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Scientific Notebook # 225

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John Walton

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Title - Debugging of TPA and EBSPAC codes

John Walton

Objective: Find bugs and general problems with above codes. Suggest fixes when possible.

Technical Approach: Stress code to produce limiting cases with known trends. Observe if code produces correct predictions

Codes: Use current version of codes as provided by R. Rice or S. Mohanty. All changes in permanent code are to be made by others.
TPA 3.1 beta

6-16-97

ebspac code on OS2 machine telnet to
big bend

stty erase ^H

begin editing "ebspac_fail.inp"

what is nset ?, = 12 table lookups for thermal loading
scenarios based on another code
Cntr - Esc bringup window list on OS2

setenv DISPLAY 129.162.200.191:0.0
cmdtool &

x5255 Wes Computer Lab

ebspac_release.inp
notice that initial Range Kutta time step
is > maximum time step

what is 2D grid system for? why does not
2-D grid match drift diameter? why is
it < container radius?

shut down advection
play with code, change funnel factor to 0.9 → 0.0
- no impact on corrode.out & there should be none

rel~~cum~~frac.out - this ~~moved peak releases~~ did not change
- because I ran code wrong JW 6/24

⇒ all releases went to zero

changed funnel 0.9 → 0.3, caused high
solubility nuclides to increase, low solubility ones did

hot change

funnel 0.9 → 0.01
for I129 the time increases but the peak is almost the same

	I-129	t peak	PFR	
funnel	0.9	0.3850 E+4	0.3948 E-4	
	0.01	0.95 E4	0.3952 E-4	
	10^{-6}	no releases		
	10^{-5}	no releases		
	10^{-4}	no release		
	10^{-3}	no release		
	10^{-2}	same as above		
	10	0.375 E4	0.4051 E-4	dissolution limited
	100	0.3750 E4	0.4051 E-4	

diffusive vs advective transport

rdiff

rdiff 5.6 E-5 → 5.6 E-4 $\frac{m^2}{yr}$

small changes in rel frac, out

rdiff → 0 exponent - does not finish
rdiff → 5.6 E-9 $\frac{m^2}{yr}$
in rel cum, out there is very little change
indicating diffusion is not important in the base case

rdiff → 5.6 e-1

saturated D ~ $10^{-9}\frac{m^2}{s}$ → $3\times10^{-2}\frac{m^2}{yr}$ → upper bound realistic value

* took a long time to run code, releases went up greatly for low solubility ones, only very slightly for high solubility ones

output intervals

200 → 20 gave no change in cum rel, out

boiling point of water

97°C → 87°C all reduced significantly

WP
2335 → 5000 more than doubles releases but fractional does not change

a mass: amount of spent fuel per waste package
8800 → 2200 no change
8800 → 0 code gave error but ran & gave strange results
8800 → 1 no change

- must not be used much
8800 → 0.001 no change

10^{-6} → no change
10^{-22} → no change
10^{+22} → no change

* how is this used ??

Runge Kutta Parameters
dt min 25 yr → 10 yr
no change

dt max 10 → 100 minor changes in 4th digit, ran in less than ½ the time.
dt max 10 → 1000 no change from 100 yr run dt

dt max → 1000yr & eps 10^{-2} → 10^{-1} & dt ini → 10

run a little faster & essentially same answers

Will set eps back to 10^{-2} but
leave faster RH settings in code

---

move to ebepac__fail.inp file

---

* tim into 49.99$\bar{9}$ → 100
slightly lower releases

49.99$\bar{9}$ → 50 gives 4th significant figure
changes, small, but ~~to~~ much larger
than it should be JW 6/24
clearly code write should know why since
49.99$\bar{9}$ was ~~[illegible]~~ baseline value

cthickl 0.1 → 0.01 gives very
minute changes in cum rel out
indicates active corrosion

---

* ctemp - note ctemp occurs in both input
files
97 → 87 no change

---

humdc 0.65 → 0.95
releases reduced by ~ factor of 2

---

film thk
$2e^{-3}$ → $2e^{-4}$ no change
$2e^{-3}$ → $2e^{-0}$ takes much longer to run

releases reduced ~ factor of 2

---

nset 1 → 2 lower releases
1 → 12 lower releases

---

look at corrode.out file

humdc 0.65 → 0.25
corrosion begins at 139.9 °C
at a much lower corrosion potential,
the corrosion never goes active why??

this leads to much lower releases. why
does it not go active at 109 °C like
the base case ??

0.65 → 0.55 corrosion begins at 113.6 °C
never goes active

NOTE: had not set film thickness back to $2E^{-3}$
thick film led to low corrosion potentials

now repeat tests

0.65 → 0.25 both corrosion and failure
begin earlier

* 0.65 → 1.0 aqueous corrosion never begins

0.65 → 0.9999 no corrosion
→ 0.9 corrosion begins at 99.84 degrees
→ 0.95 corrosion begins at 98.25 degrees
→ 0.99 no corrosion
→ 0.98 no corrosion
→ 0.97 begins at 74.28 °C
→ 0.96 begins at 97.87 °C

this looks good

ctemp → 97 → 100
only very small change in corrosion potential
no change in corrosion start time

JW 6/24
97 → 120 gives same corrosion start time but second material drops E below critical potential

note that relative humidity is read from a file "temp humd.dat"; this precludes ctemp from being used for relative humidity calculations above the boiling point - some what inconsistent as its hard wired through the external data file

if tcan > ctemp use cl conca
else
use $\frac{\text{cl conca}}{\text{cfactor}}$ → cl conc near WP

cfactor =
ctemp = boiling temperature

See Eq 2-4 in EBSPAC Manual
Tb may not be same in internal & external codes

it appears that ctemp only influences when the Cl levels move from concentrated to dilute high ctemp → more dilute waste → lower Ecorr → slower corrosion

See eq 3-2 & 3-3 for role of amassc mass of spent fuel per waste package

alteration rate limited species should be proportional to amassc when flow rates are high JW 6/24
* - try increasing funnel and then varying amassc, perhaps with all initial defective containers.

funnel 0.9 → 1000

I-129 0.1020 E3

amassc 8800 → 0.001 funnel = 1000

I-129 = 0.1020 E3 - no effect

made a new ebs flo.dat file with constant higher flow rates
~~no change~~ JW 6/24
amassc 8800 → 1E-6 no change from new baseline

what are ileach and imodel

ileach = Eq 3.2 & 3.3

imodel = Eq 2-51, Eq 2-52, or constant

* the amassc variable cancels in the code, in effect it is never used and could be eliminated by change of variable

Fuel den $10600 \frac{kg}{m^3} \rightarrow 1 \frac{kg}{m^3}$

results very strange, solubility limited
ones do not change high solubility ones
have increased release and negative remaining
fractional mass

tried turning down eps $10^{-2} \rightarrow 10^{-4} \rightarrow 10^{-6}$
sequentially,

this lowered the mass balance error but it
is still negative fractional left for high
solubility

reduced max time step to 1 yr

still gives same 1% mass balance error

---

grid
* code takes a 2-D grid but uses only
the x direction as spherical r direction
the first dr is x coordinate #1 the
other dr's are from differencing the x coordinates

only D's at the first node and the
"marker" at the drift interface appear to be used

---

* sollay variable is not used in ehsf fail f and
should be eliminated

doubled water flow rate to $0.2 \frac{m^3}{yr}$ and
that doubled release of solubility limited
nuclides but did not change high solubility ones

reduce dry rate in file ebs.flo.dat to zero
→ gives very low release
now also reduce porosity to 0 at first x grid
node
- gives same very low release

took porosity back to 0.14 & raised
diffusion coefficient to 5.6 e-5 → 5.6 e-3

made no difference at all

changed flow to $10^{-10} \frac{m^3}{time\text{-}yr}$??
no difference

changed flow to 0.1 → now much release
changed initial failures 0.1 → 1.0
10^{-5} → same very low release

---

note: initial failures may have a problem
release code does not seem to do much
when all are defectives

will only initial wet fraction release?? ever?

