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SOFTWARE RELEASE NOTICE

01. SRN Number: EBS-SRN-142	
02. Project Title: EBSPAC Development	Project No. 20-5708-572
03. SRN Title: EBSPAC Version 1.0	
04. Originator/Requestor: QA	Date: 1/9/97

05. Summary of Actions

- ■ Release of new software
- □ Release of modified software:
- □ Enhancements made
- □ Corrections made
- □ Change of access software
- ☒ Software Retirement VJ 12/10/01

06. Persons Authorized Access

Name	RO/RW	A/C/D
Sitakanta Mohanty	RW	
Dennis Vinson	RW	

07. Element Manager Approval: N. Eid/Kat Date: 1/9/98

08. Remarks:

Future versions of EBSPAC will be managed in accordance with TOP-018 by NRC Staff

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Name	RO/RW	A/C/D
Sitakanta Mohanty	RW	
Dennis Vinson	RW	

07. Element Manager Approval: N. Eid/LaS Date: 1/9/97

08. Remarks:

Future versions of EBSPAC will be managed in accordance with TOP-018 by NRC Staff

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SOFTWARE SUMMARY FORM

01. Summary Date: 1/8/97	02. Summary prepared by (Name and phone) Cathy Garcia (210) 522-5471	03. Summary Action: None
04. Software Date: 1/6/97	05. Short Title: EBSPAC Version 1.0	
6. Software Title: Engineering Barrier System Assessment Code		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch ■ Combination	10. APPLICATION AREA a. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ■ Total System PA ■ Subsystem PA ☐ Other b. Specific:
11. Submitting Organization and Address: Southwest Research Institute Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 782238-5166		12. Technical Contact(s) and Phone: Sitakanta Mohanty (210) 522-5185
13. Narrative: EBSPAC Predicts Container Life and Radionuclide Releases from the EBS.		

14. Computer Platform SUN SPARC	15. Computer Operating System: SUN OS	16. Programming Language(s): FORTRAN 77	17. Number of Source Program Statements: 5,947
18. Computer Memory Requirements: Varies	19. Tape Drives: None	20. Disk/Drum Units: Disk	21. Graphics: None
22. Other Operational Requirements None			
23. Software Availability: ■ Available ☐ Limited ☐ In-House ONLY		24. Documentation Availability: ■ Available ☐ Inadequate ☐ In-House ONLY	
Software Custodian: Sitakanta Mohanty Date: 1/14/97			

CNWRA Form TOP-4-1

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE: EBSPAC V. 1.0

May 15, 1997

EBSPAC VERSION 1.0

1. Scientific Notebook Documentation Development: CNWRA Electronic Scientific Notebook number 170 was verified; it is in the QA Records Room and it documents the EBSPAC Version 1.0 software development.

2. Programming Language: ANSI Standard FORTRAN 77 confirmed by the Software Custodian.

3. Internal Documentation: On 1/7/97, B. Mabrito reviewed portions of the EBSPAC Version 1.0 software on one of the CNWRA platforms. EBSPAC_fail and other files were reviewed and there were clear and numerous internal documentation comments meeting the requirements of TOP-018 Section 5.4.4. Printouts of screens were made and are part of the EBSPAC Version 1.0 folder documentation.

4. Software Labels and Data

a. Header Data and Format: EBSPAC Version 1.0 header data and the format were compared against TOP-018 (Revision 5 dated 4/3/97) Section 5.4.6 and found acceptable. Printout sheets of the header data and format are in the EBSPAC Version 1.0 scientific and engineering software folder in the QA Records Room.

b. NRC Data: EBSPAC Version 1.0 header NRC data and the format were compared against TOP-018, Section 5.4.6, third bullet and found generally acceptable.

c. Source Code Header: EBSPAC Version 1.0 header data was compared to TOP-018 Section 5.4.6, fourth bullet, and found generally acceptable.

5. Unique Run Identification: At the top of output files a unique identifier is created on the print out. For instance, a page of the "Calculation of Waste Package Failure Time" file printed and kept in the EBSPAC Version 1.0 QA Records Folder showed the following: "Version 1.0 Mon Jan 6 17:36:57 1997". This file was created on that date/time and it fully meets the unique run identification requirements of TOP-018, Section 5.4.5.

6. Software Analysis and Results

a. Analysis: The plusFORT programming tool was utilized as the software analysis tool on EBSPAC Version 1.0 during its development. Files of SPAG.fig were used during the development of the code. SPAG is a multi-purpose tool for analyzing and improving FORTRAN programs. It combines restructuring and re-formatting with both static and dynamic analysis in a single package. SPAG has the ability to: (i) restructure FORTRAN 66 to FORTRAN 77, (ii) identify and remove unused variables and code fragments, (iii) insert explicit type declarations for certain typed variables, (iv) convert back and forth between FORTRAN 77 and code with FORTRAN 90 extensions, (v) make re-formatted code clearer by using upper and lower case to distinguish

different types of symbols, (vi) can insert probes to perform a dynamic analysis of programs as they run, (vii) insert timing probes to identify computational hot-spots, and (ix) write out symbol table files for reference. The plusFORT reference manual, Revision B, is in Ron Janetzke's office as of 5/15/97.

b. Analysis Report: Since the software analysis of EBSPAC Version 1.0 was conducted incrementally during development and few copies of documentation were made, there is a minimum of objective evidence available. However, several selected pages have been printed out and are in the EBSPAC Version 1.0 scientific and engineering software QA Folder and they frequently reference "End of declarations inserted by SPAG" throughout the document (and have been highlighted with a blue highlighter in that folder).

c. Resolution of Comments: The developer(s) reviewed all of the warning and error messages provided by SPAG and addressed the most critical problem statements. According to developer S. Mohanty, the code analyzing software are very different from each other. Therefore, using a different analyzer, such as FOR_STUDY, may give warnings not found in SPAG.

5/15/97

CNWRA Software Developer **Date**

(Sitakanta Mohanty)

5/15/97

CNWRA Software Custodian **Date**

(Bruce Mabrito)

original to: Software Folder
cc: CNWRA Software Developer

```
-rwxrwxrwx  1 root     daemon       1624 [redacted]20 14:52 ebspac.nuc

-rwxrwxrwx  1 root     daemon        129 Jan 20 14:52 ebspacru
                                     UNIX name:    ebspacrun

-rwxrwxrwx  1 root     daemon       3124 Jan 20 14:59 ex_fail.inp
                                     UNIX name:    example_fail.inp

-rwxrwxrwx  1 root     daemon       2330 Jan 20 14:52 ex_relea.inp
                                     UNIX name:    example_release.inp

-rwxrwxrwx  1 root     daemon      68425 Jan 20 14:53 fail.f

-rwxrwxrwx  1 root     daemon        149 Jan 20 14:53 floebs.dat

-rwxrwxrwx  1 root     daemon     139251 Jan 20 14:53 release.f

-rwxrwxrwx  1 root     daemon     754061 Jan 20 15:17 tefkti.inp
```

EBSPAC VERIFICATION

EBSPAC code is one of its kind and therefore no other code can be used for an exhaustive verification of this code. Although EBSPAC has borrowed models from previously established codes, such as, SOTEC or/and SCCEX, these two codes can not be used for such verification testings because of many modifications to the models. Therefore, various intuitive verifications are conducted to demonstrate that the code behaves in some limiting cases as one would expect.

TEST 1

In the first test, the flow rate into the WP was changed. The following is the result from ebspac_release.f when all parameters are kept at the default values. In this data set summary results are presented for this standard run. Note that xnoloss is the radioactivity that would have been in the WP had there not been any release. Amwp represents the amount of radionuclide in the wp water at the end of 10000 years. Xmass represents the amount of radionuclides that have come out of the WP. Fracleft is the fraction of the radionuclides originally present in the wp is still in the wp. In other words, fracleft = 0.98 implies that 98% of that particular radionuclide has already come out. A value of 0.02 indicates that the total amount of that particular radionuclide present in the wp has come out and a maximum error is nearly 2%.

Qin = 2.086E-3 * 1.0 m3/yr

cumulative release [ci/cell] by 10000.0 years

namall	halflife(yr)	xnoloss(ci)	amwp(ci)	xmass(ci)	fracleft
CM246	0.473E+04	0.195E+02	0.191E+02	0.746E+00	0.96
PU242	0.386E+06	0.514E+04	0.523E+04	0.645E+00	1.00
U238	0.447E+10	0.104E+04	0.106E+04	0.671E-01	1.00
CM245	0.850E+04	0.182E+03	0.179E+03	0.696E+01	0.96
AM241	0.432E+03	0.193E+03	0.190E+03	0.639E+01	0.97
NP237	0.214E+07	0.202E+04	0.202E+04	0.372E+02	0.98
AM243	0.738E+04	0.198E+05	0.202E+05	0.842E+01	1.00
PU239	0.241E+05	0.763E+06	0.777E+06	0.962E+02	1.00
PU240	0.654E+04	0.575E+06	0.586E+06	0.727E+02	1.00
U236	0.234E+08	0.109E+04	0.111E+04	0.739E-01	1.00
U234	0.245E+06	0.600E+04	0.610E+04	0.387E+00	1.00
TH230	0.770E+05	0.524E+03	0.533E+03	0.116E-01	1.00
RA226	0.160E+04	0.409E+03	0.410E+03	0.543E+01	0.99
PB210	0.223E+02	0.407E+03	0.342E+03	0.718E+02	0.82
CS135	0.230E+07	0.114E+04	0.907E+00	0.116E+04	-0.02
I129	0.157E+08	0.969E+02	0.625E-02	0.986E+02	-0.02
TC99	0.213E+06	0.389E+05	0.230E+01	0.395E+05	-0.02
NI59	0.800E+05	0.107E+05	0.166E+04	0.921E+04	0.14
C14	0.573E+04	0.150E+04	0.365E-02	0.152E+04	-0.02
SE79	0.650E+05	0.112E+04	0.114E+04	0.112E-02	1.00
NB94	0.203E+05	0.185E+04	0.301E+00	0.188E+04	-0.02

zeroth yr inventory for liquid releases: 10040.5
zeroth yr inventory for gaseous releases: 8107.1

1000-yr c14 inv. for liq. rel [ci/cell:	10036.7
1000-yr c14 inv. for gaseous rel. [ci/cell]:	8104.1

The results presented below are obtained by drastically increasing the flow rate of water into the wp so that if the SF leaching is fast, then all material in the WP must come out in 10,000 years. AS seen in the last column of the output table, all radionuclides have come out of the WP and a maximum error of 1% is seen.

Qin = 2.086E-3 * 1000000.0 m3/yr

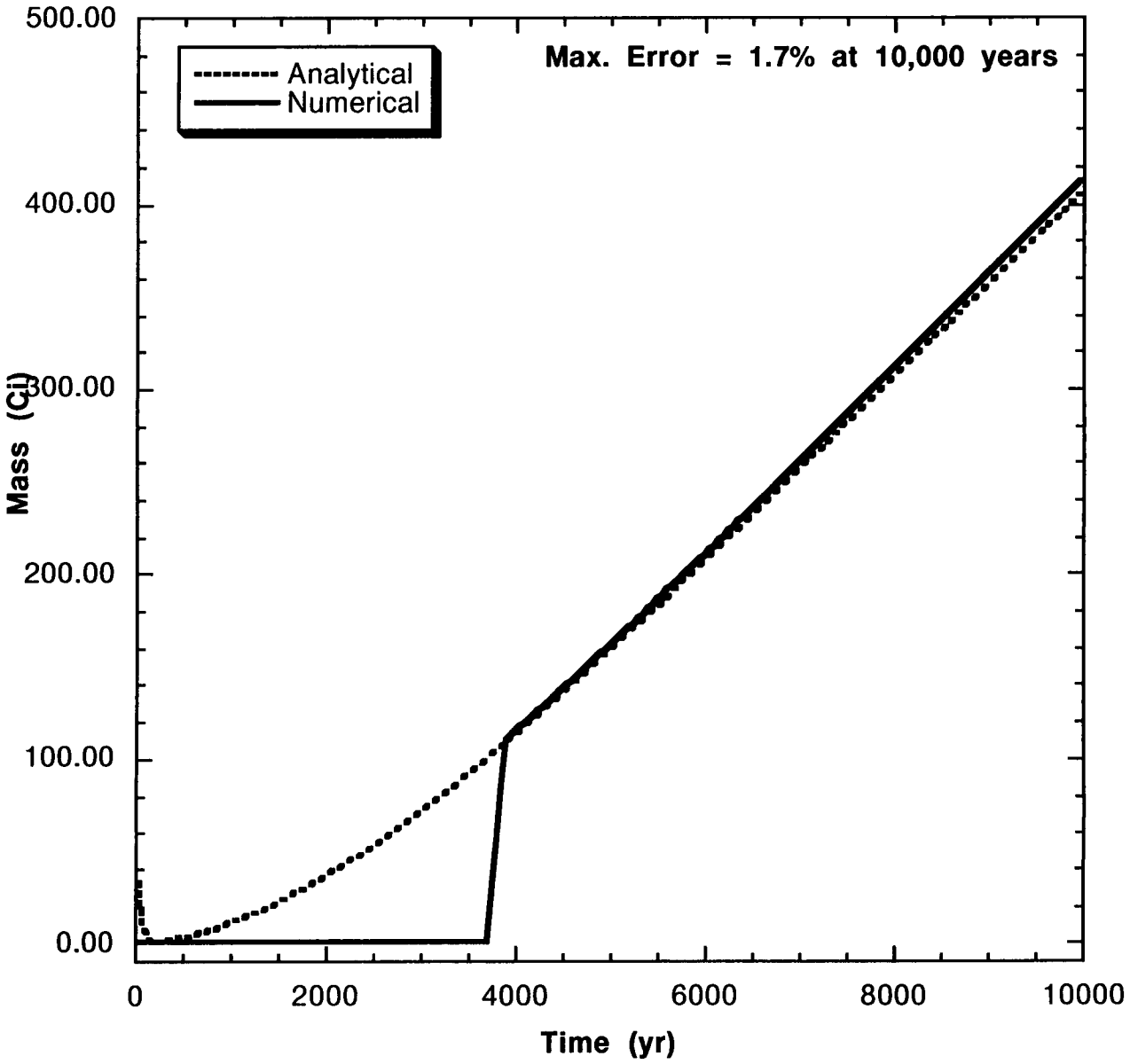
cumulative release [ci/cell] by 10000.0 years

namall	halflife(yr)	xnoloss(ci)	amwp(ci)	xmass(ci)	fracleft
CM246	0.473E+04	0.195E+02	0.587E-06	0.197E+02	-0.01
PU242	0.386E+06	0.514E+04	0.636E-02	0.519E+04	-0.01
U238	0.447E+10	0.104E+04	0.113E-03	0.105E+04	-0.01
CM245	0.850E+04	0.182E+03	0.291E-04	0.184E+03	-0.01
AM241	0.432E+03	0.193E+03	0.259E-06	0.195E+03	-0.01
NP237	0.214E+07	0.202E+04	0.240E-02	0.204E+04	-0.01
AM243	0.738E+04	0.198E+05	0.171E-02	0.200E+05	-0.01
PU239	0.241E+05	0.763E+06	0.470E+00	0.771E+06	-0.01
PU240	0.654E+04	0.575E+06	0.491E-01	0.581E+06	-0.01
U236	0.234E+08	0.109E+04	0.102E-03	0.110E+04	-0.01
U234	0.245E+06	0.600E+04	0.608E-03	0.606E+04	-0.01
TH230	0.770E+05	0.524E+03	0.201E-03	0.529E+03	-0.01
RA226	0.160E+04	0.409E+03	0.485E-06	0.413E+03	-0.01
PB210	0.223E+02	0.407E+03	0.716E-07	0.411E+03	-0.01
CS135	0.230E+07	0.114E+04	0.109E-02	0.115E+04	-0.01
I129	0.157E+08	0.969E+02	0.653E-05	0.979E+02	-0.01
TC99	0.213E+06	0.389E+05	0.241E-02	0.393E+05	-0.01
NI59	0.800E+05	0.107E+05	0.931E-03	0.108E+05	-0.01
C14	0.573E+04	0.150E+04	0.453E-05	0.151E+04	-0.01
SE79	0.650E+05	0.112E+04	0.574E-04	0.113E+04	-0.01
NB94	0.203E+05	0.185E+04	0.316E-03	0.187E+04	-0.01

zeroth yr inventory for liquid releases:	10040.5
zeroth yr inventory for gaseous releases:	8107.1
1000-yr c14 inv. for liq. rel [ci/cell:	10036.7
1000-yr c14 inv. for gaseous rel. [ci/cell]:	8104.1

TEST 2

In the second test, the numerical calculations used in the code were verified. This test involves comparing the numerical computation of the amount of radionuclides at the end of 10,000 years and the results from the analytical solution by using Bateman equation for radionuuclide chains. The numerical method, and the Bateman equation, both are used in the code. The code is faked so that no release takes place from the WP. In that case, if SF matrix leaching is fast, then all materials in the wet region in the solid portion will come to the water in the WP. Therefore the amount of radionuclide in the solid if there were no water (calculated by using analytical Bateman equation) will be same as the amount in the liquid if that material has dissolved and has come to the liquid where the amount is calculated by using the numerical method. Comparison of the mass of PB210 is presented in the figure below. In this figure, the mass of PB210 computed by Bateman equation, and the numerical method are compared in which the dotted line represents the result from the Bateman equation. The solid line shows that there is no dissolution of the solid mass until after nearly 3600 years. Then note that the solid line rises very fast to match up with the dotted curve, suggesting that the leaching time is very short (of the order of 2000 years). After this leaching period, one would expect the two curves until 10,000 years to be identical. This figure show an excellent match between these two curves and a maximum error of 1.7% is seen by the end of 10,000 years.


Max. Error = 1.7% at 10,000 years
Analytical
Numerical
Mass (Ci)
500.00
400.00
300.00
200.00
100.00
0.00
0
2000
4000
6000
8000
10000
Time (yr)

MAIN INPUT DATA FILES CORRESPONDING TO THE CODE VERIFICATION

data file 1: EXAMPLE_FAIL.INP

```
\example input file for ebspac_fail
|
\simulation time
10000.                          ! tend: simulation time length [yr]
\                         ! when iflag=1 (defined later)
\
5.682, 1.802                    ! wplen,wpdia: wp length and diameter [m]
0.1, 0.02                 ! cthick1,cthick2: wp layers 1&2 thicknesses [m]
|
\choose source of temperature data
2                         ! iflag 1: emp. equation, 2: tab.data
1                         ! nset (temp.-rel hum. relationship to use
49.9999999                ! timintv (used when iflag=2)
|
\other temperature parameters
0.                        ! age of fuel (not used in this version)
|
\Dry oxidation of wp outer overpack
5.                        ! grainr: metal grain radius [micrometer]
25                        ! nseries (terms in the infinite series)
0.7e-3                          ! gbthick [micrometer]
1.e-2                     ! constant: used in the dry oxidation equn.
|
\evaporation-condensation
0.65                      ! humdc: critical relative humidity
2.e-3                           ! filmthk: thickness of water film [m]
97.                       ! ctemp: boiling point of water [C]
|
\Corrosion Parameters(Ep: pitting potential [mV]; Erp: repassivation potential
[mV])
-584.8                          ! xipto: outer overpack Ep intercept
3.92                      ! pttemo: temp. coef. of outer overpack Ep intercept
-24.5                     ! slpto: outer overpack Ep slope
-1.1                      ! slpttemo: temp. coef. of outer overpack Ep slope
-620.3                          ! xirpo: outer overpack Erp intercept
0.47                      ! rptemo: temp. coef. of outer overpack Erp intercept
-95.2                     ! slrpo: outer overpack Erp slope
0.88                      ! slrptemo: temp. coef. of outer overpack Erp slope
200.                      ! xipti: inner overpack Ep intercept
0.                        ! pttemi: temp. coef. of inner overpack Ep intercept
-240.                     ! slpti: inner overpack Ep slope
0.                        ! slpttemi: temp. coef. of inner overpack Ep slope
422.8                     ! xirpi: inner overpack Erp intercept
-4.1                      ! rptemi: temp. coef. of inner overpack Erp intercept
-64.                      ! slrpi: inner overpack Erp slope
```

```
-0.80                    ! slrptemi: temp. coef. of inner overpack Erp slope
0.75, 0.5                ! betaox1, betahy1: beta kinetics parameters
\                          for oxygen and water for WP outer overpack
0.75, 0.5                ! betaox2, betahy2: beta kinetics parameters for
\                          oxygen and water for WP inner overpack
3.80e12, 1.6e-1              ! rkox1 [c*m/y/mol], rkhy1 [c/m2/yr]
37300., 25000.               ! gox1 [J/mol], ghy1 [J/mol]
3.0e10, 3.2                  ! rkox2 [c*m/y/m], rkhy2 [c/m2/yr]
40000., 25000.               ! gox2 [J/mol], ghy2 [J/mol]
3.15e5, 0.0, 0.0         ! aa(1,1) [C/m2/yr], aa(1,2), aa(1,3)
6.30e4, 0.0, 0.0         ! aa(2,1) [C/m2/yr], aa(2,2), aa(2,3)
-0.46                    ! eexpt: in Vshe
8.66e-3                      ! rcoef:
0.45                     ! rexpont:
2.05e-4                      ! crate2: m/yr corrosion rate
0.0                      ! xcouple, a fractional coupling strength
0.0                      ! xread
3.e-1                    ! clconc: chloride concentration [mol/L]
3.e-4                    ! clcrit1: crit. chloride conc. for 1st layer [mol/L]
2.e-3                    ! clcrit2: crit. chloride conc. for 2nd layer [mol/L]
100.                     ! cfactor: chloride dilution factor
9.0                      ! refph: reference pH
1.0, 1.0                 ! taus:deposit tortuosity,spor:deposit porosity
|
\Runge-kutta control parameters
1.e-3, 1.e0                  ! dtini, dtmax
1.e-2, 1.e-30                ! errrel (same as eps), errabs (same as tiny)
|
\end
////2000                     ! nhista (used when iflag=1)
```

data file 2: RELEASE.INP

```
\input data file for ebspac release code: ebspac_release.f
|
\Cell information
2335.                   ! xcon: number of WP
1000                    ! iscon: # of WP in scenario failure
4500.                   ! sftime: time of  scenario failure [y]
0.00                    ! deffrac: defective fraction of WPs/cell
|
\WP information
1.421, 4.572                ! dintl: wp ID, xintl: internal length [m]
4.83                    ! xvol: wp internal vol[m3]
|
\Thermal data
'temphumd.dat'              ! temfil: temp. file (output from ebspac_fail.f)
97.                     ! ctemp: BP of water at atm. condition [C]
|
\Flow parameters
'floebs.dat'                ! hydfil: flow parameters file
7.                      ! funnel: funnel factor
|
\SF  materials
\
2800.                   ! amassc: SF mass [kg]
250., 10000., 1.0E-08, 0.5    ! fuewt,fueden,fuedif,fuepor
\
\Fuel leaching
2, 9.0, 0.2, 2.e-3, 5.e-1     ! imodel,phvalue,oxgnovpr [atm],cco3 [mol/L],wetfrac
|
\ Radionuclide inventory
'ebspac.nuc'                ! elefil: nuclide names, halflife,inventory
|
\C-14 generation
0.5e-3                      ! r0z: initial radius of SF particle [m]
37.                     ! rhou: density of SF [kg mole/m^3]
1.e-5                   ! r1z: radius of the SF grain [m]
1.e-6                   ! r2z: subgrain fragment radius after trans. frac. [m]
6.1e-4                      ! thclad: thickness of cladding [m]
7.2e-4                      ! cfuel: c-14 [ci] /kg SF
4.89e-4                     ! czmetal: c-14 [ci] /kg SF in Zry clad & other
metals
2.48e-5                     ! czoxide: c-14/kg SF in initial Zry oxide & crud
6.2e-6                      ! cgap: c-14/kg SF in grain and gap
|
\NUMERICAL
\
\Grids
10, 10                      ! imax,jmax: # of grid nodes in i,j directions
\X-COOR of grid nodes
```

```
.1, .5, 1.0, 2.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0
\Y-COOR of grid nodes
.1, .5, 1.0, 2.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0
\ Note: zones apply to the above grid, zones are the same for all cell
\ZONES
4                        ! nzones: no. of zones for material types
1    1  1    1  1        ! iz,ib,jb,ie,je: for zone 1
2    2  1    2  1        ! iz,ib,jb,ie,je: for zone 2
3    3  1    3  1        ! iz,ib,jb,ie,je: for zone 3
4    4  1    10 1        ! iz,ib,jb,ie,je: for zone 4
|
\Rock parameters
0.14, 0.34, 0.34, 0.34         ! rpor(1..nzones): rock porosity
|
\ Radionuclide transport
5.6e-5, 5.6e-5, 5.6e-5, 5.6e-5      ! rdiff(1..nzones):diffusion coef. [m2/yr]
5.0                      ! driftdia [m]
|
\ Solution algorithm control parameters (Runge-Kutta)
25., 0.0, 10.                  ! dtinit [yr], dtmin [yr], dtmax [yr]
1.0e-2, 1.0e-10                ! eps, tiny
|
\output parameters
200                      ! nbt: number of time intervals for output
|
\END
```

data file 3: FLOEBS.DAT

```
scratchy1:/u01/mohanty> more floebs.dat
1.                       ! flowfactr: flow factor
0.       2.086E-03       ! time(yr) and infiltration(m^3/yr)
10000.   2.086E-03       ! time(yr) and infiltration(m^3/yr)
```

REQUIREMENT DESCRIPTION

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SOFTWARE REQUIREMENTS DESCRIPTION FOR THE ENGINEERED BARRIER SYSTEM PERFORMANCE ASSESSMENT CODE (EBSPAC)

(Revised June 14, 1996)

by
Sitakanta Mohanty
Tae Ahn
Peter C. Lichtner
Ronald W. Janetzke
Gustavo A. Cragnolino

Center for Nuclear Waste Regulatory Analyses
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Version 1.0

Approved by:

Narasi Sridhar, Manager, EBS Element
CNWRA

Revised 6/14/96

1 INTRODUCTION

This Software Requirements Description (SRD) document is the first stage in the development of the Engineered Barrier System Performance Assessment Code (EBSPAC), a numerical model for the evaluation of container life and source term. EBSPAC will be used as the source term module in the Nuclear Regulatory Commission (NRC) Total System Performance Assessment (TPA) code.

