
| Nontronite-Mg | 6.016 | 8.207 | ssatd |
| Nontronite-Na | 5.716 | 7.798 | ssatd |
| Okenite | -3.816 | -5.206 | |
| Paragonite | 0.320 | 0.436 | satd |
| Pentahydrite | -6.674 | -9.105 | |
| Petalite | 1.878 | 2.562 | ssatd |

| | | | |
|---|---|---|---|
| Phlogopite | 0.817 | 1.114 | ssatd |
| Prehnite | -2.478 | -3.381 | |
| Pseudowollastonite | -4.433 | -6.049 | |
| PuO2 | -3.957 | -5.398 | |
| Pyrolusite | 0.000 | 0.000 | satd |
| Pyrophyllite | 1.879 | 2.563 | ssatd |
| Quartz | 0.999 | 1.363 | ssatd |
| Rutile | -6.355 | -8.670 | |
| Sanidine high | 1.409 | 1.922 | ssatd |
| Saponite-Ca | 3.058 | 4.172 | ssatd |
| Saponite-H | 1.943 | 2.650 | ssatd |
| Saponite-K | 2.645 | 3.608 | ssatd |
| Saponite-Mg | 2.998 | 4.090 | ssatd |
| Saponite-Na | 2.698 | 3.681 | ssatd |
| Scolecite | 2.009 | 2.741 | ssatd |
| Sellaite | -2.765 | -3.773 | |
| Sepiolite | -0.549 | -0.749 | |
| SiO2(am) | -0.287 | -0.391 | satd |
| Sillimanite | -4.988 | -6.805 | |
| Smectite-high-Fe-Mg | -6.936 | -9.463 | |
| Smectite-low-Fe-Mg | -2.635 | -3.595 | |
| Spodumene | -2.933 | -4.002 | |
| Starkeyite | -7.061 | -9.633 | |
| Stilbite | 7.651 | 10.438 | ssatd |
| Talc | 2.783 | 3.797 | ssatd |
| Tremolite | -0.235 | -0.320 | satd |
| Tridymite | 0.827 | 1.129 | ssatd |
| Wairakite | -3.191 | -4.353 | |
| Whitlockite | -2.701 | -3.685 | |
| Wollastonite | -4.194 | -5.722 | |
| Zircon | -2.353 | -3.210 | |
| Zoisite | -5.689 | -7.761 | |

13 approx. saturated pure minerals
0 approx. saturated input solid solutions
0 saturated hypothetical solid solutions

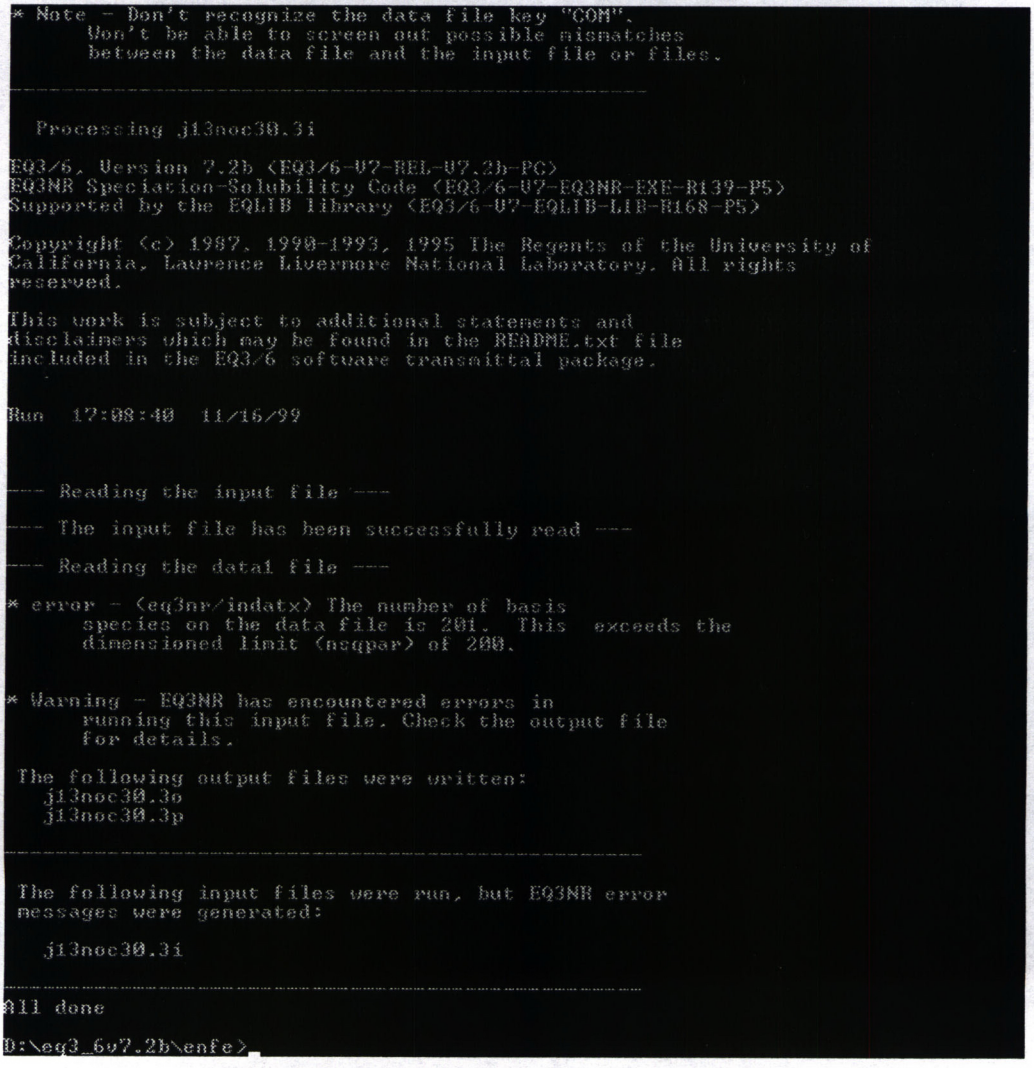
53 supersaturated pure minerals
0 supersatd. input solid solutions
0 supersatd. hypothetical solid solutions

