308
Scientific Notebook #233
Q200002070011

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JEFF BOGAN

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20-5708-762 TPA CODE

07/16/97 TITLE: QUALITY ASSURANCE OF TOTAL SYSTEM PERFORMANCE ASSESSMENT (TPA) VERSION 3.1 BETA

NAMES OF INDIVIDUALS PERFORMING THEORETICAL RESEARCH:

SITAKANTA MOHANTY

ROBERT BACA

OBJECTIVES: TO DETERMINE ANY ERRORS IN THE TPA 3.1 beta CODE AND MAKE SUGGESTIONS ON IMPROVEMENT

PROCEDURE:

CHECK DATA OUTPUT FOR REASONABLENESS BASED ON PARAMETERS - ALTERING IN THE INPUT FILES PERFORM MASS BALANCE CHECKS AND PEAK TO PEAK CHECKS ON FLUXES BETWEEN MODULES

DATA AND INFORMATION SOURCES

1) MANTEUFEL R.D. ET AL "TOTAL-SYSTEM PERFORMANCE ASSESSMENT (TPA) VERSION 3.0 CODE: MODULE DESCRIPTION AND USERS GUIDE", NRC-02-93-005, 1997

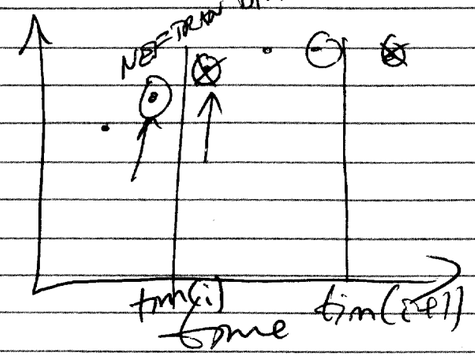
Jul 17/97 TESTED SZFT.F

problem in formatting for nefii.dat.
dispersion ≥ 1000.0 m is too much for format
in prenefmbs subroutine. These values could
conceivably occur in cases where leg are
large i.e. 10,000 or more.

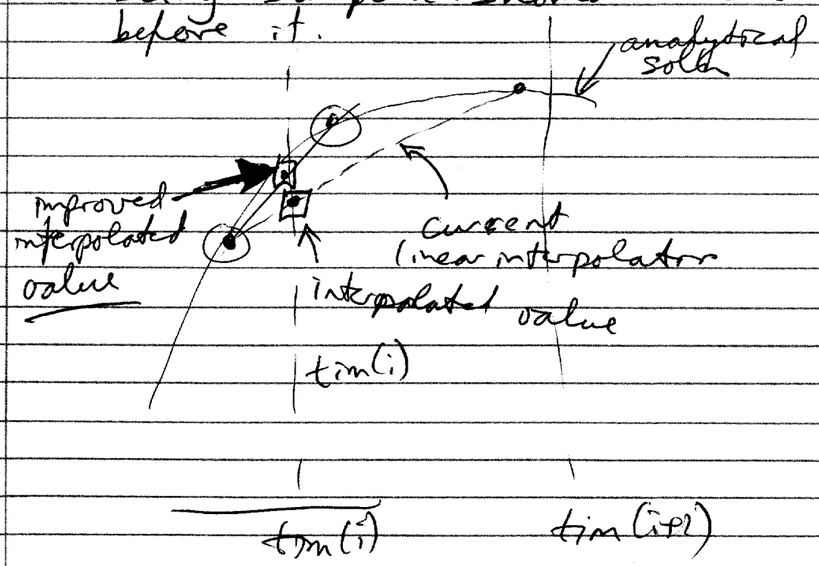
JUL 17/97

Data sampling

NEF TRAN DATA POINTS:



Currently data points are being sampled. Should add a ⊙ before it.



Jul 16 / 97

Jeff Bogan

Errors:

In uzft.f, prenefmks subroutine,

1) nefii.out should be opened as 'old' instead of 'unknown'. This will prevent any unauthorized use of the file.

2) More data should be sampled from nefmks output files. Currently there are only one data points taken one after the tim(i) value. If one before and one after the times specified in the tim() array is taken, then there is more accuracy and there is a lesser chance of introducing spurious data at the beginning and end of the data array.

3) Instead of mapping the values directly to the ciperyrintosa output array, they should be initially zeroed and then added to what is currently in the array. As it is, if nuclides share a daughter product then there one will over write the other.

e.g.

```
Am243       Cm243
  |           |
  v
      --->  Pu239
```

The last one the be determined will overwrite the previous.

Jul 17 / 97

1) In nfenv.f, all flows that are used are properly multiplied. However:
The qm3peryrperwpinsa is multiplied through my number of WP's early in the code. It retains the name 'qm3peryrperwpinsa' which is a misnomer. A solution would be to use an EQUIVALENCE routine with 'qm3peryrinsa' and then perform the scaling, or use a different array to avoid confusion later on. Similarly, when qm3peryrperwpinsahitwp is passed to nfdrip it is in terms of total flow, but when then same variable is returned as an output parameter, it is in terms of flow per WP. Again, introducing an equivalence or a new array will avoid future confusion. In addition, the variable qm3peryrperwpinsamisswp is not used.

2) Spelling mistakes occur in prenefmks subroutine (these outputted to the nefii.inp file, which may be read, so it is of some concern):

in uzft.f and szft.f search on

ARRRAY
WRITTTEN
SUMMAARY
DETERMNATION
PARAMTER

3) If Dispersion lengths are greater than 999.9m the formatting results in a ****** in the dispersion field in the file nefii.dat.

Jul 18/97

SZFT

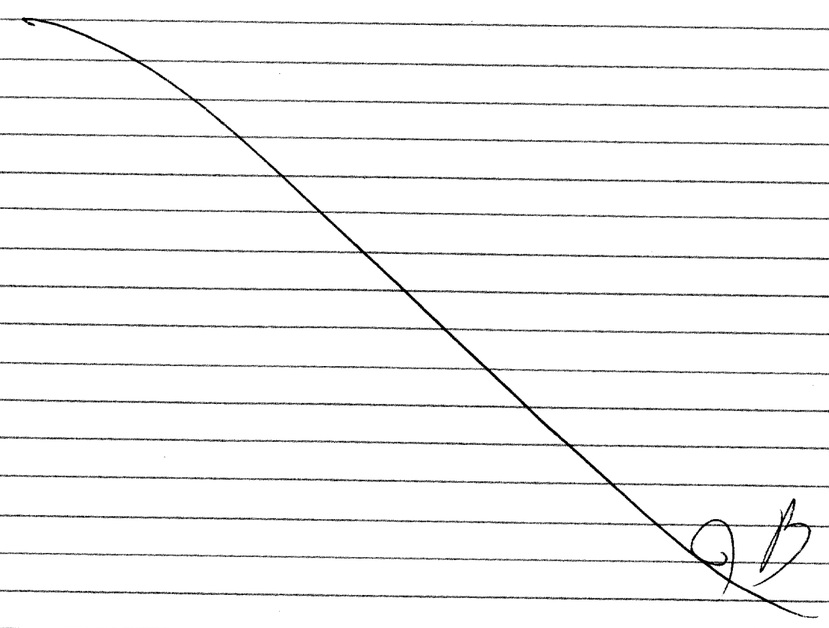
NEFTRAN CANNOT MANDLE 0.0 or less DISPERSIVITY. UZFT.F adds 0.1 to all dispersivities - this should be impented in szft.f as well. (Physically this would represent Diffusion coefficient) D*

disp = DMAX(0.1, disp)

path length is slightly longer than distance to tortuosity

5.2 km > 5

34.0 km > 30



DC. Jul 19/97

Figure 7-2 highest population ~~22000~~ 22000

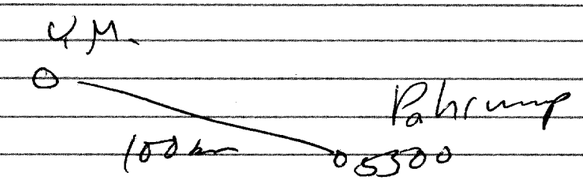
Person 2 l/day

44 000 l/day

44 m³/day

Human Consumption 16060 m³/yr.

Carrying capacity of land may change with irrigation, land reclamation etc.



do isum = 1, 4

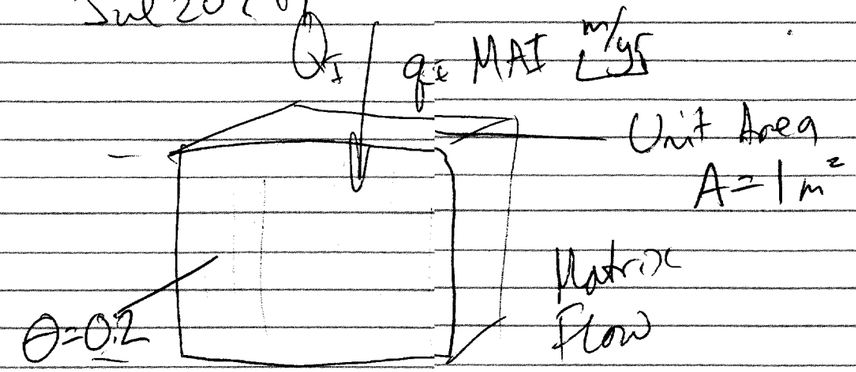
4 should be replaced w/ number of tubes

$$\left(\frac{rem}{yr}\right)_{gwi}(t) = \frac{dcf_i \times (ci/yr)(t)}{V_{dil}}$$

$$V_{dil} = MAX(MAX(Q_{MIX}, Q_{PUMP}), Q_{UZ\,ESA})$$

Control Volume (actually a flow rate)

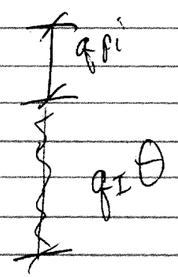
Jul 20 (97)



$V = 1\,m^3$

Pore Space $= 0.2\,m^3$

Infiltration rate $> q_I$
Precipitation ~~rot/runi~~ q_{PI}
infiltratating
if $q_{PI} <$



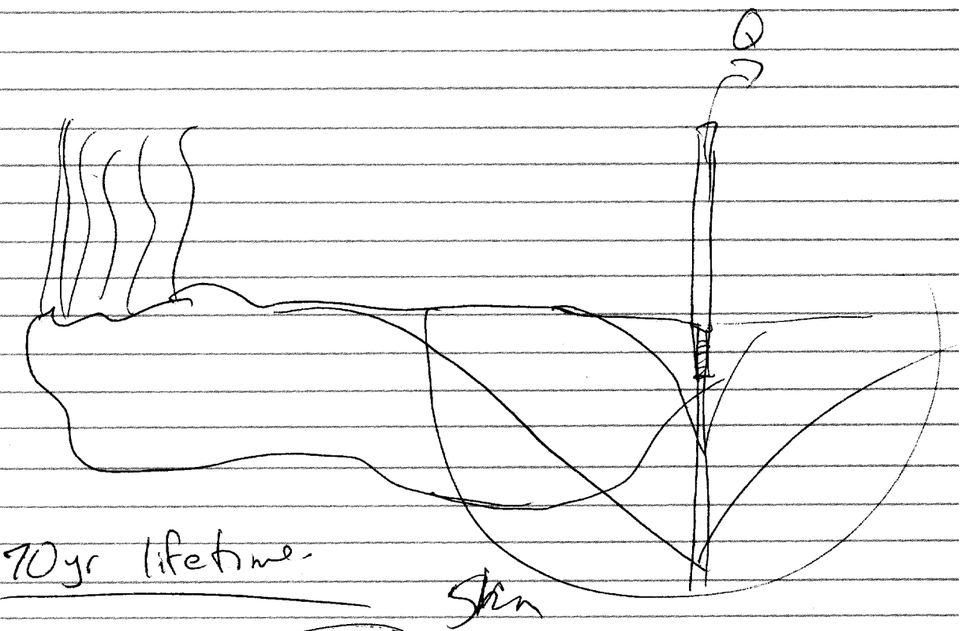
$q_{PI} > q_I\theta$ ponding/saturated flow.

(MAX) Q_{AV} 1000-3000 Q_{AV} calc'd correctly

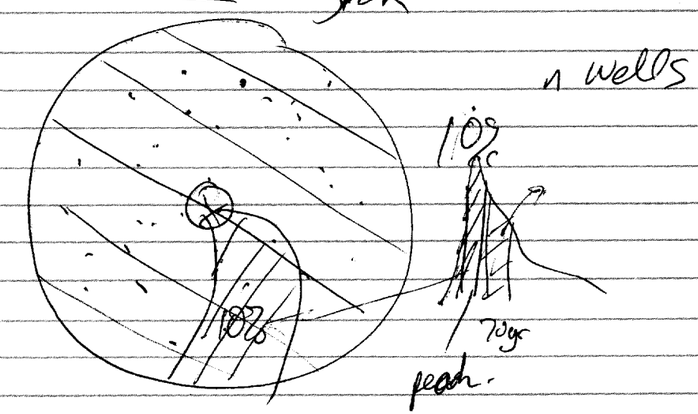
2000 ≠ {10, 100} m^3/yr

{7200, 144000} (5.0 gm) m^3/yr

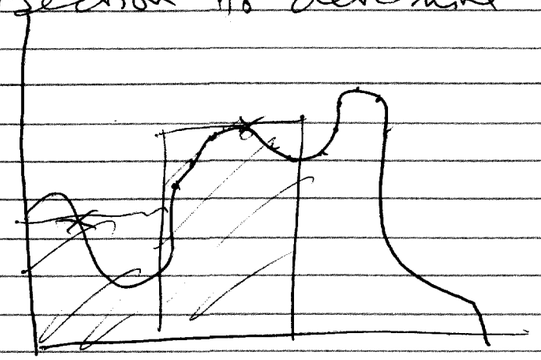
{724,000, 10.9 mil} (30.0 gm) m^3/yr



70yr lifetime.