2 SOFTWARE REQUIREMENTS DESCRIPTION: EBSPAC

This SRD briefly outlines the software function, technical bases, computational approach, program flow and user interface, hardware and software requirements, graphics, and pre- and post-processors that are relevant to the development and use of the code EBSPAC.

Because EBSPAC will be used as a module in the TPA code that will execute hundreds of Monte Carlo runs, the EBSPAC code must be based on simplified models that will allow fast computation. As a rule of thumb, the design will be such that the average execution time for a single EBSPAC run will be in the neighborhood of 22 seconds on CRAY-YMP with eight processors. With an execution time scale factor of approximately 10, this 22 cray-seconds will be equivalent to 220 seconds on a UNIX IPX machine. EBSPAC will be developed and will be placed under Center for Nuclear Waste Regulatory Analyses (CNWRA) configuration management as required by the CNWRA Technical Operating Procedure (TOP)-018.

2.1 SOFTWARE FUNCTION

The code EBSPAC will be used to provide the source term to the TPA code. The code will provide waste package failure time and the release rate of radionuclides from the engineered barrier system (EBS). The code may eventually be used to evaluate the issue of criticality in conjunction with the U.S. Department of Energy (DOE) reference waste package design proposed in the TSPA-95 report (U.S. Department of Energy, 1994, 1995). However, criticality calculations are not considered in the first version of EBSPAC. Additionally, the multipurpose canister (MPC) performance is ignored in this version in correspondence with TSPA-95 calculations.

The first iteration of EBSPAC will be based on the SCCEX code modified to be applicable to the reference design. EBSPAC will not perform calculations to address "substantially complete containment" because of a possible rule change which may eliminate subsystem requirements.

2.2 TECHNICAL BASIS: PHYSICAL AND MATHEMATICAL MODELS

The code EBSPAC will consist of a number of modules based on a simplified physical description of the underlying processes which govern the failure of the waste package and ultimate release of radionuclides. Figures 1 and 2 show a simplified conceptualization around which the EBSPAC code will be built. This includes the horizontal emplacement of the waste package instead of the vertical emplacement implemented in SCCEX and SOTEC (Cragnolino et al., 1994; Sagar et al., 1992) codes. The main modules to be included in the EBSPAC code are briefly described below. The flow diagram in Figure 3 shows various components of the EBSPAC code.

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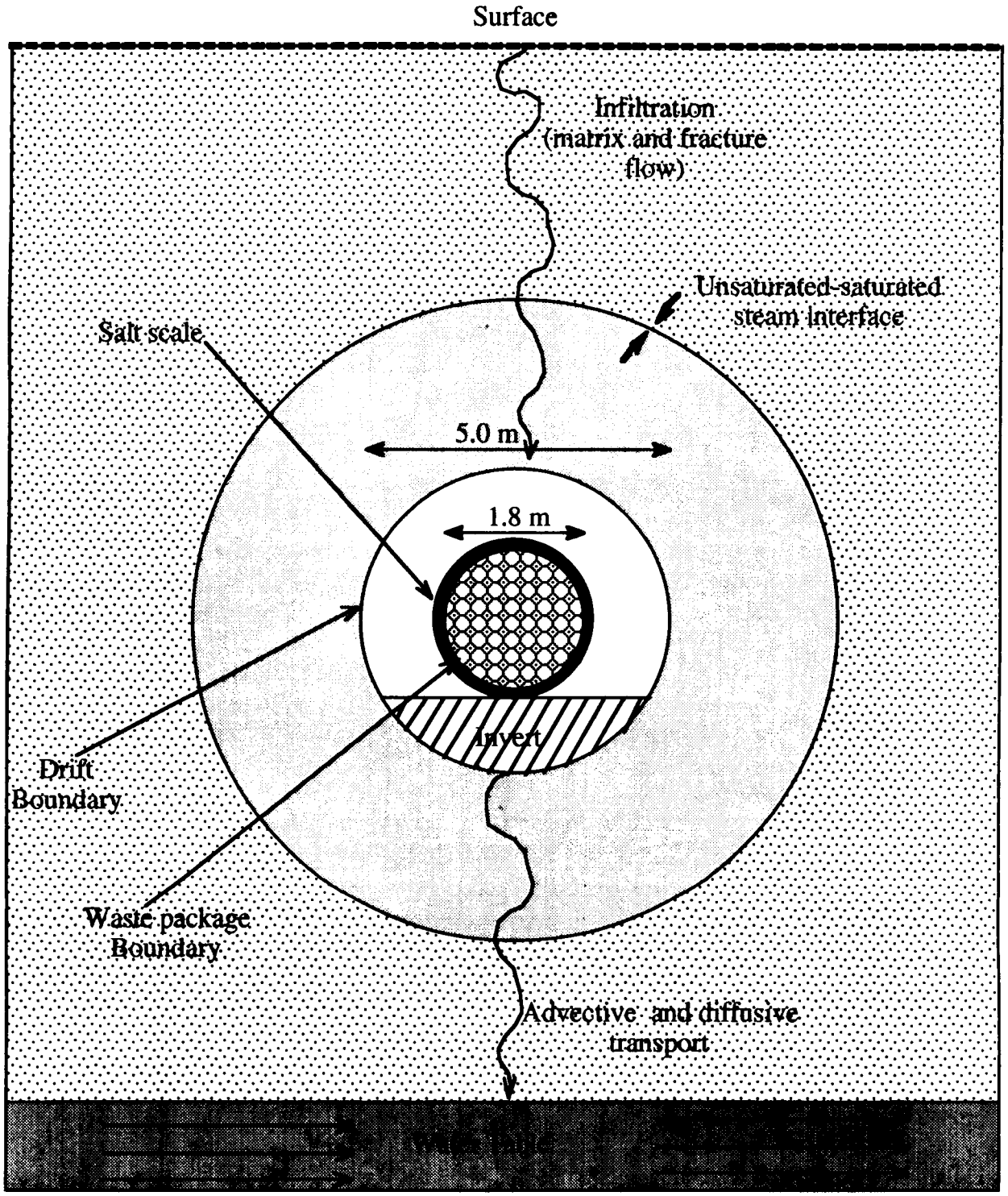

Figure 1. Conceptualization of the radionuclide release from waste packages emplaced in a horizontal drift

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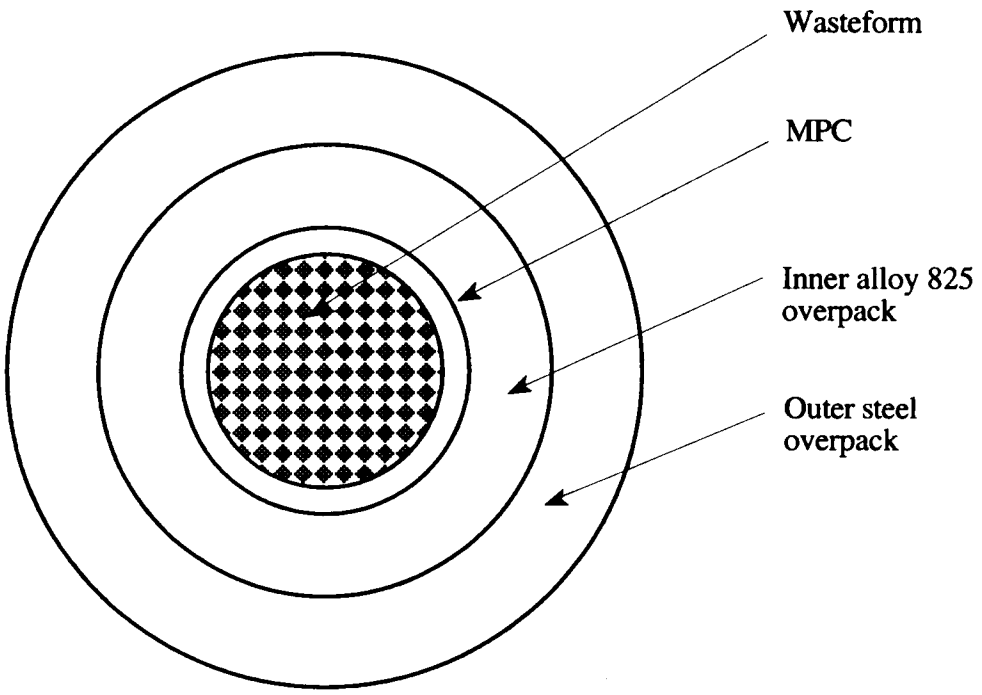

Figure 2. Schematic showing the magnified view of the cross-section of a waste package

2.2.1 Thermal Module

The thermal module will provide the temperature distribution as a function of time and position within the EBS as well as the surrounding geosphere. The thermal model will initially be based on conduction as the only heat-transfer mechanism. This module will reflect the geometry adopted in the reference design. Temperature distribution data will be stored in a file at various times, and, therefore, this module will not be called from within EBSPAC. External temperature calculation is justifiable because conduction is considered to be the dominant heat transfer mechanism and also the amount of heat to be generated by the source in the future is known deterministically. Other heat-transfer modes (convection and radiation) may be considered in future versions of EBSPAC. For example, in the absence of backfill, radiation may become an important heat transfer mechanism.

2.2.2 Environmental Module

The environmental module processes input from external data sources. These data are to include ground water composition, such as concentrations of species Na^+, Cl^-, HCO_3^-, and O_2 and pH among others, provided as functions of time. In addition, relative humidity and liquid saturation will be provided as functions of time. MULTIFLO will be used for generating fluid composition and

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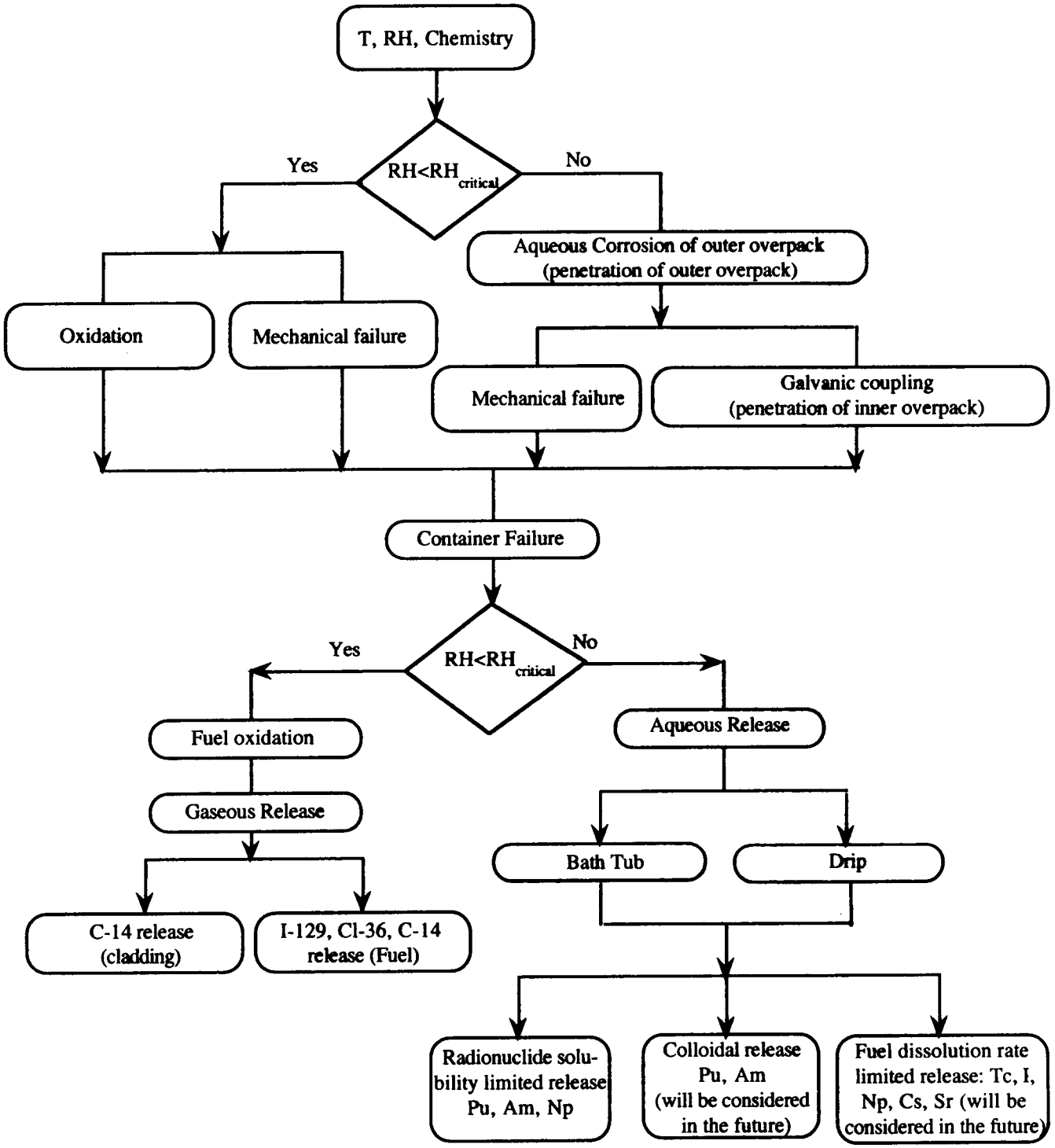

Figure 3. Flow chart showing the logic sequence of Engineered Barrier System Performance Assessment Code

species concentration data. The environmental conditions are expected to be affected significantly only by a few scenarios, including different mechanism or process of water movement (e.g., fracture flow). Calculating the environmental conditions outside the EBSPAC leaves the user with the option for using MULTIFLO only selectively. The MULTIFLO code meets the quality assurance requirements of TOP-018.

Because the onset of aqueous corrosion is dictated by the waste package surface conditions, especially the presence of a water film, the time at which the surface will be covered by a water film (i.e., the surface wetting time and area wetted) will be determined by using either the vapor-pressure gradient model (Walton et al., 1995) or the critical relative humidity and the temperature approach adopted by the DOE.

The environmental module will provide the amount of water reaching the waste package surface which will be used in determining the wetted area of this surface.

2.2.3 Corrosion Module

The corrosion module will be changed to address the DOE reference design. The basic equations (Sridhar et al., 1993; Cragnolino et al., 1994) will follow the SCCEX code with appropriate modifications to represent the DOE reference waste package materials and design. The SCCEX corrosion model includes:

- Oxidation
- General corrosion
- Localized corrosion (pitting and crevice corrosion)
- Stress corrosion cracking
- Galvanic corrosion

The corrosion process at any given time is dictated by the corrosion potential and the corresponding critical potential associated with the process. Therefore, solution chemistry and relative humidity data read in by the environmental module will also be used in this module. Galvanic corrosion becomes important only after the outer overpack is penetrated. Hence, the corrosion module will consist of two stages—that for the outer overpack and that for the inner overpack.

2.2.4 Mechanical Failure Module

The applicability of the mechanical failure models used in SCCEX, namely, yielding, buckling, and fracture models, will be evaluated from the point of view of horizontal emplacement. For the new design, fracture failure as a result of the thermal embrittlement of the steel overpack is an important failure mode to be considered. The mechanical failure model should take into account material instability due to long-term thermal exposure. A simplified calculation of waste package temperature (thermal model) and changes in mechanical properties of overpack material will be considered in EBSPAC. For the first version, priority will be given to the fracture failure.

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2.2.5 Release Rate Module

Gaseous Release

For the sake of simplicity, the gaseous release will be treated separately from the liquid release. The gaseous release will include three release modes:

(1) Prompt release: This will account for the loosely-held C-14 and I-129 on the cladding and cladding/fuel gap and grain boundaries that will be released immediately following the container failure (within the first 100 years after the failure).

(2) Oxidation of cladding: The zirconium cladding, which is a strong oxygen getter, will make this oxygen available for carbon oxidation and release of C-14. Other buried irradiated structural metal will also undergo the same process.

(3) Oxidation of UO_2: This will account for the largest amount of the inventory of the C-14 which is contained in the form of solid solutions, elemental carbon, carbides, and oxycarbides. Dry oxidation of UO_2 will also change its crystal structure, resulting in volume expansion and fracture.

These three processes have already been implemented in SOTEC (Sagar et al., 1992). These models will be implemented in EBSPAC considering more recent discussions (Ahn, 1994) where appropriate. Improved calculation efficiency will be considered because of the possibility of extending calculations to beyond 10,000 years.

Liquid Release

The liquid release will account for the radionuclides released from the fuel, production from radioactive decay of another radionuclide, losses from radioactive decay, advective flow, and diffusion. The liquid release of radionuclide from the fuel will include only congruent release option with the assumption that the radionuclides are contained in the matrix of the UO_2. The advective mass transfer will be a simple mass balance (i.e., amount out = concentration $\times$ water flow rate out of the container). The diffusive mass transfer will be assumed to be taking place from a spherical source as implemented in SOTEC. The diffusion model will consider radioactive decay. Radioactive decay chains are not considered, however. Attention will be given to improving calculation efficiency because of the possibility of extending these calculations to above 10,000 years.

During a later phase of EBSPAC code development activities, an attempt will be made to include the effects of uranylsilicates, potential secondary alteration products of the spent fuel in the expected high-silica concentration groundwater likely to encounter the waste package. Thermodynamic data is only poorly known at this time for these minerals. However, because of their large molar volumes, resulting in large positive volume changes in replacement reactions of spent fuel, formation of these alteration products could play an important role in dissolution of spent fuel.

A simplified model for formation and transport of colloids may be considered at a later phase of code development.

2.2.6 Inventory Model

The inventory in the failed waste package will be monitored by performing mass balance calculation at specified time steps. The mass balance calculation will include depletion due to decay, generation of daughter products, and mass depletion due to diffusive and advective releases.

Although SCCEX conducted performance calculations up to 1,000 years, EBSPAC will calculate source term for periods extending to 10,000 years. In concurrence with the National Academy of Sciences (NAS) recommendation, the subsystem performance requirement periods of 300 to 1,000 years will not be considered.

2.3 COMPUTATIONAL APPROACH

EBSPAC will closely follow the existing approaches in SOTEC and SCCEX in order to minimize code development time. Specific attempts will be made to address numerical oscillations by incorporating methods to minimize them. The use of faster solvers for solving a system of ordinary differential equations will be investigated and will be compared against the fourth order Runge-Kutta method currently used.

2.4 DATA FLOW AND USER INTERFACE

An initial version of the comprehensive computation flow chart has been developed for EBSPAC and is presented in Figure 4. The flow chart presents three segments of the EBSPAC code. The first column shows mainly the input data that will be obtained from the output of other codes such as MULTIFLO and ABAQUS. The second column presents the portion of the code that will calculate corrosion and mechanical failures. The third column represents release calculations for three release scenarios: (i) releases from initially defective canisters, (ii) releases subsequent to corrosion and mechanical failure, and (iii) releases from containers failed due to drilling, faulting, and volcanic activities. The fourth column represents the modules that will be used for record keeping (e.g., cumulative gas release, cumulative liquid release, inventory, etc.) and preparing data for output that can be used in TPA code.

The code is run on a UNIX system by entering the command:

ebspac [−i] < input < database . . . > output

where the square brackets designate that $-i$ need not be entered in the command line, *input* represents the input file, *output* the output file, and .... stands for possible additional options to be specified at a later date.

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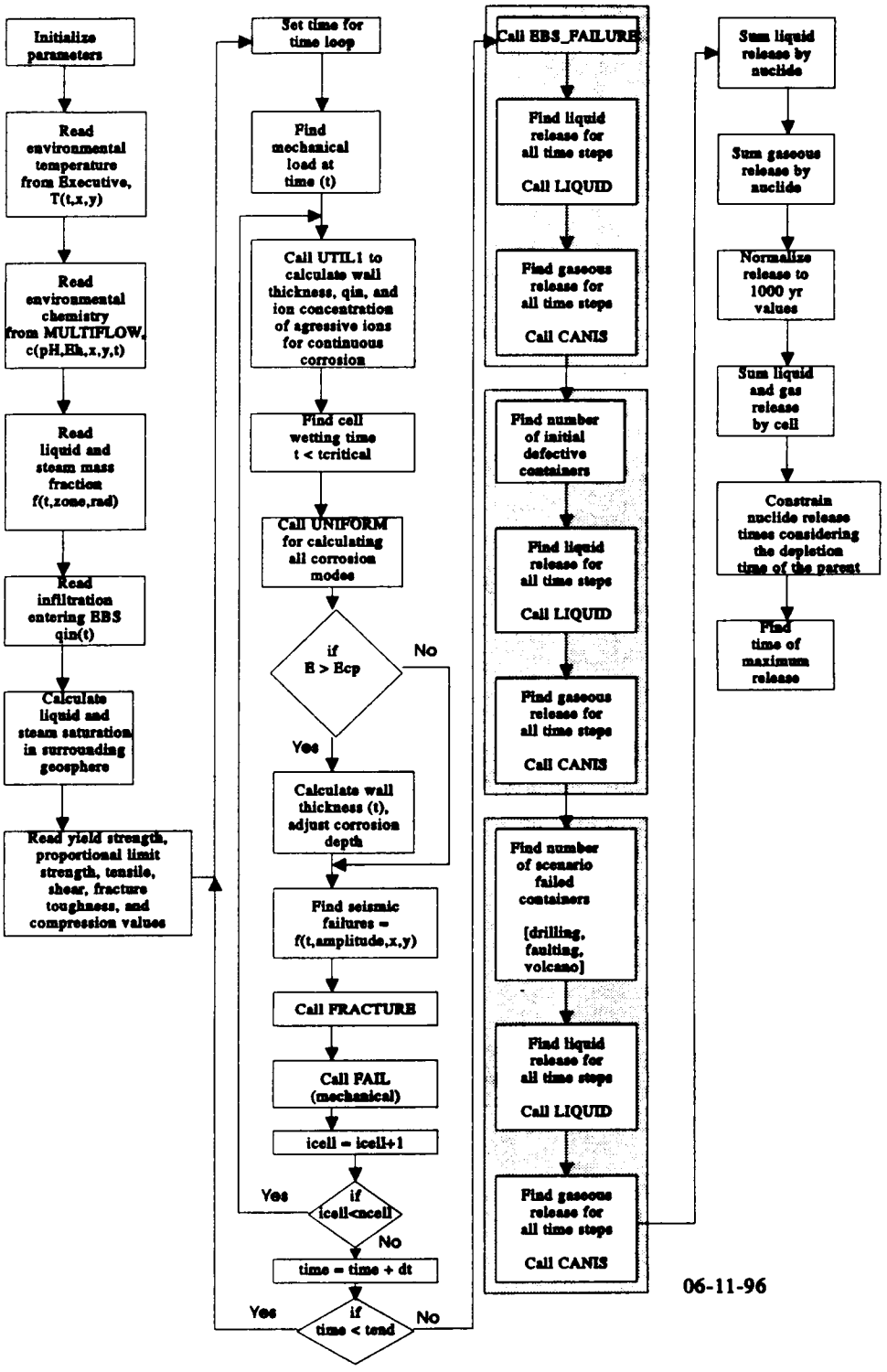

Figure 4. Proposed Engineered Barrier System Performance Assessment Code flow diagram

2.4.1 I/O

The input and output for EBSPAC will be presented in free format. Emphasis will be given to make the input file more readable and compatible to Monte Carlo sampling options to be invoked by the TPA executive code.

At the completion of program execution, the EBSPAC code will provide the following:

- Waste package failure time
- List of daughter products created before the waste package fails
- Mass of parent nuclide and mass of daughter products
- Radionuclide release rates as a function of time
- Cumulative release at the end of program execution

A partial list of input data includes:

General parameters

- Length of simulation time
- Length of waste package
- Waste package radius
- Packing radius
- External fixed boundary radius for the geosphere
- Container thickness (two types)
- Metric ton of waste per container
- Age of fuel
- Initial temperature
- Vertical extent of repository
- Spent-fuel alteration/dissolution rate
- Decay constants for radionuclides
- Initial time steps in years
- Minimum time step in years
- Ratio between evaporation and rate of water encroachment

Evaporation parameters

- Vapor diffusion coefficient
- Reference temperature for diffusion coefficient
- Geometric factor for rock
- Geometric factor for packing
- Porosity of packing for vapor diffusion
- Porosity of rock for vapor diffusion
- Water film thickness
- Dripping rate
- Concentration of NaCl in dripping water
- Initial salt around the container
- Initial scale on the container

- Funnel area for capture of darcy flow onto container
- Edge width of the circular umbrella
- Temperature at the waste package where the edge of umbrella hits
- Atmospheric pressure

Corrosion parameters

- Transfer coefficient (alpha) for oxygen reduction
- Transfer coefficient (beta) for water reduction
- Rate constant for oxygen reduction
- Rate constant for water reduction
- Activation energy for oxygen reduction
- Activation energy for water reduction
- Current density for air/steam environment
- Active current density
- Passive current density
- Nitrate/chloride ratio
- Reference pH
- Tortuosity in scale
- Porosity in scale
- Critical potentials for localized corrosion and stress corrosion cracking (E_{rp}, E_p)

Mechanical properties

- Young's modulus
- Poisson's ratio
- Yield strength
- Safety factor for uncertainties in mechanical properties
- Fracture toughness (K_{ic}, J_{ic})

This partial input list is by no means exhaustive. New parameters will be added and some of these parameters presented will be deleted during the course of EBSPAC code development.

2.5 HARDWARE AND SOFTWARE REQUIREMENTS

EBSPAC code will be a mixture of ANSI FORTRAN 77 and Fortran 90 routines with the main program being written with Fortran 90 language. Fortran 90 provides the option for compiling routines written in FORTRAN 77 language. Fortran 90 will provide significant improvement in coding (i.e., will use fewer code lines) and simplify input by making it more readable.

