

SOFTWARE CHANGE REPORT (SCR)

SCR No. (Software Developer Assigns): PA-SCR-270	Software Title and Version: TPA 3.2.2	/Project No: 20-1402-762
Affected Software Module(s), Description of Problem(s): maxntime.i, releaset.f The number of TPA executive time steps is controlled by the maxntime.i include file. All files that reference this include file specify internal time array sizes as 201. This limits the flexibility of the code in doing time step dependent studies. Releaset.f has an internal time array size of 300 to accept the executive time steps. This change should be coordinated with the change to maxntime.i.		
Change Requested by: S. Mohanty Date: 5-28-99	Change Authorized by (Software Developer): S. Mohanty <i>[Signature]</i> 7/14/99 Date: 5-28-99	
Description of Change(s) or Problem Resolution (If changes not implemented, please justify): The maxntime.i size was set to 401 and the releaset.f array size was set to 402.		
Implemented by: Ron Janetzke <i>[Signature]</i>	Date: 5-28-99	
Description of Acceptance Tests: Four cases were considered: 1) oso - seismic only at 20km, 2) fso - seismic and faulting at 20km, 3&4)fsv - seismic, faulting, and volcanic at both 10km and 20km. The standard tpa.inp file was used and no differences were found in the results compared to the runs before the change was made (10,000 years maximum and compliance, 1 vector, 7 subareas).		
Tested by: Ron Janetzke <i>[Signature]</i>	Date: 5-28-99	

SOFTWARE CHANGE REPORT (SCR)

SCR No. (Software Developer Assigns): PA-SCR-271	Software Title and Version: TPA 3.2.2	Project No: 20-1402-762
Affected Software Module(s), Description of Problem(s): ebsrel.f, uzft.f Under certain conditions the large time steps of NEFTRAN containing a transition from zero to non-zero values get interpolated to non-zero values at the smaller time steps, sometimes advancing the non-zero values in time.		
Change Requested by: S. Mohanty Date: 5-28-99	Change Authorized by (Software Developer): S. Mohanty <i>AW for Sitakanta Mohanty 7/14/99</i> Date: 5-28-99	
Description of Change(s) or Problem Resolution (If changes not implemented, please justify): The interpolation section of ebsrel.f and uzft.f were changed to reduce the undesired effect of this interpolation procedure.		
Implemented by: Rob Rice <i>[Signature]</i>	Date: 5-28-99	
Description of Acceptance Tests: A test was performed to show that the cases that had showed time of first release before the time of first failure were now successfully showing the time of first release occurring not only after the time of first failure, but also after the time corresponding to unsaturated zone and saturated zone transport. See attachment.		
Tested by: Rob Rice <i>[Signature]</i>	Date: 5-28-99	

(results for testing time stepping modifications - R.Rice)

"tpa.out"

=====

exec: Welcome to TPA Version 3.2

Job started: Wed May 12 14:55:36 1999

=====

Specified Global Parameters:

Compliance Period = 10000.0 (yr)
Maximum Simulation Time = 100000.0 (yr)
Number Of Realizations = 250

subarea 5 of 7 realization 139 of 250

exec: calling uzflow

exec: calling nfenv

exec: calling ebsfail

ebsfail: time of WP failure = 12063.5 yr

exec: failed WPs from INITIAL event = 2 at time = 999.3 yr

exec: failed WPs from CORROSION event = 652 at time = 12063.5 yr

*** failed WPs: all WPs failed ***

"szft.rlt"

(previous version-note releases before WP failure and with zero UZ and SZ travel)

Input file tpa.inp as supplied with TPA Version 3.2 Code.

Base case data set Rev 3.2 7/16/98

TPA 3.2, Job started: Wed May 12 14:55:36 1999

REALIZATION 139 SUBAREA 5

	time	Th230	I129	Tc99	C14	Se79
65	7.1645E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
66	7.4387E+02	0.0000E+00	3.8664E-11	0.0000E+00	0.0000E+00	0.0000E+00
67	7.7222E+02	0.0000E+00	1.3495E-10	0.0000E+00	0.0000E+00	0.0000E+00

"szft.rlt"

(modified version - note releases after WP failure and with UZ and SZ travel)

Input file tpa.inp as supplied with TPA Version 3.2 Code.