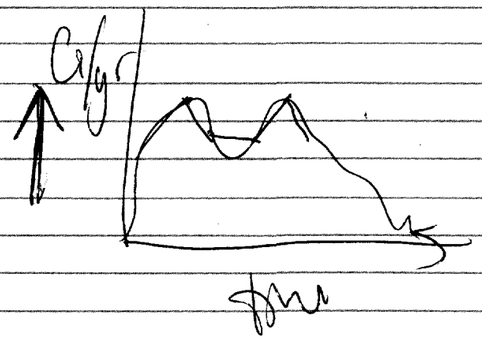
When determining Flow rates in stead of map list which just takes the intersection to determine flow rates



it would be more accurate to integrate

- Try adding a nuclide
- szft.f dilution factors have been recently updated. - check.

This could be equally applied to the radioactive Fluxs



May result in inaccuracies in the values

JUL 18/97

1) IN exec.f there is a extra data on the end of the dose converted mrem reading - in the 'rgwna.tpa' for e.g. The final two lines of these files contain extra information. which is used when importing the file into Keleidagraph. This is currently controlled by a parameter in the writedata() subroutine in exec.f, which is 1 for on, 0 for off. This should be converted to a variable so that it may be turned off and on easily, and should be defaulted to off, so as not to confuse the average user.

2) Selected parameters in the tpa.inp file were set to zero, the results are recorded. These are from the NFENV/THERMAL portion of the file.

Parameter	Result
WPLength[m]	FATAL when read of Inf / NAN occurs
WPDiameter[m]	FATAL when read of Inf / NAN occurs
EmplacementDriftDiameter[m]	NonFatal - Inf / NAN
WPSpacingAlongEmplacementDrift[m]	caught by parameter check
EmissivityOfDriftWall[-]	Division by Zero recorded, overflow/underflow when UseNfhydro2 = 0
ThermalConductivityOfFloor[W/(m-C)]	Division by Zero recorded, overflow/underflow
EffectiveThermalConductivityOfUnbackfilledDrift[W/(m-C)]	Not trapped
ThermalConductivityOfInnerStainlessSteelWall[W/m-C]	Division by zero recorded
ThermalConductivityOfOuterCarbonSteelWall[W/m-C]	Division by zero recorded
EffectiveThermalConductivityOfBasket&SFinWP[W/(m-C)]	Division by zero recorded

To avoid errors in future these should be prechecked and a error message issued with indication as to where the cause of the problem is occurring.

Jul 19/97

1) NEFTRAN cannot handle dispersion lengths of 0.0m. In uzft.f this is dealt with by the following command line

```
disp = DMAX(0.1, disp)
```

but this is not implemented in szft.f. Suggest that it be implemented in szft.f the same way.

2) dcagw.f there is a potential problem in the loading of the streamtube data:

```
do isum = 1, 4
```

could be replaced with

```
do isum = 1, numberoftubes
```

To accommodate for new data on stream tubes.

3) In uzft.f and szft.f only an approximation of 500 yr interval flow rates is used. Currently maplist is used to determine the flow rates which uses the flow rates at the period in time. To determine the true average flow rates over the 500 yr period, an integration should be done over each 500 yr period and then divided by the 500 yr time.

NFENV / THERMAL
Zero test
Nf hydro2 Thickness → N.P.

Jul 21 / 97
S. Mohanty

1) ashplume.f and nfenv.f use constants to dimension some array, Replacing these with parameter constants will allow the savings in memory, and better error checking.

2) For time periods of 100,000 years altered the parameter, maxseismicevents in exec.f from the original value of 150 to a value of 250.

3) Large infiltration rates are caused by calibrating the scaling parameter in uzflow.f to values consistant with current time scales. The file climato.inp contains the climatic variation which tend to rise to very high levels, peaking at 50,000 yrs and causing large infiltration rates. Cannot be run to times of greater than 100,000 years without causing obvious errors in flowrates. i.e. any value of more than 100,000 yrs yields flow rates with a large flow at t = 0 and zeroes for the rest of the values.

J.Bogan

July 22, 1997

S.Mohanty

1) IN exec.f there is a extra data on the end of the dose converted mrem reading - in the 'rgwna.tpa' for e.g. The final two lines of these files contain extra information. which is used when importing the file into Keleidagraph. This is currently controlled by a parameter in the writedata() subroutine in exec.f, which is 1 for on, 0 for off. This should be converted to a variable so that it may be turned off and on easily, and should be defaulted to off, so as not to confuse the average user.

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ThermalConductivityOfOuterCarbonSteelWall[W/m-C]	Division by zero recorded
EffectiveThermalConductivityOfBasket&SFinWP[W/(m-C)]	Division by zero recorded

To avoid errors in future these should be prechecked and a error message issued with indication as to where the cause of the problem is occurring.

J. Bogan

Jul 24/97
Use of Constants in dimensioning of arrays
in 11000
ashplume.f
nfcheck.f
nfenv.f

could be replaced with parameter
1) Save memory
2) Better error checking

Due to Source Code Control's confusion as to what its root is
replace 'path' with './path'

ashplume.f
ebsfail.f
ebsrel.f
exec.f
findeler.f
nfenv.f
sampler.f
seismo.f.
szft.f
uzflow.f
uzft.f.

Data
Information is added to .tpa file.
for importing information into Relerdigraph

This control by the last parameter in
write data - this should be combined into
a single parameter for easy recompilation

JUL 30, 1997

S. Mohanty

1) In the module faulto, 2*pi is given as 6.2832, this could be increased in accuracy by replacing it with m2pi = 8.0d0 * datan (1.0d0)

2) In ashplume.f and nfenv.f dimensioning is done using a constant value of 10,000 To save memory and to allow better error checking the statements, a parameter (MAXN = 10000) should be used. This eases the editing of the module in the future.

J.D.Bogan

JUL 31/97
Division by zero

WPLength[m] FATAL ERROR
WPDiameter[m] FATAL ERROR.
EnplacementDriftDiameter[m] Non-Fatal Inf/NAN
WPSpacingAlongEmplacementDrift -
caught

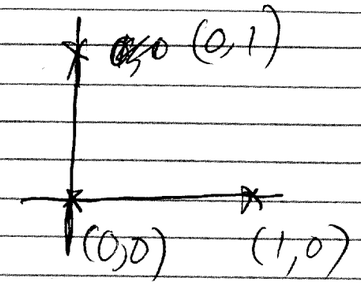
On

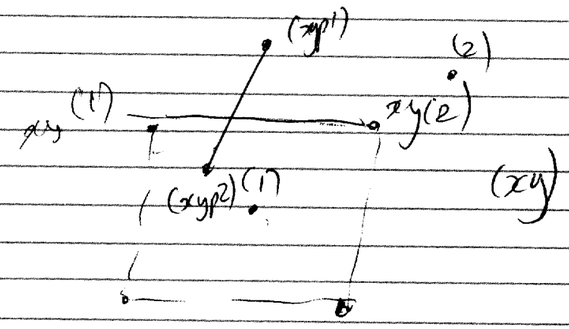
If EnplacementDriftDiameter[m] =
WPDiameter[m]

Aug 2/97

<u>fault of</u>

cos/sin / 2π





Checkin

171

4900

1700

1.4

14

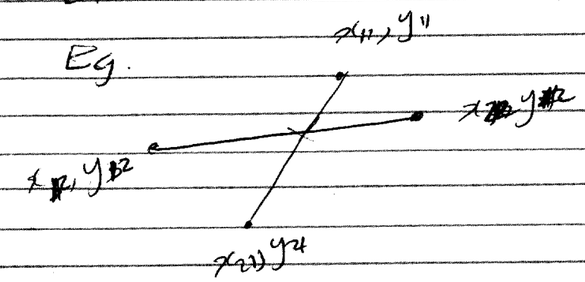
100

98

20

Line Intersection Formulation.

Eg.



$x_{11} = 0$
$y_{11} = 1$
$x_{21} = 0$
$y_{21} = 0$

$x_{12} = 0$
$y_{12} = 0$
$x_{22} = 1$
$y_{22} = 0$

a_{11} $\quad x_{21} - x_{11}$
a_{12} $\quad -(x_{22} - x_{12})$
a_{21} $\quad y_{21} - y_{11}$
a_{22} $\quad -(y_{22} - y_{12})$

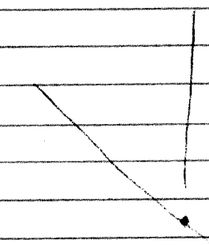
$0 - 0 \quad 0$
$1 - 0 \quad -1$
$0 - 1 \quad -1$
$0 - 0 \quad 0$

$$\begin{matrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{matrix}$$

det = 1

$$\begin{matrix} 0 & -1 \\ -1 & 0 \end{matrix}$$

For verticle lines there is a problem



Consider this an intersection

nfcn v.f.
aml ≠ 0
upspace ≠ 0
wpdia

Reflux Models

~~Thermal~~ Cn

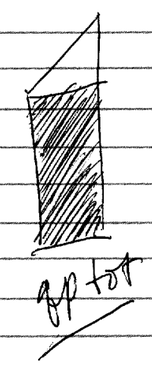
Aug 4 /97
nfhydro

parameters iSA nstm, tm()
Qm3 per Yr in SA,
Temp Rep
Qm3 per Yr in SA at Rep.

K_{THRM} Thermal Conductivity of YM Rock [W/(m-K)]
T_{BOIL} Boiling Point Of Water [C]
AML Areal Mass Loading [MTU/Acre]
dz_{REFLUX} Length of Reflux Zone [m]
J_{MAX} Maximum Flux in Reflux Zone [m/s]
V/SA_{BUCK} Perched Bucket Volume Per SA Area [m3/m2]

$$V_{BUCK} = \frac{V_{BUCK}}{SA} \times SA$$

$$f = \frac{K_{THRM}}{0.5 \times AML} \times \frac{4.04\,m^3/Acres}{m^2}$$



24

AUG 4

Ran 100 realizations successfully.

Pencil Entry photocopied for permanent record 2/8/2002 project PI

25

LHS needs → Not implemented yet.
tpa.lhs.lgd
lhs.out
lhse.out

Number of Realizations ≤ 0 →
error in sortgr.

Testing the user defined number of realizations

3-4

1-5

1, 2, 3, 4, 5

TESTED BEST

RESULTS IN *.LES FILES → OK

Pencil Entry photocopied for permanent record 2/8/2002 project PI

OK

AUG 05/97

TESTED SWITCHES → SEISMO = 0 OK

tested time values
10
* MAXTIME=100 → MATRIX INFILTRATION IS
TOO LOW FOR THE
VAN GENUCHTEN FROM DCM3D

TESTED SEISMO.

INPUT
NTIME, TIME ( )
NUMSEISMIC EVENTS ( )
TIMESEISMIC EVENTS ( )
TYPE SEISMIC EVENTS ( )

OUTPUT
CUMULATED PACKAGE FAILURE ( )

Pencil entry photocopied for permanent record 2/8/2000 project PI

BATCH RUNS
unlimit
cp tpa1.inp tpa.inp
~~tpa.e > tpa.cap~~
~~cp *.res~~
mkdir run1
cp *.res ./run1
cp *.ech ./run1
cp tpa.cap ./run1

REPEAT

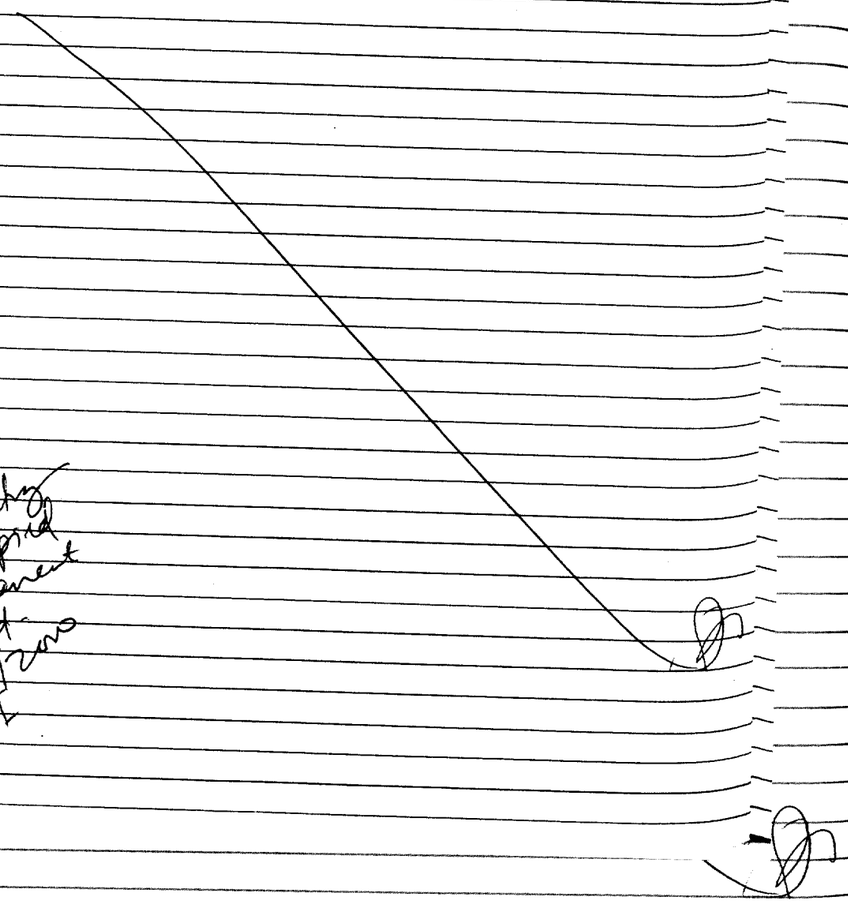
1SA 1 RUN 1 2→0
1SA 1 real 2 2→52
1SA 1 real 3 Number of Support pair 2→4
1SA 12 real 4 0,1,0 Switches
1SA 2 real 5 Rock falling dist = 1
1SA 8 real 6 switched two values in hazard curve
7SA 1 real 7 Weight wastepackage 1.27×10^5 2.5×10^7 to 5.0×10^8
1SA 1 real 8 (μ) Poisson ratio = 1.0,
1SA 2 real 9 negative in return time 500 → -500
1SA 8 real. 0 - changed hazard curve, Weight Rock P_0 → 22

Results
Run 1

Pencil Entry photocopied 2/8/2000 project PI

100,000
change time steps

get latest code



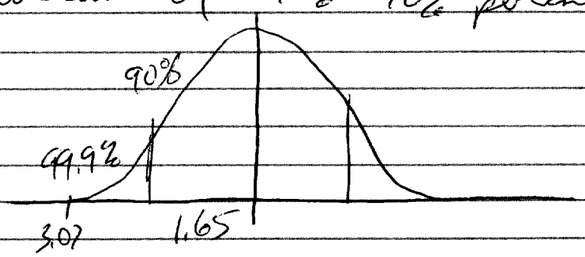
Pencil Entry
photocopied
for permanent
record.
2/8/2010
project PI

~~July~~ Aug 6 1997

ExponetForLocCorrOfOuterOverpack
(Sp) May be a spelling error.