The FORTRAN 77 portion of the code will use *do-enddo* and *include* statements as well as system-dependent calls for timing routines. The code will run on a SUN work station with the Fortran 90 compiler.

The use of Fortran 90 is justifiable for large codes because these codes, which will be audited for accuracy or will run on multiple platforms, must be developed in a controlled and standardized manner. Unlike FORTRAN 77, Fortran 90 lends itself to a fully structured approach.

Two of the undesirable features from the EBSPAC code development point of view are the structure and content of cryptic input files and the non-standard INCLUDE statement of Fortran 77. The cryptic input in FORTRAN 77 is reduced by writing a library of routines which permit free-format input using a system of keywords and free-format numerical data. Free-format means that a specific column location for data is not required. Also, both integer and floating point values could be supplied with or without decimal points or exponents. A large percentage of the previous source term code (i.e., SOTEC) was dedicated to the implementation of this free-format mechanism. The functions available in Fortran 90 eliminate the need for both of these procedures. The use of the NAMELIST statement for input provides a standardized free-format input mechanism. The MODULE concept in Fortran 90 virtually eliminates the need for INCLUDE statements altogether.

Fortran 90 will reduce the cost associated with the implementation of these functions which are necessary for the controlled development of software.

2.6 GRAPHICS

No special graphics output devices are required at this time. Output will be in the form of ascii files written in a spreadsheet-like format that can be read in by the user-preferred graphics software.

2.7 PRE- AND POST-PROCESSORS

No pre- or post-processors will be designed at this stage. The pre- and post- processors will be made a part of TPA executive code.

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SOFTWARE REQUIREMENTS DESCRIPTION FOR THE ENGINEERED BARRIER SYSTEM PERFORMANCE ASSESSMENT CODE (EBSPAC)

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Version 1.0

Approved by:

Narasi Sridhar, Manager EBS Element
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1 INTRODUCTION

This Software Requirements Description (SRD) document is the first stage in the development of the Engineered Barrier System Performance Assessment Code (EBSPAC), a numerical model for the evaluation of container life and source term. EBSPAC will be used as the source term module in the NRC Total System Performance Assessment (TPA) code.

2 SOFTWARE REQUIREMENTS DESCRIPTION (SRD): EBSPAC

This SRD briefly outlines the software function, technical bases, computational approach, program flow and user interface, hardware and software requirements, graphics, and pre- and post-processors that are relevant to the development and use of the code EBSPAC.

Because EBSPAC will be used as a module in the TPA code that will execute hundreds of Monte Carlo runs, the EBSPAC code must be based on simplified models that will allow fast computation. As a rule of thumb, the design will be such that the average execution time for a single EBSPAC run will be in the neighborhood of 22 seconds on CRAY-YMP with eight processors. With an execution time scale factor of approximately 10, this 22 cray-seconds will be equivalent to 220 seconds on a UNIX IPX machine.

2.1 SOFTWARE FUNCTION

The code EBSPAC will be used to provide the source term to the TPA code. The code will provide waste package failure time and the release rate of radionuclides from the engineered barrier system. The code may eventually be used to evaluate the issue of criticality in conjunction with the DOE reference waste package design proposed in the TSPA-95 report (U.S. DOE, 1994, 1995). However, criticality calculations are not considered in the first version of EBSPAC. Additionally, the multipurpose canister (MPC) performance is ignored in this version in correspondence with TSPA-95 calculations.

The first iteration of EBSPAC will be based on the SCCEX code modified to be applicable to the reference design.

2.2 TECHNICAL BASIS: PHYSICAL AND MATHEMATICAL MODELS

The code EBSPAC will consist of a number of modules based on a simplified physical description of the underlying processes which govern the failure of the waste package and ultimate release of radionuclides. Figures 1 and 2 show a simplified conceptualization around which EBSPAC code will be built. This includes the horizontal emplacement of the waste package instead of the vertical emplacement implemented in SCCEX and SOTEC (Cragnolino et al., 1994; Sagar et al., 1992) codes. The main modules to be included in the EBSPAC code are briefly described below. The flow diagram shown in Figure 3 shows the stages at which these major modules are called.

2.2.1 Thermal Module

The thermal module will provide the temperature distribution as a function of time and position within the EBS as well as the surrounding geosphere. The thermal model will initially be based on conduction as the only heat-transfer mechanism. This module will reflect the geometry adopted in the reference design. Temperature distribution data will be stored in a file at various times and therefore this module will not be called from within EBSPAC. External temperature calculation is justifiable because conduction is considered to be the dominant heat transfer mechanism and also the amount of heat to be generated by the source in the future is known deterministically. Other heat-transfer modes (convection and radiation) may be considered in future versions of EBSPAC. For example, in the absence of backfill, radiation may become an important heat transfer mechanism.

2.2.2 Environmental Module

The environmental module processes input from external data sources. These data are to include ground water composition, such as concentrations of species Na^+, Cl^-, HCO_3^-, and O_2 and pH among others, provided as functions of time. In addition, relative humidity and liquid saturation will be provided as functions of time. MULTIFLO will be used for generating fluid composition and species concentration data. The environmental conditions are expected to be affected significantly only by a few scenarios, including different mechanism or process of water movement (e.g. fracture flow). Calculating the environmental conditions outside the EBSPAC leaves the user with the option for using MULTIFLO only selectively.

Because the onset of aqueous corrosion is dictated by the waste package surface conditions, especially the presence of a water film, the time at which the surface will be covered by a water film (i.e., the surface wetting time and area wetted) will be determined by using either the vapor-pressure gradient model (Walton et al., 1995) or the critical relative humidity and the temperature approach adopted by the DOE.

The environmental module will provide the amount of water reaching the waste package surface which will be used in determining the wetted area of this surface.

2.2.3 Corrosion Module

The corrosion module will be changed to address the DOE reference design. The basic equations (Sridhar et al., 1993; Cragnolino et al., 1994) will follow the SCCEX code with appropriate modifications to represent the DOE reference waste package materials and design. The SCCEX corrosion model includes

- general corrosion
- localized corrosion (pitting and crevice corrosion)
- stress corrosion cracking
- galvanic corrosion

The corrosion process at any given time is dictated by the corrosion potential and the corresponding critical potential associated with the process. Therefore, solution chemistry and relative humidity data read in by the environmental module, will also be used in this module. Galvanic

corrosion becomes important only after the outer overpack is penetrated. Hence, the corrosion module will consist of two stages—that for the outer overpack and that for the inner overpack.

2.2.4 Mechanical Failure Module

The applicability of the mechanical failure models used in SCCEX, namely, yielding, buckling, and fracture models, will be evaluated from the point of view of horizontal emplacement. For the new design, fracture failure as a result of the thermal embrittlement of the steel overpack is an important failure mode to be considered. The mechanical failure model should take into account material instability due to long-term thermal exposure. A simplified calculation of waste package temperature (thermal model) and changes in mechanical properties of overpack material will be considered in EBSPAC. For the first version, priority will be given to the fracture failure.

2.2.5 Release Rate Module

Gaseous Release:

For the sake of simplicity, the gaseous release will be treated separately from the liquid release. The gaseous release will include three release modes:

(1) Prompt release: This will account for the loosely-held C-14 and I-129 on the cladding and cladding/fuel gap and grain boundaries, that will be released immediately following the canister failure. (within the first 100 years after the failure).

(2) Oxidation of cladding: The zirconium cladding, which is a strong oxygen getter, will make this oxygen available to carbon, thus forming $^{14}CO_2$ upon oxidation. Other buried irradiated structural metal will also undergo the same process.

(3) Oxidation of UO_2: This will account for the largest amount of the inventory of the C-14 which is contained in the form of solid solutions, elemental carbon, carbides, and oxycarbides. Dry oxidation of UO_2 will also change its crystal structure, resulting in volume expansion and fracture.

These three processes have already been implemented in SOTEC (Sagar et al., 1992). These models will be implemented in EBSPAC considering more recent discussions (Ahn, 1994) where appropriate.

Liquid Release:

The liquid release will account for the radionuclides released from the fuel, production from radioactive decay of another radionuclide, losses from radioactive decay, advective flow, and diffusion. The liquid release of radionuclide from the fuel will include only congruent release option with the assumption that the radionuclides are contained in the matrix of the UO_2. The advective mass transfer will be a simple mass balance (i.e., amount out = concentration x water flow rate out of the container). The diffusive mass transfer will be assumed to be taking place from a spherical source as implemented in SOTEC. The diffusion model will consider radioactive decay. Radioactive decay chains are not considered, however.

During a later phase of ESBSPAC code development activities, an attempt will be made to include the effects of uranylsilicates, potential secondary alteration products of the spent fuel in the expected high-silica concentration groundwater likely to encounter the waste package. Thermodynamic data is only poorly known at this time for these minerals. However, because of their large molar volumes, resulting in large positive volume changes in replacement reactions of spent fuel, formation of these alteration products could play an important role in dissolution of spent fuel.

A simplified model for colloids transport may be considered at a later phase of code development.

2.2.6 Inventory Model

The inventory in the failed waste package will be monitored by performing material balance calculation at specified time steps. The mass balance calculation will include depletion due to decay, generation of daughter products, and mass depletion due to diffusive and advective releases.

Although SCCEX conducted performance calculations up to 1000 years, EBSPAC will calculate source term for periods extending to 10,000 years. In concurrence with the National Academy of Sciences (NAS) recommendation, the subsystem performance requirement periods of 300 to 1,000 yr will not be considered.

2.3 COMPUTATIONAL APPROACH

EBSPAC will closely follow the existing approaches in SOTEC and SCCEX in order to minimize code development time. Specific attempts will be made to address numerical oscillations by incorporating methods to minimize them. The use of faster solvers for solving a system of ordinary differential equations will be investigated and will be compared against the fourth order Runge-Kutta method currently used.

2.4 DATA FLOW AND USER INTERFACE

A first-cut comprehensive computation flow chart has been developed for EBSPAC and is presented in Figure 4. The flow chart presents three segments of the EBSPAC code. The first column shows mainly the input data that will be obtained from the output of other codes such as MULTIFLO and temperature code such as ABAQUS. The second column presents the portion of the code that will calculate corrosion and mechanical failures. The third column represents release calculations for three release scenarios: i) releases from initially defective canisters, ii) releases subsequent to corrosion and mechanical failure, and iii) releases from containers failed due to drilling, faulting, and volcanic activities The fourth columns represents the modules that will be used for record keeping (e.g. cumulative gas release, cumulative liquid release, inventory, etc.) and preparing data for output that can be used in TPA code.

The code is run on a UNIX system by entering the command:

ebspac < input < database . . . > output

where the square brackets designate that *-i* need not be entered in the command line, input represents the input file, output the output file, and .... stands for possible additional options to be specified at a later date.

2.4.1 I/O

The input and output for EBSPAC will be presented in free format. Emphasis will be given to make the input file more readable and compatible to Monte Carlo sampling options to be invoked by the Total Performance Assessment (TPA) executive code.

At the completion of program execution, the EBSPAC code will provide the following:

- Waste package failure time
- List of daughter products created before the waste package fails
- Mass of parent nuclide and mass of daughter products
- Radionuclide release rates as a function of time
- Cumulative release at the end of program execution

A partial list of input data includes:

General parameters

- Length of simulation time
- Number of cells
- Length of waste package
- Waste package radius
- Packing radius
- External fixed boundary radius for the geosphere
- Container thickness (two types)
- Initial thermal power density
- Metric ton of waste per container
- Age of fuel
- Initial temperature
- Vertical extent of repository
- Spent-fuel alteration rate
- Decay constants for radionuclides
- Initial time steps in years
- Minimum time step in years
- Ratio between evaporation and rate of water encroachment

Evaporation parameters

- Vapor diffusion coefficient
- Reference temperature for diffusion coefficient
- Geometric factor for rock
- Geometric factor for packing
- Porosity of packing for vapor diffusion

- Porosity of rock for vapor diffusion
- Water film thickness
- Dripping rate
- Effective concentration of NaCl in dripping water
- Effective concentration of scale forming minerals in dripping water
- Scale factor for vapor pressure lowering relative to NaCl solution
- Initial salt around the container
- Initial scale on the container
- Funnel area for capture of darcy flow onto container
- Edge width of the circular umbrella
- Temperature at the waste package where the edge of umbrella hits
- Atmospheric pressure

Corrosion parameters

- Transfer coefficient (alpha) for oxygen reduction
- Transfer coefficient (beta) for water reduction
- Rate constant for oxygen reduction
- Rate constant for water reduction
- Activation energy for oxygen reduction
- Activation energy for water reduction
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- Active current density
- Passive current density
- Nitrate/chloride ratio
- Reference pH
- Tortuosity in scale
- Porosity in scale
- Critical potentials for localized corrosion and stress corrosion cracking (Erp, Ep)

Mechanical properties

- Young's modulus
- Poisson's ratio
- Yield strength
- Safety factor for uncertainties in mechanical properties
- Fracture toughness (K_{ic}, J_{ic})

This partial input list is by no means exhaustive. New parameters will be added and some of these parameters presented will be deleted during the course of EBSPAC code development.

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EBSPAC code will be a mixture of ANSI FORTRAN 77 and Fortran 90 routines with the main program being written with Fortran 90 language. Fortran 90 provides the option for compiling routines written in FORTRAN 77 language. Fortran 90 will provide significant improvement in coding (i.e., will use fewer code lines) and simplify input by making it more readable.

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The use of Fortran 90 is justifiable for large codes because these codes which will be audited for accuracy, or codes which will run on multiple platforms must be developed in a controlled and standardized manner is essential for large codes, Unlike FORTRAN 77, Fortran 90 lends itself to a fully structured approach.

Two of the undesirable features from the EBSPAC code development point of view are the structure and content of cryptic input files and the non-standard INCLUDE statement of Fortran 77. The cryptic input in FORTRAN 77 is reduced by writing a library of routines which permit free-format input using a system of keywords and free-format numerical data. Free-format means that a specific column location for data is not required. Also, both integer and floating point values could be supplied with or without decimal points or exponents. A large percentage of the previous source term code (i.e., SOTEC) was dedicated to the implementation of this free-format mechanism. The functions available in Fortran 90 eliminate the need for both of these procedures. The use of the NAMELIST statement for input provides a standardized free-format input mechanism. The MODULE concept in Fortran 90 which virtually eliminates the need for INCLUDE statements altogether.

Fortran 90 will reduce the cost associated with the implementation of these functions which are necessary for the controlled development of software.

2.6 GRAPHICS

No special graphics output devices are required at this time. Output will be in the form of ascii files written in a spreadsheet-like format that can be read in by the user-preferred graphics software.

2.7 PRE- AND POST-PROCESSORS

No pre- or post-processors will be designed at this stage. The pre- and post- processors will be made a part of TPA executive code.

3 REFERENCES

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U.S Department of Energy. 1994. Initial Summary Report for Repository/Waste Package Advanced Conceptual Design. Revision 00. CRWMS M&O Document No. B00000000-01717-5705-00015. Las Vegas, NV: TRW Environmental Safety Systems, Inc.

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Walton, J.C., and Lichtner, P.C. 1995. Quasi-Steady State Model for Coupled Liquid, Vapor, and Heat Transport: Application to the Proposed Yucca Mountain High-Level Waste Repository. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

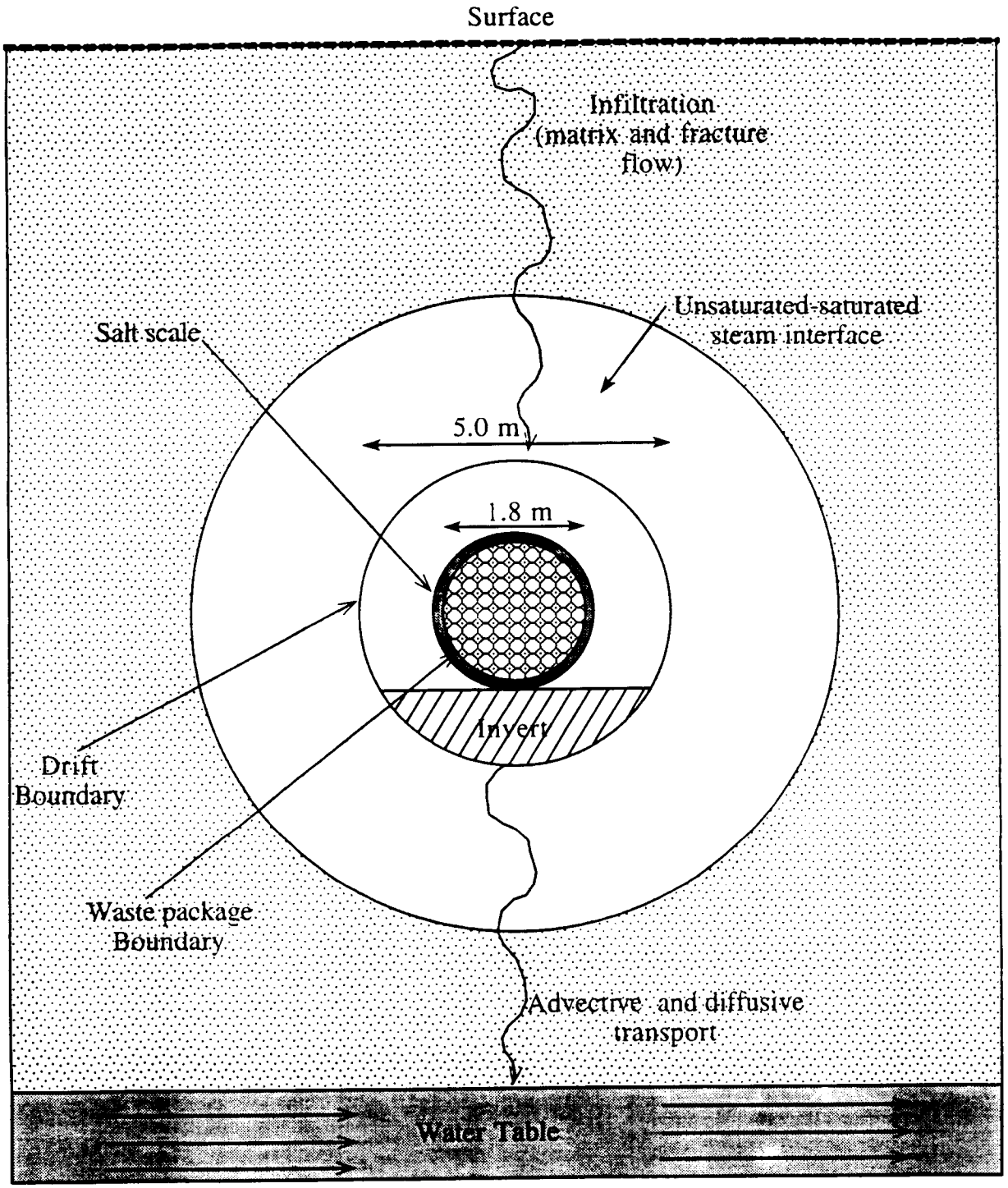

Figure 1. Conceptualization of the radionuclide release from waste packages emplaced in a horizontal drift

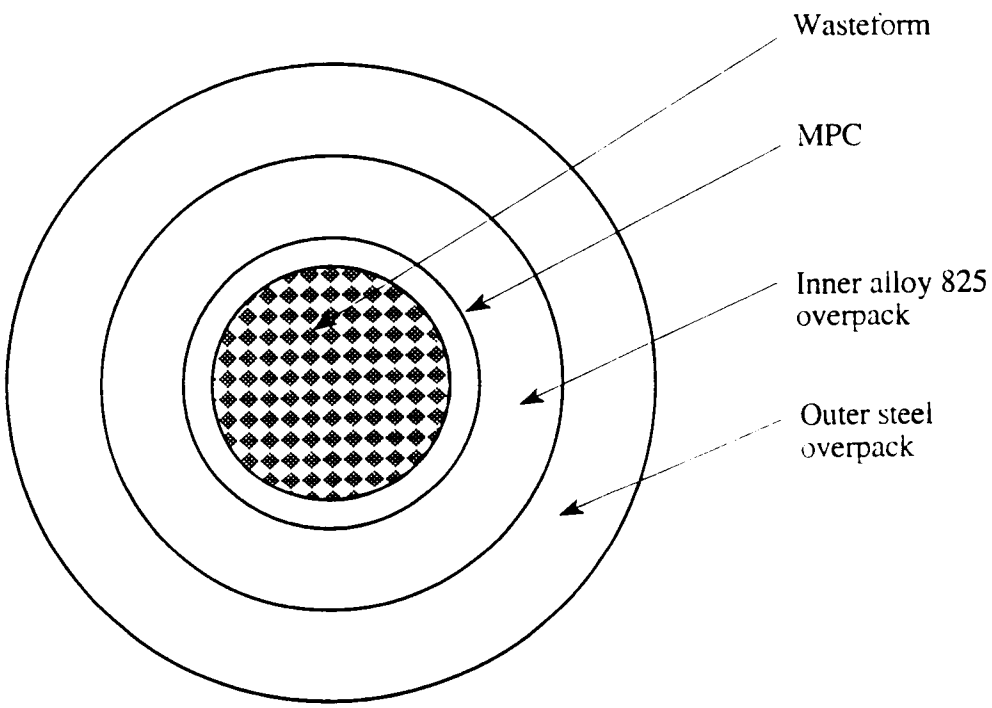

Figure 2. Schematic showing the magnified view of the cross-section of a waste package

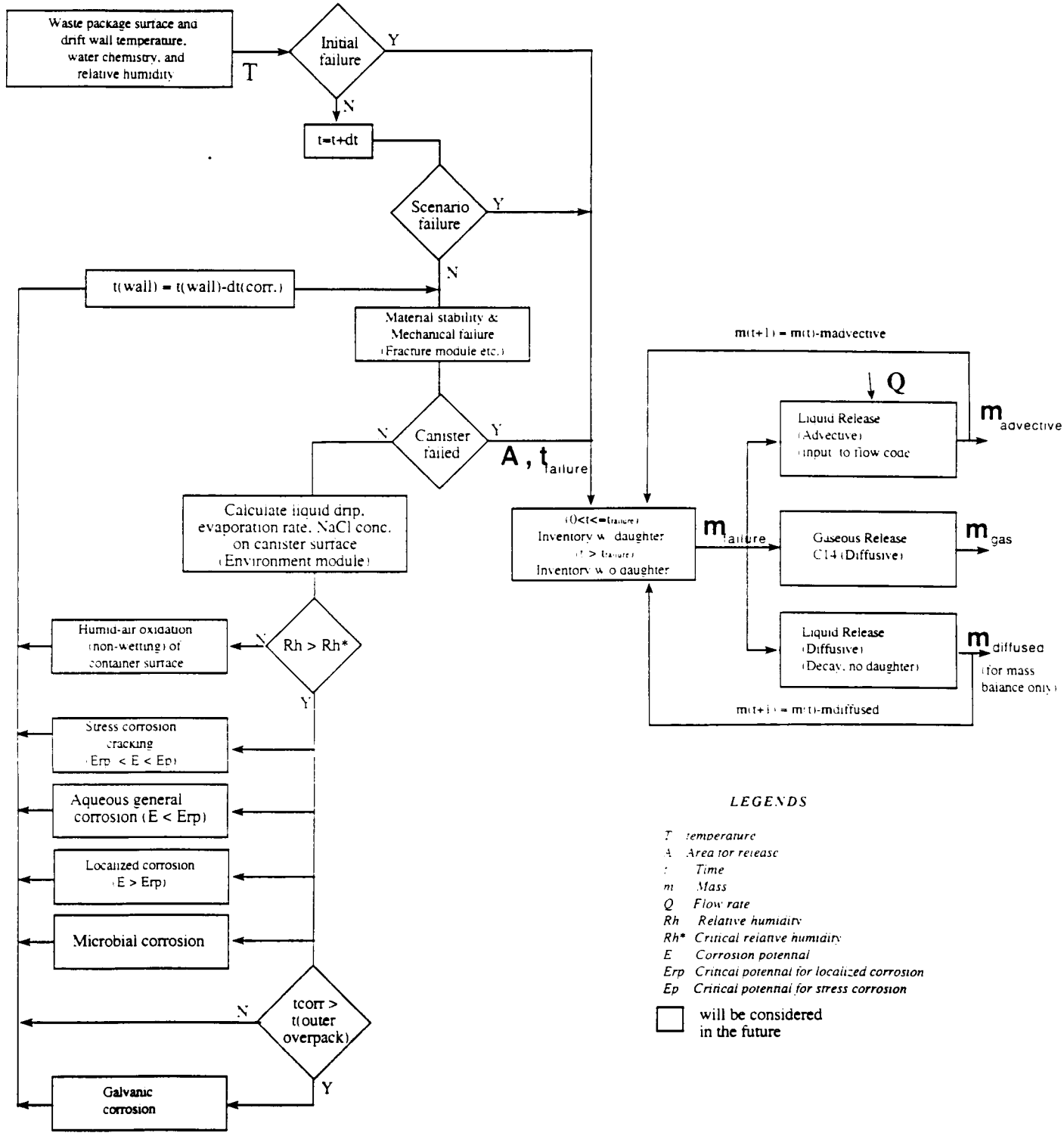

Figure 3. Flow chart showing the major components of the source term

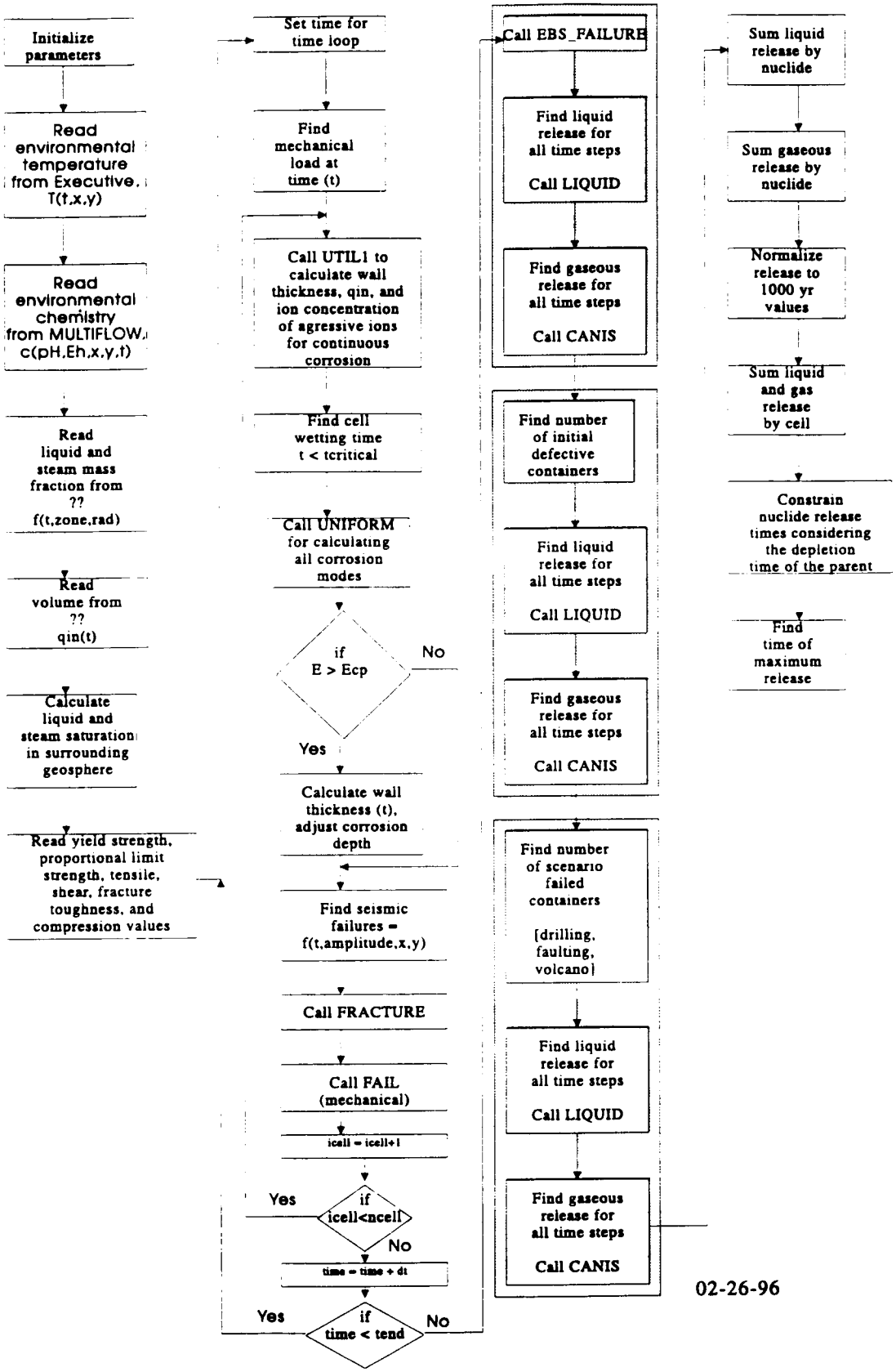

Figure 4. Proposed engineered barrier system performance assessment code flow diagram