Base case data set Rev 3.2 7/16/98

TPA 3.2.3 PVM capable, Job started: Tue May 18 16:11:54 1999

REALIZATION 139 SUBAREA 5

	time	Th230	I129	Tc99	C14	Se79
96	2.1760E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
97	2.2526E+03	0.0000E+00	8.9737E-11	0.0000E+00	0.0000E+00	0.0000E+00
98	2.3318E+03	0.0000E+00	2.1858E-10	0.0000E+00	0.0000E+00	0.0000E+00

SOFTWARE CHANGE REPORT (SCR)

SCR No. (Software Developer Assigns): PA-SCR-261	Software Title and Version: TPA 3.2.2	/Project No: 20-1402-762
Affected Software Module(s), Description of Problem(s): ebsrel.f and exec.f. Ebsrel, uzft, and szft exhibit the behavior of showing a release prior to that specified in the input array. This is due to the linear interpolator trying to compensate for disparate time steps in the two arrays.		
Change Requested by: S. Mohanty Date: 5-18-99	Change Authorized by (Software Developer): S. Mohanty <i>SW for Sitakanta Mohanty 7/14/99</i> Date: 5-18-99	
Description of Change(s) or Problem Resolution (If changes not implemented, please justify): Compensation is made for the interpolator's behavior in the critical values of release from EBS, UZ and SZ. The output arrays from each section are compared to the input arrays such that if a non-zero appears in the output before a non-zero appears in the input, it is set to zero after interpolation. No attempt was made to modify the general interpolator to handle step functions in all cases. These changes will substantiate a new version, TPA 3.2.3		
Implemented by: Ron Janetzke <i>Ron Janetzke</i>	Date: 5-18-99	
Description of Acceptance Tests: Two cases were considered: 1) EBS release before WP failure time, and 2) UZ/SZ release before EBS release. The description of the tests is attached.		
Tested by: Bob Rice <i>Bob Rice</i>	Date: 5-18-99	

vulcan → /project/tpa/doeva/var/run/ll/test2/new-tpa.e/temg

R. Rice
5/18/99

FIXING THE 2 INTERPOLATION PROBLEMS (i.e., (1) releases before the initial failure and (2) UZ/SZ releases before EBS releases)

(prepared by R. Rice 5/18/99)

from tpa.inp, 250 realizations, 100,000 yrs,
initial failure time = 1000 yr, realization 216
and subarea 7

1. Releases before initial failure

Input file: intial WP failures at 1000.0 yr (which is mapped to 999.28 yr)

Output from releaset.f before modifying the source code
(note interpolation will be from 500 to 1000 yr - see TPA release rates below):

(ebsnef.dat)
release rate [ci/yr]
11 200 ! num nucs, ntemp
CM245
5.0000E+02 0.0000E+00
1.0000E+03 2.7541E-10
1.5000E+03 1.6739E-08
2.0000E+03 1.0532E-08
2.5000E+03 9.9064E-09
3.0000E+03 7.7138E-09

Release rates passed back into the EXEC from ebsrel.f (note release rates before the 1000 yr failure time) (ebsrel.rlt) - INCORRECT MAPPING

	(time)	(release rates ->)					
54	4.6780E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
55	4.8685E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
56	5.0654E+02	3.6029E-12	1.7415E-08	2.4344E-11	3.7743E-10	3.8218E-11	
57	5.2689E+02	1.4814E-11	7.1605E-08	1.0010E-10	1.5519E-09	1.5714E-10	
58	5.4793E+02	2.6403E-11	1.2762E-07	1.7840E-10	2.7659E-09	2.8007E-10	
59	5.6968E+02	3.8382E-11	1.8552E-07	2.5934E-10	4.0208E-09	4.0714E-10	
. . .							
72	9.2895E+02	2.3627E-10	1.1420E-06	1.5965E-09	2.4751E-08	2.5063E-09	
73	9.6353E+02	2.5532E-10	1.2341E-06	1.7252E-09	2.6747E-08	2.7083E-09	
74	9.9928E+02	2.7501E-10	1.3293E-06	1.8582E-09	2.8809E-08	2.9172E-09	
75	1.0362E+03	1.4684E-09	4.1288E-06	1.0883E-08	1.1477E-07	1.6055E-08	
76	1.0744E+03	2.7261E-09	7.0782E-06	2.0393E-08	2.0536E-07	2.9901E-08	
77	1.1139E+03	4.0262E-09	1.0127E-05	3.0225E-08	2.9899E-07	4.4214E-08	
78	1.1547E+03	5.3701E-09	1.3278E-05	4.0387E-08	3.9578E-07	5.9009E-08	
. . .							