Change to imodel = 3 and $10^{3} \frac{m^3}{yr}$ water drips

Sa wetfrac = ?? ~~scenario~~ wet fraction = wetted sub area
input from input file
tftc = maximum of WP failure time or
boiling point = max (tfail, tcool)

change # WP to 1

I-129 inventory = 0.2596 $\frac{Ci}{WP}$

output is 0.2441 E3 Ci with

remaining fractional mass of -0.007

xmass is cumulative release in Ci
sumrel is cumulative release in Kg

Xno loss = Ci of nuclide times xfrac * sawet frac = ~~[illegible]~~ Inventory * wetted fraction * wetted fraction of canisters in area

I 129 1054 Ci releases
10000 packages x 0.2596 $\frac{Ci}{WP}$ * 0.8 * 0.5 = 1038.4 Ci

sawetfrac wet frac

- Can the non-wet portion ever be released ?? - it should be

* - Why is there no release without drips?

Tc 99 release = 0.426 E6 Ci released

10000 packages * 108.24 $\frac{Ci}{WP}$ * 0.8 * 0.5 = 4.33×10^5

so this is close

* problem → wet frac should not limit total release since things can change & material can settle - it should just extend leaching time

I believe wetfrac works instead of x frac in above hand calculation because its $\frac{1}{2}$ aWD & geometry drops out

⟹ code is approximately balancing mass but there is a conceptual problem

⟹ the code takes the sawetfrac and xfrac back out of inventory when calculating cumulative fractional release, - it should not do this, the non leaching stuff is part of the inventory; must rename your CFR ~~if~~ or amount remaining if everything does not count (i.e.) only leachable material counts)

change drip rate 1 $\frac{m^3}{yr}$ → 0.01 $\frac{m^3}{yr}$

I-129 → 0.26 E+4
Tc-99 → 0.107 E+7

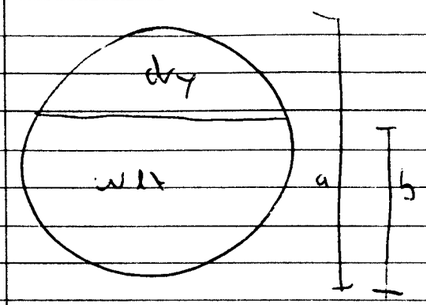
as per calculation on previous page the released is > initial inventory
* cranking eps down to 10^{-4} solves this problem

below after about 10^{-4} $\frac{m^3}{yr}$ of drip water the release calculation shuts down and only very low noise ??, numbers show up as release
run times are also much lower in the code

change to no release is between 3 and 4 $\times 10^{-4}$ $\frac{m^3}{yr}$ drip rate
U max = 2.415 this makes it look like there

is no diffusional release until
the container overflows
- not a good idea

the code is set up such that



wet frac = $\frac{b}{a}$

this determines the waste that can alter
and leach the dry stuff never
can leach

~~xvol~~ = void fraction = $\frac{xvol}{\text{total volume}}$

Vmax = total volume ?? * void fraction

⇒ making xvol low will lead to a
film treatment of leaching rather than
a bath tub except dry waste never leaches

* note major inconsistency - corrosion code allows
corrosion & failure from condensed water
but release code does not allow alteration of
spent fuel by condensed water - only leaching water
- fix by turning on routine earlier using
minimum water level

iflow = 1 means water overflows WP & allows
for diffusional release

tlt shuts off leaching using the "wu" switch
tlt = tleach + tftc = end of leaching time

tftc = max(tcool , tfail)

tleach = amount of time for fuel to all alter/leach

note: code documentation says wu keeps leaching
zero before tlt it actually sets leaching
to zero after tlt

fut is hard wired to 1.0 in a data statement

fut is defined in derivs
wleach is also in derivs

tests indicate that fuel can leach in place
and then pulse release

tried putting in no water followed by a
spike of water & it gave a spike release
but not a sharp one

---

now try setting SE & NB for tests
first make them the same

* * if scenario #s can not be met because of initial defectives (i.e. if # in scenario + # defectives > total # cans) then code fails & stops

this could be a problem with sampled variables

note: when code fails TPA may pick up the old output values if proper logic is not added to check for good finish - perhaps old output files should be deleted at start of TPA realization ??

* code will run with a negative value for scenario ~~conta~~ WPs

Examine run time vs wetfrac

0.5 → 2:11:9 user
released 0.94 E3 NB

wetfrac → 0.1 → 3:44:0 user
0.2575 E6 NB

wetfrac → 0.4 → 3:23 user time
released 0.346 E3 NB

---

repeat test after setting ebs fluid at to uniform high flow

wetfrac → 0.9 → 2.02 user time
0.3435 E3 NB, SE

wetfrac → 0.5 → 2:00 user time
0.93 E3 NB, SE

wetfrac → 0.1 → 1:57 user time
0.2556 E3 NB, SE release

** so there's clearly a problem with wetfrac in each case all the available stuff was released.

wetfrac
0.4 → 0.88 E2

0.5 → 0.24 E3

0.9 → xfrac = 0.137 | 0.184 for wetfrac = 0.9
0.13 for wetfrac = 0.1

next problem

TPA code 6-14-97

source for TPA cscherer/tpa_4st

note ebs_pac_release.f is inconsistent with geometry. It feeds 2-D cartesian but only uses x & converts it to r strangely x(1) = Δr(1) but other Δr's are taken from x(i) - x(i-1) it strongly determines edge of drift. Rd is a constant here so nuclides cannot be "sucked" from drift by high Rd but rock or cement

ps check ibs

changed I-129 to 100% gap fraction

changed U solubility to 1E-5

changed defectives from 10% to 95% then 100%

the jpa code runs correctly with 100% defectives even though ebsfail does not in stand alone mode - must have logic to handle defective + scan arr > total #

note that code gave an unacceptable mass balance error of -10% -100% for I-129
- looks like it released 2X total amount when gap fraction was high

release I-129 = 7.96E2 Ci/cell

with 100% initial defectives
currently gap fraction is 0.5
rerun to double check this # then change
Gap fraction for I & solubility for U

Cumrel.out

I-129	0.45E2 Ci/area	-0.13 fraction left
U-238	0.52E-3	1.0
U-234	0.14E-2	1.0

I-129 gap fraction 0.5 → 1.0
U solubility 1E-5 → 2E-5

I-129	0.79E2	-1.0
U238	0.104E-2	1.0
U234	0.385E-2	1.0

} looks good if doubled as it should

now increase U solubility to infinity (1000) and I gap fraction to zero

I-129	0.107E2	0.731
U-238	0.116E3	0.731
U-234	0.43E3	0.731

} mass balance error

** the problem seems to be that the alteration is subject to Xfrac, the fraction wetted but the gap inventory is not subject to xfrac, thus too much gap gets released
xfrac was ½ for the above runs so 100% gap lets it all out

Parameters are now set up for instant fail and rapid release with inodel = 3 and fast alteration rate.