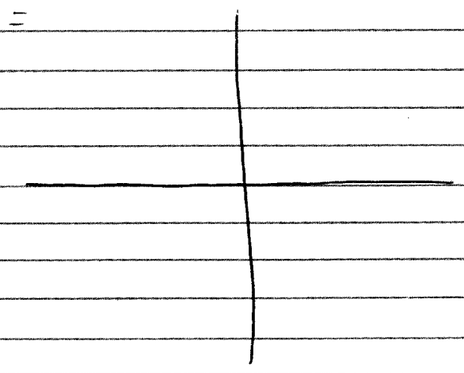
In both ~~[illegible]~~ tpu.inp and the
obsfail.f unit that it is used in.

Conversion of 10% - 90% percentile to 0.01 - 99.9% percentile

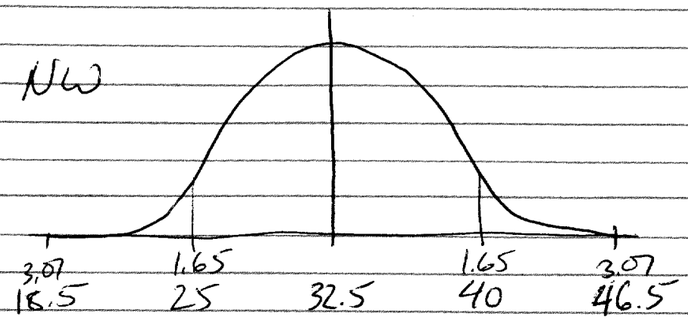


$$\sigma^2 = \left(\frac{dx}{6.18}\right)^2 \qquad 3.07$$

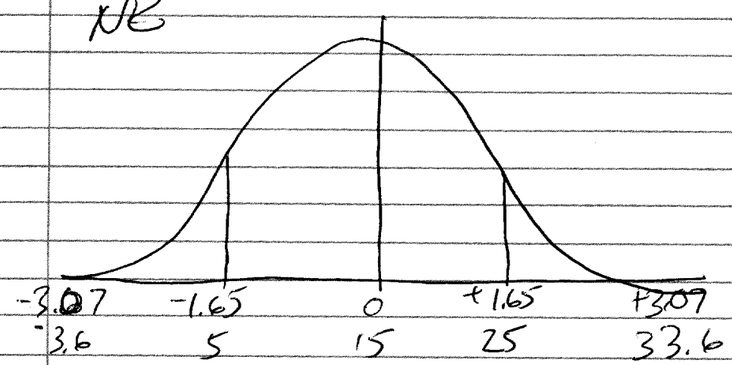
$$6.18^2\,\sigma^2 = dx^2$$
$$6.18\,\sigma =$$



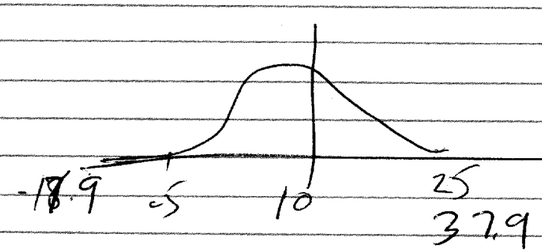
NW



NE



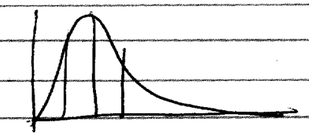
Alternate NE



-37.9 , 17.9

Lognormal Calculation

Given PP



9.0×10^{-18}, 4.0×10^{-17} as 1 SD on either side of log mean

$\log_{10}(9.0\times10^{-18}) = -17.05$
$\log_{10}(4.0\times10^{-17}) = -16.40$

log mean $= -16.725 \pm 0.325$

0.01/99.9 percentile is 3.07 SD on either side of log mean.

or -16.725 ± 0.998

-15.73, -17.72

1.9×10^{-16}, 1.9×10^{-18}

UCF 3.1×10^{-18}, 5.6×10^{-18}
-17.51 -17.25
-17.38 ± 0.13
-17.38 0.40
-16.98 -17.78
1.0×10^{-17}, 1.7×10^{-18}

BF 2.1×10^{-19}, 2.4×10^{-19}

~~2.25~~

-18.68, -18.62

-18.65 ± 0.03

-18.65 ± 0.09

-18.74, -18.56

3SD 1.8×10^{-19}, 2.8×10^{-19}

MCF 5.0×10^{-18}, 7.0×10^{-17}

-17.30, -16.15

-16.725 ± 0.575

-16.725 ± 1.765

-18.49, -14.96

~~9.1×10⁻¹⁴~~

1.1×10^{-15}, 3.2×10^{-19}

Recurrance Interval (yr) 13000 yr

↓

Time Of Next Faulting Event in Region Of Interest

pdf Finite Exponential

100, 10000, (7.69×10^{-5} 1/yr)

(1/13000)

Use Distribution OK

Aug 7 /97

Time Of Backfill Emplacement Large → OK

Increase maxntime in "maxntime.i"

and

Output Mode = 3 → Treats it as a 2

Suggest increase in

maxunit 70 to 90

in fun.i

Max Time

10000	OK
20000	OK
50000	OK
75000	nfenv Bus Error (Core Dumped)
90000	nfenv Segmentation Fault
100000	nfenv Bus Error

Suggestion - for Output Mode = 2

Warning → If number of realization is less than User Defined Lower Realization Appended.

Current tpa.inp file

Wind Direction → uniform / constant

Volcanic Event Duration

6.13e+4 / 6.31e+4

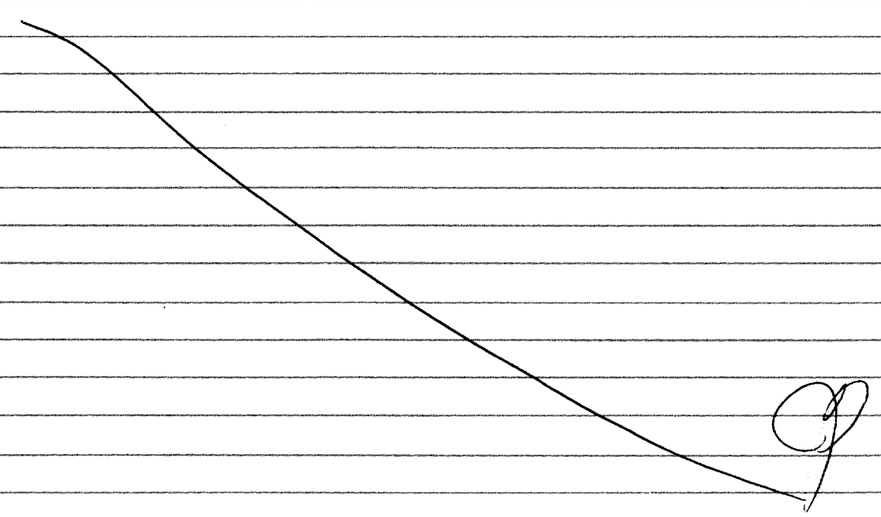
Aug 8 /97
25 realizations
testtpa → run on bigbend · latest data
~~gotta~~ Tpa806 → run on golath older data
Compare latest data to old data
→ gwtt - travel Times are lower even with extra layers

→ infilper - Infiltration rates are higher in latest data (uniform vs. loguniform infiltration pdf, same limits)

→ totdose - In both zero dose or the tail end at a late time

→ nearfld. - Average CI exactly the same for all cases

→ upsfail - Same distributions, more vary few corrosion incidents.
→ ~~cum~~ ~~elics~~ elics → ~~no numbers~~. (crashed)

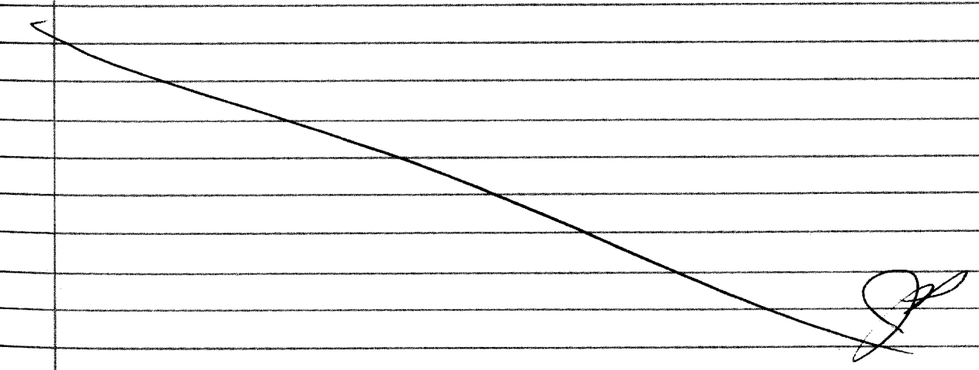


Aug 9 /97
Bombed at 24 realization of S2
memory problem disk run of out space etc. or ISA × real > Some limit

Cannot run the same version of tpa on the machine because both use the local var TPA3 ~~BETA~~ - - - thus must access the same directory for input and output.

Consistently there is no S2 release or insignificant values. Reason long residence times in the UZ. Reason for this is that there is matrix flow predominantly / infiltration is slower / WIT has dropped or repository elevation has risen → thicker layers in UZ / Stratigraphy has changed so that less permeable strata take up more of the total ~~#~~ UZ thickness / Matrix properties have been altered so that effective perm is lower. (Retardation factors, perm, thickness, dispersion - to some degree,

Run



Aug 10/97

Time to run:

Started run 10:33 am 10 realizatn
SPARC20 shipping 7 SA
196MB Mem

10:25 50 real
SPARC10 ← goloth 1 SA
176MB Mem

Aprox 5 min / SA calc.

Realization w/ ~~solution~~ fewer time steps

50 real ≈ 4 hours
12 real/hr

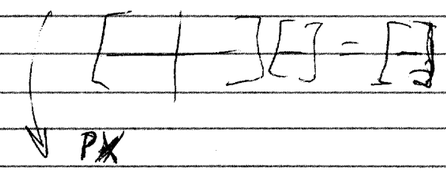
CRASHED AT 24 real → Do a postmortem on files.

Aug 11/97

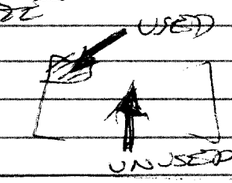
NON PORTIBLE BUT -- ~~USING~~ TO REDUCE BOUNDS ERRORS.

```
INTEGER NUMX / 20 /
REAL*4 X
POINTER (PX, X)
PX = MALLOC(4*NUMX)
  ⋮
CALL FREE(PX)
  ⋮
END
```

SOLVE THE EQUATION



ESPECIALLY USEFUL FOR MULTIDIMENSIONAL ARRAY OF LARGE SIZE



AX = C

- ELIMINATES PROBLEMS WITH OVER ALLOCATION OF MEMORY - ONLY USE WHAT YOU NEED
  MORE CONTROL - CAN ANTICIPATE MEMORY PROBLEMS TO SOME DEGREE. COMPARE FREE SPACE TO TOTAL ALLOCATED + STATIC VAR.
- NO PARAMETERS NEED ~~NOT AS MUCH~~ & EMPHASIS IS MORE ON CHECKING IF THERE IS ENOUGH MEMORY RATHER THAN IF MAX PARAMETERS HAVE BEEN EXCEEDED.

PROBLEMS.
- POINTERS ARE DIFFICULT TO WORK WITH
- CAN USE O2 optimization ~~OR~~ OR LESS, AS O3, O4 OPTIMIZE BY SOME PARAMETER PASSING ASSUPTION THEREFORE ONLY O2. or AVOID PASSING A POINTER AS AN ARC.
- ON UNIX BOXES AVAIL. MEMORY IS DIFFICULT TO FIND OUT

Aug 12/97
EDIT MAKEfile TO ALLOW
DEBUGGER TO WORK FFLAGS = -O -g
(There is a conflict between these two as linking is not performed if not a fatal conflict, however)

add -g option to linking as well

new option

tpa:
f77 -O -g execf -o ~~exec~~ tpa.e
$(OBJECTS)
make clean
make tpa.

debugger must not use a optimized version or some capabilities are lost such as line stepping and looking at local var's.

patch is usually needed

rtc_patch_area -o patch.o -size 1000000
↑ Maybe larger

execute on scratchy1 → creates patch.o

& add patch.o to OBJECT files list and recompile. (Makefile)

The number of User Defined echo runs

nfenv.f

RAN TO 50,000 yrs 30 REALIZATIONS hung up on 4th Realization

finite exponential / Return period

should this be exponential?

