308 --- Q200003150001
Scientific Notebook # 225

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John Walter

[signature]

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Title - Debugging of TPA and EBSPAC codes

John Walter

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 were to be made by others.

TPA 3.1 beta

6-16-97

ehspac code on OS2 machine telnet to
big bend

stty erase ^H

begin editing "ehspac_fail.inp"

what is nset ?, = 12 table lookups for thermal loading
screen across based on earth code
Cntr - Esc brings up window list in OS2

setenv DISPLAY 129.62.200.19[illegible]:0.0
cmdtool &

x5255 Wes Compute Lab

ehspac_release.inp
notice that initial Runge Kutta time step
is > maximum time step

what is 2D grid system for? why does not
2-D grid match drift climate? why is
it < ~~in~~ contains residue?

shut down advertising
play with code, change Funnel fcole to 0.9 → 0.0
- no impact on cocode.out & none should be none

release.out - this ~~moved~~ each release did not change
- because I ran code wrong Jw 6/24

⇒ all releases went to zero

changed Funnel 0.9 → 0.3, could high
solubility nuclides to increase, low solubility ones did

but 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	0.3880 E+4	0.3948 E-4
	0.01	0.95 E4	0.3952 E-4
	10^{-6}	no release	
	10^{-5}	no release	
	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 (dissolution limited)

diffusive vs advective transport

r diff

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

small change in vel frac, out

r diff → 0 expected - does not finish
vdiff → 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

r diff → 5.6 e-1

saturated D ~ $10^{-9} \frac{m^2}{s}$ → $3 \times 10^{-2} \frac{m^2}{yr}$ → upper bound reasonable 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 double releases but fractional does not change

amass: amount of spent fuel per waste package
8800 → 3200 no change
8800 → 0 code gave error but run & gave strange results
8800 → 1 no change

- must not be used much
8800 → 0.001 no change

10^{-36} → no change
10^{-22} → no change
10^{+22} → no change

* how is this used ??

Runge Kutta Parameters
dt init 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 → 1000 yr & eps 10^{-2} → 10^{1} & dt ini → 10

run a little faster & essentially same answer

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

move to ebspec_fast.inp file

* fin init 49.999 → 100
slightly lower releases

49.999 → 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
49.999 was ~~not~~ baseline value

cthrkl 0.1 → 0.01 gives very
minute changes in cum release
indicates active corrosion

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

humdc 0.65 → 0.45
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 104° 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~~ calculations above the boiling point - some what inconsistent as its hard wired through the external data file

if tcan ≥ ctemp use clconca
else
use clconca → cfactor · clconc new WP

cfactor =
ctemp = boiling temperature

See Eq 2-4 in EBSPAC Manual
Tb may not be same in internal Fortran code

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

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

~~trigger~~ alteration rate limited species should be proportional to amassc when flow rates are high JW 6/24
- t/v in vessels ~~and~~ funnel and then varying amassc per hour with all initial defective containers.

funnel 0.4 → 1000

I-129 0.1020 E3

amassc ~~#~~ 880 → 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 880 → 1E-6 no change from new scenario

What move i leach and i model

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

Cs-135 10640 $\frac{kg}{m^3}$ → 1 $\frac{kg}{m^3}$

results very strange solubility limited ones do not change with solubility ones have in creased release and at same 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

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grid

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

only 0's at the first node and the "marker" at the drift interface appear to be used

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* solfuy variable is not used in shaft fault 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 ehs.flo.dat to zero → gives very low release

now also reduce porosity to 0 at first dx grid node

- gives same very low release

took Porosity back to 0.14 & revised diffusion coefficient to 5.6 e-5 → 5.6 e-3

made no difference at all

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

changed flow to 0.1 → now much release
changed initial fating 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 defective

will only initial wet fraction release ?? ever ?