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Software Analysis Tools (SPAG)

pcl4

JOB 165

fail.f

For: root
Date: Wed Jan 8 15:30:58 CST 1997

Submit queue: Ethernet
Submitted: 116:47:36
Started: 116:47:36

QMS
QMS 1725 Print System **QMS 1725 (1st floor)**

```
**==EBSPAC_FAIL.spg  processed by SPAG 4.0[illegible] at 14:01 on  7 Jan 1997
      program ebspac_fail
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 aa, age, betahy1, betahy2, betaox1, betaox2, cfactor,
     &       clconc, clconca, clcrit1, clcrit2, constant1, cpass,
     &       ctemp, cthick1, cthick2, curact, d, dtini, dtmax
      real*8 dtmin, e, ecor, ecrit, eps, errabs, errrel, filmthk,
     &       garb1, gbthick, ghy1, ghy2, gox1, gox2, grainr, humd,
     &       humdc, odev, pnt, pntd
      real*8 pntf, rate, refph, rkhy1, rkhy2, rkox1, rkox2, rkqc,
     &       rthick, sfactor, sollay, spor, taus, tavg, tcan, temp2,
     &       temp3, tend, tfail, thicktot
      real*8 timintv, timr, tiny, tstart, tstop, twet, twetf, tyears,
     &       wpdia, wplen, x, xcouple, xread, y, z
      integer i, icorr, ifail, iflag, iflag1, iflag3, iflagcl, ilayer,
     &       nbad, nhist, nhista, nintv, nok, nseries, nset, nv
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------
c   Code:       EBSPAC (Engineering Barrier System Performance Assessment Code)
c
c   Part:       ebspac_fail.f.  This is one of the two parts of EBSPAC
c
C   Version:    1.0
c
c   Date:       January 6, 1997
c
C   Purpose:    The EBSPAC computer program has been developed jointly by the
c               Center for Nuclear Waste Regulatory Analyses (CNWRA) and the
c               U. S. Nuclear Regulatory Commission (NRC) for use in the
C               review of DOE's licence application for the HLW Geologic
c               Repository by the Office of NMSS, DWM.
C
C               ebspac_fail.f part of EBSPAC calculates waste package failure
c               time & ebspac_release.f part of EBSPAC calculates the rate of
c               release of nuclides from the repository in the near field.
C
C               The repository is assumed to be made up of cells and EBSPAC
c               provides results for one cell. Input to EBSPAC is read from
c               files which may either be created manually by the user or
c               generated by use of codes other than EBSPAC.
C
C   Developers: ebspac_fail.f was developed by Sitakanta Mohanty
c               at the CNWRA with assistance from Tae Ahn (NRC, 301-415-5812),
c               G. Cragnolino, P. Lichtner, & N. Sridhar
C
C   User:       Developed for use in NRC Iterative Performance Assessment
c               III. This computer code is managed under CNWRA's CODE
c               CONFIGURATION PROCEDURE. Any modifications to the source
c               code must be reported to code custodian (see below).
c               OTHER versions of this code will be released in the future.
c
C   Disclaimer: This computer code has not been formally or informally
C               verified, is known to have numerous bugs, and the model
c               embodied in it are not validated.
C
C   Contact:    Sitakanta Mohanty (210)522-5185
C               Center for Nuclear Waste Regulatory Analyses
C               Southwest Research Institute, San Antonio, Tx 78250
c-----------------------------------------------------------------
```

```
      parameter (nv=1, nintv=20000)
      external rate, bsstep, rkqc
      character*80 title1
      character*7 , mode
      character*24 fdate

      dimension odev(nv)

      common /bulk  / age, tend, x, y, z, d, filmthk, e, cthick1,
     &                cthick2, sfactor
      common /histry/ nhist
      common /thist / timr(nintv), tavg(nintv), tcan(nintv),
     &                humd(nintv)
      common /new1  / clconca, clcrit1, clcrit2, clconc(nintv),
     &                cfactor, iflagcl
      common /corrpar1/ ecor, ecrit, cpass, sollay, curact, aa(2, 3),
     &                  xread, refph, betaox1, betahy1, betaox2,
     &                  betahy2, rkox1, rkhy1, rkox2, rkhy2, gox1,
     &                  ghy1, gox2, ghy2, spor, taus, xcouple
c     common /corrpar2/ xipto, slpto, xirpo, slrpo, xipti, slpti,
c    &                  xirpi, slrpi
      common /solve / dtini, dtmax, errrel, errabs
      common /temp1 / iflag, nset, timintv, humdc, ctemp, nhista
      common /dryoxdc/ grainr, gbthick, constant1, nseries
      common /wpgmty/ wplen, wpdia
      common /wetting/ twet
      common /flags / icorr
crrrr common /cripotout/ xipto,pttemo,slpto,slpttemo,
crrrr   &                        xirpo,rptemo,slrpo,slrptemo
crrrr common /cripotin/ xipti,pttemi,slpti,slpttemi,
crrrr   &                        xirpi,rptemi,slrpi,slrptemi

      open (2, file='tefkti.inp', status='old')
c      open(2,file='../83mtu.doe',status='old')
      open (3, file='temphumd.dat', status='unknown')
c      open(9,file='fail1.inp',status='old')
      open (9, file='example_fail.inp', status='old')
      open (8, file='corrode.out', status='unknown')
      open (19, file='transition.out', status='unknown')
      open (22, file='echo_fail.dat', status='unknown')
c-----------------------------------------------------------------
c
c     nomenclature:
c
c     age:     age of the waste [yr] (not used)
c     tend:    end time for simulation
c     filmthk: thickness of water film [m] on the wp
c     cthick1: wp outer overpack initial thickness [m]
c     cthick2: wp inner overpack initial thickness [m]
c     sfactor: safety factor for uncertainties in mechanical properties
c     betaox:  beta kinetics parameter for oxygen reduction
c     betahy:  beta kinetics parameter for water reduction
c     rkox:    rate constant for oxygen reduction  [coulomb m/mole/yr]
c     rkhy:    rate constant for water redution in [coulomb/m^2/yr]
c     gox:     activation energy for oxygen rate constant [J/mole]
c     ghy:     activation energy for water reduction [j/mole]
c     aa(1,3): cpass = aa(1,1)+aa(1,2)*t+aa(1,3)*t**2
c     aa(2,3): cpass = aa(2,1)+aa(2,2)*t+aa(2,3)*t**2
c     ecrit:   critical potential for localized corrosion [volts SHE]
c     taus:    tortuosity/geometry correction for liquid diffusion
```

```
c               of oxygen through boiler scale
c       refph:  reference ph
c       spor:   porosity of scale deposited on the wp [=1.0 for liq. film]
c       dtini:  initial time step in years
c       dtmax:  maximum time step in years
c       errrel: relative error
c       errabs: absolute error
c       timr(i): representative time [yr]
c       tavg(i): average repository temperature [Celsius]
c       tcan(i): waste package surface temperature [Celsius]
c       ecor:   corrosion potential [volts SHE]
c       cpass:  passive current density [Coulomb/m^2/yr]
c       sollay: thickness of scale layer [m]
c       curact: active current density [coulomb/m^2/yr]
c       grainr: grain radius [micrometer]
c       nseries: number of terms in infinite series for wp oxidation
c       gbthick: grain bundary thickness [micrometer]
c       constant1:a constant relating matrix and grain  boundary
c               oxygen diffusion in metal
c       humdc:  critical relative humidity
c       clconca:chloride ion concentration near the WP [mol/liter]

c -------------------begin reading input data-----------------------

c top18 requirements:

        write (*, *)
     & 'EBSPAC (Engineering Barrier System Performance Assessment Code)'
        write (*, *)
     &      'This is the part of the code that computes WP Failure Time'
        write (*, *) 'Version= 1.0'
        write (*, *) fdate()

c       prepare and read input data including temperature rel. hum. history

        call input
        nhista = int(tend/timintv)
        call temphstry(iflag, nset, timr, tcan, tavg, humd, tend, nhist,
     &                 nhista, timintv)

        open (21, file='chloride.dat', status='unknown')

c-->    prepare chloride concentration data.  Remove this
c       feature when data is available from multiflo directly

        garb1 = 99999.
        title1 = 'This is replacement for peters data'

        write (21, *) title1
        write (21, *) nhist, garb1, nhist, garb1, nhist, garb1
        do 100 i = 1, nhist
          if ( tcan(i).gt.ctemp ) then
            write (21, 9001) timr(i), clconca, timr(i), clconca, timr(i)
     &                       , clconca
          else
            write (21, 9001) timr(i), clconca/cfactor, timr(i),
     &                       clconca/cfactor, timr(i), clconca/cfactor
          end if
  100   continue
```

```
      close (21)

      call chloride(iflag, nset, timr, clconc, nhist)

c     write to the data file to be read by the subsequent program(s)

      write (*, '(a58)') 'CALCULATION OF WASTE PACKAGE FAILURE TIME'
      write (*, '(80("="))')
      write (3, *) tend
      write (3, *) nhist
      write (*, '(a50,f12.0)') 'end of simulation time [yr]:', tend
      write (*, '(a50,i12)')
     &       'No. of rows of data to pass to release.f:', nhist
      write (8, '(80("-"))')
      write (8, 9004)
      write (*, '(80("-"))')
      write (*, 9004)
      write (8, 9005)
      write (8, '(80("="))')
      write (*, 9005)
      write (*, '(80("="))')

      write (3, *) 'i,timr,tcan,tavg,humd'
c      write(*,*) 'i,timr,tcan,tavg,humd'
      do 200 i = 1, nhist
        write (3, '(i5,10f12.4)') i, timr(i), tcan(i), tavg(i),
     &       humd(i)
c         write(*,'(i5,10f12.4)') i,timr(i),tcan(i),tavg(i),humd(i)
  200 continue


csm  initialize v

      do 300 i = 1, nv
        odev(i) = 0.0
  300 continue
      ilayer = 1
      pnt = 0.
      twetf = 99999.

      do 400 i = 2, nhist
        dtmin = 0.0
        eps = errrel
        tiny = errabs
crrrr    time = timr(i)
        if ( i.gt.1 ) then
          tstart = timr(i - 1)
          tstop = timr(i)
        else
          tstart = 0.
          tstop = errabs
        end if

c  calculate depth of penetration of corrosion pit.................

        temp2 = tcan(i)
        if ( humd(i).lt.humdc ) then
          tyears = tstop - tstart
          call dryoxdwp(i, tyears, temp2, grainr, nseries, gbthick,
     &                  constant1, pntd)
```

```
          pnt = pnt + pntd
          twet = timr(i)
          iflag3 = 0
          odev(1) = pnt
cssss       print*,'timr,penetration by dry oxidation =', timr(i),pnt
        else
          if ( iflag3.eq.0 ) then
            twetf = twet
            pntf = pnt
cdbg           print*,'wetting time [yr] =',twetf
cdbg           print*,'time,penetration by dry oxidation',tstart,pntf
            iflag3 = 1
          end if
          call odeint(odev, nv, tstart, tstop, eps, dtini, dtmin,
     &                dtmax, nok, nbad, tiny, rate, rkqc, ilayer,
     &                cthick1)
          pnt = odev(1)
        end if

c  test if fracture failure would occur.....................

          temp3 = tcan(i)

          if ( pnt.le.cthick1 .and. icorr.eq.1 )
     &         call mech(i, tstart, tstop, temp3, pnt, ifail)
          thicktot = cthick1 + cthick2
          rthick = thicktot - pnt

          mode = 'dry oxd'
          if ( tstop.gt.twetf ) then
            if ( ecor.gt.ecrit .and. iflagcl.eq.1 ) then
              mode = 'local  '
            else
              mode = 'general'
            end if
          end if

          write (8, 9003) ilayer, tstop, tcan(i), ecrit, ecor, iflagcl,
     &                    rthick
          write (*, 9003) ilayer, tstop, tcan(i), ecrit, ecor, iflagcl,
     &                    rthick, mode
          if ( odev(1).gt.thicktot .or. ifail.eq.1 ) then
            iflag1 = 1
            go to 500
          else
            iflag1 = 0
          end if

  400   continue

  500   continue
        write (*, '(80("="))')
        write (*, '(a42,f12.0)') 'wp wetting time [yr]:', twetf
        if ( iflag1.eq.1 ) then
          tfail = tstart
          write (3, *) tfail
          write (3, *) wplen
          write (3, *) wpdia
          write (*, '(a42,f12.0)') 'wp failure time [yr]:', tfail
        else
```

```
        tfail = tend
        write (3, *) tfail
        write (3, *) wplen
        write (3, *) wpdia
        write (*, '(a42,f12.0,a)') , '$$$ no wp failure below [yr]:',
     &          tfail, '  $$$'
       end if

       write (*, '(a42,1pe15.3)') 'penetration by dry oxidation [m]:',
     &         pntf
       write (*, '(a42,6x,a)') 'echoed inpot data in:', 'echo_fail.dat'
       write (*, '(a42,6x,a)') 'output data are in files:',
     &         'temphumd.dat and corrode.out'
       write (*, '(80("="))')

       close (2)
       close (3)
       close (9)
       close (8)
       close (19)
       close (21)

       stop

 9001  format (6(1x,1P1e10.4))
cdbg      print*, '**before odeint**',(odev(in),in=1,nv),tstart,tstop
c         write(*,121) tstart,tstop,eps,dtini,dtmin,dtmax
 9002  format ('tstart,tstop,eps,dtini,dtmin,dtmax', 20E13.3)

 9003  format (i2, 2x, 2(f10.2,1x), 2(f10.4,1x), 4x, i1, 2x, 1pe15.7,
     &         2x, a7)
 9004  format (1x, 'ilayer', 2x, 'tstop', 6x, 'tcan', 6x, 'ecrit', 6x,
     &         'ecorr', 3x, 'chloride', 3x, 'rthick'6x, 'mode')
 9005  format (1x, '     ', 2x, '[yr] ', 6x, ' [C]', 6x, '[Vshe]', 5x,
     &         '[Vshe]', 5x, 'flag', 6x, ' [m] ')
       end
**==TEMPHSTRY.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




       subroutine temphstry(iflag, nset, timr, tcan, tavg, humd, tend,
     &                      nhist, nhist3, timintv)
       implicit none
C*** Start of declarations inserted by SPAG
       real*8 ambient, col, dcan, dt, eps1, humd, tavg, tcan, tend,
     &        timintv, timr
       integer i, iflag, ii, iset, nhist, nhist3, nintv, nset
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c      Purpose: read temperature, relative humidity from a table to be
c               provided by the TPA code. Also, DOE data can be read if
c               proper data file is provided
c-----------------------------------------------------------------------
       parameter (nintv=20000)
       dimension timr(nintv), tcan(nintv), tavg(nintv), humd(nintv)
c      local arrays:
       dimension col(4, 12)
c-----------------------------------------------------------------------
```

```
c       Nomenclature:

c       maxrow: maximum number of rows provided in the temperature data file
c       timr:   time at which temperature and relative humidity
c                       data are provided [y]
c       tcan:   surface temperature of the wp outer overpack [c]
c       tavg:   temperature of thedrift wall surrounding the wp [c]
c       humd:   relative humidity near the wp surface [dimensionless]
c       nset:   correspons only to iflag = 2; it is the data set
c               that corresponds to a particular set of
c               temperature, humidity data

c       iflag   :1      use functional temp, humidity representation
c                       of DOE data
c               :2      read from a file temp,humidity
c-----------------------------------------------------------------------

c       note:  the reason we have this doe model is that the temperature is
c       calculated to 100,000 years.  But as drift surface temperature
c       is not available, therefore, a constant temperature difference
c       between wp surface and drift wall (dcan) is assumed

        if ( iflag.eq.1 ) then
          ambient = 25.
          dt = timintv
          dcan = 30.
          timr(1) = 0.0
          tavg(1) = 185.96
          tcan(1) = tavg(1) + dcan
          humd(1) = 0.16535
          do 50 i = 2, nhist3
            timr(i) = i*(dt - 1)
            tavg(i) = 185.96 - 30.694*log10(timr(i))
            tcan(i) = tavg(i) + dcan
            humd(i) = 0.16535 + 0.19391*log10(timr(i))
            if ( tavg(i).lt.ambient ) tavg(i) = ambient
            if ( humd(i).gt.1.0 ) humd(i) = 1.0
   50     continue
          nhist = nhist3
        end if

c       note:  the original data file could contain such data that the
c       temperature data at two consecutive time are the same
c       (i.e., for the lack of adequate resolution).  therefore,
c       screening is done to ensure that temperatures at two consecutive
c       times are different by at least eps1.  Also, data recorded at
c       time intervals smaller than mintime are discarded.

        if ( iflag.eq.2 ) then
          read (2, *)
          read (2, *) ((col(ii,iset),ii=1,4), iset=1, nset)
          nhist3 = int(col(1,nset))
          write (1, *) , 'nhist3=', nhist3
          eps1 = 1.E-6
          read (2, *) ((col(ii,iset),ii=1,4), iset=1, nset)
          timr(1) = col(1, nset)
          tcan(1) = col(2, nset)
          tavg(1) = col(3, nset)
          humd(1) = col(4, nset)
```

```
        nhist = 1
        do 100 i = 2, nhist3
          read (2, *) ((col(ii,iset),ii=1,4), iset=1, nset)
          if ( abs(col(2,nset)-tcan(nhist)).gt.eps1 .and. col(1,nset)
     &          - timr(nhist).gt.timintv ) then
            nhist = nhist + 1
            timr(nhist) = col(1, nset)
            tcan(nhist) = col(2, nset)
            tavg(nhist) = col(3, nset)
            humd(nhist) = col(4, nset)
          end if
          if ( i.eq.nhist3 .and. timr(nhist).lt.col(1,nset) ) then
            nhist = nhist + 1
            timr(nhist) = col(1, nset)
            tcan(nhist) = col(2, nset)
            tavg(nhist) = col(3, nset)
            humd(nhist) = col(4, nset)
          end if
  100     continue
        end if

        return
        end
**==CHLORIDE.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




        subroutine chloride(iflag, nset, timr, clconc, nhist)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 clconc, clconc1, col, time, timr, timr1, tmax, yprevious,
     &         yyyy
        integer i, iflag, ii, iset, isetp, nhist, nhist4, nintv, nset,
     &          nsetp
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c       purpose: obtain data from the chloride data file.  chloride
c       data are presented for three thermal loadings only.  chloride
c       data are based on the assumption that there is no difference
c       between backfill-no backfill, ventillation-no ventilation etc.
c-----------------------------------------------------------------------
        parameter (nintv=20000)
        dimension timr(nintv), clconc(nintv)
        dimension timr1(nintv), clconc1(nintv)
c       local arrays:
        dimension col(4, 12)
c-----------------------------------------------------------------------
c       Notes:
c       time and temperature data in the data file coming from the
c       near-field environment kti which contains chloride data do
c       not have to match with the one coming from the tef kti.
c       however, the max. simulation time (tmax) must match.

c       If the chloride concentration history is not provided until
c       tmax, then the last value provided in the chloride concentration
c       file is repeated until tmax.
c-----------------------------------------------------------------------
c       Nomenclature:
```

```
c       maxrow: maximum number of rows provided in the temperature data file
c       timr:   time at which temperature and relative humidity
c                       data are provided [y]
c       nset:   correspons only to iflag = 2; it is the data set
c               that corresponds to a particular set of chloride data

c-----------------------------------------------------------------------

        open (21, file='chloride.dat', status='old')

        if ( iflag.eq.1 ) then
          read (21, *)
          read (21, *) nhist
          write (*, *) 'nhist=', nhist
          do 50 i = 1, nhist
            read (21, *) timr(i), clconc(i)
   50     continue
          go to 300
        end if

        if ( nset.le.4 ) nsetp = 1
        if ( nset.gt.4 .and. nset.le.8 ) nsetp = 2
        if ( nset.gt.8 .and. nset.le.12 ) nsetp = 3

        read (21, *)
        read (21, *) ((col(ii,iset),ii=1,2), iset=1, nsetp)
        nhist4 = int(col(1,nsetp))
        do 100 i = 1, nhist4
          read (21, *) ((col(ii,isetp),ii=1,2), isetp=1, nsetp)
c          write(*,*) '***',i,((col(ii,isetp),ii=1,2),isetp=1,nsetp)
          timr1(i) = col(1, nsetp)
          clconc1(i) = col(2, nsetp)
  100   continue
        tmax = timr1(nhist4)
c       print*,'nhist4,tmax=',nhist4,tmax

        do 200 i = 1, nhist
          time = timr(i)
          if ( time.lt.tmax ) then
            call lint(timr1, clconc1, nintv, nhist4, time, yyyy)
            clconc(i) = yyyy
            yprevious = yyyy
          else
            yyyy = yprevious
            clconc(i) = yyyy
          end if
c          print*,'from chloride timr,clconc=',timr(i),clconc(i)
  200   continue

  300   continue
        return
        end
**==ODEINT.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997



        subroutine odeint(ystart, nvar, x1, x2, eps, h1, hmin, hmax,
```

```
     &                  nok, nbad, tiny, derivs, rkqc, ilayer,
     &                  cthick1)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 cthick1, dydx, eps, errc, h, h1, hdid, hmax, hmin, hnext,
     &         tiny, x, x1, x2, y, yscal, ystart, zero
        integer i, ieq, ilayer, maxstp, nbad, nmax, nok, nstp, nvar
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c       Purpose: subroutine implementing Runge-Kutta Integration algorithm
c-----------------------------------------------------------------------
crrrr   parameter (maxstp=50000,nmax=50,two=2.0,zero=0.0)
        parameter (maxstp=50000, nmax=50, zero=0.0)
        dimension ystart(nvar), yscal(nmax), y(nmax), dydx(nmax)
crrrr   common /wetting/twet
        external rkqc, derivs
c-----------------------------------------------------------------------

c       nomenclature:

c       nmax:   maximum number of functions
c       nvar:   a subset of nmax, i.e., nvar<nmax (# of starting values)
c       h:      step size that can be positive or negative
c       yscal:  a vector against which the error is scaled
c       hdid:   step size which was actually accomplished
c       hnext:  estimated next step size
c       eps:    accuracy to which integration to be done
c       h1:     guessed first step size
c       hmin:   minimum allowed step size (can be zero)
c       nok:    number of good steps taken
c       nbad:   number of bad steps taken (but retried and fixed)
c       ystart: this is replaced by values at the end of the
c               integration interval

c       ieq:    equation controlling step size,
c       errc:   critical error

c       Note: the user must provide a value of the derivative at the
c       starting point.
c-----------------------------------------------------------------------

        h = sign(h1, x2 - x1)
        x = x1
        nok = 0
        nbad = 0
crrrr           ifudge = 0
        do 100 i = 1, nvar
          y(i) = ystart(i)
  100   continue

  200   continue
        do 300 nstp = 1, maxstp
c          print*,y(1),ilayer
          if ( y(1).ge.cthick1 ) ilayer = 2
cdbg       print*, 'printing from odeint : before derivs'
          call derivs(x, y, dydx, ilayer)
cdbg       print*, 'printing from odeint : after derivs'
          do 250 i = 1, nvar
            yscal(i) = abs(y(i)) + abs(h*dydx(i)) + tiny
c              yscal(i)=abs(y(i)) + tiny
```

```
  250     continue
          if ( (x+h-x2)*(x+h-x1).gt.zero ) h = x2 - x
          if ( h.gt.hmax ) h = hmax
cdbg       print*, 'printing from odeint : before rkqc'
          call rkqc(y, dydx, nvar, x, h, eps, yscal, hdid, hnext, ieq,
     &              errc, derivs, ilayer)
cdbg       print*, 'printing from odeint : after rkqc'
          if ( hdid.eq.h ) then
            nok = nok + 1
          else
            nbad = nbad + 1
          end if
          if ( (x-x2)*(x2-x1).ge.zero ) then
            do 260 i = 1, nvar
              ystart(i) = y(i)
  260       continue
cssss             eps = eps / (10.**ifudge)
cssss             tiny = tiny / (10.**ifudge)
            return
          end if
          if ( abs(hnext).lt.hmin ) then
            write (*, *)
     &             'runge-kutta error messages,                    step size too small'
            write (*, *) 'time = ', x
            write (*, *) 'i, y(i), dydx(i), yscal(i)'
            do 280 i = 1, nvar
              write (*, *) i, y(i), dydx(i), yscal(i)
  280       continue
            write (*, *) 'equation controlling step size is:  ', ieq
            write (*, *) 'controlling equation error is: ', errc
            write (*, *) 'step size is: ', hdid

cssss             ifudge = ifudge+1
cssss             eps = eps * 10.
cssss             tiny = tiny * 10.
          end if

          h = hnext
  300   continue
        write (*, *) 'runge-kutta error messages'
        write (*, *) 'i, y(i), dydx(i), yscal(i)'
        write (*, *) 'time = ', x
        do 400 i = 1, nvar
          write (*, *) 'from odeint**', y(i), dydx(i), yscal(i)
  400   continue
        write (*, *) 'equation controlling step size is:  ', ieq
        write (*, *) 'controlling equation error is: ', errc
        write (*, *) 'step size is: ', hdid

cssss           ifudge = ifudge+1
cssss           eps = eps * 10.
cssss           tiny = tiny * 10.
        go to 200

c       pause 'too many steps.'

c       return
        end
**==RKQC.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997
```

```
      subroutine rkqc(y, dydx, n, x, htry, eps, yscal, hdid, hnext,
     &                ieq, errc, derivs, ilayer)
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 dydx, dysav, eps, errc, errcon, errmax, fcor, h, hdid,
     &       hh, hnext, htry, one, pgrow, pshrnk, safety, x, xsav, y,
     &       ysav
      real*8 yscal, ytemp
      integer i, ieq, ilayer, n, nmax
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
C     quality controlled runge kutta integration routine
C     from numerical recipes
C-----------------------------------------------------------------------
      parameter (nmax=50, fcor=1./15., one=1., safety=0.9,
     &           errcon=6.E-4)
      dimension y(n), dydx(n), yscal(n), ytemp(nmax), ysav(nmax),
     &          dysav(nmax)
crrrr common /wetting/twet
      external derivs
C-----------------------------------------------------------------------

c     Nomenclature:

c     x:      independent variable
c     htry:   step size to be attempted
c     n:      length of the dependent variable vector y
c     ytemp:  an array containing error estimates
c     derivs: name of the subroutine with the derivative of the eq.
c             to be integrated
c     y(i):   dependent variable vector
c     dydx:   derivative of the dependent variable
c     eps:    integration to be done with required overall tolerance eps
c     hdid:   step size which was actually accomplished
c     hnext:  estimated next stepsize
C
C-----------------------------------------------------------------------

      pgrow = -0.20
      pshrnk = -0.25
      xsav = x
      do 100 i = 1, n
        ysav(i) = y(i)
        dysav(i) = dydx(i)
  100 continue
      h = htry
  200 continue
      hh = 0.5*h
      call rk4(ysav, dysav, n, xsav, hh, ytemp, derivs, ilayer)
      x = xsav + hh
      call derivs(x, ytemp, dydx, ilayer)
      call rk4(ytemp, dydx, n, x, hh, y, derivs, ilayer)
      x = xsav + h
      if ( x.eq.xsav ) then
c       pause 'stepsize not significant in rkqc.'
        write (*, *) 'x and xsav=', x, xsav
        write (*, *) 'step size not significant'
```

```
          write (*, *) 'the code is forcibly stopped'
          stop
        end if
        call rk4(ysav, dysav, n, xsav, h, ytemp, derivs, ilayer)
        errmax = 0.
        errc = 0.
        ieq = 0

c  make this routine return the equation controlling
c  the step size, put in variable "ieq", the error is returned
c  in "errc"

        do 300 i = 1, n
          ytemp(i) = y(i) - ytemp(i)
          if ( abs(ytemp(i)/yscal(i)).gt.errmax ) then
            ieq = i
            errc = ytemp(i)
          end if
          errmax = max(errmax, abs(ytemp(i)/yscal(i)))
  300   continue

        errmax = errmax/eps
        if ( errmax.gt.one ) then
          h = safety*h*(errmax**pshrnk)
          go to 200
        else
          hdid = h
          if ( errmax.gt.errcon ) then
            hnext = safety*h*(errmax**pgrow)
          else
            hnext = 4.*h
          end if
        end if
        do 400 i = 1, n
          y(i) = y(i) + ytemp(i)*fcor
  400   continue

        return
        end
**==RK4.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




        subroutine rk4(y, dydx, n, x, h, yout, derivs, ilayer)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 dydx, dym, dyt, h, h6, hh, twet, x, xh, y, yout, yt
        integer i, ilayer, n, nmax
C*** End of declarations inserted by SPAG
        common /wetting/ twet
c-----------------------------------------------------------------------
c       Basic Runge-Kutta Method for integration
c-----------------------------------------------------------------------
        parameter (nmax=50)
        external derivs
        dimension y(n), dydx(n), yout(n), yt(nmax), dyt(nmax), dym(nmax)
        hh = h*0.5
        h6 = h/6.
        xh = x + hh
```

```
      do 100 i = 1, n
        yt(i) = y(i) + hh*dydx(i)
  100 continue
      call derivs(xh, yt, dyt, ilayer)
      do 200 i = 1, n
        yt(i) = y(i) + hh*dyt(i)
  200 continue
      call derivs(xh, yt, dym, ilayer)
      do 300 i = 1, n
        yt(i) = y(i) + h*dym(i)
        dym(i) = dyt(i) + dym(i)
  300 continue
      call derivs(x + h, yt, dyt, ilayer)
      do 400 i = 1, n
        yout(i) = y(i) + h6*(dydx(i) + dyt(i) + 2.*dym(i))
  400 continue

      return
      end
**==BSSTEP.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997



      subroutine bsstep(y, dydx, nv, x, htry, eps, yscal, hdid, hnext,
     &                  ieq, errc, derivs)
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 derivs, dydx, dysav, eps, errc, errmax, grow, h, hdid,
     &       hnext, htry, one, shrink, x, xest, xsav, y, yerr, ysav,
     &       yscal
      real*8 yseq
      integer i, ieq, imax, j, nmax, nseq, nuse, nv
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
      external derivs
      parameter (nmax=50, imax=11, nuse=7, one=1.E0, shrink=.95E0,
     &           grow=1.2E0)
      dimension y(nv), dydx(nv), yscal(nv), yerr(nmax), ysav(nmax),
     &          dysav(nmax), yseq(nmax), nseq(imax)
cssss common /wetting/twet
      data nseq/2, 4, 6, 8, 12, 16, 24, 32, 48, 64, 96/
C-----------------------------------------------------------------------
c     n:              number of variables
c     h:              r-k to advance the solution over an interval h
c     xh:
c     y(i):           dependent variables
c     dydx(i):        derivatives of dependent variables
c     yout(i):        an array containing the incremented y values
C-----------------------------------------------------------------------
C
      h = htry
      xsav = x
      do 100 i = 1, nv
        ysav(i) = y(i)
        dysav(i) = dydx(i)
  100 continue
  200 continue
      do 300 i = 1, imax
        call mmid(ysav, dysav, nv, xsav, h, nseq(i), yseq, derivs)
        xest = (h/nseq(i))**2
```

```
        call rzextr(i, xest, yseq, y, yerr, nv, nuse)
        errmax = 0.
        do 250 j = 1, nv
          errmax = max(errmax, abs(yerr(j)/yscal(j)))
  250   continue
        errmax = errmax/eps
        if ( errmax.lt.one ) then
          x = x + h
          hdid = h
          if ( i.eq.nuse ) then
            hnext = h*shrink
          else if ( i.eq.nuse - 1 ) then
            hnext = h*grow
          else
            hnext = (h*nseq(nuse-1))/nseq(i)
          end if
          return
        end if
  300   continue
        h = 0.25*h/2**((imax-nuse)/2)
        if ( x + h.eq.x ) pause 'step size underflow.'
        go to 200

        end
**==MMID.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




        subroutine mmid(y, dydx, nvar, xs, htot, nstep, yout, derivs)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 dydx, h, h2, htot, swap, x, xs, y, ym, yn, yout
        integer i, ilayer, n, nmax, nstep, nvar
C*** End of declarations inserted by SPAG
crrrr   common /wetting/twet
c-----------------------------------------------------------------
        external derivs
        parameter (nmax=50)
        dimension y(nvar), dydx(nvar), yout(nvar), ym(nmax), yn(nmax)
        h = htot/nstep
        do 100 i = 1, nvar
          ym(i) = y(i)
          yn(i) = y(i) + h*dydx(i)
  100   continue
        x = xs + h
        call derivs(x, yn, yout, ilayer)
        h2 = 2.*h
        do 200 n = 2, nstep
          do 150 i = 1, nvar
            swap = ym(i) + h2*yout(i)
            ym(i) = yn(i)
            yn(i) = swap
  150     continue
          x = x + h
          call derivs(x, yn, yout, ilayer)
  200   continue
        do 300 i = 1, nvar
          yout(i) = 0.5*(ym(i) + yn(i) + h*yout(i))
  300   continue
```

```
      return
      end
**==RZEXTR.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997



      subroutine rzextr(iest, xest, yest, yz, dy, nv, nuse)
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 b, b1, c, d, ddy, dy, fx, v, x, xest, yest, yy, yz
      integer iest, imax, j, k, m1, ncol, nmax, nuse, nv
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------
      parameter (imax=11, nmax=50, ncol=7)
      dimension x(imax), yest(nv), yz(nv), dy(nv), d(nmax, ncol),
     &          fx(ncol)
crrrr common /wetting/twet
c-----------------------------------------------------------------

      x(iest) = xest
      if ( iest.eq.1 ) then
        do 50 j = 1, nv
          yz(j) = yest(j)
          d(j, 1) = yest(j)
          dy(j) = yest(j)
   50   continue
      else
        m1 = min(iest, nuse)
        do 100 k = 1, m1 - 1
          fx(k + 1) = x(iest - k)/xest
  100   continue
        do 150 j = 1, nv
          yy = yest(j)
          v = d(j, 1)
          c = yy
          d(j, 1) = yy
          do 120 k = 2, m1
            b1 = fx(k)*v
            b = b1 - c
            if ( b.ne.0. ) then
              b = (c - v)/b
              ddy = c*b
              c = b1*b
            else
              ddy = v
            end if
            v = d(j, k)
            d(j, k) = ddy
            yy = yy + ddy
  120     continue
          dy(j) = ddy
          yz(j) = yy
  150   continue
      end if
      return
      end
**==RATE.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997
```

```
      subroutine rate(time, odev, dvdt, ilayer)