✓ examine TPA screen output
* OK note: end of TDI annual dose GW pathway is > maximum dose GW pathway
note it
and it wrote this output > baseline during lunch

* note that underflow errors occur and are never cleared

changed areal average mean annual precip at start + 0.00001 mm/yr
and multiplier for precip at glacial max to 100

* note: one cannot change ebsrel.tmp, the template file that has eps & step sizerings
recommend eps → 1E-4 & maximum step → 100yr

this is generally faster & more accurate

Failed with parameters in UZ FLOW
and that made it hard to
get the code to run

WP failure at 7551 years (for zoo WPs)
for zone # 1
8640.8 yr for zone # 2

UZ ft now takes most of the time rather than ebsnef

** note that when I interrupt ~~ed~~ ebsfail code
run ~~at~~ after first cell the code continues
executing & probably takes the ~~next~~ old results
interrupt prior to first cell finish bombs the
tpa code

— bisbend bombed
changed Cl multiplication factor to 1.0
→ no corrosion failure in area # 1

in tpa2 directory I took all the
defaults and told it to do
10 realizations overnight in the background

in tpa1 directory running the Cl multiplier = 1.0
case; gives no corrosion WP failures

change multiplier to 1000

this makes the containers fail as soon as it wets

change multiplier to 0.0001 → no corrosion failures

What is sot nef.dat file, only has
1 sub area, it's say release
but appear to be cumulative release??

note that ebs nef.dat file contains
negative release rates for I-129
and TC-99
and some others

6/20/97

tpa2 run, used given input file with
10 realizations

* code failed on subarea 3/7 realization 6/10

subscript out of range in nefmks.f
line 9141, procedure trn spt
subscript number 1 has value of -2
in array rho
77 Error in UZFT <<
NEFTRAN failure, Status = 1536

* changed time period 10,000 → 100,000 yr
and re run simulation, this
gave an error message, must increase max events
so that one can fill time period of interest
with events - sample hazard curve

changed Number Of Time Steps
201 → 501
this gave error ntim > mxntime
⇒ can't change time period

* looking at density I find that the matrix grain density is generally < rock bulk density & this is impossible

$\rho_b = (1-\phi)\rho_s$

PTn has a grain density of only 1400 $\frac{kg}{m^3}$??

change to LHS sampling & turn printout to 1 from 0

* ⇒ code does not work with LHS

shut off LHS now only change is full output mode

* ⇒ code stopped with error
  Error in iget unit number
  iopen > maxunit
  iopen = 71
  max unit = 70
  need to increase size of maxunit

changed annual average mean precip from 1 to 10 ⇒ 0.1 to 1.0

* now the code runs 10 realizations OK

also changed time period to 100,000 yr and changed Seismic Hazard Curve 0.1 500 → 0.1 1000 to avoid array size problem

TPA source code

cp -r ~cscherer/tpamaster620/*

to get source code

make tpa to make tpa executable

in tpa2 directory trying to run 100,000 yrs
error
  Bus Error
  Error in U2FT
  NEFTRAN Failure, Status = 2560

tried resetting to 1 realization

- the code takes a very long time to run for 100,000 years, may not be viable
  ebs rel and uz ft appear to cause the problem

in tpa1 examining influence of initial infiltration rate → 0.0001 $\frac{mm}{yr}$

in tpamaster620 directory try reproducing the fatal error to check in NEFTRAN

NEFTRAN
KSC = ilast - ic

ilast is defined when subroutine adjb is called
it can be = IS2, NCMP
its a mess of a code, upped

the initial infiltration to 9 - 10 mm/yr
to try to face NEFTRAN failure

it looks like NEFTRAN fails on chain #5
ending in PB 210 PB 210 has
a very short half life, try increasing it to
a higher H
22.3 years initially

- the increase was over written

nefiyuz.vel = input water velocities to neftran

c ~~she~~ scherer / tpu_4st/

- trial a 100,000 yr run, got held
up in NEFTRAN unsaturated run, run
for ≥ 40 minutes CPU, finally killed it
in first sub area

* may have to place time limitations on code runs
neftran never can get through 100,000 yr
w/o excessive run times

* may want to eliminate Pb-210 it's in secular
equilibrium with Ra 226 anyway
so nothing is lost

6-24-97

tried Failing Neftran input Files

Couldn't fix ~~sa~~ negative subscript with Rd changes in Pb210

try changing ½-life exponent
2 → 3 → 4 → 5 → 6

"Subscript number 1 has value -2 in array rho"

message does not go away until half life ~~z~~ exponent is at least 10^6
$t_{\frac{1}{2}}$ = 0.22 E6

invent.f has all radionuclide properties

gave up on checking this because of machine operating system problems

John Walton

TPA and EBSPACK code testing results:

B= bug that should be fixed
S= suggestion or minor problem
W= appears to work properly

EBSPACK: Overall the code authors have done an excellent job of putting these codes together in a short period of time based on previous codes.

1. (S) In sample input file initial Runge-Kutta time step (25 yr) is > maximum time step (10 yr). Examined time stepping throughout the week and found that a) 100 yr maximum time steps give faster run times with no loss of accuracy (limited tests) and b) the eps parameter should be reduced from 1e-2 to 1e-4 to ensure good mass balance. Making both changes appears improve mass balance and increase run times.
de Jun 6/24

2. (W) Changed flow rate, funnel factor, alteration, and solubilities and examined cumulative fractional releases. This allows testing of a vareity of limiting cases where release is alteration controlled (high solubility radionuclides) and solubility controlled (low solubility) radionuclides. In every case the code worked correctly. Mass balance errors in the range of 10% could be obtained unless the eps parameter was reduced. Lowering the eps parameter to 1e-4 or less reduced mass balance errors to < 2%.

3. (W) Changed diffusion coefficients and flow rates to switch between advection and diffusion controlled release. The default diffusion parameters give insignificant diffusional release. The code appears to work correctly.

4. (S) Note that in the relcum.out file the fraction remaining is actually the fraction that can be released that remains - not the total fraction remaining. This is a bit misleading as it is assumed in the code that portions of areas and portions of containers will never wet and thus never have liquid release. The never released fractions are not counted in the fraction remaining.

5. (S) The variable amassc, the mass of spent fuel in a container is read into the code then multiplied and divided in a manner such that is makes no difference in the final results. This is misleading and it would be preferable to simply remove it from the code. Actual inventories are obtained from the ebsnuc.dat file.

6. (S) Changing the timintv variable from 49.9999 to 50 changes the output results in the third of fourth significant figure. This is a small difference but perhaps greater than it should be. Larger changes in this variable cause about the same change in results.

7. (W) Changing the humdc variable influences aqueous corrosion times in the correct manner.

8. (S) The ebsfail code inputs a two dimensional grid but actually uses a one dimensional spherical grid. The spherical grid is based on the x coordinates. The first x coordinate is the first delta r but the rest of the delta r's are obtained by differencing the x coordinates. The location of the backfill/rock interface is calculated in the code and difficult to determine by the analyst. This makes it difficult to change backfill to rock properties in the input file.

9. (S) Separate treatment of advection and diffusion is a hold over from SOTEC. It does not allow diffusionally released radionuclides to be flushed out of the rock and backfill during high flow periods. The diffusion should either be eliminated or coupled with the advective release.

10. (S) Only a fraction of each container is subject to wetting and release even at time=infinity using the current "bathtub" conceptual model. Since container corrosion continues over time, all mass on wetted containers should eventually be subject to release. It would be preferable to make all spent fuel subject to liquid release even with the bathtub model (perhaps by just increasing the release period subject to the fraction wetted. This option in the code can be effectively bypassed by increasing the wetted fraction to 1.0 and lowering the internal volume of the container. These parameter changes effectively switch the conceptual model from a bathtub to a dripping mode. The ability to switch conceptual models with input parameters is a good design feature in the code.

11. (S) The sollay variable is not used in the ebsfail code and should probably be eliminated.

12. (S) EBSPAC fails with an internal stop when the # of defectives + # scenario failures > total number of waste packages. The TPA code does not allow this to happen. EBSPAC could have some logic to handle this problem.

13 (S) The ebsfail code allows corrosion of the canister to begin when water can condense on the metal at relative humidity less than one. The ebsrelease code does not allow the spent fuel to alter until drips begin (and container has corroded). This is inconsistent. If condensed water can corrode the steel, it can also corrode the spent fuel. The ebsrelease code could be modified easily to be consistent with the assumptions in ebsfail.

14. (S) The code internal documentation says that the variable "wu" keeps leaching to zero before tlt. It actually sets leaching to zero after tlt.