Change to inctbl = 3 and to $\frac{m^3}{yr}$ water drips
in 6/24

Sa wetfrac = ??, Sa area wet fraction = Wetted sub area
in set for input file
tftc = maximum of wp failure time or
backing pont = 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

cumulative
xmass is release in Ci

Smass is cumulative release in Kg

Xno loss = Ci of nuclide times xfrac * sawet frac = ~~Ci~~ Inventory * Wetted fraction * wetted fraction of canister in area

I 129 1054 Ci release $\frac{Ci}{WP}$ $\frac{\text{sawetfrac}}{\text{wetfrac}}$

10000 packages x 0.2596 $\frac{Ci}{WP}$ * 0.8 * 0.5 =

1038.4 Ci

- 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 $\frac{1}{2}$ a WP & geometry drops out

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

⟹ the code takes the sa wetfrac 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 for amount remaining if everything does not count (i.e. only leachable material counts)

change drip rate | $\frac{m^3}{Yr} \rightarrow 0.01 \frac{m^3}{Yr}$

I-129 → 0.26 E+4

Tc-99 → 0.107 E+1

as per calculation on previous page the released is > initial inventory

* cranking eps down to 10^{-4} solves this problem

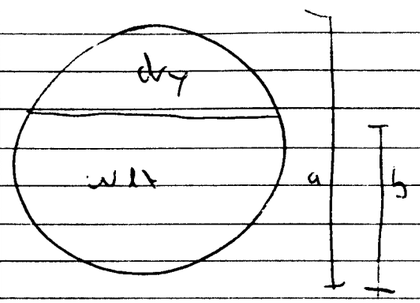
below after about $10^{-4} \frac{m^3}{Yr}$ of drip water the release calculation shuts down and only very low noise ?? numbers show up as release run times are also much lower in the code

change to no release = between 3 and 4 $\times 10^{-4} \frac{m^3}{Yr}$ drip rate

v 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



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

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

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

V_{max} = 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 leaking water - fix by turning on container early using minimum water level

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

tlt shuts off leaching using the "wet" switch

tlt = tleach + tfc = end of leaching time

tfc = max(tcorr, tfail)

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

note: code documentation says we keep 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 dcms which is also in dcmsis

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

trivial option is no water followed by a spike of water & it gave a spike release but not a sharp one

---

now try setting SE & WB 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 test is not added to check for good finish - perhaps old output files should be deleted at start of TPA execution ??

* code will run with a negative value for scenario cans 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 fluxdat 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 wet frac in each case all the available stuff was released.

wetfrac
0.4 → 0.88 E2

0.5 → 0.24 E3

0.9 → x frac = 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

make ebs pac_release.f is inconsistent with geometry. It feeds 2-D cartesian but only uses x & can't use it in 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 however so nuclides cannot be "sucked" from drift by high Rd host rock or cement

ps check jobs

changed I-129 to 100% sup fraction

changed U solubility to 1E-5

changed defaults from 10% & 95% thru 100%

the fpa code runs correctly with 100% Defectives even though ebsfail does not in stand alone mode - must have logic to handle defectives seen as > total #

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

release I-129 = 7.96E2 Ci/cell

with 100% and defectives
Currently sup fraction is 0.5
return to double check # when change
Sup fraction for I & Solubility for U

Summary out		
I-129	0.45E2 Ci	~0.13 fraction left
U-238	0.52 E-3	1.0
U-234	0.14E-2	1.0

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

I-129	0.79 E2	~1.0
U238	0.104 E-2	1.0
U 234	0.385 E-2	1.0

looks good if doubled unit should be 0

now increase U solubility to infinity (100%) and I sup fraction to zero

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

** The problem seems to be that the alteration is subject to Xfer, the fraction withdl but the sup inventory is not subject to xfer, thus too much sup gets released
xfer was 1/2 for the above runs so 100% sup lets it all out

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

✓ examine TPA screen output
*OH note: end of TDI annual dose GW pathway is > maximum dose GW pathway
note it
and it made this output > burden during lunch

* note that underflow errors occur and are never cleared

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

notes one cannot change reservoir. tmp, the tem plate file that has eps & step sizes/ranges
recommend eps → 1E-4 & maximum step → 100yr

this is specific finite element accurate

failed with parameters in UZ FLOW
and that make it hard to
get the code to run

WP failure at 7551 years (for 200 WP's)
for zone # 1
8640.8 yr for zone # 2

u z ft now takes most of the time rather than ebsrel

* * note that when I interrupt ebsfail code
run stall after first call the code continues
executing & probably takes the next elt results
interrupt prior to first call finish bombs the
tpa code

bis band bomb

changed CL multiplication factor to 1.0
⇒ no corrosion failure in area # 1

in tpa 2 directory I took all the
defaults and told it to do
10 realizations overnight in the background

in tpa 1 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 waits

change multiplier to 0.0001 ⇒ no corrosion failures

what is set ref. dat file, only has
1 sub area, it's say release
but appear to be cumulative release ??