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 cfactor, clconc, clconca, clconcb, clcrit1, clcrit2,
     &       crate, dvdt, humd, odev, tavg, tcan, time, timr, tin, xin
      integer i, iflagcl, ilayer, nhist, nintv, nv
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------
c     this returns derivatives for the main calculations
c-----------------------------------------------------------------
      parameter (nintv=20000)
      parameter (nv=1)
crrrr         common /bulk/ age,tend,x,y,z,d,filmthk,e,cthick1,cthick2,sfactor
      dimension odev(nv), dvdt(nv)
      common /thist / timr(nintv), tavg(nintv), tcan(nintv),
     &                humd(nintv)
crrrr         common /corrpar1/ecor,ecrit,cpass,sollay,curact,
crrrr     &           aa(2,3),xread,refph,betaox1,betahy1,
crrrr     &              betaox2,betahy2,rkox1,rkhy1,rkox2,rkhy2,
crrrr     &           gox1,ghy1,gox2,ghy2,spor,taus,xcouple
c     common /corrpar2/ xipto, slpto, xirpo, slrpo, xipti, slpti,
c    &                  xirpi, slrpi
crrrr         common /solve/dtini,dtmax,errrel,errabs
      common /histry/ nhist
      common /new1  / clconca, clcrit1, clcrit2, clconc(nintv),
     &                cfactor, iflagcl
crrrr common /wetting/twet
c-----------------------------------------------------------------

c     nomenclature:

c     timr(i):representative time in years
c     tcan(i):waste package surface temperature in Celsius
c     nintv:  this is used in stead of nhist when simulation is to be done
c             for large time, especially when empirical temp, rh are used
c     nhist:  number of time intervals at which temperature, rh are stored
c     time:   time at which linear interpolation is done for the temp.
c     tin:    interpolated temperature
c     nv:     size of the vector odev
c     odev:   dependent variable
c     clconc: chloride ion concentration near the WP [mol/liter]
c     crate:  corrosion rate in m/yr
c     dvdt:   derivative of the dependent variable
c-----------------------------------------------------------------

      xin = 0.8
      call lint(timr, tcan, nintv, nhist, time, tin)
      call lint(timr, clconc, nintv, nhist, time, clconcb)
      do 100 i = 1, nv
        odev(i) = max(odev(i), 0.)
  100 continue

      call corrode(tin, time, xin, clconcb, crate, ilayer, clcrit1,
     &             clcrit2, iflagcl)

      dvdt(1) = crate

c     print*, 'from rate: time,tin,dvdt(1)=', time,tin,dvdt(1)
```

```
      return
      end
**==CORRODE.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997



      subroutine corrode(temp, time, xin, clconcb, crate, ilayer,
     &                   clcrit1, clcrit2, iflagcl)
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 aa, age, bb, berp, berp0, berp1, betahy, betahy1,
     &       betahy2, betaox, betaox1, betaox2, cathod, cbulko2,
     &       cfarad, clconcb, clcrit1, clcrit2, conv, cpass
      real*8 crate, crate2, cthick1, cthick2, curact, curhy, curmax,
     &       curox, d, ddw, delt, dense1, dense2, do2w, dzc, e, ecor,
     &       ecor1, ecrit, ecthdr
      real*8 eec, eexpt, erp0, erp00, erp01, filmthk, ghy, ghy1, ghy2,
     &       gox, gox1, gox2, ph, pttemi, pttemo, rcoef, refph,
     &       rexpont, rgas, rkhy
      real*8 rkhy1, rkhy2, rkox, rkox1, rkox2, rptemi, rptemo,
     &       sfactor, slpti, slpto, slpttemi, slpttemo, slrpi, slrpo,
     &       slrptemi, slrptemo, sollay, spor, taus, tdiff
      real*8 temp, tend, time, tk, tkref, twet, wtmol1, wtmol2, x,
     &       xcouple, xgas, xin, xipti, xipto, xirpi, xirpo, xkh,
     &       xko2, xread, xxx1
      real*8 xxx2, xxx3, y, yko2, yyy1, z, zc, zo2
      integer i, icorr, iflagcl, ilayer
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------
c     corrosion rate & corrosion potential in the water film on the wp
c-----------------------------------------------------------------
      common /bulk  / age, tend, x, y, z, d, filmthk, e, cthick1,
     &                cthick2, sfactor
      common /corrpar1/ ecor, ecrit, cpass, sollay, curact, aa(2, 3),
     &                  xread, refph, betaox1, betahy1, betaox2,
     &                  betahy2, rkox1, rkhy1, rkox2, rkhy2, gox1,
     &                  ghy1, gox2, ghy2, spor, taus, xcouple
c     common /corrpar2/ xipto, slpto, xirpo, slrpo, xipti, slpti,
c    &                  xirpi, slrpi
      dimension bb(6)
      common /wetting/ twet
      common /cripotout/ xipto, pttemo, slpto, slpttemo, xirpo,
     &                   rptemo, slrpo, slrptemo
      common /cripotin/ xipti, pttemi, slpti, slpttemi, xirpi, rptemi,
     &                  slrpi, slrptemi
      common /prate / rcoef, rexpont, crate2, eexpt
      common /flags / icorr
c-----------------------------------------------------------------
c     ecrit:  critical potential for localized corrosion (volts SHE)
c     refph:  reference ph
c     aa(1,3):        cpass = aa(1,1)+aa(1,2)*T+aa(1,3)*T**2
c     aa(2,3):        cpass = aa(2,1)+aa(2,2)*T+aa(2,3)*T**2
c     bb(6):  ecrit = bb(1)+bb(2)*T+bb(3)*T**2+
c                     bb(4)* Log10(molar chloride)+bb(5)*no3/Cl+
c                     bb(6)*(ph-phref)
c     xipto:  outer overpack Ep intercept
c     pttemo: temp. coef. of outer overpack Ep intercept
```

```
c       slpto:  outer overpack Ep slope
c       slpttemo:temp. coef. of outer overpack Ep slope
c       xirpo:  outer overpack Erp intercept
c       rptemo: temp. coef. of outer overpack Erp intercept
c       slrpo:  outer overpack Erp slope
c       slrptemo:temp. coef. of outer overpack Erp slope
c       xipti:  inner overpack Ep intercept
c       pttemi: temp. coef. of inner overpack Ep intercept
c       slpti:  inner overpack Ep slope
c       slpttemi:temp. coef. of inner overpack Ep slope
c       xirpi:  inner overpack Erp intercept
c       rptemi: temp. coef. of inner overpack Erp intercept
c       slrpi:  inner overpack Erp slope
c       slrptemi:temp. coef. of inner overpack Erp slope
c       betaox1, betahy1: beta kinetics parameters for oxygen and water
c                       for WP outer overpack
c       betaox2, betahy2: beta kinetics parameters for oxygen and water
c                        for WP inner overpack
c       tkref:  reference temperature [k]; kinetic data is for 25 celsius,
c               therefore use only that temperature here
c       rgas:   universal gas constant [j/mole*k]
c       xgas:   partial pressure of oxygen
c       xkh:    Henry's law constant for oxygen solubility
c       eec:    previous ee
c       cfarad: faraday constant [coulomb/equivalent]
c       rkox:   rate constant for oxygen reduction  (coulomb m/mole/yr)
c       gox:    activation energy for oxygen rate constant (J/mole)
c       sollay: thickness of scale layer (m)
c       filmthk:thickness of water film in m prior to effluent creation
c       taus:   tortuosity/geometry correction for liquid diffusion
c                       of oxygen through boiler scale
c       spor:    porosity of scale deposited on the wp [=1.0 fir liq. film]
c       betaox: beta kinetics parameter for oxygen reduction
c       ghy:    activation energy for water reduction (J/mole)
c       rkhy:   rate constant for water redution in (coulomb/m^2/yr)
c       curox:  current density for oxygen reduction
c       curhy:  current density for hydrogen ion reduction
c       cathod: cathodic current density
c       do2w:   diffusion coefficient of oxygen in aqueous sol.[m^2/yr]
c       zo2:    # of electrons involved in the process/mole
c       ddw:    diffusivity of molecular oxygen in water at 25 C
c       wtmol1: molecular weight of outer layer [kg/mole]
c       wtmol2: molecular weight of inner layer [kg/mole]
c       dense1: density of outer layer [kg/m^3]
c       dense2: density of inner layer [kg/m^3]
c       crate:  corrosion rate of the outer overpack [m/yr]
c       crate2: corrosion rate of the inner overpack[m/yr]
c       xread:  previous bb(1) is now xread so that bb(1) etc. are properly
c               assigned to obtain xread
c       cpass:  passive current density in Coulomb/m^2/yr
c       ecor:   corrosion potential (volts SHE)
c       xcouple:a fraction representing degree of coupling bet. two layers
c       cbulko2:outer oxygen concentration in moles per m^3 of water
c       tk:     temperature in kelvin
c       temp:   temperature in celcius
c       time:   time in years
c       xxx1,xxx2,xxx3,yyy1:    local intermediate variables

c       note:   xin->   mole fraction water vapor on waste package surface
c-----------------------------------------------------------------
```

```
      cfarad = 96485.
      rgas = 8.3144
      ddw = 0.063
      dense1 = 7860.
      wtmol1 = 0.05585
      dense2 = 8140.
      wtmol2 = 0.05747

      sollay = 0.0
      ph = refph
      tkref = 273.15 + 25.
      tk = 273.15 + temp

      if ( ilayer.eq.1 ) then
        betaox = betaox1
        betahy = betahy1
        rkox = rkox1
        rkhy = rkhy1
        gox = gox1
        ghy = ghy1

c-->     critical potentials data for outer layer (A516 steel)
c         xipto = -584.8
c         pttemo = 3.92
c         slpto = -24.5
c         slpttemo = -1.1
c         xirpo = -620.3
c         rptemo = 0.47
c         slrpo = -95.2
c         slrptemo = 0.88

        erp00 = xipto + pttemo*temp
        berp0 = slpto + slpttemo*temp
        erp01 = xirpo + rptemo*temp
        berp1 = slrpo + slrptemo*temp
        erp0 = erp01 + xread*(erp00 - erp01)
        bb(1) = erp0
        bb(2) = 0.0
        bb(3) = 0.0
        berp = berp1 + xread*(berp0 - berp1)
        bb(4) = berp
        ecrit = bb(1) + bb(4)*log10(clconcb)
c         divide by 1000. to convert from mV to V
        ecrit = ecrit/1000.
        cpass = aa(1, 1) + aa(1, 2)*tk + aa(1, 3)*tk*tk
      else
        betaox = betaox2
        betahy = betahy2
        rkox = rkox2
        rkhy = rkhy2
        gox = gox2
        ghy = ghy2

c-->     critical potentials data for inner layer (Alloy 825)
c         xipti = 200.
c         pttemi = 0.
c         slpti = -240.
c         slpttemi = 0.
c         xirpi = 422.8
```

```
c           rptemi = -4.1
c           slrpi = -64.
c           slrptemi = -0.80

            erp00 = xipti + pttemi*temp
            berp0 = slpti + slpttemi*temp
            erp01 = xirpi + rptemi*temp
            berp1 = slrpi + slrptemi*temp
            erp0 = erp01 + xread*(erp00 - erp01)
            bb(1) = erp0
            bb(2) = 0.0
            bb(3) = 0.0
            berp = berp1 + xread*(berp0 - berp1)
            bb(4) = berp
            ecrit = bb(1) + bb(4)*log10(clconcb)
c             divide by 1000. to convert from mV to V
            ecrit = ecrit/1000.
            cpass = aa(2, 1) + aa(2, 2)*tk + aa(2, 3)*tk*tk

          end if

c         print*,'erp0,berp,clconcb=',erp0,berp,clconcb

          if ( cpass.lt.0. ) then
            write (*, *) '-ve passive current density =', cpass
            stop 'bad passive current density'
          end if

c-->      calculate oxygen concentration against metal using  temperature,
c-->      henry's law, amount of air present, passive current density, and
c-->      thickness of water film

          yyy1 = (1./tkref - 1./tk)/rgas

c         partial pressure of oxygen over the solution; this is a constant
c         here because we are assuming that the o2 in the atmosphere is
c         in equilibrium with the liquid film on the waste package.
c         xgas=0.21*(1.0-xin)
c         cbulko2=xgas*henry*1000.

          xgas = 0.21
          ecthdr = 14612.
          do2w = ddw*exp(ecthdr*yyy1)
          xkh = exp(0.2984 - (5.59617*10.**3)/tk + (1.04967*10.**6)/tk/tk)
          cbulko2 = xgas*xkh*1000.

c-->      estimate corrosion potential by equating oxygen reduction plus
c-->      hydrogen evolution with passive current density

          delt = 2.0
          xxx1 = betahy*cfarad/(rgas*tk)
          xko2 = rkox*exp(gox*yyy1)
c         is k298 assumed to be 1.0 ?
          xxx2 = xko2*max(sollay, filmthk)/(4.0*cfarad*do2w*taus*spor)
          zo2 = 4.0
          xxx3 = betaox*zo2*cfarad/(rgas*tk)

          if ( ilayer.ne.2 ) then
            eec = 0.
            do 50 i = 1, 15
```

```
            yko2 = rkhy*exp(ghy*yyy1)
            curhy = -yko2*exp( - xxx1*eec)

c           note: oxygen current must be constrained to < diffusion
c           limited current curmax. since cathodic current is negative,
c           take the maximum value to get the lowest absolute value

            curmax = -4.*cfarad*do2w*taus*spor*cbulko2/max(sollay,
     &                filmthk)
            xko2 = rkox*exp(gox*yyy1)
            curox = -xko2*cbulko2*exp( - xxx3*eec)
     &              /(1.0 + xxx2*exp(-xxx3*eec))
            curox = max(curmax, curox)
            cathod = -(curox + curhy)
            if ( cathod.gt.cpass ) then
              eec = eec + delt
            else
              eec = eec - delt
            end if
            delt = delt/2.0
   50     continue

c-->   ensure that the summation of all currents equal to zero,
c-->   newton-raphson method is used as an additional step

          do 100 i = 1, 10
            yko2 = rkhy*exp(ghy*yyy1)
            curhy = -yko2*exp( - xxx1*eec)
            curmax = -4.*cfarad*do2w*taus*spor*cbulko2/max(sollay,
     &                filmthk)
            xko2 = rkox*exp(gox*yyy1)
            curox = -xko2*cbulko2*exp( - xxx3*eec)
     &              /(1.0 + xxx2*exp(-xxx3*eec))
            curox = max(curmax, curox)
            cathod = -(curox + curhy)
            zc = cpass - cathod
            dzc = -xxx1*curhy - xxx3*curox/(1 + xxx2*exp(-xxx3*eec))
            if ( abs(zc).le.1.0E-8 ) go to 150
            eec = eec - zc/dzc
  100     continue

          write (*, *) 'corrosion potential not converging in 10 ',
     &                 'iterations.'

c-->    now compare potentials with critical potentials

  150     continue
          ecor1 = eec
        end if
        if ( ilayer.ne.1 ) then
          eec = ecor1
cssss      eexpt = -0.46
          eec = eec*(1. - xcouple) + xcouple*eexpt
c          print*,'xcouple,eec,ecrit=',xcouple,eec,ecrit
        end if
        ecor = eec
        iflagcl = 0
c       print*,clconcb,clcrit1,iflagcl
        if ( ilayer.eq.1 .and. clconcb.gt.clcrit1 ) iflagcl = 1
        if ( ilayer.eq.2 .and. clconcb.gt.clcrit2 ) iflagcl = 1
```

```
        if ( eec.ge.ecrit .and. iflagcl.eq.1 ) then
          icorr = 1
          if ( ilayer.eq.1 ) then
c              rexpont=0.45
c              rcoef=8.66e-3
            tdiff = time - twet
            if ( tdiff.le.1E-8 ) tdiff = 1.E-8
            crate = rcoef*rexpont*tdiff**(rexpont - 1)
c                                              ! m/yr corrosion rate
c              print*,'time,twet=',time,twet
          else
            crate = crate2
          end if

cdbg       if(time.gt.2700) write(9,*) time,eec,ecrit,crate
        else
          icorr = 0
          if ( ilayer.eq.1 ) then
            conv = wtmol1/dense1/cfarad/2.
          else
            conv = wtmol2/dense2/cfarad/2.25
          end if
          crate = cpass*conv

cdbg       if(time.gt.2700) write(9,*) time,eec,ecrit,crate
        end if

c       penetration (mm)= 8.66 t**0.45 with t in yr.
c       print*, 'time,temp,ecrit,eec,crate=', time,temp,ecrit,eec,crate

        return
        end
**==LINT.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




        subroutine lint(xa, ya, n1, n, x, y)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 h, x, xa, y, ya
        integer k, khi, klo, n, n1
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c       subroutine for linear interpolation
c-----------------------------------------------------------------------
c       nomenclature:
c       xa:     vector of length n of x values (independent variable)
c       ya:     vector of length n of y values
c       n:      length of xa and ya vectors
c       x:      x value at which interpolation is required
c       y:      returned value of dependent variable corresponding to x value
c-----------------------------------------------------------------------
        dimension xa(n1), ya(n1)
c-----------------------------------------------------------------------

        if ( xa(1).lt.xa(n) ) then
c  increasing order list
```

```
        if ( x.le.xa(1) ) then
          y = ya(1)
        else if ( x.ge.xa(n) ) then
          y = ya(n)
        else
          klo = 1
          khi = n
   20     continue
          if ( khi - klo.gt.1 ) then
            k = (khi + klo)/2
            if ( xa(k).gt.x ) then
              khi = k
            else
              klo = k
            end if
            go to 20
          end if
          h = xa(khi) - xa(klo)
          if ( h.eq.0. ) pause 'bad xa input.'
          y = ya(klo) + (x - xa(klo))/h*(ya(khi) - ya(klo))
        end if
c  decreasing order list
      else if ( x.ge.xa(1) ) then
        y = ya(1)
      else if ( x.le.xa(n) ) then
        y = ya(n)
      else
        klo = 1
        khi = n
   50   continue
        if ( khi - klo.gt.1 ) then
          k = (khi + klo)/2
          if ( xa(k).lt.x ) then
            khi = k
          else
            klo = k
          end if
          go to 50
        end if
        h = xa(khi) - xa(klo)
        if ( h.eq.0. ) pause 'bad xa input.'
        y = ya(klo) + (x - xa(klo))/h*(ya(khi) - ya(klo))
      end if

      return
      end
**==MECH.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




      subroutine mech(jj, time1, time2, temp, penet, ifail)
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 age, cdepth, cthick1, cthick2, d, e, filmthk, penet,
     &       sfactor, strss, temp, tend, time1, time2, x, y, yieldstr,
     &       z
      integer ifail, jj
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
```

```
c       subroutine to test WP for mechanical failure by fracture due to residual
c       stress associated with welds in the presence of a flaw of a given depth
c       produced by localized corrosion
c-----------------------------------------------------------------------
        common /bulk  / age, tend, x, y, z, d, filmthk, e, cthick1,
     &                  cthick2, sfactor
crrrr   common /wpgmty/ wplen,wpdia
c-----------------------------------------------------------------------
c       nomenclature:
c       temp:           temperature at the wp surface [c]
c       ifail:          =0: wp not failed; =1: wp failed
c       cdepth:         crack depth or the depth of a corroded pit [m]
c       penet:
c       strss:          tensile component of the residual stress [Pa]
c       yieldstr:       yield strength of A516 Grade 55 steel [Pa]
c       pi:             the constant pi
c       r:
c       sfactor:        safety factor considering the increase of yield
c                       strength at the welds
c-----------------------------------------------------------------------

c       debugging parameters jj, time1, time2

crrrr   print*, jj,time1,time2

        ifail = 0
crrrr        pi = 4. * atan(1.)
        sfactor = 1.5
        yieldstr = 205.E6

c       limit temperature to the applicable range of the stress equ.

        if ( temp.lt.25. ) temp = 25.
        if ( temp.gt.100. ) temp = 100.
        cdepth = penet
        strss = yieldstr*sfactor

        call fracfail(strss, cdepth, ifail)
cssss
c       print*
c       print*,'punifo,cdepth,clt,strss=',punifo,cdepth,clt,strss
c       print*,'time1,penet',time1,penet
c       print*

        return
        end
**==FRACFAIL.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




        subroutine fracfail(strss, cdepth, ifail)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 cdepth, dki, dkic, pi, strss, yfunc, yvalue
        integer ifail
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c       fracture failure analysis based on stress intensity calculation
c-----------------------------------------------------------------------
```

```
c       nomenclature:
c       cdepth:         crack depth or the depth of a corroded pit [m]
c       yvalue:         geometry factor
c       dkic:           fracture toughness of A516 Grade 55 steel
c                        =250  [MPa-m**0.5]
c       yfunc:          a function call
c       strss:          tensile component of the residual stress [Pa]
c       pi:             the constant pi
c       ifail:
c-----------------------------------------------------------------------

        pi = 4.*atan(1.)
        dkic = 250.E6
        yvalue = yfunc(cdepth)
        dki = strss*yvalue*(pi*cdepth)**.5
        if ( dki.gt.dkic ) ifail = 1
cssss
c       print*
c       print*,'dki,yvalue,cdepth=', dki,yvalue,cdepth
c       print*

        return
        end
**==YFUNC.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




        real*8 function yfunc(tt)
        implicit none
C*** Start of declarations inserted by SPAG
        real alow, atop, tt, xx, yy
        integer i
C*** End of declarations inserted by SPAG
        dimension xx(30), yy(30)
c-----------------------------------------------------------------------
c       function subprogram to determine the geometry factor for the
c       fracture toughness failure criterion. This geometry value is for
c       a surface crack in hollow cylinder, circular on outer area.
c       this value is calculated by using nasa flagro program.
c-----------------------------------------------------------------------

c       store the table data

        xx(1) = 0.00001
        xx(2) = 0.00005
        xx(3) = 0.0001
        xx(4) = 0.0002
        xx(5) = 0.0005
        xx(6) = 0.00075
        xx(7) = 0.001
        xx(8) = 0.002
        xx(9) = 0.003
        xx(10) = 0.004
        xx(11) = 0.005
        xx(12) = 0.006
        xx(13) = 0.007
        xx(14) = 0.008
        xx(15) = 0.009
```

```
      xx(16) = 0.0095
      xx(17) = 0.0097
      xx(18) = 0.0098
      xx(19) = 0.0099
      xx(20) = 0.00995
      yy(1) = 0.8817
      yy(2) = 0.8826
      yy(3) = 0.8837
      yy(4) = 0.8858
      yy(5) = 0.8923
      yy(6) = 0.8977
      yy(7) = 0.9030
      yy(8) = 0.9247
      yy(9) = 0.9463
      yy(10) = 0.9681
      yy(11) = 0.9899
      yy(12) = 1.0118
      yy(13) = 1.0338
      yy(14) = 1.0559
      yy(15) = 1.0780
      yy(16) = 1.0891
      yy(17) = 1.0935
      yy(18) = 1.0958
      yy(19) = 1.0980
      yy(20) = 1.0991

c     find location for tt

      if ( tt.le.xx(1) ) then
        yfunc = yy(1)
        return
      end if

      if ( tt.ge.xx(20) ) then
        yfunc = yy(20)
        return
      end if

      do 100 i = 1, 20
        if ( tt.le.xx(i) ) go to 200
100   continue

200   continue
      atop = xx(i)
      alow = xx(i - 1)
      yfunc = (tt - alow)/(atop - alow)*(yy(i) - yy(i-1))

      return
      end
**==INPUT.spg  processed by SPAG 4.00Aa at 14:01 on  7 Jan 1997




      subroutine input
      implicit none
C*** Start of declarations inserted by SPAG
      real*8 aa, age, betahy1, betahy2, betaox1, betaox2, cfactor,
     &       clconc, clconca, clcrit1, clcrit2, constant1, cpass,
```

```
     &        crate2, ctemp, cthick1, cthick2, curact, d, dtini
        real*8 dtmax, e, ecor, ecrit, eexpt, errabs, errrel, filmthk,
     &        gbthick, ghy1, ghy2, gox1, gox2, grainr, humdc, pttemi,
     &        pttemo, rcoef, refph, rexpont
        real*8 rkhy1, rkhy2, rkox1, rkox2, rptemi, rptemo, sfactor,
     &        slpti, slpto, slpttemi, slpttemo, slrpi, slrpo, slrptemi,
     &        slrptemo, sollay, spor, taus, tend, timintv
        real*8 wpdia, wplen, x, xcouple, xipti, xipto, xirpi, xirpo,
     &        xread, y, z
        integer iflag, iflagcl, nhista, nintv, nseries, nset
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c       purpose: read input parameters
c       most variables are passed in common blocks and all the input is simple
c       non-formatted and could be easily upgraded at a later date.
c-----------------------------------------------------------------------
        parameter (nintv=20000)
        common /bulk  / age, tend, x, y, z, d, filmthk, e, cthick1,
     &                  cthick2, sfactor
crrrr           common /thist/timr(nintv),tavg(nintv),tcan(nintv),humd(nintv)
        common /corrpar1/ ecor, ecrit, cpass, sollay, curact, aa(2, 3),
     &                    xread, refph, betaox1, betahy1, betaox2,
     &                    betahy2, rkox1, rkhy1, rkox2, rkhy2, gox1,
     &                    ghy1, gox2, ghy2, spor, taus, xcouple
c       common /corrpar2/ xipto, slpto, xirpo, slrpo, xipti, slpti,
c     &                  xirpi, slrpi
        common /solve / dtini, dtmax, errrel, errabs
        common /temp1 / iflag, nset, timintv, humdc, ctemp, nhista
        common /dryoxdc/ grainr, gbthick, constant1, nseries
        common /new1  / clconca, clcrit1, clcrit2, clconc(nintv),
     &                  cfactor, iflagcl
        common /wpgmty/ wplen, wpdia
        common /cripotout/ xipto, pttemo, slpto, slpttemo, xirpo,
     &                     rptemo, slrpo, slrptemo
        common /cripotin/ xipti, pttemi, slpti, slpttemi, xirpi, rptemi,
     &                    slrpi, slrptemi
        common /prate / rcoef, rexpont, crate2, eexpt
c-----------------------------------------------------------------------
c       nomenclature:
c       age:       age of the waste in years at time of emplacement in years
c       tend:      end time for simulation
c       d:         vapor diffusion coefficient [m^2/yr]
c       filmthk:   thickness of water film [m] on the wp
c       e:         evaporation rate [m^3/yr]
c       cthick1:   wp outer overpack initial thickness [m]
c       cthick2:   wp inner overpack initial thickness [m]
c       sfactor:   safety factor for uncertainties in mechanical properties
c       grainr:    grain radius [micrometer]
c       nseries:   number of terms in infinite series for wp oxidation
c       gbthick:   grain bundary thickness [micrometer]
c       constant1: a constant relating matrix and grain boundary
c                       diffusivities
c       betaox:    beta kinetics parameter for oxygen reduction
c       betahy:    beta kinetics parameter for water reduction
c       rkox:      rate constant for oxygen reduction [coulomb m/mole/yr]
c       rkhy:      rate constant for water redution in [coulomb/m^2/yr]
c       gox:       activation energy for oxygen rate constant [J/mole]
c       ghy:       activation energy for water reduction [J/mole]
c       aa(1,3):   cpass = aa(1,1)+aa(1,2)*T+aa(1,3)*T**2
c       aa(2,3):   cpass = aa(2,1)+aa(2,2)*T+aa(2,3)*T**2
```

```
c       ecrit:     critical potential for localized corrosion [volts SHE]
c       refph:     reference ph
c       taus:      tortuosity/geometry correction for liquid diffusion
c                       of oxygen through boiler scale
c       spor:      porosity of scale deposited on the wp (=1.0 for liq. film)
c       dtini:     initial time step [yr]
c       dtmax:     maximum time step [yr]
c       errrel:    relative error
c       errabs:    absolute error
c       ecor:      corrosion potential [volts SHE]
c       cpass:     passive current density [Coulomb/m^2/yr]
c       sollay:    thickness of scale layer [m]
c       curact:    active current density in [coulomb/m^2/yr]
c       timr(i):   representative time [yr]
c       tavg(i):   average repository temperature [Celsius]
c       tcan(i):   waste package surface temperature [Celsius]
c-----------------------------------------------------------------

c-->  read basic control parameters

c     first card is a comment line
        read (9, *)

c  end time of simulation in years. simulations always start
c  at time = 0 years

        read (9, *)
        read (9, *)
        read (9, *) tend
        write (22, *) 'tend = ', tend

c-->  container size and geometry

        read (9, *)
        read (9, *)
        read (9, *) wplen, wpdia
        write (22, *) 'wplen,wpdia', wplen, wpdia
        read (9, *) cthick1, cthick2
        write (22, *) 'cthick1,cthick2 = ', cthick1, cthick2

c--> thermal  section

        read (9, *)
        read (9, *)
        read (9, *) iflag
c       there are total of 12 sets of tabular, i.e, nset = 12 maximum
        read (9, *) nset
        write (22, *) 'iflag,nset=', iflag, nset
c       time interval for screening input data
        read (9, *) timintv
        write (22, *) 'timintv=', timintv
c       read(9,*) nhista        ! used only when iflag is one
c       write(22,*) 'nhista=', nhista

c-->  age of the waste [y]

        read (9, *)
        read (9, *)
        read (9, *) age
        write (22, *) 'age [y] = ', age
```

```
c-->  dry oxidation at the wp overpack outer surface

        read (9, *)
        read (9, *)
        read (9, *) grainr
        read (9, *) nseries
        read (9, *) gbthick
        read (9, *) constant1
c                           grain boundary diffusivities
        write (22, *) 'grainr,nseries=', grainr, nseries
        write (22, *) 'gbthick,constant1=', gbthick, constant1

c-->  liquid condensation

        read (9, *)
        read (9, *)
        read (9, *) humdc
        read (9, *) filmthk
        read (9, *) ctemp
        write (22, *) 'humdc,filmthk,ctemp= ', humdc, filmthk, ctemp

c-->    corrosion parameters

        read (9, *)
        read (9, *)
        write (22, *)
        write (22, *) 'corrosion parameters'
        write (22, *)

c       outer overpack

        read (9, *) xipto
        read (9, *) pttemo
        read (9, *) slpto
        read (9, *) slpttemo
        read (9, *) xirpo
        read (9, *) rptemo
        read (9, *) slrpo
        read (9, *) slrptemo

        write (22, *) 'xipto,pttemo=', xipto, pttemo
        write (22, *) 'slpto,slpttemo=', slpto, slpttemo
        write (22, *) 'xirpo,rptemo=', xirpo, rptemo
        write (22, *) 'slrpo,slrptemo=', slrpo, slrptemo

c       inner overpack

        read (9, *) xipti
        read (9, *) pttemi
        read (9, *) slpti
        read (9, *) slpttemi
        read (9, *) xirpi
        read (9, *) rptemi
        read (9, *) slrpi
        read (9, *) slrptemi

        write (22, *) 'xipti,pttemi=', xipti, pttemi
        write (22, *) 'slpti,slpttemi=', slpti, slpttemi
        write (22, *) 'xirpi,rptemi=', xirpi, rptemi
```

```
      write (22, *) 'slrpi,slrptemi=', slrpi, slrptemi

      read (9, *) betaox1, betahy1
      read (9, *)
      read (9, *) betaox2, betahy2
      read (9, *)
      write (22, *) 'betaox1, betahy1 = ', betaox1, betahy1
      write (22, *) 'betaox2, betahy2 = ', betaox2, betahy2
      read (9, *) rkox1, rkhy1
      read (9, *) gox1, ghy1
      read (9, *) rkox2, rkhy2
      read (9, *) gox2, ghy2
      write (22, *) 'rkox1,rkhy1,gox1,ghy1= ', rkox1, rkhy1, gox1,
     &               ghy1
      write (22, *) 'rkox2,rkhy2,gox2,ghy2= ', rkox2, rkhy2, gox2,
     &               ghy2
      read (9, *) aa(1, 1), aa(1, 2), aa(1, 3)
      read (9, *) aa(2, 1), aa(2, 2), aa(2, 3)
      write (22, *) 'aa11 ... aa13 = ', aa(1, 1), aa(1, 2), aa(1, 3)
      write (22, *) 'aa21 ... aa23 = ', aa(2, 1), aa(2, 2), aa(2, 3)
      read (9, *) eexpt
      read (9, *) rcoef
      read (9, *) rexpont
      write (22, *) 'eexpt,rcoef,rexpont=', eexpt, rcoef, rexpont
      read (9, *) crate2
      read (9, *) xcouple
      read (9, *) xread
      write (22, *) 'crate2,xcouple,xread=', crate2, xcouple, xread
      read (9, *) clconca
      read (9, *) clcrit1
      read (9, *) clcrit2
      write (22, *) 'clconca=', clconca
      write (22, *) 'clcrit1=', clcrit1
      write (22, *) 'clcrit2=', clcrit2
      read (9, *) cfactor
      write (22, *) 'cfactor=', cfactor
      read (9, *) refph
      write (22, *) 'refph = ', refph
      read (9, *) taus, spor
      write (22, *) 'taus, spor = ', taus, spor

c-->  numerical solver control parameters

      read (9, *)
      read (9, *)
      read (9, *) dtini, dtmax
      write (22, *) 'dtini, dtmax= ', dtini, dtmax
      read (9, *) errrel, errabs
      write (22, *) 'errrel, errabs = ', errrel, errabs
      write (22, *)
     &             '-------------------------------------------------'

      return
      end
**==DRYOXDWP.spg  processed by SPAG 4.00Aa at 14:02 on  7 Jan 1997



      subroutine dryoxdwp(ipr, tyears, tempc, grainr, nseries,
```

```
     &                    gbthick, constant1, penetd)
        implicit none
C*** Start of declarations inserted by SPAG
        real*8 constant1, ddd1, ddd2, dfsvtygb, dfsvtym, gbthick,
     &         grainr, penetd, pi, rgas1, sum, temp1, tempc, timehr,
     &         tyears, xxx1
        integer ipr, nnn, nseries
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c       nomenclature:
c       pi:             the constant pi
c       tempc:          temperature in celcius
c       temp1:          tempc in kelvin
c       dfsvtym:        matrix diffusivity
c       dfsvtygb        grain boundary diffusivity
c       constant1:      a constant relating matrix and grain  boundary
c                       oxygen diffusivity in metal
c       grainr:         grain radius [micrometer]
c       gbthick:        grain bundary thickness [micrometer]
c       tyears:         time in years
c       thour:          tyears in hours
c       nseries:        number if terms in infinite series for wp oxidation
c                       boundary diffusivities
c       Note:
c       Dg:     Dm/constant1
c       rgas1:  universal gas constant
c               = 1.987 (cal)/(g mol)(K)
c               = 4.184e-3*1.987 (kJ)/(g mol)(K)
c-----------------------------------------------------------------------

c       debudding parameter ipr
c       print*, ipr

c       print*,'grainr,gbthick,constant1=',grainr,gbthick,constant1

        pi = 4.*atan(1.)
        rgas1 = 1.987

c       constant1 = 1.e-2
c       nseries = 25
c       gbthick = 0.7e-3                ! [micrometer]

        temp1 = 273. + tempc
        xxx1 = 169./(4.184E-3*rgas1*temp1)
c       print*, 'rgas1,temp1,xxx1=',rgas1,temp1,xxx1
        if ( xxx1.gt.65. ) xxx1 = 65.
        dfsvtym = 575.E-6*exp( - xxx1)
        dfsvtym = dfsvtym*1.E12*60*60
        dfsvtygb = dfsvtym/constant1
        ddd1 = 4.*dfsvtym/(grainr*gbthick*dfsvtygb)

        timehr = tyears*365.*24.
        sum = 0.
        do 100 nnn = 1, nseries
          ddd2 = dfsvtym*nnn**2*pi**2*timehr/grainr**2
          if ( ddd2.gt.65. ) ddd2 = 65.
          sum = sum + exp( - ddd2)
c          print*, 'ddd1,ddd2,exp(-ddd2)=',ddd1,ddd2,exp(-ddd2)
  100   continue
```

```
      penetd = 1./sqrt(ddd1*sum)

c     convert from micrometer to meter:

      penetd = penetd/1.E6

c     print*,'@dryoxdwp:- ipr,tyears,tempc,diffvty,penetd'
c    * ,ipr,tyears,tempc,dfsvtygb,penetd

      return
      end
```