Output after modifying the source code (ebsrel.f):

Release rates passed back into the EXEC from ebsrel.f (ebsrel.rlt) - CORRECT MAPPING

	(time)	(release rates ->)					
71	8.9549E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
72	9.2895E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
73	9.6353E+02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
74	9.9928E+02	2.7501E-10	1.3293E-06	1.8582E-09	2.8809E-08	2.9172E-09	
75	1.0362E+03	1.4684E-09	4.1288E-06	1.0883E-08	1.1477E-07	1.6055E-08	
76	1.0744E+03	2.7261E-09	7.0782E-06	2.0393E-08	2.0536E-07	2.9901E-08	
77	1.1139E+03	4.0262E-09	1.0127E-05	3.0225E-08	2.9899E-07	4.4214E-08	
78	1.1547E+03	5.3701E-09	1.3278E-05	4.0387E-08	3.9578E-07	5.9009E-08	

2. UZ/SZ releases before EBS releases:

Source rates supplied as input files to NEFTRAN (before modifying the source code)

(sotnef.dat)

I129

3175.8204973364	0.
3286.0907144946	0.
3400.0754560992	0.
3517.8998483377	9.8971841428645D-08
3639.6932323550	7.7239182033730D-07
3765.5893062373	1.4684963920474D-06

and

NEFTRAN output file

(nefii.dis)

I129

100000.0000000000	4.7261773262568
0.0000E+00	0.0000E+00
1.1786E+03	0.0000E+00
3.5359E+03	1.0315E-09
5.8932E+03	6.6366E-07
8.2505E+03	1.1363E-06
1.0608E+04	1.1647E-06
1.2965E+04	9.5676E-07
1.5322E+04	7.2090E-07

Release rates passed back into the EXEC from szft.f (note times mapped back to
TPA times from 1179 to 3536 yr based on the NEFTRAN output file nefii.dis)
(below value are form szft.rlt) - INCORRECT MAPPING

	(time)	(release rates ->)					
76	1.0744E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
77	1.1139E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
78	1.1547E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
79	1.1969E+03	0.0000E+00	8.0136E-12	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
80	1.2405E+03	0.0000E+00	2.7096E-11	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
81	1.2856E+03	0.0000E+00	4.6821E-11	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

108	3.2861E+03	0.0000E+00	9.2219E-10	1.0000E-05	0.0000E+00	0.0000E+00
109	3.4001E+03	0.0000E+00	9.7207E-10	2.0841E-05	0.0000E+00	0.0000E+00
110	3.5179E+03	0.0000E+00	1.0236E-09	2.2258E-05	0.0000E+00	0.0000E+00
111	3.6397E+03	0.0000E+00	3.0207E-08	2.3722E-05	0.0000E+00	0.0000E+00
112	3.7656E+03	0.0000E+00	6.5596E-08	2.5236E-05	0.0000E+00	0.0000E+00
113	3.8957E+03	0.0000E+00	1.0218E-07	2.6801E-05	0.0000E+00	0.0000E+00

Output after modifying the source code (uzft.f) - CORRECT MAPPING:

Release rates passed back into the EXEC from szft.f (szft.rlt)

	(time)	(release rates ->)				
107	3.1758E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
108	3.2861E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
109	3.4001E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
110	3.5179E+03	0.0000E+00	1.0236E-09	2.2258E-05	0.0000E+00	0.0000E+00
111	3.6397E+03	0.0000E+00	3.0207E-08	2.3722E-05	0.0000E+00	0.0000E+00
112	3.7656E+03	0.0000E+00	6.5596E-08	2.5236E-05	0.0000E+00	0.0000E+00
113	3.8957E+03	0.0000E+00	1.0218E-07	2.6801E-05	0.0000E+00	0.0000E+00

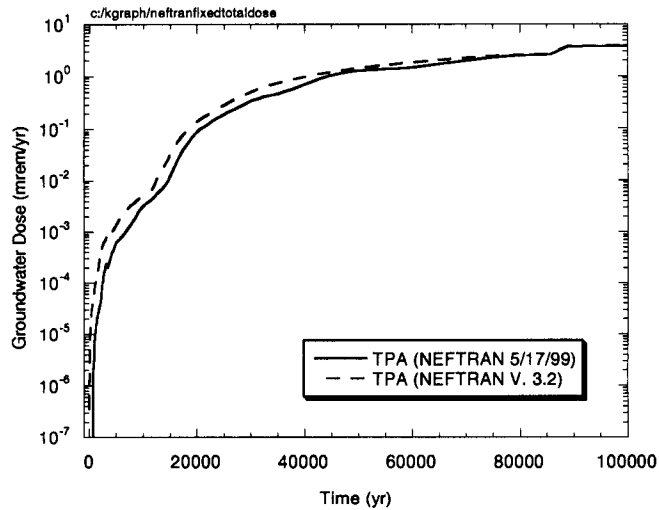
SOFTWARE CHANGE REPORT (SCR)