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

6/20/94

tpa1 run, used given input file with
10 realizations

* code failed on subarea 3/1 realization 6/10

subscript out of range in nefmks.f
line 9141, procedure transpt
subscript number 1 has value of -2
in array rho
?? Error in UZFT <<
NE FTRAN 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 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 $1400 \frac{lb}{ft^3}$??

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 10,000 yr and changed Seismic Hazard Curve 0.1 500 ⇒ 0.1 1000 to avoid array size problem

TPA source code

cp -r ~cscherer/tpa_master_b20/* .

to get source code

make tpa to make tpa executable

in tpa1 direct transport 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

also rel and u2ft appear to cause the problem

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

in tpa_master_b20 directory try reproducing the fatal error in NEFTRAN

NEFTRAN

KSC = ilast - 1

ilast is defined when subroutine addit is called

it can be = JS2, NCMP

it's a max of a code, upped

the initial inflation to 9 - 10 mm
to try to fool 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 #
22.3 years initially

- the inverse was over written

neftrans.dat = input with solubility to neftran

~~Cost~~ scheuer / tpa_4st/

- trial a 100,000 yr run, got held
up in NEFTRAN maximum run time
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 Neptun input File

Could not Fix ~~in~~ negative subscript with Rd changes in Ph210

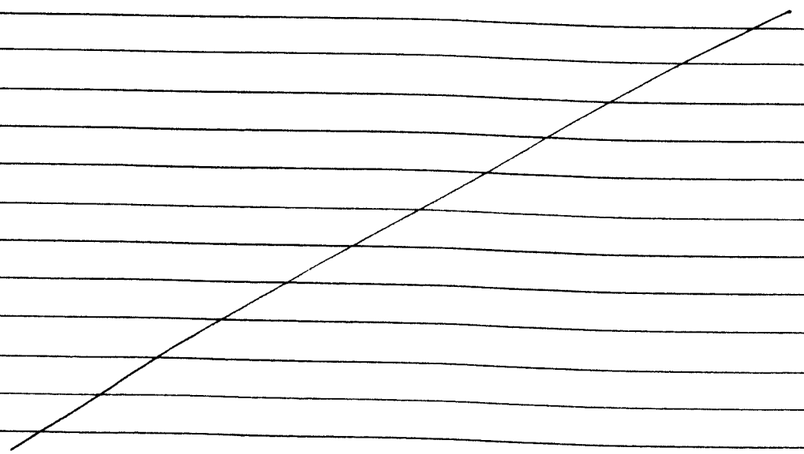
try changing ½-life exponent
2 → 3 → 4 → 5 → 6

"Subscript number 1 has value -2 in area, rho"

message does not go away until half life 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.
dc Jm 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-228.

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 fmt wen

- all input files *.inp that should have had up dated 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 fal.inp have been truncated

ls -lct lists files by modification date

ebs tr he.inp file contains 6 variable names and 4 columns ; it appears that j 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 tvh.dat
ebs flo.dat
ebs puc.nuc

notepad *.dat except stvm tube.dat have been up dated

why is stvm tube.dat not updated
should dat name be changed
new office # 226

Ip 225 ~ 129.162.200.225
at office # A226 (Ray G)

chl cr idemf.dat gives Eing, chloride data it is updated and appears reasonable

temp humd.dat is up dated and appears reasonable

stnef.dat appears to be an ebs Rel output sent to nef trans - is this really used ?

ebsflo.dat is up dated contains time, dsp rate data

* Note: after calling SZ ft 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

sstnef elbsflo chlori demf
maxrel lbstrh echo_fail
ebsnef temphumd
- are updated each area

ebsnuc multiclo climate
- 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 ##
ebsfail nefii uz

climate updates each realization

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

---

between areas only # wash packages and # scenario failures changed

a diff crossing 2 realizations showed only # contaminated, scenario # & scenario time differs

web

ISZ & NCMP = ILAST

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

ILAST - IC < 0 is the problem

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

ISZ = N1 - 1
N1 = N x (11 + NC(11) + 1
NX = # blocks in les
NC = # catcher blocks

so ISZ = ILAST = # blocks + # catcher blocks in les 1 ??