5-7-95

```
**==RELEASE.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996
      program release
      implicit none
cssss     IMPLICIT NONE
c-----------------------------------------------------------------
c   Code:       EBSPAC (Engineering Barrier System Performance Assessment Code)
c
c   Part:       ebspac_release.f.  This is one of the two parts of EBSPAC
c
C   Version:    1.0
c
c   Date:       January 6, 1997
c
C   Purpose:    The EBSPAC computer program has been developed jointly by the
c               Center for Nuclear Waste Regulatory Analyses (CNWRA) and the
c               U. S. Nuclear Regulatory Commission (NRC) for use in the
C               review of DOE's licence application for the HLW Geologic
c               Repository by the Office of NMSS, DWM.
C
C               ebspac_fail.f part of EBSPAC calculates waste package failure
c               time. ebspac_release.f part of EBSPAC calculates the rate of
c               release of nuclides from the repository in the near field.
C
C               The repository is assumed to be made up of cells and EBSPAC
c               provides results for one cell. Input to EBSPAC is read from
c               files which may either be created manually by the user or
c               generated by use of codes other than EBSPAC.
C
C   Developers: ebspac_fail.f was developed by Sitakanta Mohanty
c               at the CNWRA with assistance from Tae Ahn (NRC, 301-415-5812),
c               G. Cragnolino, P. Lichtner, N. Sridhar, and R. Janetzke (CNWRA)
C
C   User:       Developed for use in NRC Iterative Performance Assessment
c               III. This computer code is managed under CNWRA's CODE
c               CONFIGURATION PROCEDURE. Any modifications to the source
c               code must be reported to code custodian (see below).
c               OTHER versions of this code will be released in the future.
c
C   Disclaimer: This computer code has not been formally or informally
C               verified, is known to have numerous bugs, and the model
c               embodied in it are not validated.
C
C   Contact:    Sitakanta Mohanty (210)522-5185
C               Center for Nuclear Waste Regulatory Analyses
C               Southwest Research Institute, San Antonio, Tx 78250
c-----------------------------------------------------------------

C*** Start of declarations inserted by SPAG
      real amass, amass0, amassc, amassl, c14inv, ccfr, cco3, cftime,
     &     cfuel, cgap, ci1000, con3, con4, cstore, ctemp
      real relrate, cumrel, cumrfuel, cumrzirc, cvol, czmetal,
     &     czoxide, deffrac, dr, dt, wetfrac, floref, flow, fueden
      real fuedif, fuewt, funnel, gscmrl, oxgnovpr, phvalue, qin, r0,
     &     rdrift, r0z, radu, radsg, dcoefm, flowfactr, rhouz, rpor,
     &     rr
      real sc14, sftime, simtimex, sumc14, crf, drf, sumre1, sumre2,
     &     sumre3, rlrate1, rlrate2, rlrate3, tcan, tavg, tcaqu,
     &     tcool, temp1, temp2, tfail, tflo, tftc, thclad, thetim
      real amwp1, amwp2, amwp3
      real time1, tleach, tlt, totalc14, trid, ttemp, vmax, watrel,
```

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pcl5

JOB 1740

release4.f

For: **scratchy1!mohanty**
Date: **Mon Jan 6 14:35:55 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 07:08:03 1991
Started: Wed Nov 13 07:08:03 1991