SCR No. (Software Developer Assigns): PA-SCR-260	Software Title and Version: TPA 3.2.2	Project No: 20-1402-762
Affected Software Module(s), Description of Problem(s): nefmks.f subroutines SETUP and CATCH. The dispersion of long paths is unduly controlled by the mixing zone source length. <i>along</i>		
Change Requested by: T. McCartin Date: 5-14-99	Change Authorized by (Software Developer): S. Mohanty Date: 5-14-99 <i>SW for Subhanta Mohanty 5/14/99</i>	
Description of Change(s) or Problem Resolution (If changes not implemented, please justify): subroutine SETUP: cc rwj 8-21-97 New line from T. McCartin via fax. cc SIGIR=SQRT(2.0*ALPHA(I)*VELISO(I,IR)/DT) cc rwj 5-14-99 "IF" block from T. McCartin via telecon. cc SIGIR=SQRT(2.0*ALPHA(I)*(VELISO(I,IR)**2)/path(i)) IF (LTOLX .EQ. 0) THEN SIGIR=SQRT(2.0*ALPHA(I)*(VELISO(I,IR)**2)/Y) ELSE SIGIR=SQRT(2.0*ALPHA(I)*(VELISO(I,IR)**2)/path(i)) END IF subroutine CATCH: cc rwj 8-25-97 New line from T. McCartin via telecon. cc V1 = VELISO(K,IR) + (-GA)*SQRT(2.0*ALPHA(K)*VELISO(K,IR)/DT) cc rwj 9-3-97 Add **2 for veliso per T. McCartin. cc rwj 5-14-99 "IF" block from T. McCartin via telecon. cc V1 = VELISO(K,IR) + cc & (-GA)*SQRT(2.0*ALPHA(K)*VELISO(K,IR)**2/path(k)) IF (LTOLX .EQ. 0) THEN V1 = VELISO(K,IR) + & (-GA)*SQRT(2.0*ALPHA(K)*VELISO(K,IR)**2/Y) ELSE V1 = VELISO(K,IR) + & (-GA)*SQRT(2.0*ALPHA(K)*VELISO(K,IR)**2/path(k)) END IF		
Implemented by: Ron Janetzke <i>Ron Janetzke</i>	Date: 5-14-99	
Description of Acceptance Tests: Five pages are attached. 1) Plots from original NEFTRAN code show dose increase for subarea 7 and Np237 release rates for all subareas with subarea 7 far above the others. 2) Plots from original NEFTRAN code showing 4 nuclides with a range of Rd values, indicating the early release is more pronounced with higher Rd values. 3) Same as 2) with small dispersion length showing early release for large Rd value nuclides eliminated. 4) Same as 2) with modified NEFTRAN code showing early release for large Rd value nuclides eliminated. 5) Before and after plots for total GW dose, and peak GW dose.		
Tested by: Rob Rice <i>Rob Rice</i>	Date: 5-18-99	

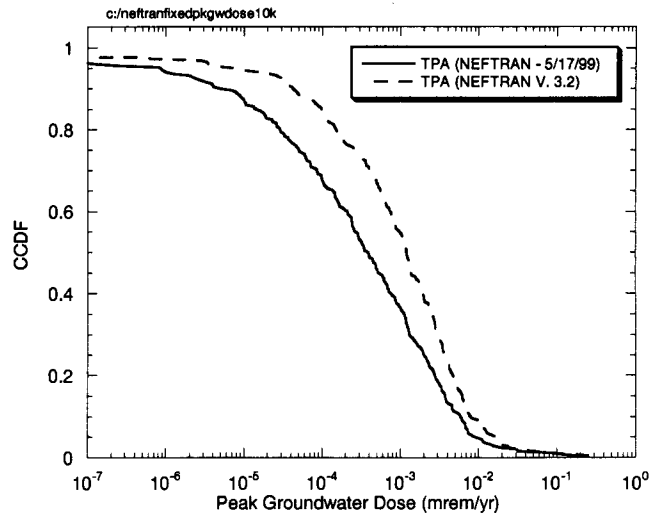
Testing After NEFTRAN Fixed

5/18/99
R. Rice

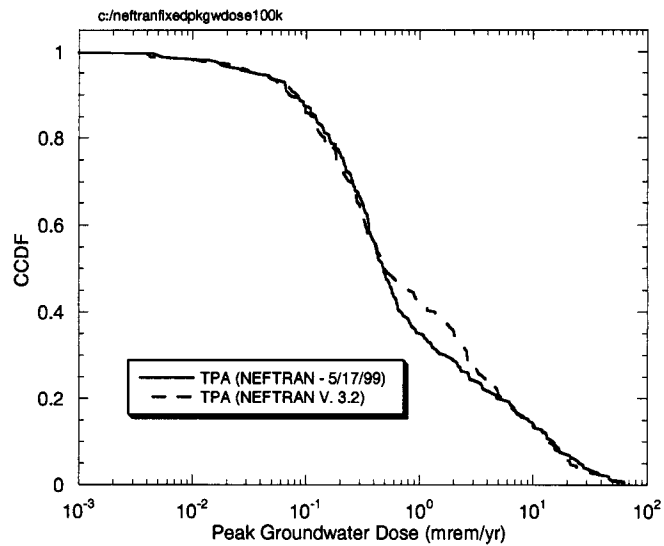
TPA Results for Total Groundwater Dose Using the Updated NEFTRAN and NEFTRAN from the TPA Version 3.2 Code