--- Summary of Gases ---

| Gas | Fugacity | Log fugacity |
|---|---|---|
| Al(g) | 1.7109-191 | -190.7668 |
| B(g) | 8.2545-204 | -203.0833 |
| BF3(g) | 6.9348E-39 | -38.1590 |
| C(g) | 1.0290-189 | -188.9876 |
| C2H4(g) | 7.6560-238 | -237.1160 |
| CH4(g) | 1.2360-145 | -144.9080 |
| CO(g) | 1.9593E-48 | -47.7079 |
| CO2(g) | 1.0000E-03 | -3.0000 |
| Ca(g) | 1.9408-151 | -150.7120 |
| Chlorine | 3.6800E-29 | -28.4342 |
| Cu(g) | 1.9037E-84 | -83.7204 |
| Fluorine | 2.2747E-82 | -81.6431 |
| H2(g) | 6.2726E-42 | -41.2025 |
| H2O(g) | 2.5975E-02 | -1.5854 |
| H2S(g) | 6.6119-144 | -143.1797 |
| HCl(g) | 7.5370E-19 | -18.1228 |
| HF(g) | 6.6879E-14 | -13.1747 |
| K(g) | 3.1066E-77 | -76.5077 |
| Li(g) | 7.2720E-92 | -91.1383 |
| Mg(g) | 3.3438-129 | -128.4758 |
| Nitrogen | 3.1745E-20 | -19.4983 |
| NH3(g) | 2.1341E-69 | -68.6708 |
| NO(g) | 5.4688E-26 | -25.2621 |
| NO2(g) | 3.6449E-20 | -19.4383 |
| Na(g) | 2.5005E-75 | -74.6020 |
| O2(g) | 1.9953E-01 | -0.7000 |
| Pb(g) | 1.8339E-74 | -73.7366 |
| S2(g) | 2.4774-230 | -229.6060 |
| SO2(g) | 1.0844E-56 | -55.9648 |
| Si(g) | 4.4352-220 | -219.3531 |
| SiF4(g) | 8.7958E-37 | -36.0557 |
| Tc2O7(g) | 2.5085E-70 | -69.6006 |
| Ti(g) | 1.7681-237 | -236.7525 |
| TiCl4(g) | 4.7775E-92 | -91.3208 |
| U(g) | 6.3293-301 | -300.1986 |
| U2Cl10(g) | 2.1206-254 | -253.6735 |
| U2Cl8(g) | 1.7865-256 | -255.7480 |
| U2F10(g) | 8.4970-162 | -161.0707 |
| UCl(g) | 4.1974-257 | -256.3770 |
| UCl2(g) | 8.3273-212 | -211.0795 |
| UCl3(g) | 3.6185-164 | -163.4415 |
| UCl4(g) | 8.5144-134 | -133.0698 |
| UCl5(g) | 1.0308-140 | -139.9868 |

```
UCl6(g)                     2.3185-142   -141.6348
UF(g)                       7.9154-242   -241.1015
UF2(g)                      7.3415-201   -200.1342
UF3(g)                      1.6757-153   -152.7758
UF4(g)                      5.6457-103   -102.2483
UF5(g)                      8.7123E-94    -93.0599
UF6(g)                      1.3239E-98    -97.8782
UO(g)                       4.8725-216   -215.3122
UO2(g)                      8.7995-132   -131.0555
UO2Cl2(g)                   1.4139E-79    -78.8496
UO2F2(g)                    9.0425E-67    -66.0437
UO3(g)                      6.3089E-79    -78.2000
UOF4(g)                     1.6399E-80    -79.7852

--- Reading the input file ---

--- No further input found ---

         Start time = 16:41:37  11/16/99
           End time = 16:41:40  11/16/99

          Run time =    3.65     seconds
         User time =    3.65     seconds
          Cpu time =    3.65     seconds

Normal exit
```