Will alway give exactly one event

Aug 13/97
J. Walton Memo concerning mass balance error in Tc99 and I129 in cumrel.res file. Similar error observed may or may not be the same error

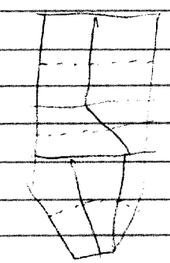
Input file tpa.inp as supplied with TPA Version 3.1beta4 Code.
Not a basecase dataset. Use only for beta testing.
TPA 3.1beta4, Job started: Wed Aug 20 16:37:41 1997
Cumulative Releases from EBS, UZ, and SZ by Nuclide
Summed Over All Subareas - Values for Each Vector

vector unitless	nuclide unitless	ebscumrl Ci	uzcumrl Ci	szcumrl Ci
1	Cm246	6.4984167E+00	0.0000000E+00	0.00000000E+00
1	U238	7.1408379E+02	6.8464094E+02	6.88497139E+00
1	Cm245	8.0340714E+01	1.2135767E-10	3.77140622E-18
1	Am241	4.2085286E+02	8.9422210E-08	3.22922667E-18
1	Np237	1.9665626E+03	1.5194738E+02	1.22751793E-01
1	Am243	8.2275903E+03	2.8298753E-09	4.88903488E-17
1	Pu239	2.8550562E+03	4.5080921E-02	1.44430440E-08
1	Pu240	1.2879426E+03	3.1809570E-03	1.99687515E-09
1	U234	2.6125778E+03	2.5021782E+03	2.44932159E+01
1	Th230	3.5127038E+02	4.1561302E-01	2.44691569E+00
1	Ra226	2.9834725E+02	2.5846030E-01	1.99928852E+00
1	Pb210	2.9738990E+02	2.8131249E+00	2.00131447E+00
1	Cs135	7.7552594E+02	1.6132512E-09	3.11170260E-17
1	I129	2.9512969E+01	2.9165915E+01	1.77513799E+01
1	Tc99	1.1976658E+04	1.2001329E+04	7.00240332E+03
1	Ni59	4.8138455E+03	4.6591791E+02	1.66303302E-01
1	C14	4.8748272E+02	0.0000000E+00	0.00000000E+00
1	Se79	7.2134203E+02	6.0928948E+02	9.66599837E+00
1	Nb94	6.6346934E+02	6.4574532E+02	1.99107494E+01
1	Cl36	2.5309143E+01	2.4725215E+01	7.63798597E-01

TT_{uz} = 340 yrs
TT_{sz} = 11,000 yrs

ashout.res - there are values for ash in the

Aug 14
Increasing number of subareas
7 → 14
current maxnsuba = 100 → OK



Took points half way up on vertical ~~to~~ sides of sub-areas.

UZFT
Double Inlet Area
" Layers thickness

Had to increase maxmv. 500 → 600
in mva.i

used in mv.f. recompiled.

~~SP~~ 600 → 1000

/net/scratchy1/~~janetzke~~ export/home/janetzke/tpa/prod

~~Solve~~ After ~~Before~~ code is frozen, before sendout

Check: 7 subarea 20000 yr

rgsnaitpa OK

Sep 2/97
problem in
:releasetif

~~3~~ empirical view of negative rdecay values:

liquel
↓
odeint(ystart ...)

y = ystart
↓
~~call~~ derivs(x, y ...)

rkqc(y ...)
↓
derivs(x, y ...)

amtl = y

amtl(~~5,4~~) is summed

to xxx2. → this value is

used to obtain dissip.

dissipxx is dissip for amt(5,4)

some amtl values are negative. If enough become negative then the sum becomes negative.

rdecay is dissipxx

Creations Sep 8/97

bt.f
Graphing beta distribution vs. logtriangular curve matching
input BETATRI.DAT (beta parameters
output

aft.f · extracts data from nefii.out file
input nefii.out
output NEFTRAN_CI.OUT → can be plotted in xplot

~~mb~~ mb.f · mass balance · integrates values from ~~a~~*_CI.OUT files

input *_CI.OUT file
MB_HL.DAT

output MB_NUC.OUT ← straight integration
MB_NUCOR.OUT ← reverses the effect of linear decay so a proper mass balance can be done.

sotout.f · creates neftran input files for specific values to ~~a~~ test neftran as a standalone.

input sotnef.dat
sot.inp

output sotnef.dat (replaces data)

th.f - creates a portion of the thickness tpa.inp file based on a data file
input Thickness.dat
output thickness.inp

---

alterations

failt.f, releaset.f, exec.f } minimized number of files open at one time

odest.f. - verification

JUL 31, 97

S. Mohanty

1) szft.f claims that this is an invalid set of subareas. However, they appear to be valid. This is the subareas as extracted from the tpa.inp file:

```
subarea
2
ZONE T="ZONE ONE SUBAREA", I=5, F=POINT
          547400.0        4076200.0
          548600.0        4076200.0
          548600.0        4077040.0
          547400.0        4077040.0
          547400.0        4076200.0
ZONE T="ZONE TWO SUBAREA", I=5, F=POINT
          547400.0        4077040.0
          548600.0        4077040.0
          548600.0        4079050.0
          547400.0        4079050.0
          547400.0        4077040.0
```

It yields this error:

```
 ***>>> Error in getunints <<<***
a line from the centroid to a point
outside the subarea intersects the
subarea more than once
subarea =   1
number of intersections =   2

subarea coordinates
(x  1,y  1) =      547400.00000000    4076200.0000000
(x  2,y  2) =      548600.00000000    4076200.0000000
(x  3,y  3) =      548600.00000000    4077040.0000000
(x  4,y  4) =      547400.00000000    4077040.0000000
x(centroid) =     548000.00000000
y(centroid) =     4076620.0000000

point outside the subarea
 (x,y) =      548600.00000000
4076170.9677419
```


2) In nfenv.f, subroutine nfhydro, there is a calculation for the total volume of water hitting the WP in a time step, calculated as the the flow rate at the beginning of the time step multiplied by the time step. This is slightly inaccurate as the true volume is an average of the flow rates from successive step multiplied by the time step This may cause larger inaccuracies for large time steps.

J.D. Bogan

Aug 1, 97

S. Mohanty

In szft.f, the module must determine where on a subarea the flow tube intersects with the sides of the subarea. It does this by tracing a straight line from the centroid of the subarea to a point outside the subarea, on the same flowline going through the centroid. In the case where the subarea contains verticle sides, the line intersection subroutine will insist that an intersection occurs on the verticle side closest to the flowline, whether there is one or not. This will immediately cause a fatal error.

2) Suggest bounds checking on

WeightPercentageOfRockFallThatHitsWPforSEISMO (It can more than 100.0%)
ProbabilityForNWOrientationOfFaults {0,1}
FractionOfTimeVolcanicEventIsExtrusive {0,1}

J.Bogan

Aug 4, 97

S. Mohanty

1) There is an error in the comments in szft.f

c qm3peryrinsafromsz(ntim) = input, double precision, flow rate [m^3/yr] from
c saturated zone
c ciperyrinsafromsz(mxntime,inucl) = input, double precision, nuclide source
c from saturated zone at critical group of subarea [ci/yr]

both of these should read 'output' instead of 'input'

2) In exec.f, when determining the number of waste packages, a conversion is done from the fraction of waste packages disrupted to the integer number of waste packages disrupted. In this case the number of waste packages is rounded to the nearest value. In the case where many are rounded up, it is possible to obtain a total number of waste packages disrupted greater than the total.

- J.Bogan

Aug 05 / 97

1) Number of realizations less or equal to 0 yields an error in sortqr. Should be trapped earlier.

2) Using a maximum time of 100 or less yields an error. 'Matrix infiltration is too low for the Van Genuchten curve from DCM3D'

- J. Bogan

Aug 11/ 97

S. Mohanty

1) The following error should be trapped with a separate routine that checks that the intersection number might be zero.

```
***>>> Error in getunints <<<***
a line from the centroid to a point
outside the subarea intersects the
subarea more than once
subarea =   1
number of intersections =   0

subarea coordinates
(x  1,y  1) =      547472.01000000    4079323.7000000
(x  2,y  2) =      548069.24000000    4079136.5000000
(x  3,y  3) =      547847.27000000    4077816.2000000
(x  4,y  4) =      547318.40000000    4077934.0000000
x(centroid) =     547677.12059000
y(centroid) =     4078568.1323160

point outside the subarea
 (x,y) =     548069.24000000    4078751.8682681
```

2) A warning should be issued in the case in which the OutputMode=2 (User Defined) and the number of realizations is less the UserDefinedLowerRealizationAppended parameter. The warning should state that there will be no output to the *.ech files.

3) For OutputMode=1,2 maxunit should be increased from 70 to 90. This is defined in the include file, 'fu2.i'.

ISSUES RELATED TO TPA.INP file

1) There may be a typing mistake in either Weldy etal (1997) or the tpa.inp file for VOLCANO. The VolcanicEventDuration in Weldy (1997) is 6.31e4, while in tpa.inp it is 6.13e4.

2) Again in VOLCANO, WindDirection has been changed from a uniform distribution to a constant, while retaining the parameters from the uniform distribution.

Currently
tar file: /bscr3/jbogan/jbogan.tar.Z

will be maintained on tape

Contains: XPlot "canvas" files
and Data relating to verification
and quality assurance of
TPA 3.1 code.

Mar 13/98

Mean of Peak Total Dose (rem/yr)

			Prob.
10000 yr			
(Nominal)	Basecase (run 1b)	8.805×10^{-4}	0.949
	Volcano (run 3b)	7.001×10^{0}	0.001
	Faulting (run 5b)	9.564×10^{-4}	0.050
50000 yr			Prob.
(Nominal)	Basecase (run 1)	1.646×10^{-2}	0.745
	Volcano (run 3)	1.670×10^{0}	0.005
	Faulting (run 5)	1.675×10^{-2}	0.250

These are results of runs performed with seismo included in the basecase at 20 km for dose and release calculations

More complete descriptions of runs can be obtained from documentation of R. Rice.

10000 yr - 200 realizations
50000 yr - 400 realizations

~jbogan/ccdr runs

These are descriptions of the files found in this directory.

relnnn.dat files are copied from relgwgs.res files in the ~rrice/tparuns respective directory. dosnnn.dat files are copied from totdose.res. There are a number of nomenclatures used both for the dat files and the ccdf res files

The program tccdf.e produces three files tpkdccdf.res, tdosccdf.res, and trelccdf.res. tpkdccdf.res contains the peak values from totdose.res, sorted into a CCDF. tdosccdf.res contains the total dose from the totdose.res files for each realization, sorted into a CCDF. The trelccdf.res file has the releases from relgwgs.res sorted into a CCDF. For each run tpkdccdf.res and trelccdf.res are retained and copied for use later. The first four characters are retained in the filename and the last changed to avoid loss. A summary of the nomenclature for the rename of the result files are given here

run1 - _50k.000
run3 - _50k.00v
run5 - _50k.f00
total of run1, run3 and run5 - _50k.tot

run1b - _10k.000
run3b - _10k.00v
run5b - _10k.f00
total of run1b, run3b and run5b - _10k.tot

Source files are renamed to the relv10.dat where v represents a volcanic scenario with maximum time at 10000 years. f represence scenarios in which faulting occurs and 0 represents basecase.

tccdf.inp instructs tccdf.e on how to weight the files that are to be run through the program tccdf.e. The current probabilities are as follows. For 10000 yrs, 0 = 0.949, v = 0.001, f = 0.050. For 50000 yr 0 = 0.745, v = 0.005, f = 0.250.
These were used for the total CCDF's described in the list of runs.

Mar 13/98

Description of procedure to produce CCDF plots ~~for~~ and ~~total~~ CCDF

Copy ~~tpkdcc~~ totdose.res and relgwgs.res ~~from~~ tpa directories and rename to some meaningful nomenclature such as dosv10.dat for volcanic scenario with a maximum time of 10k years (totdose) and keep similar consistancy with the release file. To determine individual CCDF's edit the tccdf.inp file to include 1 release file and one dose file ~~for each~~ for the scenario of interest, thus this would have a probability of 1.000 ...

1 ~~dose file~~ Release files
~~1.00000~~
1.0000 'rel050.dat'

1 ~~dose file~~ Dose files

1.0000 'dos050.dat'
(eof)

run ~~tccdf.exe~~ tccdf.e with this tccdf.inp file. These will produce 3 *.res files. Copy these files to some other file name that indicates that it is a single CCDF. Repeat this procedure for each scenario of interest.

Then TCCDF must be used to provide a weighted mean of the

values in the release and dose files

Once a set of probabilities have been set up enter them into the tccdf.inp file.

~~3 dose files~~ 3 Release files

0.75 'rel050.dat'
0.15 'relv50.dat'
0.10 'relf50.dat'

repeated for dose

run the tccdf.e command and copy the res files to some meaningful file name such as tpkd_50k.tot

Import these result files into a spreadsheet with two columns for each result file. leave a column between each for calculations. Once a set has been imported, manually multiply the CCDF colum that have been weighted with 1.000 in the tccdf.inp file by their probability in the tccdf.inp file used for the total.

Graph this out on a log to log scale.

Mar 16/98

Automatic generation of CCDF's in tccdf.f quality assurance.