15 (B) The wetfrac variable is improperly translated from height fraction to volume fraction in ebsrelease. This results in errors of up to ~a factor of 10 that are propagated throughout TPA. (Note: this has already been fixed and had to do with a radians vs degrees problem).

16. (B) The "gap fraction" (actually just a lumped initial release fraction) is not multiplied by the volume fraction wetted as is the case with the rest of the inventory in liquid release. This allows gap inventory to be released even when dry. The amount of error involved depends upon input variables but could be up to 10-20% and is propagated throughout TPA.

TPA Code Testing:

1. (B) Individual code output files are deleted by TPA between realizations but not between respository areas (currently 7 areas are used). If a code (e.g., ebsfail, ebsrelease) fails during the first area the TPA code stops with an error. If the code fails during the second or later area (e.g., with an internal stop because of a numerical problem) then TPA appears to read the old output file from the previous area and goes upon its merry way. This allows false answers to propagate (e.g., area 3 results are used for area 4). Problem can be solved by deleting all output files in the repository areas loop.

2. (B) The TPA runs are most generally stopped by a negative subscript in neftran. Increasing the half-life of Pb-210 seems to eliminate the problem at least in some cases. Perhaps Pb-210 can be eliminated from the transport codes in TPA since it is in secular equilibrium with Ra-226? If results from Pb are desired it could be put back in at the dose model stage by setting its activity equal to Ra-226.

3. (S) The TPA code runs too slowly when the time is increased to 100,000 years. Each area was taking > 45 minutes and the major problem is in neftran. We need to find a method for speeding up neftran. Unfortunately I have no suggestions at to how.

4. (S) TPA sample input files has examples where the rock grain density is < typical rock bulk density. This is unlikely to be correct and should be checked.

6/24/97 JW

Check code input - does TPA go to all codes properly ??

interrupted a run in first area

- all input files *.inp that should have had updated dates & times

climato.inp had a table going from 0 to 100,000 yr in steps of 1,000 yr

notes comment lines in ebs fail.inp have been truncated

ls - lct lists files by modification date

ebs trhc.inp file contains 6 variable names and 4 columns ; it appears that i and cl conc are missing
second line contains # lines in file ?? plus 3 other unknown variables = 4444
- a place holder ??

ebs rel.inp - comments have been preserved

- reads ebs trh.dat
ebs flo.dat
ebspac.nuc

note: all *.dat except strm tube.dat have been updated

why is strm tube.dat not updated
should ~~AA~~ name be changed

new office # 226

IP 225 → 129.162.200.225
at office # A226
(Ray G)

chlor idemf.dat gives time, chloride data
it is updated and appears reasonable

temp hmd.dat is updated and appears reasonable

sat nef.dat appears to be an sat ebs rel output sent to nef tran - is this really used ?

ebsflo.dat is updated contains time, drop rate data

* Note: after calling SZFT if there is no release it says
" There is no UZ release"
change to SZ if possible

Office # A250
129.162.200.19
called stud 8

text edit & gives a text editor

DAT files

sotnef elbsflo chlori demf
maxrel ebstrh echo_fail
ebsnef temphumd
- are updated each area

ebsnuc multiflo climato

- are updated each realization

strm tube.dat is not updated

* would be nice to have a consistent nomenclature for these files

- some are debugging parameters, some are read by other codes

of the .inp files

nefii ebs trhc } update each area
ebsrel nefii iz
ebsfail nefii uz

climato updates each realization

*.in files
watrel is the only one updated with
TPA runs

between areas only # waste packages and
scenario failures changed

a diff crossing 2 realizations
showed only # containers, scenario # &
scenario time differences

web

IS2 & NCMP = ILAST

IC may be depth of penetration / ΔX of last block??

ILAST - IC < 0 is the problem

since NCMP > IS2 the
problem must be with IS2 or IC

IS2 = N1 - 1
N1 = NX(1) + NC(1) + 1
NX = # blocks in leg
NC = # catcher blocks

so IS2 = ILAST = # blocks + # catcher blocks in leg 1 ??

DSMX = maximum distance from boundary that
is affected

what we α dx, pore in nafton ??

IC = DSMX / DX(LG)

= max distance affected / length of leg

DSMX = Σ DIS = Σ VA * TS

TS = time step
VA = ??, some type of velocity

when VA gets too high we have problems

- initially 40 seconds are needed to run usft, change climate time ~~steps~~ steps 500 → 1000 yr

~34 s cpu time

6/25

in 625a directory
cp -r c scherer / tpa623 / *
to get codes fresh

- type in unlimit at command prompt

fn2.i - change file units open at once

u2ft.f controls time steps
change to append mode in tpa.inp
.ech is input
.res is code output

initial 500yr time steps
time nofmkse → 22u 0:23

generate input file by interupting first area in first realization

changed u2ft.f 500d0 → 2500d0
years
recompile tpa code

now time it takes is 5u
⇒ run time is ~ to climate time step

climate code outputs flow over the entire sub area in m^3/yr

line 592 in release t, f

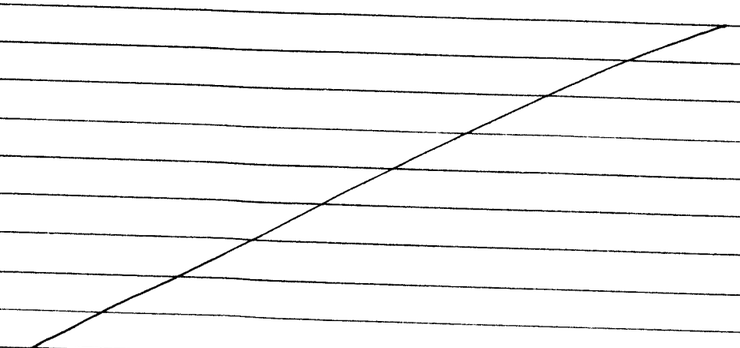
Fraction of Flow Hitting Waste Package

* ash movo, f

loops from 1 to 43 nuclides
are hard coded
- should use 1, max nucs vol
which currently = 43 instead
of hard coding 43

* dcags, f loops from 1 to 43
in do loops ; change to ~~max~~ 43 to
max nucl

* dcagw also has the same problem



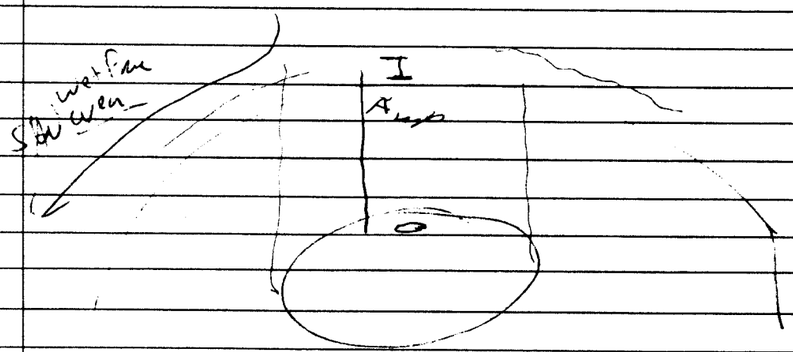
8/24/99 JCW

10 realization run finished

Flow Factor = 0.3
Fmult Factor = 0.1
Sub Area Wet Fraction = 0.5
initial defectives 0.10 & 0.01

this resulted in considerable reductions in dose

i ft p t takes one outside of CNWRA

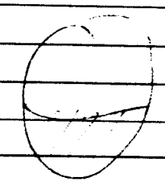


SA wetfrac = frac of cont. that can wet at all

flow * area based infiltration = drip rate = flow * i * area

Fmult = flow diversion factor, always < 1
= other reasons why dripping water does not
get into waste package = flow factors
Fmult = capillary barrier diversion *
* runs down sides of drift
* actually enters hole in WP