TPA Results for 10,000 year Peak Groundwater Dose Using NEFTRAN from 5/17/99 and NEFTRAN from the TPA Version 3.2 Code



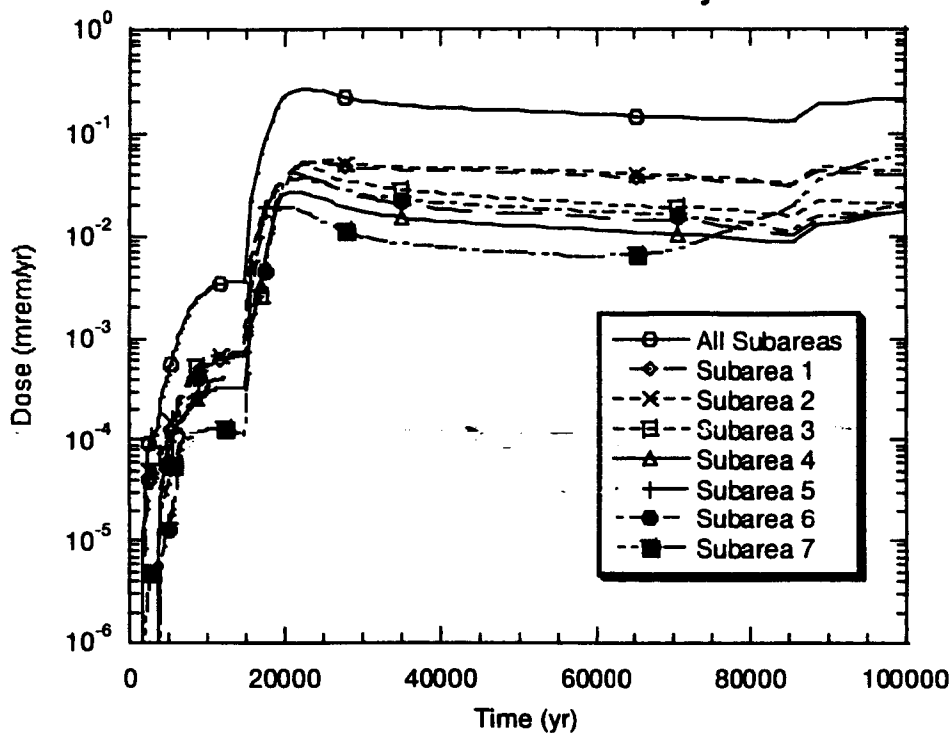
TPA Results for 100,000 year Peak Groundwater Dose Using NEFTRAN from 5/17/99 and NEFTRAN from the TPA Version 3.2 Code



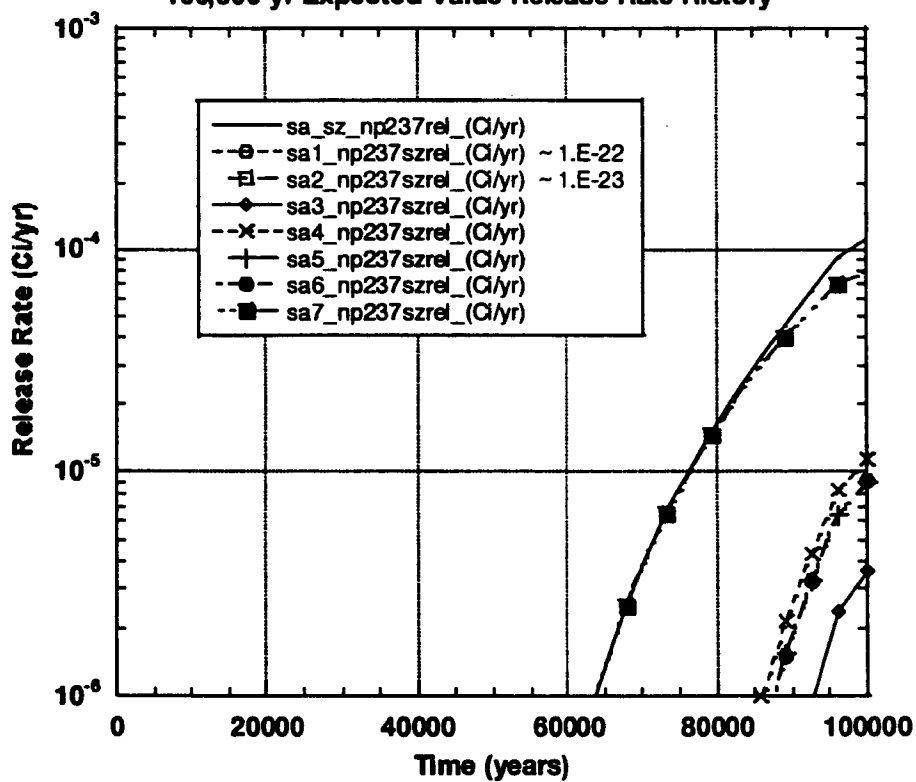
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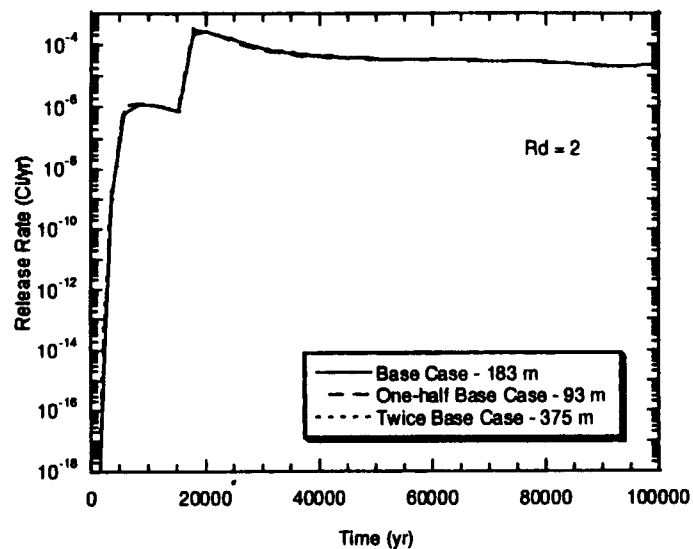
Dose From the Mean Value Data Set by Subarea