QMS 3825 Print System

59/195

Software Analysis Tool Run by Software Developer
1/8/97

```
**==RELEASE.spg  processed by SPAG 4.00Aa  19:34 on  9 Dec 1996
      program release
      implicit none
cssss      IMPLICIT NONE
c-----------------------------------------------------------------
c   Code:       EBSPAC (Engineering Barrier System Performance Assessment Code)
c
c   Part:       ebspac_release.f.  This is one of the two parts of EBSPAC
c
C   Version:    1.0
c
c   Date:       January 6, 1997
c
C   Purpose:    The EBSPAC computer program has been developed jointly by the
c               Center for Nuclear Waste Regulatory Analyses (CNWRA) and the
c               U. S. Nuclear Regulatory Commission (NRC) for use in the
C               review of DOE's licence application for the HLW Geologic
c               Repository.
C
C               ebspac_fail.f part of EBSPAC calculates waste package failure
c               time. ebspac_release.f part of EBSPAC calculates the rate of
c               release of nuclides from the repository in the near field.
C
C               The repository is assumed to be made up of cells and EBSPAC
c               provides results for one cell. Input to EBSPAC is read from
c               files which may either be created manually by the user or
c               generated by use of codes other than EBSPAC.
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C
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c
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c               embodied in it are not validated.
c
C   Contact:    Sitakanta Mohanty (210)522-5185
C               Center for Nuclear Waste Regulatory Analyses
C               Southwest Research Institute, San Antonio, Tx 78250
c-----------------------------------------------------------------

C*** Start of declarations inserted by SPAG
         real amass, amass0, amassc, amassl, c14inv, ccfr, cco3, cftime,
     &       cfuel, cgap, ci1000, con3, con4, cstore, ctemp
         real relrate, cumrel, cumrfuel, cumrzirc, cvol, czmetal,
     &       czoxide, deffrac, dr, dt, wetfrac, floref, flow, fueden
         real fuedif, fuewt, funnel, gscmrl, oxgnovpr, phvalue, qin, r0,
     &       rdrift, r0z, radu, radsg, dcoefm, flowfactr, rhouz, rpor,
     &       rr
         real sc14, sftime, simtimex, sumc14, crf, drf, sumre1, sumre2,
     &       sumre3, rlrate1, rlrate2, rlrate3, tcan, tavg, tcaqu,
     &       tcool, temp1, temp2, tfail, tflo, tftc, thclad, thetim
         real amwp1, amwp2, amwp3
         real time1, tleach, tlt, totalc14, trid, ttemp, vmax, watrel,
```

```
     &        wleach, ws, xco, xcon, dryfr[illegible]tsize
        integer nbt
        integer i, ichns, icoun, idefco, iiso, imax, imodel, iscon,
     &          itim, itime, itype, izone, jmax, k, maxbin, maxchn
        integer maxele, maxi, maxj, maxmem, maxnuc, maxnxm, maxste,
     &          maxtim, mtot, icfcon, nelem, noxz, nr, ntemp,
     &          numiso, numwp
        integer nzones
        real xlarge, xxx, ppor
        real vsmall, sum
        real dtinit, dtmax, dtmin, eps, tiny
        real xnoloss, xnolosst,xmass, rlmass, amwp
        integer errnum
        integer ncon, kcon, icon, nchns, ni
        real rmaxc14
        real tmaxc14
        real sol, rd, rde, amall, halflife, curall, fggap
        integer itemp
        real xlint, ylint, zlint
        real wplen, wpdia, driftdia
        real c14rate
        real pi, xvol, dintl, xlintl, xfrac, rintl, waterht
        real fuepor
        real dtt1
        real ntype1, ntype2, ntype3
cssss           REAL*8 alam, atoms, atall, am
        real alam, atoms, atall, am
        real vabs, voidfrac
        integer nremain
        real oxwidth
        real sum1, iflaguo24
        real diff
        real dist, marker
        real xtemporary, gwtotalc14
        integer kc14, ic14
        real pleft

        logical lxaust
        character*6 tmpnam
        character*8 timeyr
        character*80 errmsg
        character*3 elem
        character*6 namall
        character*24 fdate
C*** End of declarations inserted by SPAG
C----------------------------------------------------------------------
Cccccc
        parameter (maxchn=50)
        parameter (maxele=50)
        parameter (maxmem=10)
        parameter (maxnuc=50)
        parameter (maxnxm=maxnuc*maxmem)
        parameter (maxste=300)
        parameter (maxtim=500)
        parameter (maxbin=500)
        parameter (maxi=20, maxj=30)

        real fracre(maxchn, maxmem, maxste)
        real cumrelease(maxchn, maxmem, maxste)
        real maxrel(maxchn, maxmem)
```

```
      real timrel(maxchn, maxmem)
      real tregular(maxbin)

      common /ccont2/ deffrac
      common /ccont5/ sftime, iscon
      common /ccoro1/ cftime, tcaqu, icfcon
      common /cgeom / cvol, xcon, funnel, mtot
      common /cnucl1/ elem(maxele), namall(maxnuc, maxmem)
      common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
     &                amall(maxnuc, maxmem), halflife(maxnuc, maxmem),
     &                curall(maxnuc, maxmem), fggap(maxnuc, maxmem),
     &                kcon(maxele, maxnuc), icon(maxele, maxnuc),
     &                rd(maxnuc, maxmem), ni(maxnuc), nchns,
     &                ci1000(maxnuc, maxmem)
      common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                ccfr(maxnuc, maxmem), tleach, nelem,
     &                amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                amassl(maxnuc), tlt, tftc
      common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi, 4),
     &                rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                ppor(maxi)
      common /array1/ sumre1(maxnuc, maxmem, maxste),
     &                sumre2(maxnuc, maxmem, maxste),
     &                sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                rlrate1(maxnuc, maxmem, maxste),
     &                rlrate2(maxnuc, maxmem, maxste),
     &                rlrate3(maxnuc, maxmem, maxste),
     &                amwp1(maxnuc, maxmem, maxste),
     &                amwp2(maxnuc, maxmem, maxste),
     &                amwp3(maxnuc, maxmem, maxste)
      common /cnume1/ simtimex, imax, jmax
      common /cnume2/ xco(maxi), nzones, izone(maxi, maxj)
      common /cnum3 / diff(maxi)
      common /crhyd1/ rpor(maxi), flowfactr, flow, tflo(maxtim),
     &                floref(maxtim)
      common /cther0/ ntemp
      common /cther1/ ttemp(maxtim), tcan(maxtim)
      common /cther2/ ctemp
      common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc
      common /c14   / sc14(maxbin), sumc14(maxbin), gscmrl(maxbin),
     &                lxaust
      common /icarbon/ noxz
      common /rcarbon1/ r0z, rhouz, radu, radsg
      common /rcarbon2/ cfuel, czmetal, czoxide, cgap
      common /outpt / nbt
      common /rkutta/ eps, tiny, dtinit, dtmin, dtmax

      common /cumu  / crf(maxnuc, maxmem), drf(maxnuc, maxmem)
      common /wpvol / wplen, wpdia, driftdia, xvol, dintl, xlintl
      common /leach / imodel, phvalue, oxgnovpr, cco3, xfrac
      common /leach1/ wetfrac
      common /oxidized/ oxwidth
      common /uo24width/ sum1, iflaguo24
      common /driftwall/ marker

      dimension xlint(2), ylint(2), zlint(2)
      dimension c14rate(maxbin)
      dimension xnoloss(maxnuc, maxmem), xmass(maxnuc, maxmem, maxste)
     &          , rlmass(maxnuc, maxmem, maxste),
```

```
      &          amwp(maxnuc, maxmem, ma[redacted]e),xnolosst(maxste)
C-----------------------------------------------------------------------

c       nomenclature:
c
C       maxi:           max number of x- or r-dir nodes
C       maxj:           max number of y- or theta dir nodes
C       deffrac:        fraction of initially failed packages
C       idefco:         integer value of the same thing
C       sftime:         time at which scenario causes container failures in a cell
C       tcaqu:          time at which aqueous condition begins in  the cell
C       cftime:         corrosion failure time [y]
C       icfcon:         number failed containers in the cell due to corrosion
C       age:            age of pit
C       cvol:           cell volume
C       xcon:           num of packages in a cell
C       wplen:          length of package
C       wpdia:          diameter of waste package
C       rspher:         inner radius of spherical source for diffusion out of wp
C       funnel:         area above waste package where water is assumed to funnel
C                       into waste package.
C       mtot:           total number of containers in the cell
C       drf:            rate of release, gram moles per year
C       rd:             retardation factor for each isotope
C       dcoefm:         molecular diffusion coeficients for pack and rock [m^2/yr]
C       tfail:          time of wp failure, years
C       tcool:          time at which wp drops below boiling pt, years
C       tleach:         time span for all u to be converted, years
C       qin:            inflow of water to canister, [l/y]
C       wetfrac:        position (height) of the outlet as a fraction of the wp id
C       dryfrac:        fraction of the fuel available for dry oxidation
C       vmax:           maximum water volume in wp before overflow [l]
C       dt:             timestep [yr]
C       amass0 :        mass of fuel [kg]; amassc assigned to amass0
C       amass(k, i):    solid mass of each radionuclide in fuel matrix [kg]
C       namall:         radionuclide name
C       elem:           element name
C       v:              volume of water in canister, liters
C       vmin:           initial v
c       atall:          inventory of radionuclides [atoms];
c                       obtained by converting curall(k,i) in ci
C       sumrel:         release history:1=defective,2=scenario,3=normal
C                       failure in the cell, the results are overwritten in
C                       sumrel(maxnuc,maxmem,time step)
C       rlrate:         release rate history:1=defective,2=scenario,3=normal
C                       failure in the cell, the results are overwritten in
C                       rlrate(maxnuc,maxmem,time step)
C       time1,2,3:      times corresponding to releases for each type of
C                       container failure
C       nr:             number of zones for diffusion cal. (same as imax)
C       dr:             delta x
C       ci1000(chain,member):   1,000 years inventory in curies
c       simtimex:       maximum simulation time [y]
C       imax:           nodes in x (or r) direction
C       jmax:           nodes in y (or theta) direction
C       xco:            x (or r) coordinates
C       yco:            y (or theta) coordinates
C       nzones:         number of material zones
C       izone(i,j):     zone number of node (i,j)
C       ppor:           porosity at nodes outside the wp
```

```
C       ntflo:          num of entries in flow table
C       rpor:           porosity:: three layers damaged, disturbed, host rock
C       flow:           cell wise flow loading
C       tflo:           time of table entry i for floref
C       floref:         reference flow at tflo
C       ntemp:          num of entries in time versus temp table
C       ttemp(time):    times in table at which temperatures are given
C       tcan(time):     wp surface temp at above times
C       ctemp           crit. temp.[C] for the onset of liquid flow  around wp
C       dcoefm:         molecular diffusion coefficient in rock and packing
C       fuewt:          formula wt for spent fuel
C       fueden:         fuel density
C       fuedif:         fuel diffusion coefficient
C       amassc:         initial mass of uranium oxide fuel, kg
C       sc14:           c14 release rate [ci/kg SF]
C       sumc14:         cumulative c-14 release from the cell as a function of time [ci]
C       rhouz:          density of uo2 kg mole/m^3
C       oxz:            number of moles of uo2 oxidized/mole o (not o2)
C       rOz:            radius of SF particle [m]
c       radu:           initial radius of uo2 grain [m]
C       radsg:          subgrain radius after transgranular fracture [m]
C       thclad:         thickness of cladding, m
C       cfuel:          ci c14 / kg of fuel in fuel
C       czmetal:        ci c14 / kg of fuel in zirconium cladding
C       czoxide:        ci c14/kg of fuel in initial zirconium oxide and crud
C       cgap:           ci of c14 / kg of fuel in grain boundary and gap
C       gscmrl:         gaseous cumulative release
C       lxaust:         flag indicating c14 inventory is exhausted.
C       iscon:          scenario container numbers by cell
c       nremain:        remaining waste packages after initially defective ones
C       idefco:         defective container numbers
C       sftime:         scenario container failure time
C       cftime:         corrosion failure time [y]
C       maxchn:         max number of decay chains
C       maxele:         max number of elements (radionuclides)
C       maxnuc:         max number of isotopes
C       maxmem:         max number of enteries in table: age, prob of failure
C       maxste:         max number of time steps
C       maxtim:         max (time-data set) values
C       maxbin:         max number of c14 bins
C-----------------------------------------------------------------------
c       Notes:

C       -> defective container time is zero

C       -> formula for convertng from curies -> atoms is as follows:
c              activity(bq) == lamda x N,
c              where, lamda == log(2.0)/halflife (sec);
c             1 ci == 3.7e10 bq
C             3.7e10*365*24*3600/alog(2.0) == 1.6834e18
c             xnoloss(k,i) == atoms(k,i)/(halflife(k,i)*1.6834E18)
C
c       -> waste dissolution and transport three types:initial defective
C          containers (1), failures by scenario(2), and corrosion/buckling
C          failures(3). liqrel called 3 times
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
C+++++++++++++++++++++++++ open output files ++++++++++++++++++++++++++++
```

```
C  files:
c        input:  release4.inp
C        output: inv1000.out, relcum.out, relfrac.out, maxrel.dat,
C                ebs14.dat, treleasel.out,ebsnef.dat, maxc14.dat
C        output file numbers;
C                nunit(1) = unit 5        nunit(2) = unit 6
C                nunit(3) = unit 10      nunit(4) = unit 11
C                nunit(5) = unit 12       nunit(6) = unit 13
C                nunit(7) = unit 14       nunit(8) = unit 16
c                nunit(9) = unit 17

c       cumc14.out:     cum. release of c14 with time
c       ratec14.out:    time history of c14 release with time
c       release.out:    cum. liquid rel. for all r.n. w/ time
c       maxrel.dat:     maximum fractional release
c       inv1000.out:    no loss inventory of r.n. at 1000 yr
c       treleasel.out:  same as ebsnef.dat, but has cumulative releases
c                       in stead of release rates
c       relcum.out:     cumulative release and cumulative release fraction
c       relfrac.out:    normalized release for ebs release standards
C-----------------------------------------------------------------------
c top18 requirements
        write(*,*) 'EBSPAC (Engineering Barrier System Performance Assessment Code)'
        write(*,*) 'This is the release part of the EBSPAC code'
        write(*,*) fdate()

        call opnfil(20, 'ebsnef.dat', 'replace', .true., errnum, errmsg)
        if ( errnum.ne.0 ) stop ' opening ebsnef.dat '
        open (1, file='echo_release.out', status='unknown')
        open (21, file='cumc14.out', status='unknown')
        open (22, file='ratec14.out', status='unknown')
        open (23, file='inv1000.out', status='unknown')
        open (25, file='relcum.out', status='unknown')
        open (24, file='relfrac.out', status='unknown')
        open (26, file='treleasel.out', status='unknown')
        open (28, file='release.out', status='unknown')
        open (29, file='dignostic.out', status='unknown')
        open (40, file='maxrel.dat', status='unknown')

C++++++++++++++++++   initialize  and prepare input ++++++++++++++++++


        vsmall = 1.E-20
        pi = 4.*atan(1.)
        timeyr = 'time(yr)'

        call init
        call input

c       assign diffusion coefficients to grid nodes from zone data

        do 100 i = 1, nr
          dcoefm(i) = diff(izone(i,1))
          ppor(i) = rpor(izone(i,1))
cssss      print*,'dcoefm(i',')=',dcoefm(i)
  100   continue

c       calculate volume of maximum sustainable liquid in the wp
C
```

```
        do 200 icoun = 1, maxste
          do 150 ichns = 1, nchns
            do 120 iiso = 1, ni(ichns)
              sumre1(ichns, iiso, icoun) = 0.
              sumre2(ichns, iiso, icoun) = 0.
              sumre3(ichns, iiso, icoun) = 0.
              rlrate1(ichns, iiso, icoun) = 0.
              rlrate2(ichns, iiso, icoun) = 0.
              rlrate3(ichns, iiso, icoun) = 0.
              amwp1(ichns, iiso, icoun) = 0.
              amwp2(ichns, iiso, icoun) = 0.
              amwp3(ichns, iiso, icoun) = 0.
  120       continue
  150     continue
  200   continue

C++++++++++++++++++++++++++   radionuclide input data  ++++++++++++++++++++++++++++

        write (1, *)
        write (1, *) 'data echo: initial inventory of all nuclides'
        write (1, *)

        do 300 k = 1, nchns
          do 250 i = 1, ni(k)
            write (1, *) k, i, namall(k, i), curall(k, i), '[ci/wp]'
  250     continue
          write (1, *)
  300   continue

C       time for onset of condensation

        do 400 i = 2, ntemp
          temp1 = tcan(i - 1)
          temp2 = tcan(i)
cssss           IF ( temp2.LT.temp1 .AND. temp1.LE.ctemp) GO TO 500
          if ( temp2.le.temp1 .and. temp1.le.ctemp ) go to 500
  400   continue

  500   continue
        tcaqu = ttemp(i - 1)

        write (1, *) 'time to reach below boiling point [yr]=', tcaqu

C+++++++++++++++++ container failure of each type +++++++++++++++++

        idefco = int(mtot*deffrac + 0.005)
        write (1, *) 'mtot,idefco:', mtot, idefco

        nremain = mtot - idefco

        if ( iscon.gt.nremain ) then
          print *, '!!!Warning:-bad numbers for scenario failure'
          print *, 'make sure tpa code has right logic'
          print *, 'program forced to stop'
          stop
        end if

        if ( cftime.lt.sftime ) then
          icfcon = nremain
```

```
          iscon = 0
        else
          icfcon = nremain - iscon
        end if

C-->    loop over failure types: 1-defective, 2-scenario, 3-corrosion
C       modify this later so that in the future, all runs can be done
C       in one lapse.

        ntype1 = 0
        ntype2 = 0
        ntype3 = 0

        do 600 itime = 1, ntemp
          sumc14(itime) = 0.
          c14rate(itime) = 0.
  600   continue

        do 800 itype = 1, 3

          if ( itype.eq.1 ) then
            tfail = 0.
            numwp = idefco
          end if

          if ( itype.eq.2 ) then
            tfail = sftime
            numwp = iscon
          end if

          if ( itype.eq.3 ) then
cssss             tfail=min(simtimex, cftime)
            tfail = cftime
            numwp = icfcon
          end if
          write (*, *)
          write (*, *)
          write (*, 9007)
          write (*, '(a42,i10)') 'failure type:', itype
          write (*, '(a42,i10)') 'number of failed wp:', numwp
          write (*, '(a42,f12.0)') 'wp failure time [yr]:', tfail

C+++++++++++++++++++ inside the waste package ++++++++++++++++++++

          amass0 = amassc
          tcool = tcaqu
          write (*,'(a42,f12.0)') 'onset of flow [yr]:', tcaqu
          if (itype.eq.2.and.numwp.eq.0) then
            write(*,*)
            write(*,*) 'no release due to scenario failure ',
     &          'because it occurred after corrosion failure'
            write(*,*)
          endif
          waterht = wetfrac*dintl
          rintl = dintl/2.
          voidfrac = xvol/(pi*rintl**2*xlintl)
          if ( voidfrac.gt.1. ) then
            print *, 'voidfrac=', voidfrac
            print *, '!!!!!!program forcibly stopped for wrong data!'
            stop
```

```
          end if
          xxx = (rintl - waterht)/rintl
          vabs = rintl**2*xlintl*acos(xxx)
          xfrac = vabs/(pi*rintl**2*xlintl)
          vmax = vabs*voidfrac
          write (1, *) 'rintl,waterht=', rintl, waterht
          write (1, *) 'xlintl,xxx=', xlintl, xxx
          write (1, *) 'xfrac,vmax=', xfrac, vmax

          do 650 itime = 1, ntemp
            sc14(itime) = 0.
  650     continue
          if ( numwp.gt.0 ) then

C+++++++++++++++++++++ calculate gas releases +++++++++++++++++++++++++

            sum1 = 0.0
            iflaguo24 = 0
            call gasrel(rhouz, r0z, radu, radsg, tfail, thclad, tcan,
     &                  ttemp, cfuel, czmetal, czoxide, cgap, sc14,
     &                  cumrfuel, cumrzirc, maxtim, oxwidth)

C-->        multiply results (amassc[kg/wp] x numwp) prior to output

            do 660 itime = 2, ntemp

c12/13/96       brought the next if statement from outside to inside
c                of the do loop
C-->        mass balance check for gas releases

            if ( ttemp(itime).gt.tcaqu ) then
              dryfrac = 1. - xfrac
            else
              dryfrac = 1.
            end if

               write(1,*), 'ttemp,sc14,dryfrac=',ttemp(itime),
     &                  sc14(itime),dryfrac
c12/13/96       modified by the multiplying dactor dry frac
              c14rate(itime) = c14rate(itime) +
     &                  sc14(itime)*numwp*amassc*dryfrac
  660       continue
cdbg                  print*, 'numwp,amassc',numwp,amassc

            totalc14 = (cfuel + czmetal + czoxide + cgap)
     &                *(idefco + iscon + icfcon)*amassc
            write (1, *)
            write (1, *) 'cfuel, czmetal, czoxide, cgap', cfuel,
     &                   czmetal, czoxide, cgap
            write (1, *) '%%% initial c14 inventory [ci]=', totalc14
            write (1, *) 'normalized cumulative gaseous releases'
            write (1, *) 'cumrfuel,cumrzirc = ', cumrfuel, cumrzirc

c           gaseous c14 goes only to gas module and not neftran

C++++++++++++++++++ calculate liquid release ++++++++++++++++++++++++

c       spherical-equivalent radius of the wp and drift of wp length

            r0 = 0.5*(0.5*wpdia**2 + wpdia*wplen)**0.5
```

```
            rdrift = 0.5*(0.5*driftdia**2+driftdia*wplen)**0.5
            dist = r0
            do 680 i = 1, nr
              dist = dist + dr(i)
              if ( dist.gt.rdrift ) then
                dist = dist - dr(i)/2.
                marker = i
                go to 700
              end if
  680       continue
  700       continue
            qin = flow*flowfactr*funnel

            write (1, *)
            write (1, *) 'tfail,tcool, numwp = ', tfail, tcool, numwp
            write (1, *) 'qin,xfrac, vmax = ', qin, xfrac, vmax
            write (1, *) 'amass0 = ', amass0
            write (1, *) 'liquid phase release'
            write (1, *) 'release (ci), release/initial inventory '
            write (1, *)

            call liqrel(xfrac, xvol, dt, tcool, r0, dist, amass0, vmax,
     &                  tfail, qin, itype, simtimex, tavg)
          end if
          if ( itype.eq.1 ) ntype1 = numwp
          if ( itype.eq.2 ) ntype2 = numwp
          if ( itype.eq.3 ) ntype3 = numwp

  800   continue

c+++++++++++++++approximate mass balance check-up++++++++++++++++++++

c        calculate inventory at simtimex

        write (1, *) 'no-loss inventory at [y]=', simtimex

        do itemp = 1, ntemp
           do 900 k = 1, nchns
             do 850 i = 1, ni(k)
c             curies to atoms
              atall(k, i) = curall(k, i)*(halflife(k,i)*1.6834E18)
              alam(k, i) = alog(2.0)/halflife(k, i)
  850        continue
  900      continue

           call decay(ttemp(itemp), atall, atoms, alam)

c          total no-loss cell inventory at max. time
           do 1000 k = 1, nchns
             do 950 i = 1, ni(k)
c-->           convert atoms to curies
               xnoloss(k, i) = atoms(k, i)/(halflife(k,i)*1.6834E18)
               xnoloss(k, i)=xnoloss(k, i)*(ntype1+ntype2+ntype3)*xfrac
               if(k.eq.5.and.i.eq.4) xnolosst(itemp)=xnoloss(k,i)
  950        continue
 1000      continue
        enddo

c-->    cumulative mass released
```

```
      do 1100 itemp = 2, ntemp

        do 1050 k = 1, nchns
          do 1020 i = 1, ni(k)
            xmass(k, i, itemp) = sumre1(k, i, itemp)
     &        *ntype1 + sumre2(k, i, itemp)
     &        *ntype2 + sumre3(k, i, itemp)*ntype3
            rlmass(k, i, itemp) = rlrate1(k, i, itemp)
     &        *ntype1 + rlrate2(k, i, itemp)
     &        *ntype2 + rlrate3(k, i, itemp)*ntype3
            amwp(k, i, itemp) = amwp1(k, i, itemp)
     &        *ntype1 + amwp2(k, i, itemp)*ntype2 + amwp3(k, i, itemp)
     &        *ntype3

c-->        convert from kg/cell to ci/cell

            xmass(k, i, itemp) = xmass(k, i, itemp)
     &        *3.576095996E8/halflife(k, i)/amall(k, i)
            rlmass(k, i, itemp) = rlmass(k, i, itemp)
     &        *3.576095996E8/halflife(k, i)/amall(k, i)
            amwp(k, i, itemp) = amwp(k, i, itemp)
     &        *3.576095996E8/halflife(k, i)/amall(k, i)
            if(k.eq.5 .and. i.eq.4) write(29,9009) ttemp(itemp),
     &        xnolosst(itemp),amwp(k,i,itemp),xmass(k,i,itemp)
 1020     continue
 1050   continue

 1100 continue

      write (25, 9001)
      write (*, *)
      write (*, 9008)
      write (*, 9001) simtimex
      write (*, 9007)
      write (*, 9006)
      write (*, 9008)
      do 1200 k = 1, nchns
        do 1150 i = 1, ni(k)
          pleft = (xnoloss(k,i)-xmass(k,i,ntemp))/xnoloss(k,i)
          write (*, 9002) namall(k, i), halflife(k, i), xnoloss(k, i),
     &                    amwp(k, i, ntemp), xmass(k, i, ntemp),pleft
          write (25, *) namall(k, i), xmass(k, i, ntemp),pleft
 1150   continue
 1200 continue
      write (*, 9008)