DSMX = maximum distance from boundary that is affected

what we & dx, pass in nfrm ??

IC = DSMX / DX(LG)

= max distance affected / length of leg

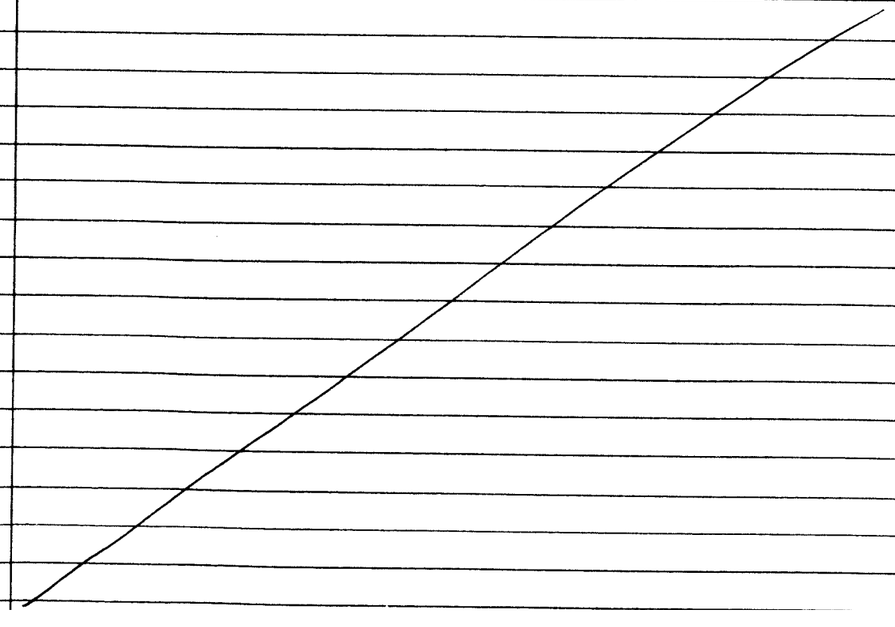
DSMX = Σ DIS = Σ VA * TS

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

when VA gets too high use hard problems

- initially 40 seconds are needed to run ust + change climate
time ~~step~~ steps 500 → 1000 yr

~34 s cpu time



6/25

in 625a directory
cp -r c s cheren/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 capped make in tpa.inp
.exh is input
.res is code output

initial 500 yr time steps
time not take → 22m 0:23

generate input file by interpting first area in
first realization

changed u2ft.f 50000 → 250000
years
recompile tpa code

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

---

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

line 592 in release.f

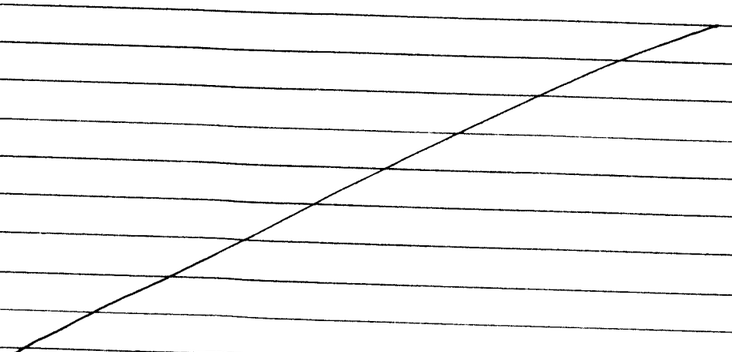
Fraction of Flow Hitting Waste Package

* ash movo.f

loops from 1 to 43 nuclides
are hard coded
- should use 1, maxnucs vol
which currently = 43 instead
of hard coded as 43