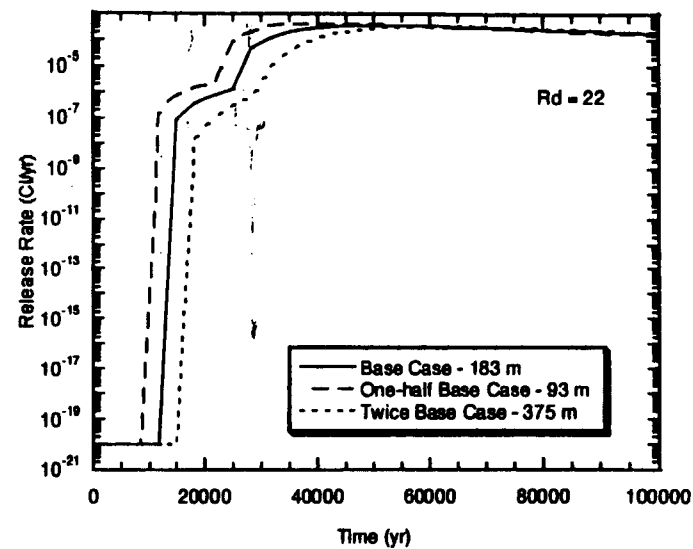
Release From SZ Np237
100,000-yr Expected-Value Release Rate History



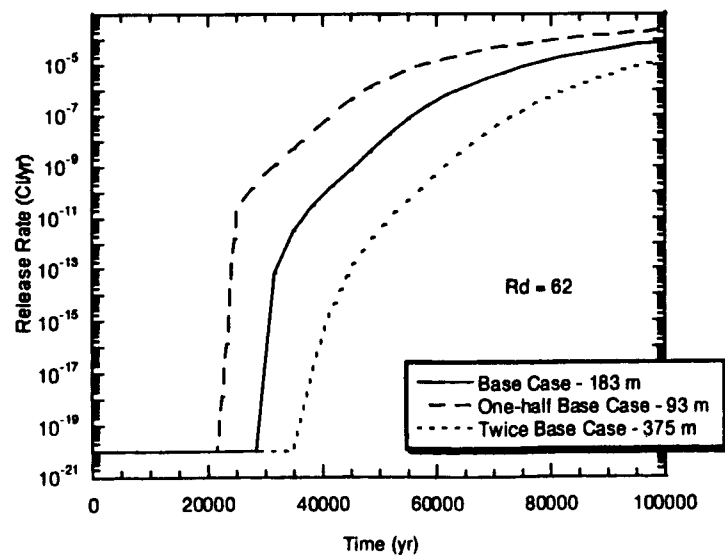
**I-129 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths**