* pit holes clogged

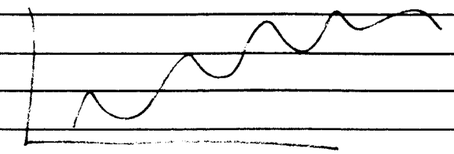


put all flow factors up to 1.0 made all initial defectives, increased infiltration to check TDA mass balance also reduced starting repository temperature

** us ft & sz ft give no release when total time 1e4 > 2e4 even though release occurs at 1e4 yr total time

flow rates into the areas go way up for 2e4 yr runs

** uz flow down keeps increasing flow rates when total time > 10,000 yr



** → when neftran input file "ftuz f program sees high flow it eliminates too many legs and there is no transport through uz solution - have it just copy ebs rel output to nef iscz input file

after maximum release run usft.ech has lots of I ~129 but sz ft.ech has none

cum rel ires is cumulative release to AE from ebs, us zone, sat zone

Ci/wp 307
7125 wp's

0.2596 Ci/wp * 7125 wp =

```
10c10
< 0
---
> 1
14c14
< 0
---
> 1
18c18
< 0
---
> 1
104c104
< 1
---
> 3
122c122
< 2
---
> 0
126c126
< 1
---
> 2
136c136
< 9.9, 10.0
---
> 1, 10.0
1080c1080
< 1.0
---
> 0.3
1092c1092
< 1.00
---
> 0.10
1103c1103
< 100.                    ! set a large number (999.) to start flow at time=0 yr
---
> 97.                     ! set a large number (999.) to start flow at time=0 yr
1146c1146
< 1.000
---
> 5.e-1
1273c1273
< 1.00
---
> 0.0
```

this is a diff between my input file and tpa623 default input file

note: also set high $\frac{1}{2}$ life for Pb-210 to keep nuftran from bombing w/ negative subscript

		EBS	UZ	SZ
1	Cm246	2.6056394E+02	2.3536470E+01	2.0038291E+01
1	U238	2.7476227E+02	8.2964892E+01	5.7475475E+01
1	Cm245	1.7080162E+03	1.5435296E+02	1.3744190E+02
1	Am241	1.8722565E+05	1.6710797E+04	4.1817533E+03
1	Np237	1.8183511E+04	6.6675494E+03	3.7016835E+03
1	Am243	1.8242838E+05	1.7594621E+04	1.5525556E+04
1	Pu239	3.8099821E+04	5.1511287E+03	4.6376628E+03
1	Pu240	3.9084217E+04	5.0108295E+03	3.9887331E+03
1	U234	1.0328079E+03	0.0000000E+00	0.0000000E+00
1	Th230	2.1333622E+03	0.0000000E+00	0.0000000E+00
1	Ra226	7.0055060E+02	0.0000000E+00	0.0000000E+00
1	Pb210	5.7666206E-02	0.0000000E+00	0.0000000E+00
1	Cs135	7.1245394E+03	0.0000000E+00	0.0000000E+00
1	I129	2.0880238E+03	0.0000000E+00	0.0000000E+00
1	Tc99	2.5304569E+05	0.0000000E+00	0.0000000E+00
1	Ni59	4.9159834E+04	0.0000000E+00	0.0000000E+00
1	C14	1.5571508E+04	0.0000000E+00	0.0000000E+00
1	Se79	7.5297761E+03	0.0000000E+00	0.0000000E+00
1	Nb94	3.2780829E+02	0.0000000E+00	0.0000000E+00
1	Cl36	2.4205453E+02	0.0000000E+00	0.0000000E+00

Cumulative release from run -

* note that lower nuclides don't get out - but should

Changed flow-initial infiltration to 1.0 to 1.1 & now nuftran won't run at all

Changed to 1-10, the default mm/yr

* we frequently get no or too low release from nuftran

6-27-91 JM

~ v rice / tpab24 / cales / nefmkf

- Increased flow rates by one order of magnitude in stream tube dat

rel cum. vol

		EDSPAC	N2FT	S2FT
1	Cm246	1.4459441E+03	2.0642920E-05	2.0334405E-05
1	U238	2.0133681E+04	8.1111241E+02	8.0612305E+02
1	Cm245	7.2664689E+03	1.8086279E-04	1.7819318E-04
1	Am241	1.3630332E+08	1.7383378E-02	1.6929456E-02
1	Np237	4.0193435E+04	2.6611919E+04	2.6555797E+04
1	Am243	8.8642212E+05	2.9630291E+00	2.9233803E+00
1	Pu239	1.8455960E+07	8.1745458E+04	8.1022050E+04
1	Pu240	2.9377007E+07	7.0141686E+04	6.9501913E+04
1	U234	9.5511745E+04	3.7666415E+03	3.7434366E+03
1	Th230	4.6258775E+02	1.1407530E+01	1.1855582E+01
1	Ra226	2.9618029E+01	3.3683807E+00	3.3931707E+00
1	Pb210	2.4481410E+01	1.0389190E+01	7.5774955E+00
1	Cs135	2.1585527E+04	1.8872853E+03	1.8781065E+03
1	I129	1.8438107E+03	1.6091877E+03	1.6093532E+03
1	Tc99	7.7755753E+05	6.6740783E+05	6.6743612E+05
1	Ni59	1.5508968E+05	2.5211267E+04	2.5118534E+04
1	C14	7.9725979E+04	0.0000000E+00	0.0000000E+00
1	Se79	2.3936491E+04	4.9031488E+03	4.8872545E+03
1	Nb94	2.2963566E+02	1.2881140E+02	1.2840490E+02
1	Cl36	7.3976723E+02	6.3574944E+02	6.3578518E+02

97%
95%
C14
none
85.6%

Note that mass is lost between EDSPAC & NEFTRAN

mass loss can be by export in one case

increased I, Tc ½ life → ∞ to eliminate decay

1 curie vs N

1	Cm246	1.5434507E+03	2.4299441E-04	2.3705083E-04
1	U238	2.3526478E+04	3.4353957E+03	3.4062535E+03
1	Cm245	7.7155440E+03	2.1281156E-03	2.0769601E-03
1	Am241	1.6436098E+08	2.0422170E-01	1.9525812E-01
1	Np237	3.8073945E+04	5.4921036E+04	5.4792826E+04
1	Am243	9.4179410E+05	2.7400191E+01	2.6816372E+01
1	Pu239	3.1068448E+07	6.2991933E+05	6.2168284E+05
1	Pu240	5.0022588E+07	5.4937956E+05	5.4187169E+05
1	U234	1.1164089E+05	1.5968010E+04	1.5832067E+04
1	Th230	4.4571233E+02	5.5296970E+01	5.8532892E+01
1	Ra226	1.7730783E+01	1.7957232E+01	1.8153515E+01
1	Pb210	1.3843217E+01	6.1839023E+01	3.6343809E+01
1	Cs135	2.4419258E+04	6.1512569E+03	6.1104750E+03
1	I129	1.9496706E+03	1.9510650E+03	1.9499247E+03
1	Tc99	8.9325682E+05	8.8030592E+05	8.8041688E+05
1	Ni59	1.7506539E+05	7.0999759E+04	7.0655202E+04
1	C14	9.0811720E+04	0.0000000E+00	0.0000000E+00
1	Se79	2.6997922E+04	1.3041078E+04	1.2986477E+04
1	Nb94	2.5260958E+02	2.4399960E+02	2.4275692E+02
1	Cl36	8.3376064E+02	8.3399935E+02	8.3434802E+02