* changes.f loops from 1 to 43
in do loops; change to 43 to
maxnucl

* decay.w also has the same problem



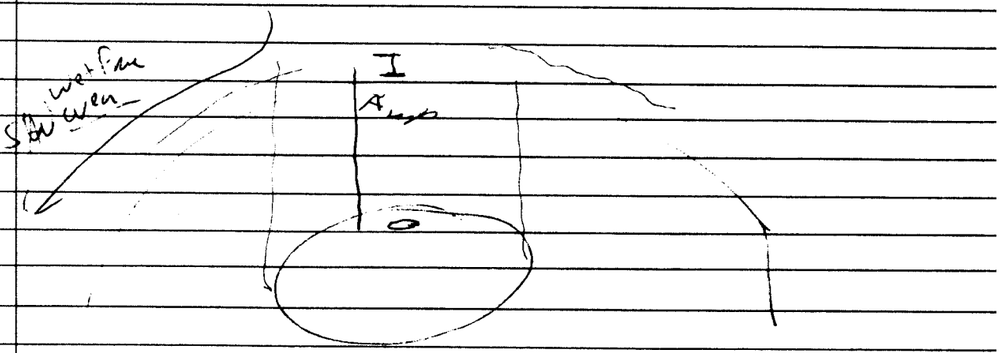
8/24/97 Flow

10 realizations run finished

Flow Factor = 0.3
Fmult Factor = 0.1
Sub Area Wet Fraction = 0.15
initial diameter 0.10 ± 0.01

this results in considerable reduction in dose

i.f.p takes one units of CYLWAT

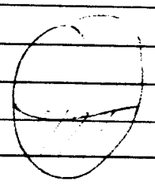


SAwetfac = fraction of cont. that can wet/drip

flow * area based infiltr = drip rate - flow * fix area

Fmult: flow diversion factor, always ≤ 1
= other realms with drips might flow out
of the waste package = 1.0 for this
Fmult = Capillary barrier diversion *
* runs down side of drift
* actually enters hole in WP

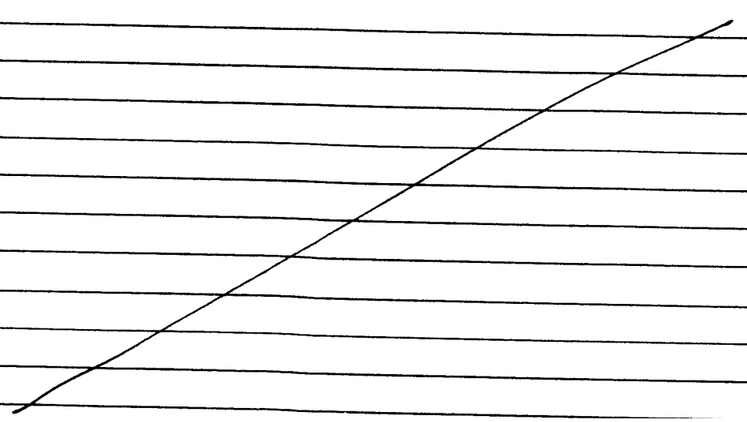
* gif hits closed



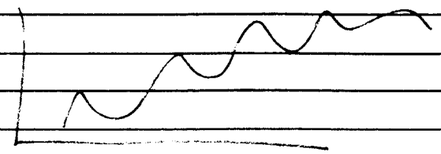
Put all flow factors up to 1.0 mode
all initial elevations, increased
initial storm to check TDA mass balance
also reduced starting recession coefficient

** WSft 52 ft gives no release when
total time 164 > 264 even though
release occurs at 164 in total time

flow rules into the areas so way up
for 264 in time



** WZ flow dim drops increasing
flow rates when total time > 16 time yr



** → when return input file "AtwZ"
program sees high flow it
eliminates too many less and
there is no transfer through WZ
solution - have it just copy
to by val output to ref WSZ input f.h

after maximum release rate
WSft rech has sub of I = 129
but 52 ft rech still none

Cum Val vol is cumulative release to AE
from ebs, WS zone, Sat zone

Cif WP 307
7125 wpl

0.2596 $\frac{Cif}{wp}$ * 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 ½ life for Pb-210 to keep neptun from bombing w/ negative subscript

		EOS	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	3.7018835E+03
1	Am243	1.8242838E+05	1.7594821E+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	5.7668206E-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	2.5304589E+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 unc -