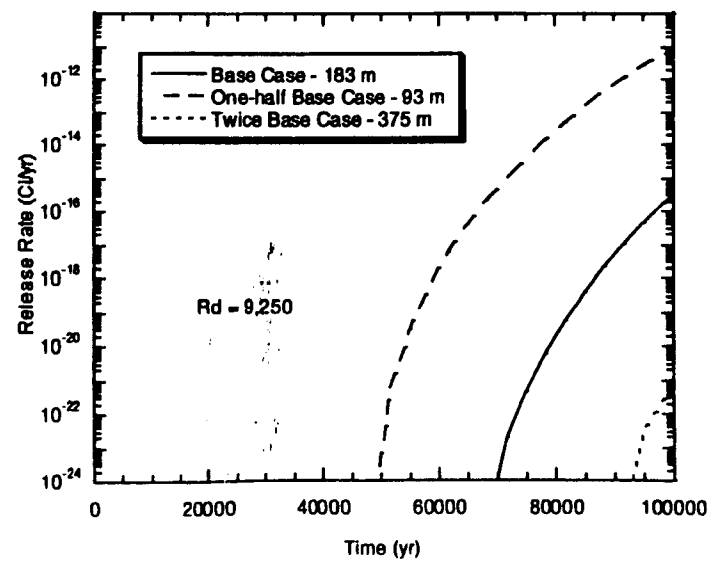
**Se-79 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths**