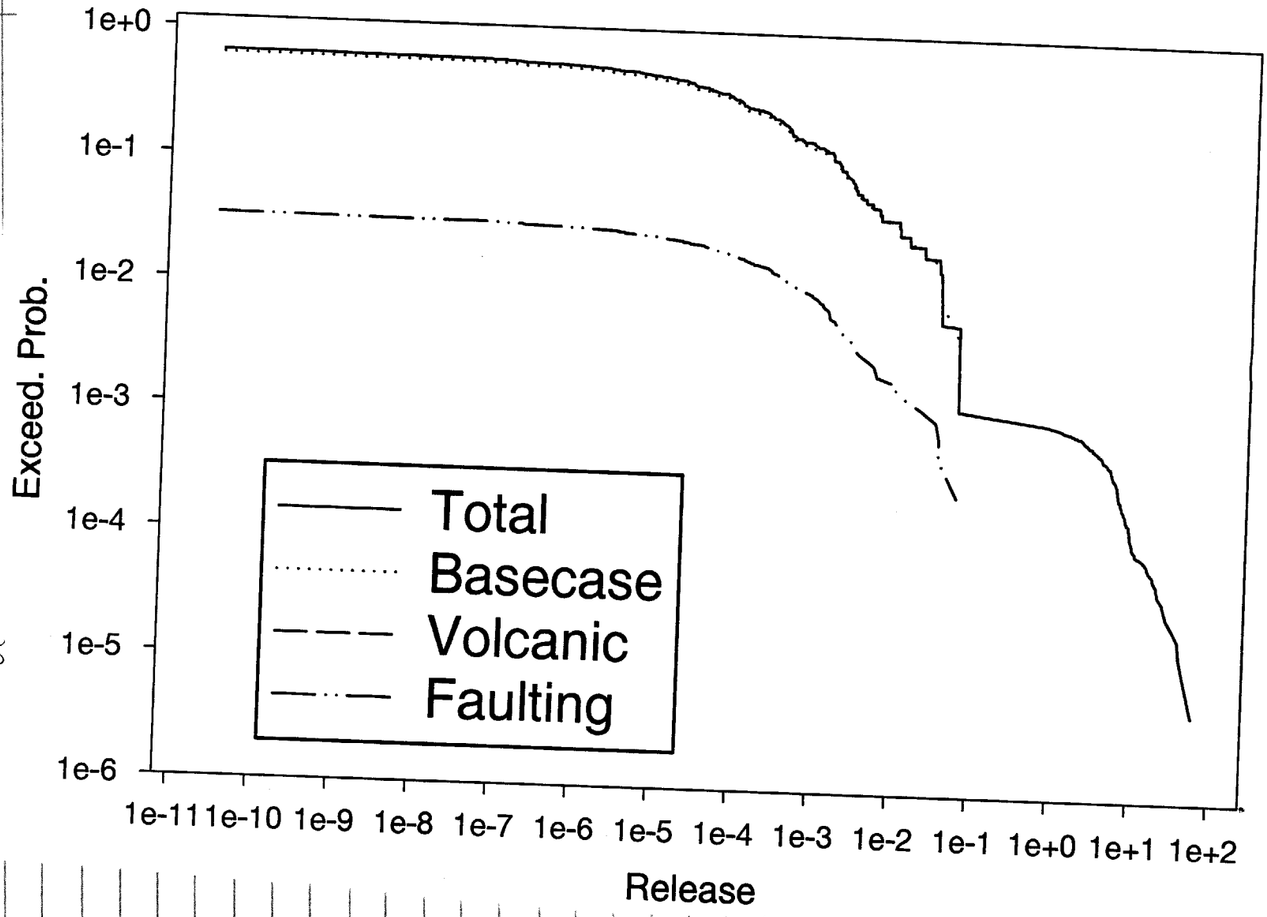
50000 yr test
Compared mean values with those calcula earlier. Mean value appear the same.

	basecase	volcanic	faulting
Mean values:	0.016464	0.67	0.016752

value same as on pg 51 of this notebook
edited tccdf.f is in ~jbogan/TPA313/ccdf

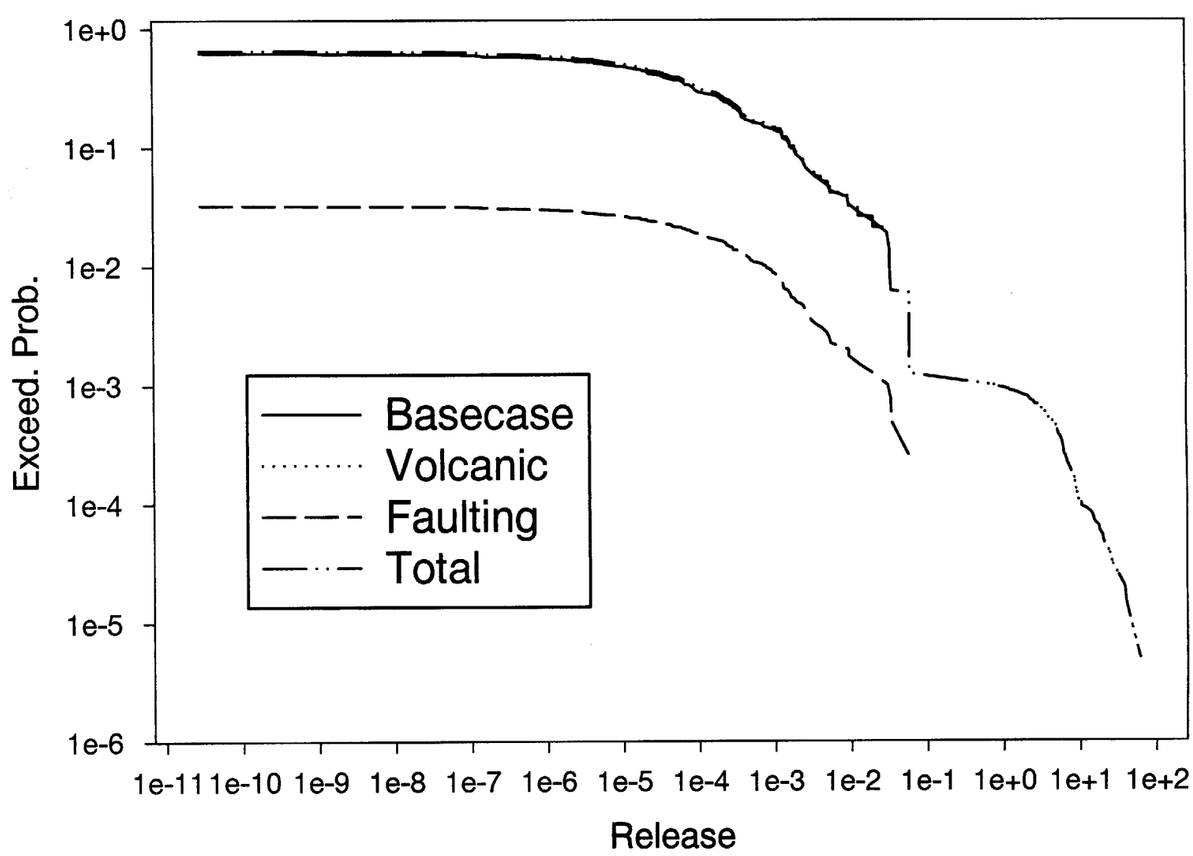
Visual Comparison reveal that these two are the same

Test 10000 yr - Automatically computed CCDF's



MAR 16/98

Test 10000 yr - Manually computed CCDF's



MAR 16 1998

Compiled nefmks.f 3.1.3 for Windows NT / Intel and UNIX / Sun Solaris on respective platforms. There had to be some editing done on the nefmks FORTRAN program in order for it to run properly. It was compiled with the make file writen from the original PC port of TPA 3.1.1 with minor modifications. The UNIX version was timed with a stopwatch and executed with the time command. The NT version was just timed with a stopwatch. UNIx numbers represent average performance with only one other major program running at the time and some 4 other users at the time. The NT version had two other programs running in the background. THis was tested to determine if the other programs had any significant effect on the performance and times were 5% quicker with no other programs running in the background. The nefii.inp file was editted in order to alter the execution times and computational effort. The difference in velocity between legs has a strong influence over execution times. The recorded times are below

	UNIX - BigBend				Windows NT - 200 MHz MMZ Intel
Test	Actual time	%CPU	user	system	Actual time
TEST 1	3:46s	39%	92.0u	0.0s	3:53s
TEST 2	11:48s	46%	324.0u	8.0s	14:40s
TEST 3	0:41s	26%	11.0u	0.0s	0:40s

TEST 1 - Velocity in legs
leg 1 - 0.157E+03
leg 2 - 0.779E+02
leg 3 - 0.187E+04

TEST 2
leg 3 - 0.477E+04

TEST 3
leg 3 - 0.477E+03

MAR 19/98

TEST OF REPETITIVE INPUT/OUTPUT
results of time repio.e
FORTRAN PROGRAM repio.f.

	Machine	User	System	CPU%	Actual
	skippy	24u	6.0s	46%	1:06s
	goliath	31u	3.0s	38%	1:04s
1st run	bigbend	14u	1.0s	25%	0:59s
2nd run		21u	0.0s	28%	1:14s
1st run	PC	—	—	aprox. 99%	20sec
2nd run		—	—	99%	21sec

```
c Program: Repetitive Input / Output
c Purpose: To test the input and output functions effieciency
c
c234567890
      program rep
      character*8 repstr
      real*4 repreal
      open (UNIT=1, FILE='repio.dat', STATUS='UNKNOWN')
      do j = 1, 40
        do i = 1, 10000
          write(1, 9000) 'Test: ', 3.2432525e20
        end do
        rewind(UNIT=1)
      end do
      close (UNIT=1)
      open (UNIT=2, FILE='repio.dat', STATUS='OLD')
      do j = 1, 40
        do while (.true.)
          read(2, 9000, end = 20) repstr, repreal
        end do
 20     continue
        rewind(UNIT=2)
      end do
      close(UNIT=2)
 9000 format (a10, e16.7)
      end
```

May 25/98

COPIED FILES FROM

/bscr3/mohanty/A-tpa3.2dev/

TO DETERMINE ANY PROBLEMS AS GAP FRACTION APPROACHES 1.0000 SOME RESULTING VALUE BECOME NEGATIVE THAT ARE NOT NORMALLY NEGATIVE.

COPYIED TO

/bscr3/jbogam/releaset_neg

---

releaset.f ebsrel.inp

RELEASET.F POSSIBLE ERRORS

- does not appear to add up and check that the addition of WP affected is not greater than the total number of WP. It will, however, check that individual numbers are not greater than the total i.e. idefect = 2336, if Total WP = 2335 will yeild an error. This actually works properly but there is no indication when a number is eliminated after corrosion failure - If event occurs after corrosion failure (all packets fail) then the value is set equal to zero with no warning.

Problem with negative values in releaset.f results were corrected with the last update mentioned before on (p 60)

Read over code - go to attached code for (tpa development directory) details (releaset.f) To gain information on the behavior of output ran a series of tests

---

Tested ranges of parameters for releaset.

~~peak~~ Base case 1 has seism3 = 2335 WP fail (All fail)

is the basecase
changes done one by one eg. flow factor 0.91 changed to flow factor = 0.2 and executed releaset.f.

Altered values in ebsrel.inp one at a time by a factor of ten in each direction if possible with some variation to test robustness of releaset.f. Values for the basecase are given on the next page (p 62) A single parameter was changed in each case, releaset.f executed, then the basecase was copied to the input file and another value was changed. A file containing all release rates over time for I-129 with 50% gap fraction specified was kept for each run. This (I-129) was used for comparison as it is a simple nuclide with no daughter products

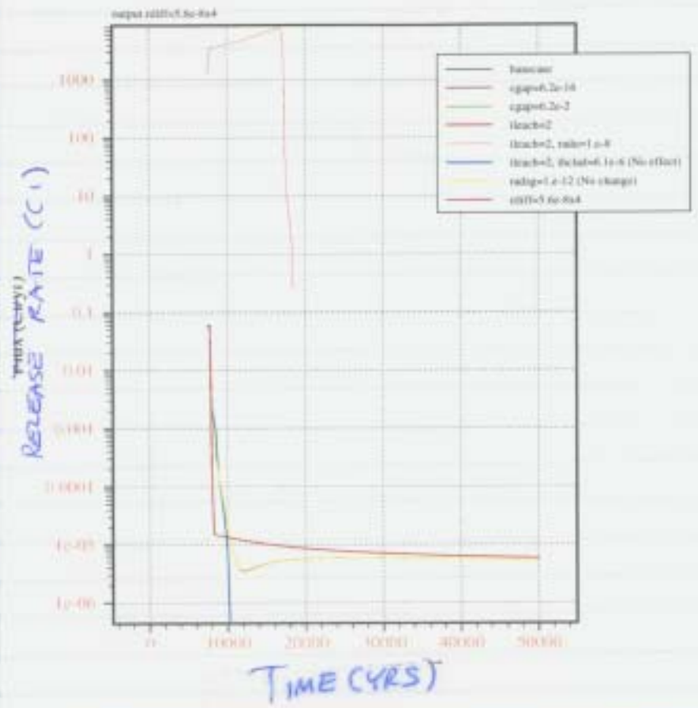
(ebsrel.inp)
basecase data file for releaset.f

```
\input data file for ebspac release code in tpa: releaset.f
|
\Cell information
2335., 1.0, 0                    ! xcon: # of WP; sawetfrac: wetted subarea; bathflow: flow model
0.        0                      ! defect,idefect:  initially defectime time [yr] & WPs affected
4500.     0                      ! sftimef,isconf:  faulting failure [yr] & WPs affected
3800      0                      ! sftimev,isconv:  volcano fail time [yr] & WPs affected
1000.     0                      ! seismt1,seismp1: first seismic failure time [yr] & WP affected
3500.     0                      ! seismt2,seismp2: second seismic failure time [yr] & WP affected
7500.     2335                   ! seismt3,seismp3: third seismic failure time [yr] & WP affected
15000.    0                      ! seismt4,seismp4: fourth seismic failure time [yr] & WP affected
|
\WP information
1.421, 4.572                     ! dintl: wp ID, xintl: internal length [m]
4.83                             ! xvol: wp internal vol[m3]
|
\Thermal data
'ebstrh.dat'                     ! temfil: temp. file (output from ebspac_fail.f)
97.                              ! ctemp: BP of water at atm. condition [C]
|
\Flow parameters
'ebsflo.dat'                     ! hydfil: flow parameters file
1.0, 0.9                         ! fmult; fow: fraction of flow into the wp
|
\SF  materials
\
9760.                            ! amassc: SF mass per WP [kg]
10600., 1                        ! fueden,ileach (1:particle,2:grain)
\
\Fuel leaching model paramters
5.e-1                            ! wetfrac(1): ht. fraction of wet SF in initially def. WPs
5.e-1                            ! wetfrac(2): ht. fraction of wet SF in faulting failure WPs
5.e-1                            ! wetfrac(3): ht. fraction of wet SF in volcanic failure WPs
5.e-1                            ! wetfrac(4): ht. fraction of wet SF in seismt1 failure WPs
5.e-1                            ! wetfrac(5): ht. fraction of wet SF in seismt2 failure WPs
5.e-1                            ! wetfrac(6): ht. fraction of wet SF in seismt3 failure WPs
5.e-1                            ! wetfrac(7): ht. fraction of wet SF in seismt4 failure WPs
5.e-1                            ! wetfrac(8): ht. fraction of wet SF in corrosion failure WPs
2                                ! imodel: leaching model
9.0, 0.2, 2.e-3                  ! phvalue,oxgnovpr [atm]; cco3 [mol/L]: used if imodel=1
20.1                             ! usrlrate:[kg/yr/m2]: used if imodel=3
|
\ Radionuclide inventory
'ebspac.nuc'                     ! elefil: nuclide names, halflife,inventory
|
```