Increased T parameters and tried again

Tc was retarded in the fractures & wrong data not balance mass as well

Tc did not have instant jump release, Iodine did

now do 2 runs changing time step increment

in 625b change increment to 1.0

time step factor = 100

Cm246	6.1[illegible]471E+02	4.8047[illegible]E-05	4.6717495E-05
U238	2.2571884E+04	2.4912219E+03	2.4848472E+03
Cm245	3.3527810E+03	4.2551628E-04	4.1393660E-04
Am241	1.0539764E+07	1.6001192E-02	1.5272494E-02
Np237	3.3717556E+04	2.6140778E+04	2.6060529E+04
Am243	4.0086608E+05	6.0739371E+00	5.9251353E+00
Pu239	1.4095223E+07	1.8654670E+05	1.8360013E+05
Pu240	2.0495276E+07	1.5818450E+05	1.5558922E+05
U234	1.0673335E+05	1.1565447E+04	1.1441791E+04
Th230	1.7069100E+03	3.2968739E+01	3.5318721E+01
Ra226	4.1200500E+02	9.5593439E+00	9.6831510E+00
Pb210	3.9474705E+02	3.3040654E+01	1.9361854E+01
Cs135	2.5720233E+04	5.2645920E+03	5.2204503E+03
I129	9.8321841E+02	1.0009697E+03	1.0012697E+03
Tc99	8.5631252E+05	8.5491912E+05	8.5455760E+05
Ni59	1.8205110E+05	6.4477600E+04	6.4080676E+04
C14	8.2207982E+04	0.0000000E+00	0.0000000E+00
Se79	2.8003594E+04	1.2120613E+04	1.2056084E+04
Nb94	2.2227757E+02	2.1418817E+02	2.1298485E+02
Cl36	8.7368754E+02	8.8831034E+02	8.8815691E+02
	EPS	U2FT	S2FT

>200% error

1.018

1.185

1.016

time step factor = 1.0

cumulative release

Cm246	1.8678806E+02	1.5352726E-05	1.4906913E-05
U238	2.1877222E+04	2.4031618E+03	2.3776467E+03
Cm245	1.0423821E+03	1.3683106E-04	1.3287815E-04
Am241	2.8686817E+06	4.6450237E-03	4.4323477E-03
Np237	1.2188991E+04	9.0619158E+03	9.0324662E+03
Am243	1.2100721E+05	1.9183607E+00	1.8692480E+00
Pu239	4.3754144E+06	5.8468592E+04	5.7527979E+04
Pu240	6.1439234E+06	4.9157294E+04	4.8344561E+04
U234	1.0342409E+05	1.1155136E+04	1.1038425E+04
Th230	1.3995140E+03	3.1315940E+01	3.3579660E+01
Ra226	3.3297654E+02	9.0332917E+00	9.1475854E+00
Pb210	3.1806800E+02	3.1301560E+01	1.8321122E+01
Cs135	1.9858111E+04	4.1649429E+03	4.1307374E+03
I129	3.6241344E+02	3.7853392E+02	3.7851791E+02
Tc99	8.3547556E+05	8.3692348E+05	8.3660301E+05
Ni59	1.4374027E+05	5.2170885E+04	5.1860752E+04
C14	6.4052251E+04	0.0000000E+00	0.0000000E+00
Se79	2.2052645E+04	9.7920355E+03	9.7420993E+03
Nb94	2.2155085E+02	2.1268125E+02	2.1149713E+02
Cl36	6.8878085E+02	7.1936003E+02	7.1913838E+02
	EPS	U2	S2

2% error

I error ~264%

factor = 10

Cm246	7.0378371E+02	5.7977670E-05	5.6322855E-05
U238	2.3082134E+04	2.5690565E+03	2.5417564E+03
Cm245	3.8276848E+03	5.1438726E-04	4.9986977E-04
Am241	1.1927881E+07	1.8086211E-02	1.7258117E-02
Np237	3.8261829E+04	3.0046263E+04	2.9956041E+04
Am243	4.5829463E+05	7.2929376E+00	7.1094945E+00
Pu239	1.6071081E+07	2.1973933E+05	2.1624484E+05
Pu240	2.3383936E+07	1.8600018E+05	1.8294202E+05
U234	1.0913977E+05	1.1925904E+04	1.1798908E+04
Th230	1.7801542E+03	3.3718085E+01	3.6139190E+01
Ra226	4.3525979E+02	9.7604117E+00	9.8844073E+00
Pb210	4.1730952E+02	3.3708376E+01	1.9751271E+01
Cs135	2.6710770E+04	5.5066966E+03	5.4610002E+03
I129	1.1072320E+03	1.1333296E+03	1.1329256E+03
Tc99	8.5787748E+05	8.5790644E+05	8.5855289E+05
Ni59	1.8883128E+05	6.7123134E+04	6.6715340E+04
C14	8.5190528E+04	0.0000000E+00	0.0000000E+00
Se79	2.9056259E+04	1.2606309E+04	1.2540183E+04
Nb94	2.2198514E+02	2.1351716E+02	2.1232033E+02
Cl36	9.0659760E+02	9.2127674E+02	9.2196542E+02

factor = 1

Cm246	1.1283806E+03	9.4082585E-05	9.1348931E-05
U238	2.1895717E+04	2.4046925E+03	2.3791568E+03
Cm245	6.1471033E+03	8.3480326E-04	8.1074510E-04
Am241	1.7973544E+07	2.8899942E-02	2.7578204E-02
Np237	6.1289684E+04	4.8988853E+04	4.8851344E+04
Am243	7.3669899E+05	1.1845275E+01	1.1542457E+01
Pu239	1.6726024E+07	2.2949936E+05	2.2582253E+05
Pu240	2.4103116E+07	1.9374382E+05	1.9054665E+05
U234	1.0351066E+05	1.1162271E+04	1.1043479E+04
Th230	1.3851638E+03	3.1334044E+01	3.3599319E+01
Ra226	3.3300379E+02	9.0382504E+00	9.1526149E+00
Pb210	3.1805782E+02	3.1318726E+01	1.8331152E+01
Cs135	1.9893645E+04	4.1672341E+03	4.1329972E+03
I129	1.7322865E+03	1.8168302E+03	1.8167521E+03
Tc99	8.3618437E+05	8.3762401E+05	8.3729980E+05
Ni159	1.4406677E+05	5.2260164E+04	5.1949285E+04
C14	6.4073225E+04	0.0000000E+00	0.0000000E+00
Se79	2.2073657E+04	9.7987047E+03	9.7486937E+03
Nb94	2.2155050E+02	2.1268087E+02	2.1149675E+02
Cl36	6.8944953E+02	7.2003563E+02	7.1982307E+02

EBS UZ SZ

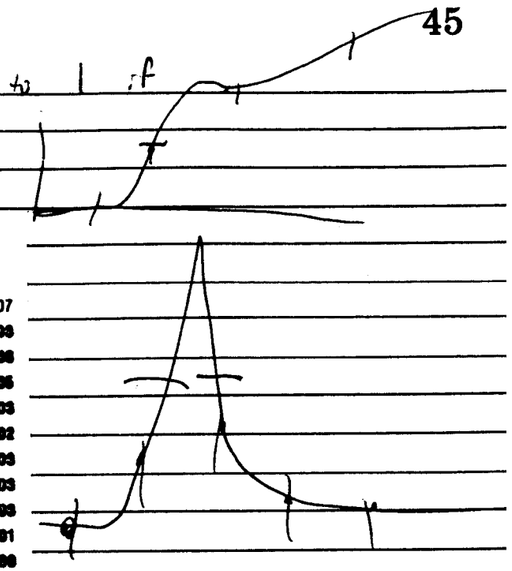
ratio factor = 10

	EBS	UZ	SZ
Cm246	1.5354970E+03	1.2452894E-04	1.2088911E-04
U238	2.3073064E+04	2.5683298E+03	2.5410390E+03
Cm245	8.3211970E+03	1.1037899E-03	1.0725968E-03
Am241	2.5731380E+07	3.8752284E-02	3.6977258E-02
Np237	8.0562868E+04	6.3562209E+04	6.3376308E+04
Am243	1.0018941E+06	1.5705649E+01	1.5309848E+01
Pu239	2.2449037E+07	3.0336409E+05	2.9852664E+05
Pu240	3.2703516E+07	2.5664084E+05	2.5241096E+05
U234	1.0909756E+05	1.1922478E+04	1.1795522E+04
Th230	1.7506979E+03	3.3708784E+01	3.6129438E+01
Ra226	4.3480426E+02	9.7577749E+00	9.8817518E+00
Pb210	4.1686800E+02	3.3699093E+01	1.9745740E+01
Cs135	2.6685026E+04	5.4993498E+03	5.4537092E+03
I129	2.2859617E+03	2.3216605E+03	2.3208692E+03
Tc99	8.5766815E+05	8.5769328E+05	8.5833491E+05
Ni159	1.8907043E+05	6.7192254E+04	6.6784381E+04
C14	8.5280095E+04	0.0000000E+00	0.0000000E+00
Se79	2.9098415E+04	1.2622739E+04	1.2556514E+04
Nb94	2.2198266E+02	2.1351474E+02	2.1231795E+02
Cl36	9.0796863E+02	9.2283319E+02	9.2332123E+02