**Using the same input file, j13noc30.3I, an EQ3 run was done using the V8.R6 thermodynamic database. An error message was encountered, as seen in the following screen capture:**



**November 17, 1999**

The calculations conducted by Stockman used a thermodynamic database modified, originally by P. Cloke, from the EQ3 data0.alt file (data0.alt.V8.R5) and the SKB EQ3 database (data0.b19.skb). The following are the comment lines in the data0.nuc.R8a file used by Stockman:

*data0.nuc.R8a*
*THERMODYNAMIC DATABASE*
*11-25-98 HWStockman creates this DB by starting with data0.nuc.R8, then adding molar volumes estimated for Trevorite (NiFe2O4), pyrolusite, baddelyite and zircon. Reference:*
*Roberts, W. L., Jr., Rapp, G. R., Jr., and Weber, J. 1974. Encyclopedia of Minerals. New York, New York: van Nostrand Reinhold Co. TIC Cat. No. 238571. Gives densities: (g/cm^3)*
*Baddeleyite: meas 5.739+/-0.005 (calc 5.825) (pp 46-47)=> V0PrTr=V0PrTr*
*Zircon: meas 4.65 (4.6-4.7) (calc 4.668) (pp 689-690)*
*Pyrolusite: meas 5.06 (calc 5.148) (p 500)*
*Trevorite: meas 5.165 (calc 5.24) (pp 624-625) NOTE HWS uses molar Vol of magnetite for consistency with calc. sent to INEEL, in F03_2022_alln_scratch.xls Mol Vol = 44.524 for Trevorite.*
*(following PLC's example, we use measured crystal densities if available)*
********Original comments from PLCloke's *nuc.R8 database below**********
*This data base is a composite of data0.alt.V8.R5 and data0.b19.skb, as revised by P. L. Cloke on 31-mar-98. It was specially modified for evaluation of nuclear criticality needs on the Yucca Mt. Project. Six EQ3NR runs were made using input data for elements in J13 well water and components of the current design for waste glass packages. Three runs were saturated with air, at pH 4, 7.41, and 10. The other three were for highly reducing conditions, log fO2 = -80, and carbonated limited to the solubility of atmospheric CO2 in water, 1.0 E-5 m. Solid and solution species appearing on the outputs and which constituted less than 0.1% of dissolved elements, or whose affinities did not exceed 1.0 E-10, on any of the outputs, were deleted from this data base.*

*The lanthanide data from the .skb data base replaced those in the .alt file in those cases in which there was overlap, except for the lanthanide metals. This includes replacing data for LnO2H, LnO+, and LnO2- by the .skb data for Ln(OH)3, Ln(OH()2+, and Ln(OH)4-, respectively. Ce++++ was added as well as more data for Y. Lanthanide data in the .skb base that aren't in the .alt base were added. LnPO4.xH2O, to which .skb assigned a value of 10 to x, was changed to LnPO4.H2O, in keeping with the formula for rhabdophane (and in keeping with the XRD pattern). Added limited Rh data on basis of data in Latimer, 1952, and NBS Technical Note 270.*

*Exceptions: The .skb data for Pm were not entered. Divalent lanthanide data were not entered.*

*Output package: eq3*

*Data set:* *nuc8*

The EQ3 calculations done yesterday used the data0.com file. A new EQ3 run was made using the data0.alt file, using Stockman's j13noc30.3I input file, for comparison with Stockman's results.

**The run, using the data file GEMBOCHS.V2-EQ8-DATA0.ALT.R2 failed with a lot of error messages, some of which are shown below:**

```
* note - (eq3nr/arrsin) The species "H2(aq)                    "
     has a required concentration near   100.00     molal.

---- Reconsider your choice of input constraints ----

* note - (eq3nr/arrsin) The species "Al+++                     "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "Fe++                      "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "HCO3-                     "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "Mn++                      "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "H2(aq)                    "
     has a required concentration near   100.00     molal.

--- Reconsider your choice of input constraints ---

* note - (eq3nr/arrsin) The species "Al+++                     "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "Fe++                      "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "HCO3-                     "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "Mn++                      "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "H2(aq)                    "
     has a required concentration near   100.00     molal.

---- Reconsider your choice of input constraints ----

* note - (eq3nr/arrsin) The species "Al+++                     "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "Fe++                      "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "HCO3-                     "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "Mn++                      "
     has a required concentration near   100.00     molal.

* note - (eq3nr/arrsin) The species "H2(aq)                    "
     has a required concentration near   100.00     molal.

----- Reconsider your choice of input constraints -----
```

**The cause of the error messages is not known.**

**Entries into Scientific Notebook No. 185 for the period October 1, 1999, to December 31, 1999, have been made by**

**Roberto T. Pabalan / Date**

**No original entry into this Scientific Notebook has been removed.**