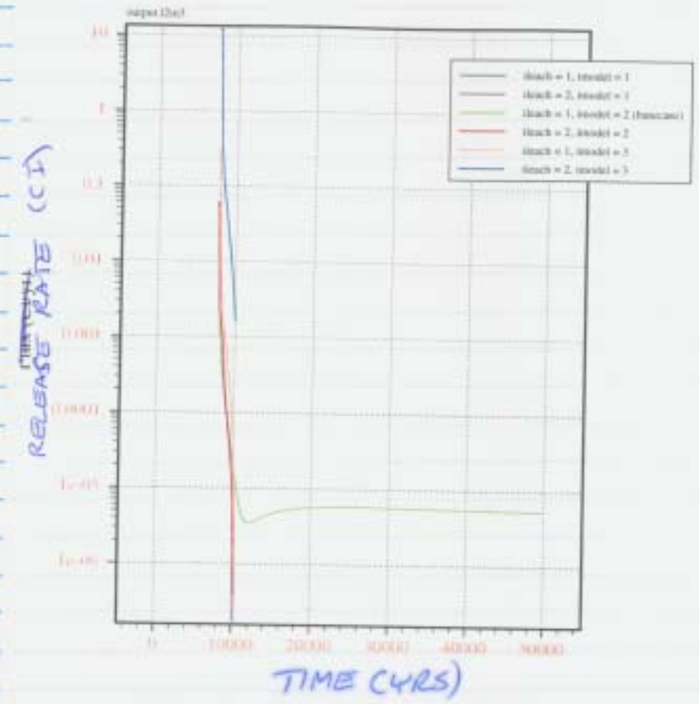


```
\C-14 generation
.5e-3                            ! r0z: initial radius of SF particle [m]
1.e-5                            ! radu: radius of the SF grain [m]
1.e-6                            ! radsg: subgrain fragment radius after trans. frac. [m]
5.e-3                            ! claddingcorfact: cladding correction factor
6.1e-4                           ! thclad: thickness of cladding [m]
7.2e-4                           ! cfuel: C-14 [ci] /kg SF
4.89e-4                          ! czmetal: C-14 [ci] /kg SF in Zyr. clad & other metals
2.48e-5                          ! czoxide: C-14/kg SF in initial Zry oxide & crud
6.2e-6                           ! cgap: C-14/kg SF in grain and gap
|
\NUMERICAL
\
\Grids
10, 10                           ! imax,jmax: # of grid nodes in i,j directions


\X-COOR of grid nodes
.1, .5, 1.0, 2.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0
\Y-COOR of grid nodes
.1, .5, 1.0, 2.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0
\ Note: zones apply to the above grid, zones are the same for all cell
\ZONES
4                                ! nzones: no. of zones for material types
1    1  1    1  1                ! iz,ib,jb,ie,je: for zone 1
2    2  1    2  1                ! iz,ib,jb,ie,je: for zone 2
3    3  1    3  1                ! iz,ib,jb,ie,je: for zone 3
4    4  1    10 1                ! iz,ib,jb,ie,je: for zone 4
|
\Rock parameters
0.14, 0.14, 0.14, 0.14           ! rpor(1..nzones): rock porosity
|
\ Radionuclide transport
5.6e-5, 5.6e-5, 5.6e-5, 5.6e-5   ! rdiff(1..nzones):diffusion coef. [m2/yr]
5.0                              ! driftdia [m]
|
\ Solution algorithm control parameters (Runge-Kutta)
25., 0.0, 10.                    ! dtinit [yr], dtmin [yr], dtmax [yr]
1.0e-2, 1.0e-10                  ! eps, tiny
|
\output parameters
200                              ! nbt: number of time intervals for output
|
\END
```



The basecase is shown in gellow/black
These were cases in which there was
some question as to weather the parameter
had any effect on the release rate
All values before the release of nuclide
at the failure due to seismic event 3 are
zero, and do not appear on this log graph.



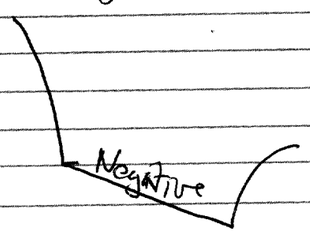
In those cases all combanations
of leaching and particle/grain models
were tested with the basecase
parameters

There is consern regarding the slight dip shown in the basecase as it drops and athen rises in release rate Certain parameters where shown to increase this effect.

These are as follows.

cladding correction factor (claddingcorfact)
radial diffusion coefficient (rdiff)
radius of particle (rOz) in leach 1
(radu) in leach 2

where the is a sharp dip a ~~the~~ recognizable pattern along in the release rate roughly shown as the following:



This maybe due different releases initiating i.e. liquid release because of advection dominated release with a transition to diffusion dominated or increase contribution from diffusion Advection dominated

6

Summary of the Testing for TPA 3.2 Beta version

June 11, 1998

1) Imodel = 4, compared result from a test done with Imodel = 2, to observe the differences in the implementation. Read over code to look for observable errors. The effects of the IModel=4 are in the scientific notebook

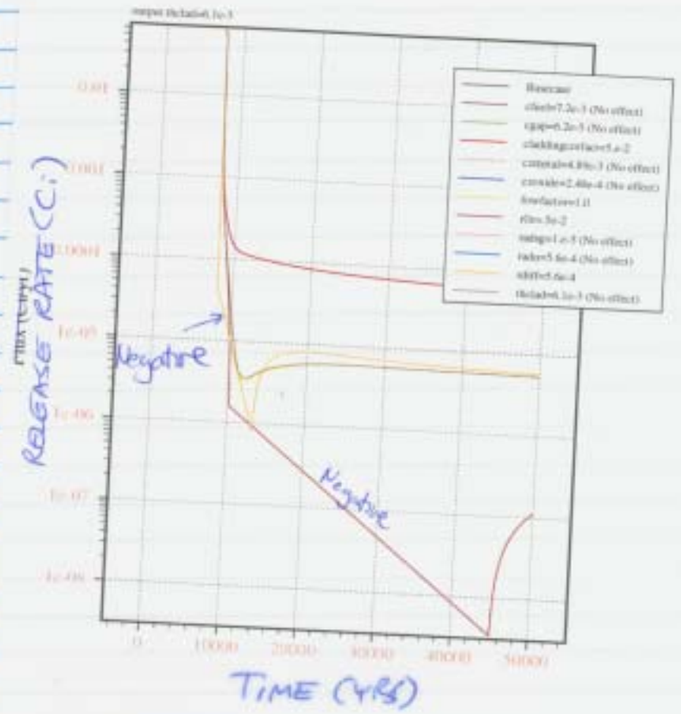
2) ebsfilt.f module - parameters transfered correctly. Checked that the variables that are derived from other variables are calculated correctly. Performed a sensitivity analysis on the values input into the top line of numbers in the esbfilt.inp file. For a 3.2 m thickness layer of cementitious material there will be no release under the flow conditions in the basecase tpa.inp file, in the 50000 yr time span specified in the tpa.inp file. The release is assumed to be delayed to such a degree that the release does not appear in any large quantity in the given time span. For thinner layer however there will be release in the 50000 year time span, for instance for a 0.3 m thick layer.

3) Aqueous release of gap fraction - tested the transfer of variables to the releaset.f module. Generated output for 5 different gap fraction and looked at the results and the intermediate files for signs of reasonable values. The tests showed no sign of error in the files. From 0.001 to 0 to 1.0.

4) Initially defective time specified in the input file. Tested with various values, from 0.0 to 1.0 for the fraction of Wp initial failed. and value for time of initial failure from 500 to 30000. Tested initial failure that occurred after corrosion failure with no errors or unresonable results. The other test were various in nature. Checked to see if the case in which all events occur at the same time effects the initial defect.

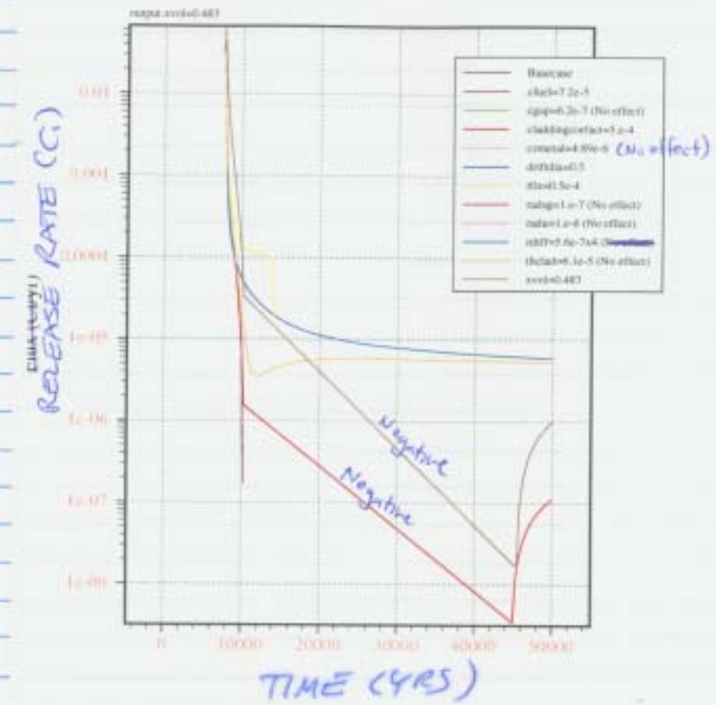
The procedure for all testing was to, as much as possible, start with the tpa.inp file and alter the values in that file. Repetitive testing or testing derived parameters, were the only cases in which this procedure was not used. In that case one run if tpa code was performed and then any alteration were performed on the files. The information in the ebsrel.ech and ebsrel.rlt files were examined in the case of modules. The standalones were examined through the inp and dat files that are used to interface with the exec code.

- J. Bogan



Increase factors by ten

Higher diffusion ~~rates~~ coefficients resulted in the sharp transitions but average values were similar



decrease factors by ten

May 27/98

output files from releaset.f

Unit	file	array in releasetf
21	cumc14.out	ttemp sumc14
28	cumrelease.out	tregular, cumrelease(1-) for chn=4, ni=5
29	dignostic.out	ttemp, xnoloss, amwp, xmas
1	echo_release.out	selected data.
27	frac-relrate.out	tregular, fracre
23	mv1000.out	ttemp ci1000
22	ratec14.out	ttemp, c14rate
25	relcum.out	namall, halflife, xnoloss, amwp, xmas
24	relfrac.out	namall, tregular, maxrel
26	trelease1.out	ttemp, xmas
40	maxrel.dat	namall, timrel, maxrel
20	ebsnef.dat	tregular, fracre

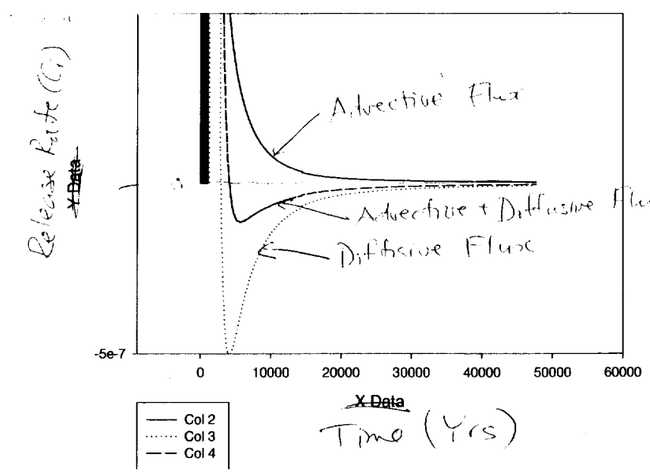
June 2/98

RELEASET.F: An explaination for the dip after peak and negative values in ebsnef.dat

There was some concern over a decrease in the release rate after the initial peak caused by release due to a failure. There was some indication that immediatelly after the release due to failure the release rates decreased then increased gradually again. The cause for this was assumed to be correct behaviour but, cause for some concern because there are some indications that the release rate actually reverse themselves and nuclides flow back into the ebspac zone. To determine the exact cause, the source of the output was traced back into the code and the arrays dumped into a file. The release rates for the parameters for TC99 are shown in the graph.