problem appears in or before abs vel since #'s match up before that

note tpa sets Δt ratio to 1 if input value is <1

set time factor = 1.0 50 steps



	EBS	UZ	SZ
Cm246	1.5939596E+01	5.9035996E-07	5.7209951E-07
U238	1.8569065E+04	1.8829231E+03	1.8617604E+03
Cm245	1.3602568E+02	6.1073462E-06	5.9184420E-06
Am241	2.0537243E+04	5.8237688E-05	5.5135590E-05
Np237	4.8848080E+03	2.3914905E+03	2.3758634E+03
Am243	8.6368124E+03	5.3505153E-02	5.2005260E-02
Pu239	6.4434300E+05	2.9654243E+03	2.9049308E+03
Pu240	4.4031757E+05	1.8829607E+03	1.8454768E+03
U234	8.7713652E+04	8.7380054E+03	8.6395925E+03
Th230	2.5408057E+02	2.3292205E+01	2.5071584E+01
Ra226	7.3962000E+00	6.5118227E+00	6.6004860E+00
Pb210	2.6976795E+00	2.2450367E+01	1.3155404E+01
Cs135	7.3449420E+02	5.1893097E+01	5.1172456E+01
I129	1.2968403E+02	1.2411066E+02	1.2407512E+02
Tc99	8.5298717E+05	8.3645807E+05	8.3668709E+05
Ni159	1.2839583E+04	3.7545454E+03	3.7271684E+03
C14	3.5413003E+03	0.0000000E+00	0.0000000E+00
Se79	1.5843016E+03	5.9361836E+02	5.8988386E+02
Nb94	2.0852630E+02	1.9913822E+02	1.9794011E+02
Cl36	5.0679637E+01	4.8177962E+01	4.8176561E+01

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Cm246	1.1283806E+03	9.4082585E-05	9.1348931E-05
U238	2.1895717E+04	2.4046925E+03	2.3791568E+03
Cm245	6.1471033E+03	8.3480326E-04	8.1074510E-04
Am241	1.7973544E+07	2.8899942E-02	2.7578204E-02
Np237	6.1289684E+04	4.8988853E+04	4.8851344E+04
Am243	7.3669899E+05	1.1845275E+01	1.1542457E+01
Pu239	1.6726024E+07	2.2949936E+05	2.2582253E+05
Pu240	2.4103116E+07	1.9374382E+05	1.9054665E+05
U234	1.0351066E+05	1.1162271E+04	1.1043479E+04
Th230	1.3851638E+03	3.1334044E+01	3.3599319E+01
Ra226	3.3300379E+02	9.0382504E+00	9.1526149E+00
Pb210	3.1805782E+02	3.1318726E+01	1.8331152E+01
Cs135	1.9893645E+04	4.1672341E+03	4.1329972E+03
I129	1.7322865E+03	1.8168302E+03	1.8167521E+03
Tc99	8.3618437E+05	8.3762401E+05	8.3729980E+05
Ni159	1.4406677E+05	5.2260164E+04	5.1949285E+04
C14	6.4073225E+04	0.0000000E+00	0.0000000E+00
Se79	2.2073657E+04	9.7987047E+03	9.7486937E+03
Nb94	2.2155050E+02	2.1268087E+02	2.1149675E+02
Cl36	6.8944953E+02	7.2003563E+02	7.1982307E+02

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Cm246	1.5220931E+02	1.0764172E-05	1.0450764E-05
U238	2.0105043E+04	2.1516821E+03	2.1284336E+03
Cm245	8.7702095E+02	9.6487963E-05	9.3702574E-05
Am241	1.9198535E+06	2.9774441E-03	2.8400085E-03
Np237	1.1953179E+04	7.8512800E+03	7.8211101E+03
Am243	9.8161658E+04	1.3444681E+00	1.3099547E+00
Pu239	2.6392060E+06	2.8578337E+04	2.8104114E+04
Pu240	3.3502509E+06	2.3469009E+04	2.3071710E+04
U234	9.5017869E+04	9.9868092E+03	9.8787442E+03
Th230	4.0571887E+02	2.7587862E+01	2.9618063E+01
Ra226	5.2079746E+01	7.8810383E+00	7.9835207E+00
Pb210	4.6124870E+01	2.7329835E+01	1.5992912E+01
Cs135	3.1213951E+03	5.2516547E+02	5.2049421E+02
I129	3.6421796E+02	3.6208429E+02	3.6201440E+02
Tc99	8.0059342E+05	7.9843507E+05	7.9832058E+05
Ni159	3.0725363E+04	9.9743097E+03	9.9103351E+03
C14	1.2317342E+04	0.0000000E+00	0.0000000E+00
Se79	4.5789464E+03	1.8571392E+03	1.8469654E+03
Nb94	2.2008846E+02	2.1148782E+02	2.1027765E+02
Cl36	1.4425013E+02	1.4251781E+02	1.4243524E+02

2aa

	EBS	UZ	SZ
Cm246	1.0265299E+03	7.5643475E-05	7.3415894E-05
U238	2.1401993E+04	2.2988524E+03	2.2741859E+03
Cm245	5.5818964E+03	6.7162859E-04	6.5198952E-04
Am241	1.6614937E+07	2.3469183E-02	2.2392754E-02
Np237	5.5091758E+04	4.1702478E+04	4.1581292E+04
Am243	6.7010820E+05	9.6176515E+00	9.3683906E+00
Pu239	1.5143004E+07	1.9065975E+05	1.8756525E+05
Pu240	2.1905138E+07	1.6085590E+05	1.5817190E+05
U234	1.0118461E+05	1.0670820E+04	1.0556054E+04
Th230	1.2527895E+03	3.0072856E+01	3.2233407E+01
Ra226	2.9936456E+02	8.6812120E+00	8.7895289E+00
Pb210	2.8622290E+02	2.9963968E+01	1.7553997E+01
Cs135	1.8019199E+04	3.5192351E+03	3.4899276E+03
I129	1.5660512E+03	1.5523864E+03	1.5525397E+03
Tc99	8.5622275E+05	8.5368945E+05	8.5352422E+05
Ni59	1.2964092E+05	4.4116424E+04	4.3849653E+04
C14	5.8026356E+04	0.0000000E+00	0.0000000E+00
Se79	1.9923125E+04	8.3034187E+03	8.2602252E+03
Nb94	2.1991905E+02	2.1154721E+02	2.1036835E+02
Cl36	6.2206287E+02	6.1660439E+02	6.1655723E+02

Conclusion - order of magnitude error or more based on time step changes

could not run tpa with >2aa time steps because relcum t has a 300 step limit

* # time intervals from ebspac ≠ # time intervals from tpa - this is incorrect and leads to unnecessary interpolation loss

- this is the variable nbt

ebsnef.dat gets time steps from nbt

Sotnef.dat uses tpa time steps

the map list is due to ebs rel. f file and is not needed if variables are made the same by writing tpa variable to bottom of release t code.