**Np-237 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths**

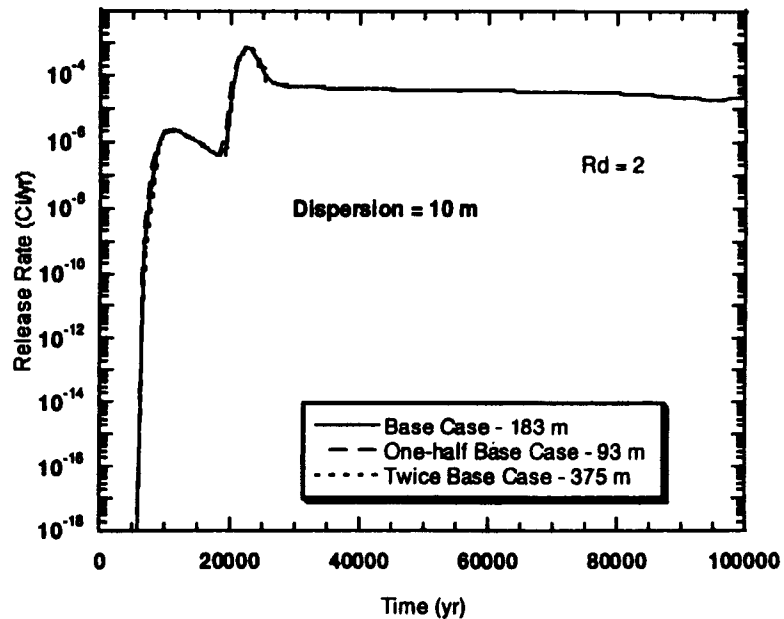


**Th-230 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths**



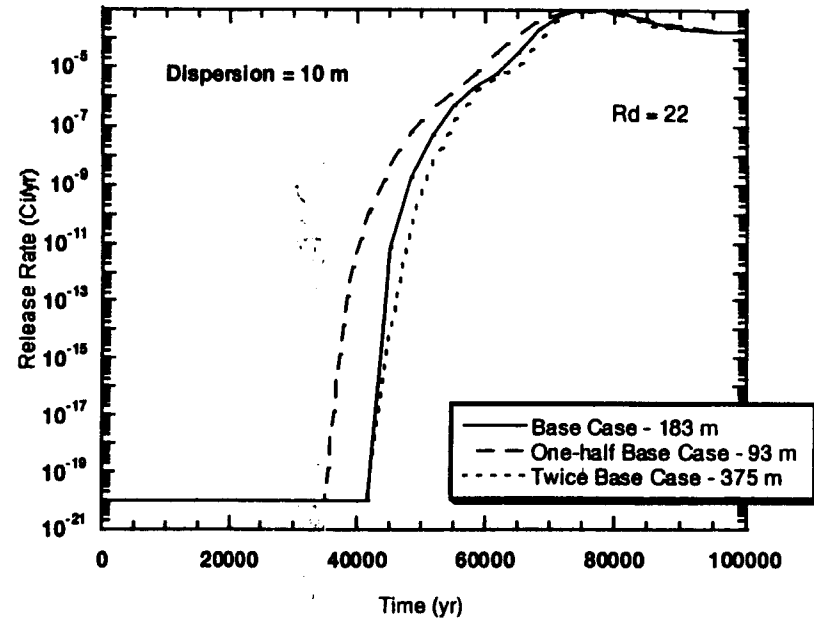
Dispersion Length = 10 m

I-129 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths



No Np-237 Release

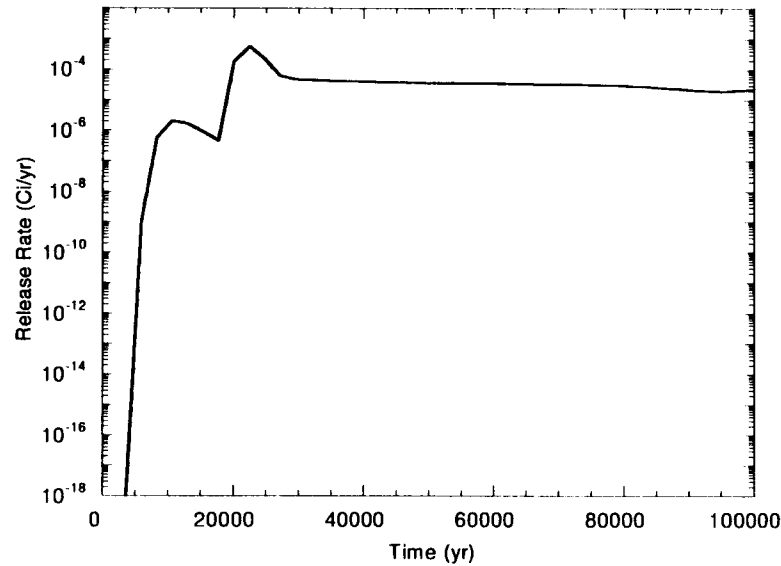
Se-79 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths



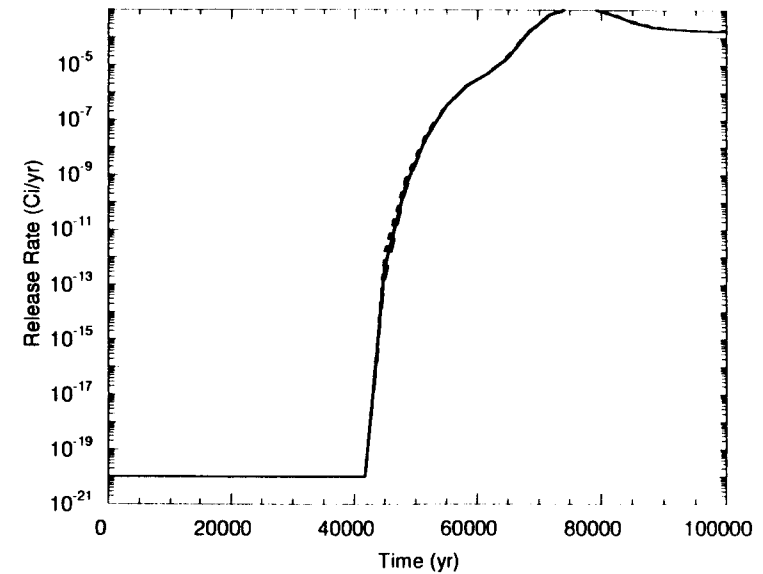
No Th-230 Release

Mean Value Data Set

**I-129 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths (new NEFTRAN 5/17/99)**



**Se-79 Saturated Zone Release Rates From Subarea 7
with Varying Mixing Lengths (new NEFTRAN 5/17/99)**



No Np-237 Release

No Th-230 Release

SOFTWARE CHANGE REPORT (SCR)

SCR No. (Software Developer Assigns): PA-SCR-259	Software Title and Version: TPA 3.2.2	Project No: 20-1402-762
Affected Software Module(s), Description of Problem(s): <p>At the time of delivery of TPA3.2 three versions of the TPA code were under development (TPA3.2, TPA3.2PCbeta, and TPA3.2PVMbeta). It is desirable from a development and configuration control point of view to have only one version of the TPA code. These three versions were merged to form the TPA3.2.2. No algorithmic changes were made and as far as the disparate platforms permit, none of the results changed. It was necessary to change all modules that used system calls or shell commands in order to interface them to the new system interface technique where all system calls are handled by a set of system independent interface routines in file zportpc.f.</p> <p>Reader.f, sampler.f and exec.f were changed to enable the PVM interface with PARJOB the PVM executive.</p>		
Change Requested by: Mohanty Date: 1-4-99	Change Authorized by (Software Developer): Date: 4/21/99 S. Mohanty	
Description of Change(s) or Problem Resolution (If changes not implemented, please justify): <p>A system independent set of routines located in zportpc.f was implemented to handle system utility functions for the SUN and PC platforms.</p>		
Implemented by: <i>R. Janetzke</i> M. Muller & R. Janetzke	Date: 2-18-99	
Description of Acceptance Tests: <p>The TPA3.2.2 code was tested with 29 different input files. The results of these runs were compared to the same runs on the PC platform. All differences were attributed to the differences in the machine CPU architecture and compiler extensions. A complete description of the testing is in CNWRA scientific notebook 310 authored by J. Menchaca.</p>		
Tested by: <i>J. Menchaca</i> J. Menchaca	Date: 3-5-99 <i>John W. Menchaca</i> 4/28/99	