Release rates consist of advective flux and diffusive flux which are added together to obtain the release rates. They are determined in subroutine derivs. These passed back to odeint at the intervals on the time steps as a block values with in a larger array which contains other information on the flow and release rates. The release rates from all events are combined, units are converted from kg to Ci, then values are determined for regular interval specified in the ebspac.inp file. These are then output to ebsnef.dat file in column format.

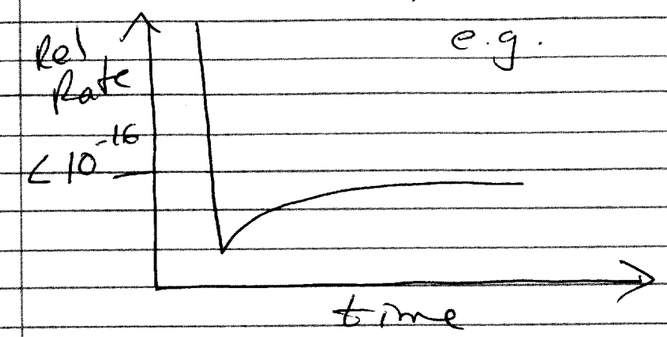
The negative values, although unusual, are consistant with the mathematics that are used to determine the diffusive flux, which is a movement of a solution following a negative gradient. If there is a higher level of nuclides outside the waste package and the resulting diffusive flux is greater than the advective, then there will be a migration of nuclide back into the waste package. If this is decided to be a unreasonable or unrealistic that may cause problems in other modules, then there should be some check for negative values that automatically sets the value to zero in that case.



The case of these negative values there are values in the ebstel.inp file that yeild negative values. There may be an implicit assumption that is being violated as diffusion coefficients increase. This should be investigated - ~~or~~ In the interests of time the diffusive flux term in the code may be elimated if this is felt to be the case, until such time as this can be thoroughly researched.

June 2/98

In releaset.f
Explaination of other dip - small (notch) in cases of very low diffusion



line 2087 (or thereabouts)
If amass(ielem) ~~greater~~ less than 1.0E-20)

ccfr = 1.0E-20

ccfr is used to calculate adflux

ccfrd = ccfr * vwnow/vfull

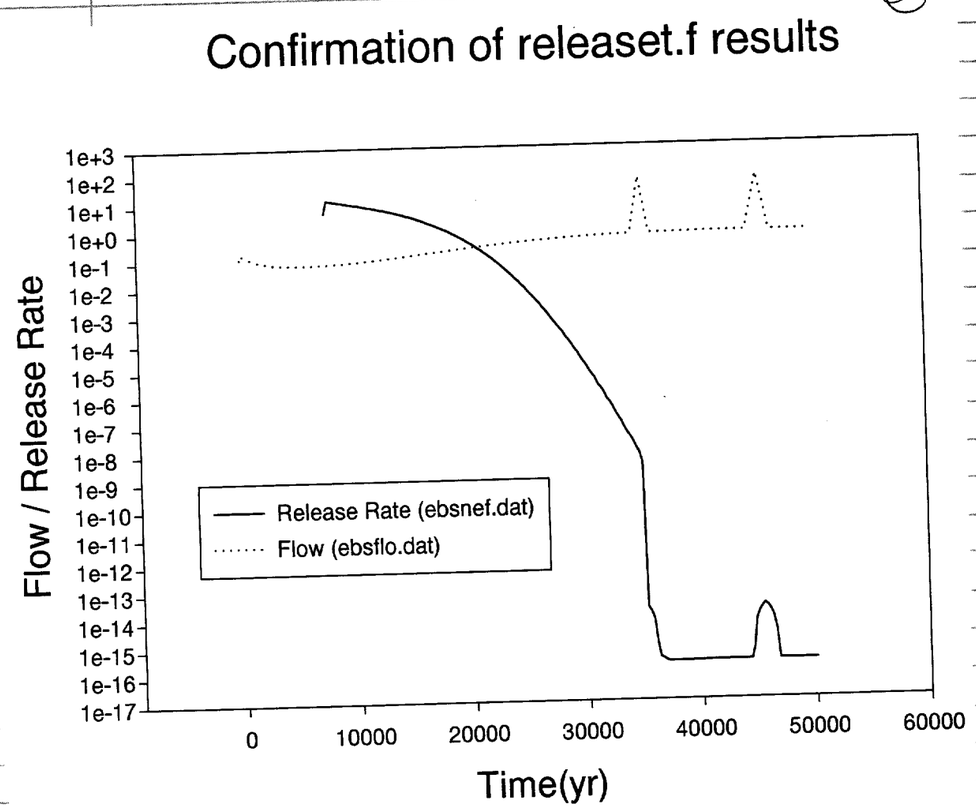
adflux = ccfr * qout

or. adflux = 1.0e-20 * qout.

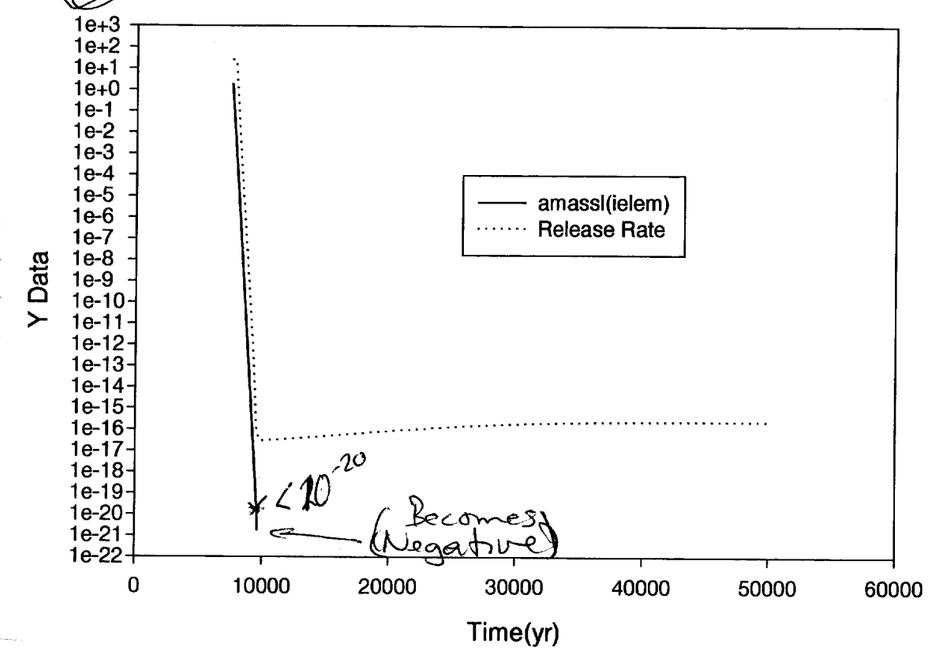
at low diffusion rates.
Therefore ~~the release rates are~~ flux is a constant ~~multiple~~ factor times the flow rate through the waste package.

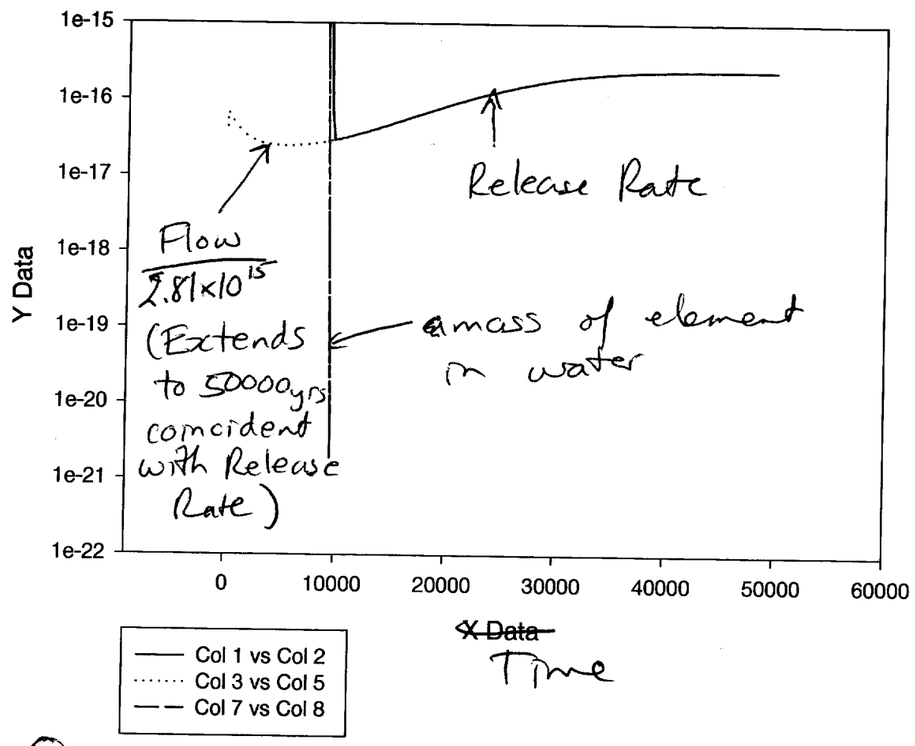
June 3/98

The conclusion that there are ~~constant~~ constant values being ~~factored~~ by the grout to produce low values was confirmed by adding spikes of larger flow in the ~~ebsflo.dat~~ ebsflo.dat file and observing these spikes in the resulting graph of the ~~flow~~ release rates



amassl is the total mass of the specific element in the water. More convincing proof of this can be shown in the following graph as the dip occurs as amassl becomes less than 1e-20.



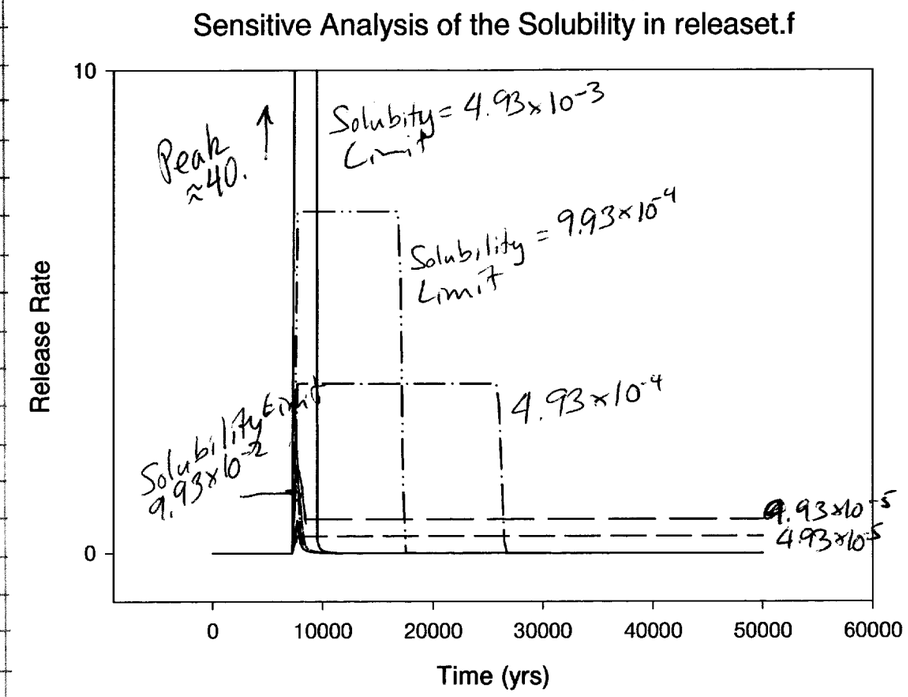


The flow rate as taken from ebsflo.dat was plotted then factored by a constant that would match the values at 50,000 yrs with the release rate, so at least values at 50000 would be coincident. It can be clearly seen that as amass1 of the nuclide decreases below 1.0×10^{-20} release rates change from a factor of amass1 to the flow rate in the WP.

June 4

6

limit



run3 - imodel=3 (usrlrate)
rund - Diffusion
runevent - time and number of WP failed for all was tested
runf - Runs with the code altered - the name given is a variable name in the releaset.f code
runfr - Flow rate
rungap - Gap fraction
runi - solubility limits
runk - imodel=3, usrlrate
runlm - leach model
runn - various runs performed with higher extremes
runs - values smaller by a factor of 10
runu - values larger by a factor of 10

odeint returns nbad=23 indication of step size change for numerical solver.

description of derivs subroutine in releaset and varidble, dydx and its organization.