John Walton

TPA and EBSPACK code testing results:

B= bug that should be fixed
S= suggestion or minor problem
W= appears to work properly

EBSPACK: Overall the code authors have done an excellent job of putting these codes together in a short period of time based on previous codes.

1. (S) In sample input file initial Runge-Kutta time step (25 yr) is > maximum time step (10 yr). Examined time stepping throughout the week and found that a) 100 yr maximum time steps give faster run times with no loss of accuracy (limited tests) and b) the eps parameter should be reduced from 1e-2 to 1e-4 to ensure good mass balance. Making both changes appears improve mass balance and decrease run times.

2. (W) Changed flow rate, funnel factor, alteration, and solubilities and examined cumulative fractional releases. This allows testing of a vareity of limiting cases where release is alteration controlled (high solubility radionuclides) and solubility controlled (low solubility) radionuclides. In every case the code worked correctly. Mass balance errors in the range of 10% could be obtained unless the eps parameter was reduced. Lowering the eps parameter to 1e-4 or less reduced mass balance errors to < 2%.

3. (W) Changed diffusion coefficients and flow rates to switch between advection and diffusion controlled release. The default diffusion parameters give insignificant diffusional release. The code appears to work correctly.

4. (S) Note that in the relcum.out file the fraction remaining is actually the fraction that can be released that remains - not the total fraction remaining. This is a bit misleading as it is assumed in the code that portions of areas and portions of containers will never wet and thus never have liquid release. The never released fractions are not counted in the fraction remaining.

5. (S) The variable amassc, the mass of spent fuel in a container is read into the code then multiplied and divided in a manner such that is makes no difference in the final results. This is misleading and it would be preferable to simply remove it from the code. Actual inventories are obtained from the ebsnuc.dat file.

6. (S) Changing the timintv variable from 49.9999 to 50 changes the output results in the third of fourth significant figure. This is a small difference but perhaps greater than it should be. Larger changes in this variable cause about the same change in results.

7. (W) Changing the humdc variable influences aqueous corrosion times in the correct manner.

8. (S) The ebsfail code inputs a two dimensional grid but actually uses a one dimensional spherical grid. The spherical grid is based on the x coordinates. The first x coordinate is the first delta r but the rest of the delta r's are obtained by differencing the x coordinates. The location of the backfill/rock interface is calculated in the code and difficult to determine by the analyst. This makes it difficult to change backfill to rock properties in the input file.

9. (S) Separate treatment of advection and diffusion is a hold over from SOTEC. It does not allow diffusionally released radionuclides to be flushed out of the rock and backfill during high flow periods. The diffusion should either be eliminated or coupled with the advective release.

10. (S) Only a fraction of each container is subject to wetting and release even at time=infinity using the current "bathtub" conceptual model. Since container corrosion continues over time, all mass on wetted containers should eventually be subject to release. It would be preferable to make all spent fuel subject to liquid release even with the bathtub model (perhaps by just increasing the release period subject to the fraction wetted. This option in the code can be effectively bypassed by increasing the wetted fraction to 1.0 and lowering the internal volume of the container. These parameter changes effectively switch the conceptual model from a bathtub to a dripping mode. The ability to switch conceptual models with input parameters is a good design feature in the code.

11. (S) The sollay variable is not used in the ebsfail code and should probably be eliminated.

12. (S) EBSPAC fails with an internal stop when the # of defectives + # scenario failures > total number of waste packages. The TPA code does not allow this to happen. EBSPAC could have some logic to handle this problem.

13 (S) The ebsfail code allows corrosion of the canister to begin when water can condense on the metal at relative humidity less than one. The ebsrelease code does not allow the spent fuel to alter until drips begin (and container has corroded). This is inconsistent. If condensed water can corrode the steel, it can also corrode the spent fuel. The ebsrelease code could be modified easily to be consistent with the assumptions in ebsfail.

14. (S) The code internal documentation says that the variable "wu" keeps leaching to zero before tlt. It actually sets leaching to zero after tlt.

15 (B) The wetfrac variable is improperly translated from height fraction to volume fraction in ebsrelease. This results in errors of up to ~a factor of 10 that are propagated throughout TPA. (Note: this has already been fixed and had to do with a radians vs degrees problem).

16. (B) The "gap fraction" (actually just a lumped initial release fraction) is not multiplied by the volume fraction wetted as is the case with the rest of the inventory in liquid release. This allows gap inventory to be released even when dry. The amount of error involved depends upon input variables but could be up to 10-20% and is propagated throughout TPA.

TPA Code Testing:

1. (B) Individual code output files are deleted by TPA between realizations but not between respository areas (currently 7 areas are used). If a code (e.g., ebsfail, ebsrelease) fails during the first area the TPA code stops with an error. If the code fails during the second or later area (e.g., with an internal stop because of a numerical problem) then TPA appears to read the old output file from the previous area and goes upon its merry way. This allows false answers to propagate (e.g., area 3 results are used for area 4). Problem can be solved by deleting all output files in the repository areas loop.

2. (B) The TPA runs are most generally stopped by a negative subscript in neftran. Increasing the half-life of Pb-210 seems to eliminate the problem at

least in some cases.

3. (S) The TPA code runs too slowly when the time is increased to 100,000 years. Each area was taking > 45 minutes and the major problem is in neftran. I tried increasing the time step in the neftran infiltration input from 500 to 2500 years and neftran run times went from 23 seconds cpu time to 4-5 seconds cpu time. This is at least one method of making neftran run faster.

4. (S) TPA sample input files has examples where the rock grain density is < typical rock bulk density. This is unlikely to be correct and should be checked.

5. (B) When the time frame of the simulations is increased from 10,000 to 20,000 or 50,000 years, uzflow gives flow rates into the repository areas that appear to be on an ever increasing sine wave pattern leading to unrealistic infiltration rates. The code results should not spirial upward indefinitely.

6. (B) When infiltration rates are very high neftran in the unsaturated zone gets too few legs in the input file (prepared by uzft.f) and stops execution. When this occurs no release is predicted/allowed from the system just when releases should be greatest. For high flow situations ebspac output results can be sent directly to the saturated zone run.

7. (S) ashmovo.f, dcags.f, and dcagw.f have a number of do loops ranging from 1 to 43 nuclides. Rather than hard code the loop range it might be preferable to use the maximum nuclides variable available in the codes.

8. (W) Traced the flow of water through the system and this appears to be working correctly with exception noted above.

9. (W) Checked mass balance between subsystems (EBS, UZ, SZ) and mass balance errors are generally < 2%.

10. (B) Changing the time step ratio in tpa from the default (100) to values of 10, 1 and some other values resulted in cumulative release changes at (EBS, UZ, SZ) of around 1000% or more in some cases. Since one does not know a priori when the greatest action is, it is probably best to use a multiplier of 1.0. Someone needs to investigate how many time steps will be required to obtain needed accuracy in mass balance in tpa.

The major problem seems to come in prior to neftran. One area to examine is in releaset. releaset writes an output file using a number of time steps hard wired into its template input file. The is the variable nbt. It would be preferable (but require some coding) to have ebspac use the same time steps as tpa. Alternatively one might hard code nbt to be the same value used in tpa and make the tpa time steps of constant duration.

At a minimum the time step problem needs to be resolved. I examined its influence on cumulative release but it is likely that peak releases are more sensitive to the issue.

One solution to the time step problem, especially for peaks is to integrate releases in EBS PAC then use the integrated release to calculate the time averaged release rates. This will cause fewer mass balance errors and give a better defined output result

Right now I believe the pac gives an instantaneous release rate

This scientific notebook contains a record of tests conducted on the EBSPAC and TPA Exciter by John Walton, a consultant, and former employee, of the CNARA. In my opinion this notebook has not been maintained in full accordance with QAP-001. In particular some entries have not been signed or initialed by the user. However, there is sufficient information contained herein that similar tests could be conducted by another, qualified engineer.

Gordon Wittmeyer

3/14/2000