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

Changed flow-induced infiltration to 1.0 to 1.1 & now neptun won't run well

Changed to 1-10, the default mm/yr

we frequently get no or too low release from neptun

6-27-91 JH

~ Vrice / tpa624 / cases' nefmtf

- Increased flow rates by one order of magnitude & ran to be dat

rel cum. rels

		EDSPAC	NZFT	SZFT
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	2.6811919E+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 set by Xfmt in one cases

increased I, Tc ½ life → ∞ to eliminate decay

1 case run

1	Cm246	1.5434507E+03	2.4298441E-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	5.4187189E+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	6.1512589E+03	6.1104750E+03
1	I129	1.9498706E+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	8.3378064E+02	8.3399035E+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 gap release, Tdue di

now do 2 runs changing time step increment

in 625b change increment to 1.0

time stp fact=1.00

Cm246	6.1666471E+02	4.8047488E-05	4.6717495E-05
U238	2.2571884E+04	2.4912219E+03	2.4648472E+03
Cm245	3.3527810E+03	4.2551628E-04	4.1393660E-04
Am241	1.0539784E+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	1.0873335E+05	1.1565447E+04	1.1441791E+04
Th230	1.7069100E+03	3.2968739E+01	3.5318721E+01
Ra226	4.1200500E+02	9.5593439E+00	9.8831510E+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	8.5455780E+05
Ni59	1.8205110E+05	6.4477600E+04	6.4080876E+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	2.1296485E+02
Cl36	8.7368754E+02	8.8831034E+02	8.8815891E+02
	EPS	U2FT	S2FT

>20% error

~1.18

~1.175

1.016

time stp fact=1.0

Cumulative release

Cm246	1.8678806E+02	1.5352726E-05	1.4806913E-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	2.1288125E+02	2.1149713E+02
Cl36	6.8878085E+02	7.1936003E+02	7.1913838E+02
	EPS	U2	S2

2% error

I error ~264%

fact = 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	2.3791588E+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	3.0993193E+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	8.3818437E+05	8.3762401E+05	8.3729980E+05
Ni59	1.4406677E+05	5.2260184E+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	8.8944953E+02	7.2003583E+02	7.1982307E+02

EBS UZ SZ

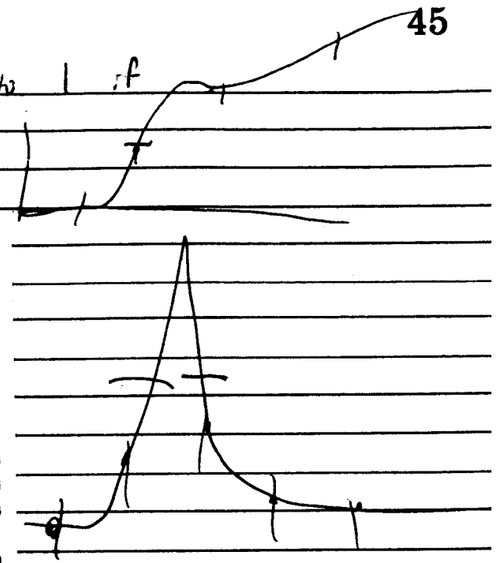
ratio back = 10

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

	EBS	UZ	SZ
Cm246	1.5354970E+03	1.2452894E-04	1.2088611E-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	2.9852684E+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	3.6129436E+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	2.2859817E+03	2.3216605E+03	2.3208692E+03
Tc99	8.5766815E+05	8.5769328E+05	8.5833491E+05
Ni59	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	9.0796893E+02	9.2283319E+02	9.2332123E+02

make tpg 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	5.9184428E-06
Am241	2.0537243E+04	5.8237688E-05	5.5135598E-05
Np237	4.8848080E+03	2.3914905E+03	2.3758634E+03
Am243	8.6368124E+03	5.3505153E-02	5.2005268E-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	6.6004868E+00
Pb210	2.6978795E+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	8.3668708E+05
Ni59	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	8.0878637E+01	4.8177982E+01	4.8178561E+01

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Cm246	1.1283806E+03	9.4082585E-05	9.1348931E-05
U238	2.1895717E+04	2.4046925E+03	2.3791588E+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	8.3818437E+05	8.3762401E+05	8.3729980E+05
Ni59	1.4406677E+05	5.2260184E+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	8.8944953E+02	7.2003583E+02	7.1982307E+02