~~derivs~~ dydx currently is containing 4 separate blocks of data

n nuclides examined

dydx(1) = net change in flow

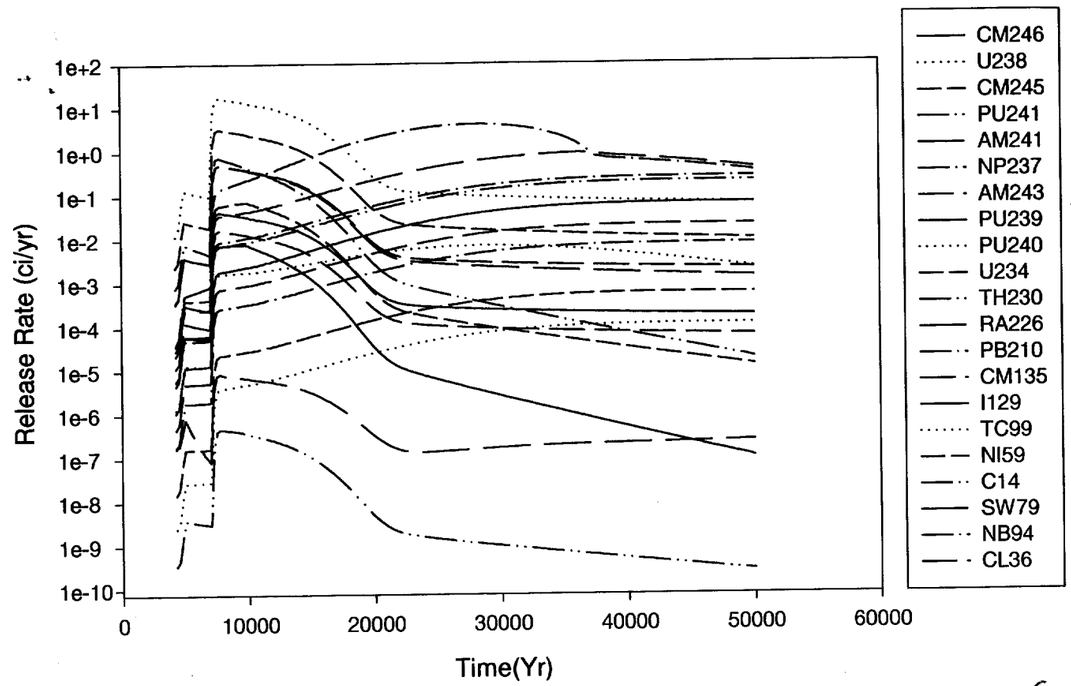
dydx(n2, n≠2) = rate change of mass of nuclide in wp including leaching, decay, decay of any parent, advective flux, dispersion flux

dydx(, n≠3) = rate change of mass of nuclide in wp including decay, decay of of any parent, advective flux, dispersive flux

dydx(1, n4) = rate change of mass of nuclide in wp including advective flux, and dispersive flux.

Sure 7

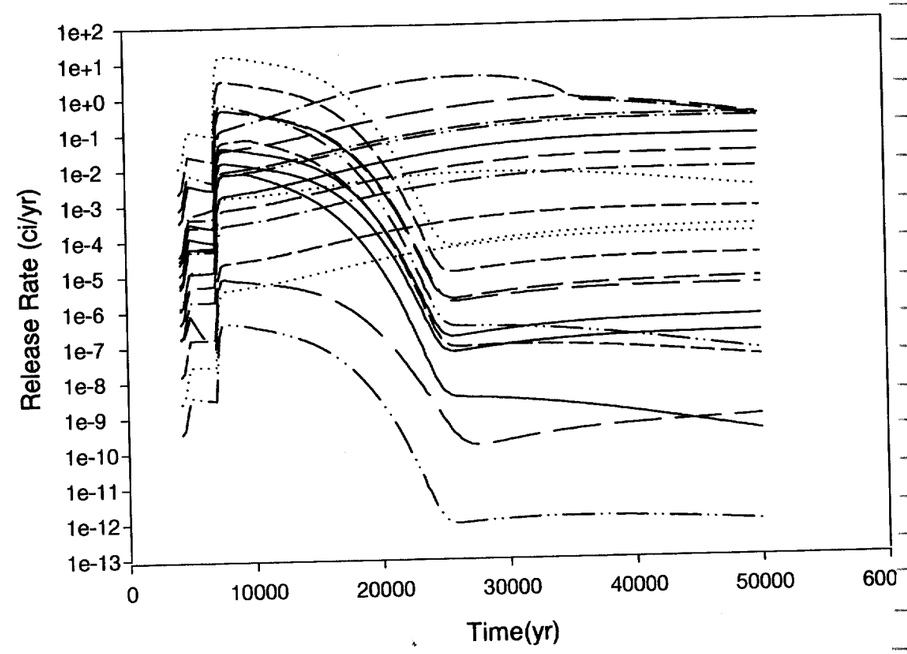
Imodel = 2 (without PU238)



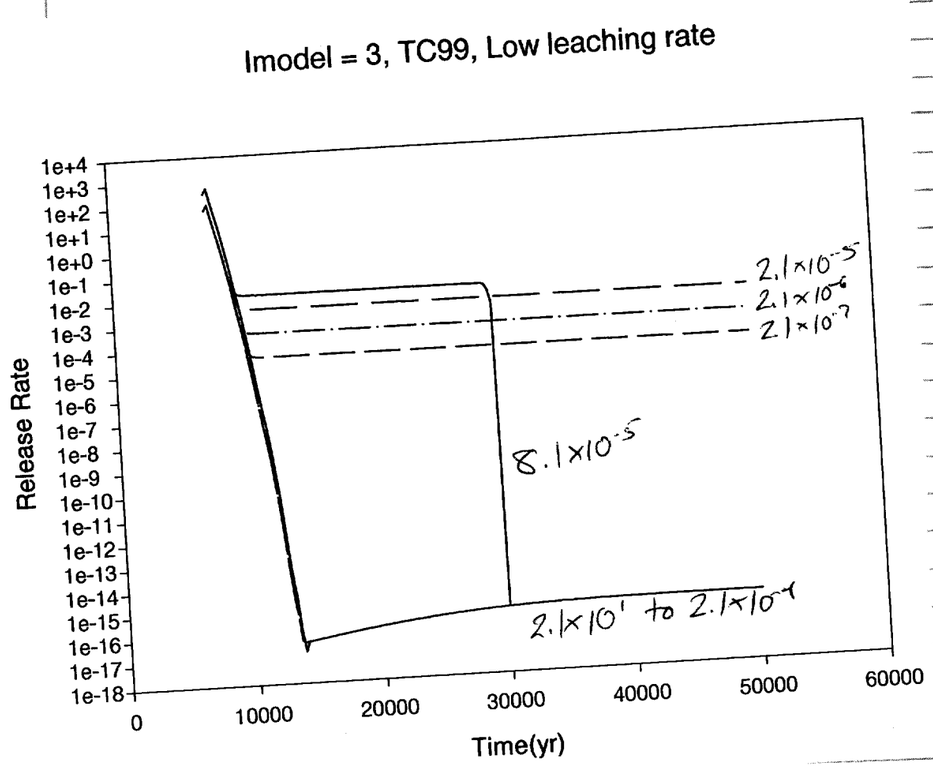
The effect of the newly implemented Model 4 is shown here. Pu 238 was excluded because it had very small amounts and distorted the semi log plot

6

Imodel=4 (without PU238)

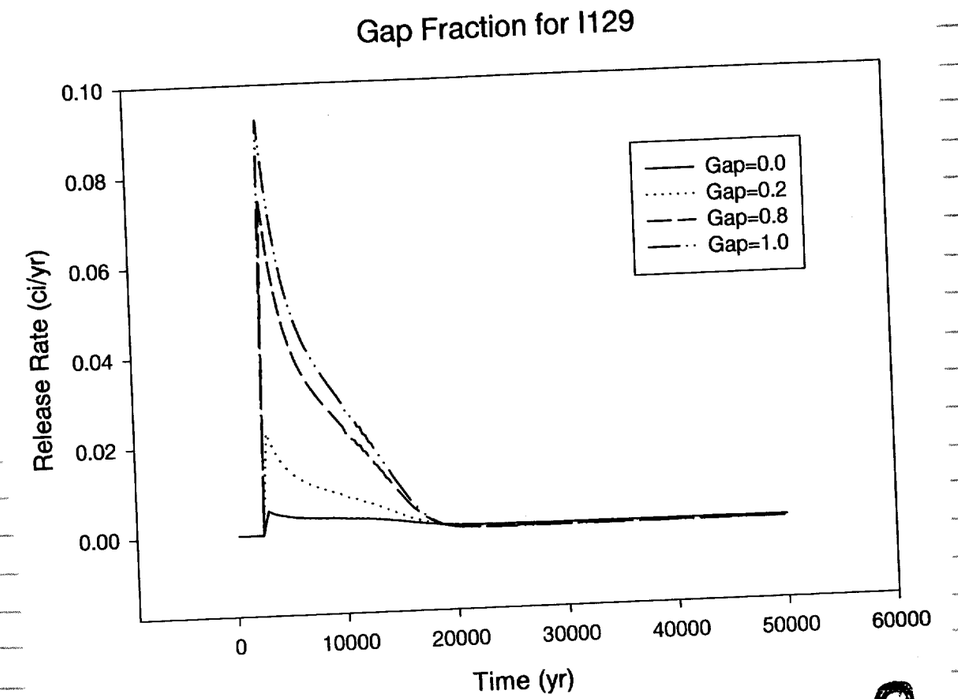


The trend here ~~is to~~, for the parameters used ~~on~~ page 62 and 63 of this notebook, ~~was to~~ is apparent in the above plot. In general there is a change in the plot, therefore, without specific knowledge of the principles involved the most that can be determined is that there the switch is operating correctly.



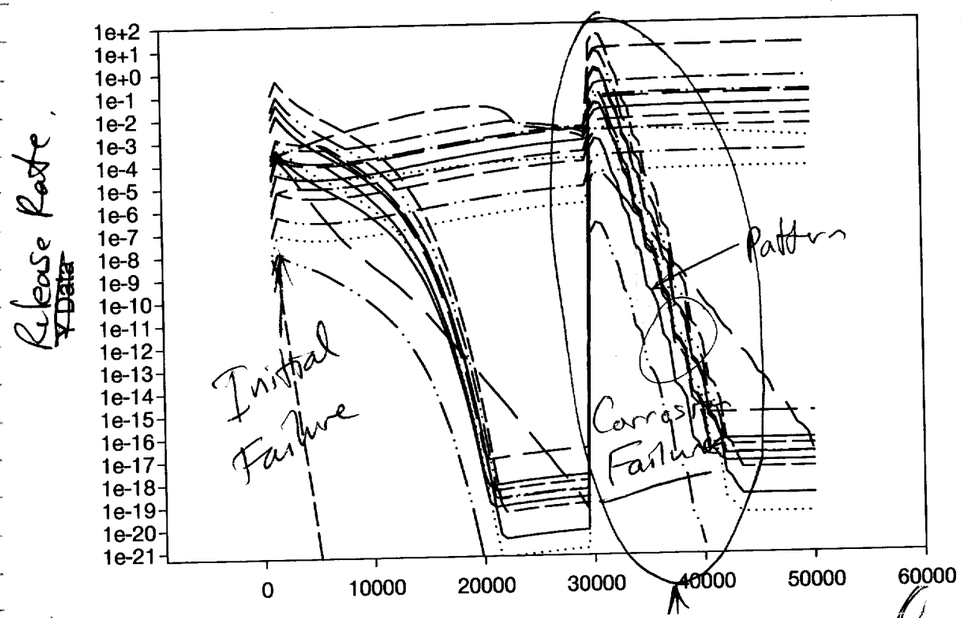
Low leaching rates were tested
Note the transition between quick exhaustion of the WP and a continuous flat release at low leaching rates. at leach rate 8.1×10^{-5}

June 10, 98



Tested gap fraction for Release.

June 10



There is a pattern that occurs in later releases. This is ~~probably~~ an effect of log plot with linear interpolation occur at the larger time steps, not an error.

Bug report

If the initially defective Faction of Wp / Cell is set to 1.0, Then any non-zero value input into the Initially Defective Time is ignored and zero is used. This can be confirmed by setting up these parameter as described and then examining either the ebsrel.ech file or ebsrel.inp for for the Time of initial failure.

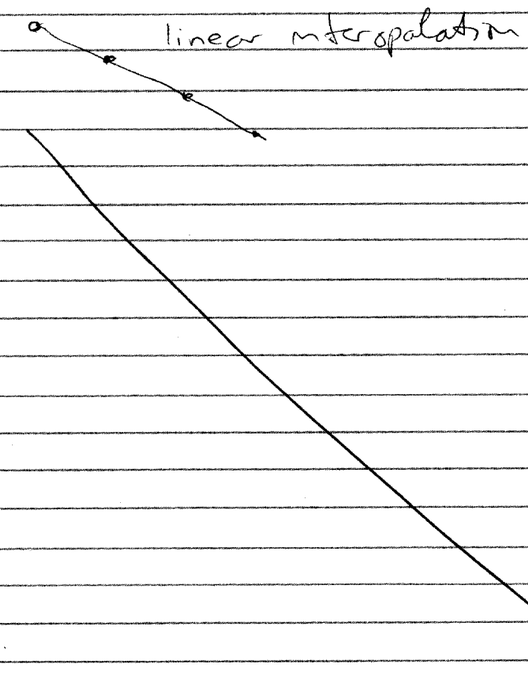
June 12, 1998

1) The ebsfilt.def file should be eliminated as it only is used for the title line. This could be quickly and simply outputted as a line of text from the ebsrel.f code. This would be an improvement over the current design.

2) Standalone was tested by compiling it with the Makefile in the codes directory. The executable was then deleted and the tpa program then produced a file io error when run.

- J.Bogan

Explanation.



Changed values in ebstch.dat to values that are ~~do~~ randomly placed and releasetf mentioned that Runge Kutta step-size is too small, but continued with the run. This can be observed by cp'ing

Sm

I am submitting this scientific notebook to QA because Jeff Bogan does not work with us anymore. This submission fulfills the recent call for submitting the scientic notebooks not currently in use. However, I will need in the future to ~~consult~~ use/refer to this volume for gathering information relevant to the TPA code development.

Sitakanta Mohanty
2/07/2000
Sm

This notebook has been prepared in conformance with CNWRA QA procedures except on pages 24-28 in which entries were made in pencil.

Gordon Wittmeyer
2/8/2000