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Cm246	1.5220931E+02	1.0764172E-05	1.0450764E-05
U238	2.0105043E+04	2.1518621E+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	2.3071716E+04
U234	9.5017869E+04	9.9868092E+03	9.8787432E+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	3.6421798E+02	3.6208429E+02	3.6201440E+02
Tc99	8.0059342E+05	7.9843507E+05	7.9832058E+05
Ni59	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	2.2068465E+02	2.1148782E+02	2.1027765E+02
Cl36	1.4425913E+02	1.4251781E+02	1.4243524E+02

2aq

	FEBS	U2	S2
Cm246	1.0265299E+03	7.5643475E-05	7.3415894E-05
U238	2.1401993E+04	2.2988524E+03	2.2741859E+03
Cm245	5.5818984E+03	6.7162859E-04	6.5198952E-04
Am241	1.6814937E+07	2.3489183E-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	8.2206287E+02	6.1660439E+02	6.1655723E+02

Conclusion - code of mag nitude error or more based on time step changes

could not run tpa with ≥ 2aq time steps because release has a 300 step limit

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

- this is the variable nbt

ebs.ref.dat gets time steps from nbt

Sut ref.dat uses tpa time steps

the map list is due to ebs.ref.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%.

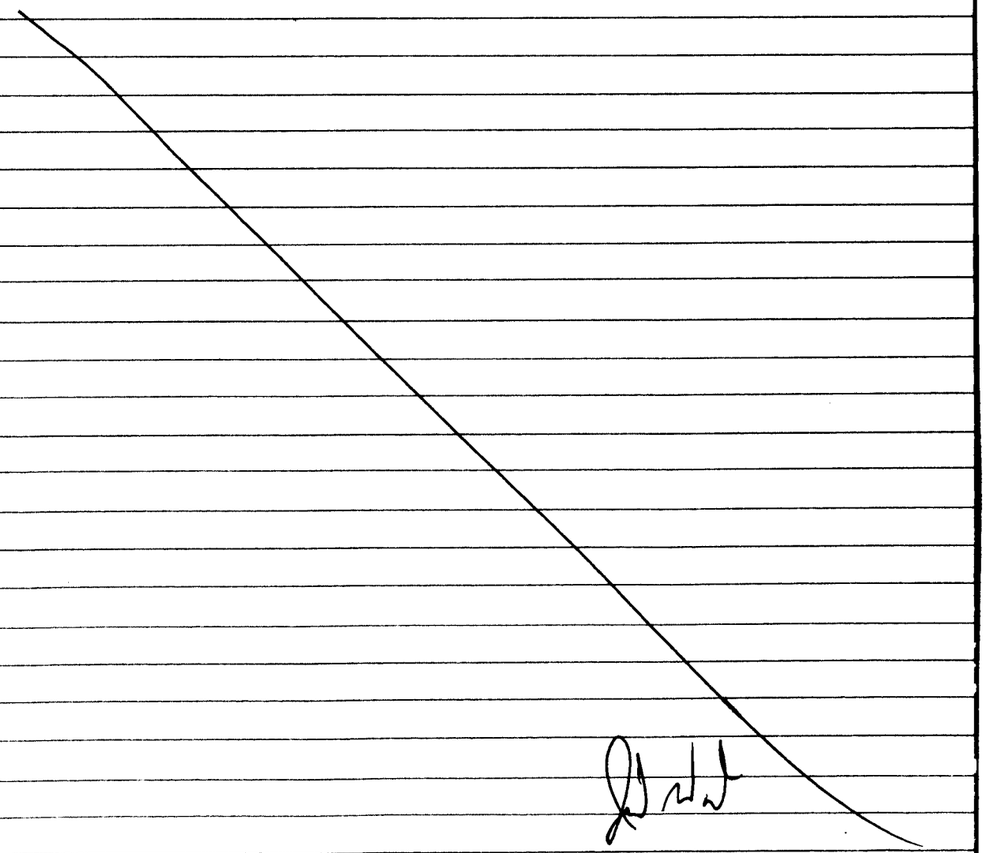
10. (B) Changing the time step ratio in tpa from the default (100) to values of 10, 1 and some other values resulted in cumulative release changes at (EBS, UZ, SZ) of around 1000% or more in some cases. Since one does not know a priori when the greatest action is, it is probably best to use a multiplier 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 Cooler 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