      write (26, *) 'cumulative release with time [ci/cell]'
      do 1300 k = 1, nchns
        do 1250 i = 1, ni(k)
          write (26, *) namall(k, i)
          do 1220 itemp = 2, ntemp
            write (26, *) ttemp(itemp), xmass(k, i, itemp)
 1220     continue
 1250   continue
 1300 continue

      write (1, *) 'ntype1+ntype2+ntype3=', ntype1 + ntype2 + ntype3

c     cumulative gas release
```

```
        sum = 0.0
        do 1400 itime = 2, ntemp
          dtt1 = ttemp(itime) - ttemp(itime - 1)
          sum = sum + c14rate(itime)*dtt1
cssss           sum= c14rate(itime)*dtt1
          sumc14(itime) = sum
 1400   continue

cccc    stop

C+++++++++++++++++  equal interval outputs of releases ++++++++++++++++++++

C   count number of isotopes for the ebsnef.dat file

        numiso = 0
        do 1500 k = 1, nchns
          do 1450 i = 1, ni(k)
            numiso = numiso + 1
 1450     continue
 1500   continue

        xtsize = simtimex/nbt

        do 1600 k = 1, nchns
          do 1550 i = 1, ni(k)
            cumrel = 0.
            relrate = 0.

            do 1540 itim = 1, nbt
              watrel = 0.0
              thetim = itim*xtsize
              tregular(itim) = thetim
              do 1510 itemp = 2, ntemp
                if ( ttemp(itemp).ge.thetim ) then
                  xlint(1) = ttemp(itemp - 1)
                  xlint(2) = ttemp(itemp)
                  ylint(1) = rlmass(k, i, itemp - 1)
                  ylint(2) = rlmass(k, i, itemp)
                  call lint(xlint, ylint, 2, 2, thetim, relrate)
                  zlint(1) = xmass(k, i, itemp - 1)
                  zlint(2) = xmass(k, i, itemp)
                  call lint(xlint, zlint, 2, 2, thetim, cumrel)
                  go to 1520
                end if
 1510         continue

 1520         continue
              fracre(k, i, itim) = relrate
              cumrelease(k, i, itim) = cumrel

 1540       continue
 1550     continue
 1600   continue

c-->    write cumulative release output for graphics plots

        write (28, 9004) timeyr, ((namall(k,i),i=1,ni(k)), k=1, nchns)
        do 1700 itim = 1, nbt
          write (28, 9005) tregular(itim),
     &                     ((cumrelease(k,i,itim),i=1,ni(k)), k=1,
```

```
     &                    nchns)
 1700   continue

        write (20, '(a)') 'release rates from ebspac'
        write (20, '(2i11,2x,a)') numiso, nbt, 'num nucs, ntemp'

        do 1800 k = 1, nchns
          do 1750 i = 1, ni(k)
C          loop over time steps
            tmpnam = namall(k, i)
 1720       continue
            if ( tmpnam(1:1).eq.' ' ) then
              tmpnam = tmpnam(2:)
              go to 1720
            end if

            write (20, '(a6)') tmpnam

            do 1740 itim = 1, nbt
              write (20, 9003) tregular(itim), fracre(k, i, itim)
 1740       continue
 1750     continue
 1800   continue

C+++++++++++++++++ maximum fractional release with time ++++++++++++++++++++

        call decay(1000.D0, atall, atoms, alam)
        write (23, *) 'k,i,1000 yr inventory, ini. inv./cell'
        do 1900 k = 1, nchns
          do 1850 i = 1, ni(k)
            ci1000(k, i) = atoms(k, i)/(halflife(k,i)*1.6834E18)
            ci1000(k, i) = ci1000(k, i)*mtot
            write (23, *) k, i, namall(k, i), ci1000(k, i), curall(k, i)
 1850     continue
 1900   continue

c-->    find fractional releases

C-->    find maximum fractional release for all nuclides

        do 2000 k = 1, nchns
          do 1950 i = 1, ni(k)
            maxrel(k, i) = 0.0
            timrel(k, i) = 0.0
            do 1920 itim = 1, nbt
              xlarge = fracre(k, i, itim)/ci1000(k, i)
              if ( xlarge.gt.maxrel(k,i) ) then
                maxrel(k, i) = xlarge
                timrel(k, i) = tregular(itim)
              end if
 1920       continue
 1950     continue
 2000   continue

C-->    find maximum fractional release of c14
        kc14 = 0
        ic14 = 0
        do 2100 k = 1, nchns
          do 2050 i = 1, ni(k)
            if ( namall(k,i).eq.'  C14 ' ) then
```

```
              kc14 = k
              ic14 = i
cssss              c14inv=ci1000(k,i)
cssss              IF (c14inv.le.vsmall) c14inv = vsmall
              go to 2200
            end if
 2050     continue
 2100   continue

 2200   continue
        xtemporary = atall(kc14, ic14)
        gwtotalc14 = curall(kc14, ic14)*mtot + totalc14
        write(*,'(a50,f12.1)')
     &         'zeroth yr inventory for liquid releases:',
     &         curall(kc14,ic14)*mtot
        write(*,'(a50,f12.1)')
     &         'zeroth yr inventory for gaseous releases:',totalc14
        if ( kc14.ne.0 .and. ic14.ne.0 ) then
          atall(kc14, ic14) = gwtotalc14*halflife(kc14, ic14)*1.6834E18
          call decay(1000.D0, atall, atoms, alam)
          c14inv = atoms(kc14, ic14)/(halflife(kc14,ic14)*1.6834E18)
          if ( c14inv.le.vsmall ) c14inv = vsmall
        write(*,'(a50,f12.1)')
     &         '1000-yr c14 inv. for liq. rel [ci/cell:',
     &         ci1000(kc14,ic14)
        write(*,'(a50,f12.1)')
     &         '1000-yr c14 inv. for gaseous rel. [ci/cell]:',
     &         c14inv-ci1000(kc14,ic14)
        end if
        atall(kc14, ic14) = xtemporary

        rmaxc14 = 0.0
        tmaxc14 = 0.0
        write (21, *) 'time [yr]    cumulative c14 release [ci]'
        write (22, *) 'time [yr]    c14 release rate [ci]'
        do 2300 itime = 1, ntemp
          write (21, *) ttemp(itime), sumc14(itime)
          write (22, *) ttemp(itime), c14rate(itime)
          xlarge = c14rate(itime)/c14inv
          if ( xlarge.gt.rmaxc14 ) then
            rmaxc14 = xlarge
            tmaxc14 = ttemp(itime)
          end if
 2300   continue

C-->    write maximum fractional releases to file maxc14.dat

        write (40, *) 'title: maximum fractional release of c14'
        write (40, *) 'tmaxc14 [yr]     rmaxc14 [fraction]'
        write (40, *) tmaxc14, rmaxc14
        write (40, *)
        write (40, *)

        write (40, *) 'maximum fractional release of all nuclides'
        write (40, *) ' name      timrel (year)    maxrel (fraction)'

        do 2400 k = 1, nchns
          do 2350 i = 1, ni(k)
            if ( k.eq.kc14 .and. i.eq.ic14 ) maxrel(k, i) = maxrel(k, i)
     &           *ci1000(k, i)/c14inv
```

```
            write (40, *) namall(k, i), t[illegible]el(k, i), maxrel(k, i)
 2350     continue
 2400   continue

        print *,
     &  'output files: release.out, ebsnef.dat, relcum.out, relfrac.out'
     &  , 'maxrel.dat, ebs14.dat, maxc14.dat, ratec14.out, inv1000.out'

        stop
 9001   format (15x, 'cumulative release [ci/cell] by'f10.1, ' years')
 9002   format (5x, a8, 4(4x,e10.3),2x,f8.2)

 9003   format (1x, f15.7, 1x, e15.7)

 9004   format (a8, 50(a6,1x))
 9005   format (1P50(e10.3,1x))
 9006   format (6x, 'namall', 4x, 'halflife(yr)', 4x, 'xnoloss(ci)', 4x,
     &          'amwp(ci)', 4x, 'xmass(ci)',2x,'fracleft')

 9007   format (80('-'))
 9008   format (80('='))
9009    format(4(2x,e10.3))
        end
**==LIQREL.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine liqrel(xfrac, xvol, dtt, tcool, r0, dist, amass0,
     &                    vtmp, tfail, qin, itype, tend, tavg)
C-----------------------------------------------------------------------
C       liquid source-term model
C-----------------------------------------------------------------------
        implicit none
cssss      IMPLICIT NONE
C*** Start of declarations inserted by SPAG
        real xvol
        real amass, amass0, amassl, ccfr, ci1000, con3, con4, cstore,
     &       derivs, dcoefm, dr, dt, dtinit, dtmax, dtmin, dtt, eps,
     &       xfrac, pi, qin
        real qout, qtmp, r0, crf, drf, rkqc, rr, srate, sumre1, sumre2,
     &       sumre3, rlrate1, rlrate2, rlrate3, t, tcan, tavg, tcool,
     &       tend, tfail, tftc, time, time1
        real amwp1, amwp2, amwp3
        real tiny, tleach, tlt, tmass0, tmp, trid, tstart, tstop, ttemp,
     &       vmax, vmin, volw, vtmp, wleach, ws, ystart
        integer i, ifailt, itype, j, k, maxele, maxi, maxmem, maxnuc,
     &          maxnxm, maxste, maxtim, nbad, nelem, nok, nr
        integer ntemp, nvar
        integer ncon, kcon, icon, nchns, ni
        real sol, rd, rde, amall, halflife, curall, fggap
        real r0z, rhouz, radu, radsg
cssss      REAL*8 alam, atoms, atall, am
        real alam, atoms, atall, am
        real fuewt, fueden, fuedif, fuepor, amassc
        real sareap, sareat, uo2rate
        real sum
        integer kmax, kount
```

```
      integer it
      integer iflaga
      real dydx
      real dxsav, xp, yp
      real timintv, addtime
      integer idisplay
      real oxwidth
      real ppor
      real dist, marker
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
      parameter (maxele=50, maxmem=10, maxnuc=50)
      parameter (maxnxm=maxnuc*maxmem)
      parameter (maxste=300, maxtim=500)
      parameter (maxi=20)

      real dissipxx, rdpxx, adflux(maxnuc, maxmem),
     &     diffusion1(maxnuc, maxmem), diffusion2(maxnuc, maxmem)
      dimension dydx(200)
      dimension ystart(200)
      common /cther1/ ttemp(maxtim), tcan(maxtim)
      common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc
      common /cther0/ ntemp
      common /rcarbon1/ r0z, rhouz, radu, radsg
      common /path  / kmax, kount, dxsav, xp(200), yp(100, 200)
      common /damvalues/ rdpxx, dissipxx, adflux, diffusion1,
     &                   diffusion2
      common /rkutta/ eps, tiny, dtinit, dtmin, dtmax
      common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
     &                amall(maxnuc, maxmem), halflife(maxnuc, maxmem),
     &                curall(maxnuc, maxmem), fggap(maxnuc, maxmem),
     &                kcon(maxele, maxnuc), icon(maxele, maxnuc),
     &                rd(maxnuc, maxmem), ni(maxnuc), nchns,
     &                ci1000(maxnuc, maxmem)
      common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                ccfr(maxnuc, maxmem), tleach, nelem,
     &                amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                amassl(maxnuc), tlt, tftc
      common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi, 4),
     &                rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                ppor(maxi)
      common /array1/ sumre1(maxnuc, maxmem, maxste),
     &                sumre2(maxnuc, maxmem, maxste),
     &                sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                rlrate1(maxnuc, maxmem, maxste),
     &                rlrate2(maxnuc, maxmem, maxste),
     &                rlrate3(maxnuc, maxmem, maxste),
     &                amwp1(maxnuc, maxmem, maxste),
     &                amwp2(maxnuc, maxmem, maxste),
     &                amwp3(maxnuc, maxmem, maxste)

      common /cumu  / crf(maxnuc, maxmem), drf(maxnuc, maxmem)
      common /oxidized/ oxwidth
      common /driftwall/ marker

      external derivs, rkqc
C-----------------------------------------------------------------------

c     Nomenclature:
```

```
C       r0z:            radius of SF particle [m]
C       amass0:         mass of fuel [kg]; amassc assigned to amass0
C       amass(k,i):     solid mass of each radionuclide in fuel matrix [kg]
c       amassl(ielem):  mass of element ielem in water
C       ccfr:           conc. at volw (mass/vol)
C       ci1000:         1,000 years inventory of radionuclides in [ci]
c       con3:           coefficient for diffusion calculation
C       cstore:         concentration in cell, gm/l
c       derivs:         name of derivative subroutine for mass balance in wp
C       dcoefm:         mol. diffusion coeficient of packing & rock [m^2/yr]
C       dr:             delta x
C       dt:             timestep, years
c       dtinit:         initial time step used in the R-K algorithm
c       dtmax:          maximum allowed timestep
c       dtmin:          minimum allowed timestep
c       dtt:            time intervals (in the data from external temp module)
C       eps:            integration accuracy for runge kutta integration
C       xfrac:          fraction of fuel exposed
c       pi:             the constant pi
C       qin:            inflow of water to canister, m^3/yr
C       qout:           flow rate out of wp [l/y]
c       qtmp:           maximum of qin and a very small flow rate
C       r0:             effective spherical radius of canister
C       drf:            rate of release, gram moles per year
c       crf:            cumulative release at a given time [yr]
c       rkqc:           name of a subroutine
C       srate:          spent fuel matrix dissolution rate [kg/m2/yr]
c       sumre1:         crf for itype = 1
c       sumre2:         crf for itype = 2
c       sumre3:         crf for itype = 3
c       rlrate1:        drf for itype = 1
c       rlrate2:        drf for itype = 2
c       rlrate3:        drf for itype = 3
C       t:              time [yr]
C       tcan(time):     wp surface temperature [C]
c       tavg(time):     drift wall temperature [C]
C       tcool:          time at which wp drops below boiling point
c       tend:           end time for simulation run
C       tfail:          time of wp failure [yr]
c       tftc:           maximum of wp fail time or boiling point
C       time1,2,3:      times corresponding to releases for each type of
C                       container failure
c       tiny:           a small number needed for odeint subroutine
C       tleach:         time span for all u to be converted, years
c       tlt:            absolute time until which leaching takes place
c                       i.e., tleach+tftc
c       tmass0:         remaining mass after leaching at each time step
c                       (initially same as amass0)
c       trid:           array containing coefficients for the tridiagonal matrix
c                       in the diffusion calculation
c       tstart:         beginning time for odeint subroutine
c       tstop:          end time for odeint subroutine
C       ttemp(time):    times in table at which temperatures are given
c       vmin:           initially volw=vmin
C       vmax:           maximum water volume in wp before it overflows, liters
C       vtmp:           maximum water volume in canister, m^3
c       wleach:         rate of radionuclide release (congruent dissolotion)
c       ystart:         array containing all dependent variables for odeint
c       ifailt:         a flag indicating quick release  of gap inventory
```

```
C       itype:          1=defective can r=scenario can run,3=normal failure run
c       maxele:         array dimension for maximum number of elements
C       maxi:           max number of x- or r-dir nodes
c       maxmem:         array dimension for maximum number of members in a chain
c       maxnuc:         array dimension for maximum number of nuclides
C       maxste:         max number of time steps
C       maxtim:         max (time-data set) values
c       nbad:           number of bas steps but corrected later in the R-K method
C       nelem:          number of elements
c       nok:            number of steps accepted in the R-K calculations (see odeint)
C       nr:             number of zones for diffusion cal. (same as imax)
C       volw            volume of water in canister, m^3
C       ntemp:          num of entries in time versus temp table
c       nvar:           an index for number of variables being solved in odeint
c       ncon(ielem):    number of chains in which isotopes of element ielem occur
c       kcon(ielem,l):  chain identifier among all chains in which element ielem
c                       occurs; l is the index for all chains with ielem
c       icon(ielem,l):  position of ielem in the chain kcon(ielem,l)
c       nchns:          number of chains
c       ni
c       sol(ielem):     solubility limit of the element ielem
C       rd:             retardation factor for each isotope
c       rde
c       amall:          molecular weight of radionuclides
c       halflife:       half life of radionuclides [yr]
c       curall          radionuclide inventory per WP in curies
c       fggap:          gap fraction of each radionuclide
c       alam:           coefficient of decay for each radionuclide
c       atoms:          number of atoms of radionuclides at time t
c       atall:          number of atoms in the initial inventory curall curies
c       am:             mass of each radionuclide in the wp water at time t
C       fuewt:          formula wt for spent fuel
C       fueden:         fuel density
C       fuedif:         fuel diffusion coefficient
c       fuepor:         porosity in between SF particles
C       amassc:         initial mass of uranium oxide fuel, kg
c       sareap:         total surface area from one SF particle
c       sareat          total internal surface area in the wetted portion of sf
c       uo2rate:        leaching rate of sf matrix radionuclide [kg/yr]

C  note: solubility is in kg/m^3 = mg/l to be input in radionuclide
C        data file
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

        pi = 4.*atan(1.)
        iflaga = 0

Cjw  make sure time constant for water in can is not too fast

        qtmp = max(qin, 1.E-6)
        if ( vtmp/qtmp.lt.5. ) then
          vmax = 5.*qtmp
        else
          vmax = vtmp
cqqqq     print*,'vtmp/qtmp, and vmax=',vtmp/qtmp,vmax
        end if
```

```
        write (1, *) 'above:vmax,vtmp,qtmp', vmax, vtmp, qtmp

C  constant in transient diffusion equation

        con3 = 4*pi*(r0 + dr(1)/2)**2*dcoefm(1)*ppor(1)/dr(1)
        con4 = 4*pi*(dist)**2*dcoefm(marker)*ppor(marker)/dr(marker)

        write (1, *) 'ppor(marker),con3,con4=', ppor(marker), con3, con4

C set up the tridiagonal matrix for diffusive flux calculation

        call setdif(r0)

C calculate uo2 matrix leachng time

        tmass0 = amass0*xfrac
        tftc = amax1(tfail, tcool)

        write (1, *) 'amass0=', amass0
        addtime = 0.0
        timintv = 50.
        do 100 i = 2, ntemp
          time = ttemp(i)
          if ( time.gt.tftc ) then
            tavg = tcan(i)
            addtime = time - tftc
            dtt = ttemp(i) - ttemp(i - 1)
            if ( iflaga.eq.0 ) then
              timintv = dtt
              iflaga = 1
            end if
c       print*,'time,tcool,tftc,timintv,tavg=',
c     &         time,tcool,tftc,timintv,tavg

            call leachrt(tavg, srate)

c-->        waste matrix surface area and leach rate/unit mass UO2

cssss       sareap = 4.*pi*((r0z-oxwidth)**2+(3.*r0z**2*oxwidth-3.
cssss     &                    *r0z*oxwidth**2+oxwidth**3)/radu)

            write (1, *) , 'grain radius [m]         :', radu
            write (1, *) , 'grain oxidation depth [m]:', oxwidth

            sareap = 4.*pi*(radu - oxwidth)
     &              **2 + (3.*radu**2*oxwidth - 3.*radu*oxwidth**2 +
     &              oxwidth**3)/radu**3*(4.*pi*radu**2)

c-->        waste matrix leach rate from total wet mass of UO2/wp

cssss       sareat = (amass0*xfrac) * saream
            sareat = sareap*(amass0*xfrac)/(4./3.*pi*radu**3*fueden)
            uo2rate = srate*sareat
            write (1, *) 'time,amass0,sareat,srate,uo2rate,tmass0'
            write (1, *) time, amass0, sareat, srate, uo2rate, tmass0

            tmass0 = tmass0 - uo2rate*dtt
            if ( tmass0.lt.0. ) then
              if ( time.le.tftc + timintv ) then
                addtime = amass0*xfrac/uo2rate
```

```
            else
              addtime = addtime - abs(tmass0)/uo2rate
            end if
            go to 200
          end if
          write (1, *) 'time,amass0,xfrac,uo2rate,tmass0'
          write (1, *) time, amass0, xfrac, uo2rate, tmass0
        end if
  100   continue

  200   continue
        tleach = addtime
        tlt = tleach + tftc
        write (*, '(a42,f12.0)') 'sf leaching time span [yr]:', tleach
        write (*, '(a42,f12.0)') 'sf leaching onset time [yr]:', tftc
        write (*, '(a42,f12.0)') 'sf leaching will end  at [yr]:', tlt
        write (*, 9001)

        do 300 k = 1, nchns
          do 250 i = 1, ni(k)

C-->       convert curies/wp -> atoms/wp

c          activity(bq)=lamda x N;
C          lamda->alog(2.0)/halflife (sec); 1 ci -> 3.7e10 bq
c          the next line is equivalent to: atall(k, i)=curall(k, i)
c     &     *3.7E10*(365*24*3600*halflife(k,i))/alog(2.0)

           atall(k, i) = curall(k, i)*(halflife(k,i)*1.6834E18)

C-->       calculate decay coefficient [1/yr]

           alam(k, i) = alog(2.0)/halflife(k, i)

  250     continue
  300   continue

C       set minimum value of water in wp to a small value

        if ( vtmp.ne.vmax ) then
          tmp = vtmp/qtmp
          vmin = (5. - tmp)*qtmp
        else
          vmin = 1.e-6
        end if

        volw = vmin

        write (1, *) 'aliqrel-namall,am241i(kg),it,crf,am(kg),volw'

        ifailt = 0

        do 400 k = 1, nchns
          do 350 i = 1, ni(k)
            am(k, i) = 1.E-20
            crf(k, i) = 1.E-20
  350     continue
  400   continue

        write (1, *) 'volw=', volw
```

```
      sum = 0.0
      idisplay = 0

      do 600 it = 2, ntemp

        t = ttemp(it)
        dt = t - ttemp(it - 1)
        tavg = tcan(it - 1)

cssss         tavg=tcan(it)

C       set inventory for quick release at tfail

        if ( t.gt.tfail .and. t.gt.tftc ) then

          if ( ifailt.eq.0 ) then
            ifailt = 1

            call decay(t - dt, atall, atoms, alam)

C               radionuclides in grain+gap [kg]

            do 410 k = 1, nchns
              do 405 i = 1, ni(k)
                am(k, i) = am(k, i) + fggap(k, i)*(atoms(k,i)/6.02E23)
     &                     *amall(k, i)*0.001
  405         continue
  410       continue
            ystart(1) = volw
            j = 1
            do 420 k = 1, nchns
              do 415 i = 1, ni(k)
                j = j + 1
                ystart(j) = am(k, i)
                write (1, *) 'ystart(', j, ')=', ystart(j)
  415         continue
  420       continue

            do 430 k = 1, nchns
              do 425 i = 1, ni(k)
                j = j + 1
                ystart(j) = crf(k, i)
                write (1, *) 'ystart(', j, ')=', ystart(j)
  425         continue
  430       continue
            nvar = j
          end if

C  ode solver from numerical recipes

          tstart = t - dt
          tstop = t
          kmax = 100
          dxsav = (tstop - tstart)/20.

          call odeint(ystart, nvar, tstart, tstop, eps, dtinit, dtmin,
     &                dtmax, nok, nbad, tiny, derivs, rkqc, xfrac,
     &                xvol, tfail, qin, vmax, amass0, r0z, tavg, qout,
     &                dydx, it)
```

```
cssss       if (it.eq.ntemp-31)
            volw = ystart(1)
            j = 1

            do 460 k = 1, nchns
              do 440 i = 1, ni(k)
                j = j + 1
                am(k, i) = ystart(j)
  440         continue
  460       continue
            do 480 k = 1, nchns
              do 470 i = 1, ni(k)
                j = j + 1
                crf(k, i) = ystart(j)
  470         continue
  480       continue

            do 500 k = 1, nchns
              do 490 i = 1, ni(k)
                j = j + 1
                drf(k, i) = dydx(j)
  490         continue
  500       continue

C             limit the flux and concentration to positive

            do 520 k = 1, nchns
              do 510 i = 1, ni(k)

                if ( am(k,i).lt.0.0 ) am(k, i) = 0.0

                if ( crf(k,i).lt.0.0 ) crf(k, i) = 0.0
  510         continue
  520       continue

C           cumulative release of all nuclides [kg/wp]

            do 540 k = 1, nchns
              do 530 i = 1, ni(k)
                if ( itype.eq.1 ) then
                  amwp1(k, i, it) = am(k, i)
                  sumre1(k, i, it) = crf(k, i)
                  rlrate1(k, i, it) = drf(k, i)
                end if
                if ( itype.eq.2 ) then
                  amwp2(k, i, it) = am(k, i)
                  sumre2(k, i, it) = crf(k, i)
                  rlrate2(k, i, it) = drf(k, i)
                end if
                if ( itype.eq.3 ) then
                  amwp3(k, i, it) = am(k, i)
                  sumre3(k, i, it) = crf(k, i)
                  rlrate3(k, i, it) = drf(k, i)
                end if
                if ( k.eq.5 .and. i.eq.4 .and. idisplay.eq.0 ) then
                  write (*, 9002)
                  write (*, 9003)
                  write (*, 9005)
                  write (*, 9002)
```

```
              end if
              if ( k.eq.5 .and. i.eq.4 ) write (*, 9004) t, crf(k, i),
     &             rdpxx, dissipxx, adflux(k, i), diffusion1(k, i),
     &             diffusion2(k, i)
  530       continue
  540     continue
          idisplay = idisplay + 1
          if ( idisplay.gt.21 ) idisplay = 0

          if ( t.gt.tend ) go to 700

        end if

        time1(it) = t

  600   continue

  700   continue
        return
 9001   format (80('-'))
 9002   format (80('.'))

 9003   format (4x,'time', 4x,'cwpwater', 5x, 'rgenerate', 5x, 'rdecay',
     &          6x, 'rconv', 5x, 'rdiff_r0', 4x, 'rdiff_ebs')
 9005   format (5x, '[yr]', 6x, '[kg]', 7x, '[kg/yr]', 5x,
     &          '[kg/yr]', 5x, '[kg/yr]', 5x, '[kg/yr]',
     &          5x, '[kg/yr]')

 9004   format (f10.1, 1P6e12.3)
        end
**==DERIVS.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine derivs(t, y, dydx, xfrac, xvol, tfail, qin, vmax,
     &                    amass0, tavg, qout, dtd, it)
        implicit none
cssss       IMPLICIT NONE
        integer it
        real xvol
C*** Start of declarations inserted by SPAG
        real amass, amass0, amassl, amt1, amt2, ccfr, ccfrd, ci1000,
     &       con1, con3, con4, concn, cstore, dam, dcoefm, difflux1,
     &       difflux2, diffusion1, diffusion2, dr, dt, dtd, dvdt, dydx
        real xfrac, fut, qin, qout, rdp, rf, adflux, rr, srate, sumre1,
     &       sumre2, sumre3, rlrate1, rlrate2, rlrate3, t, tavg, tfail,
     &       tftc, time1, tleach
        real amwp1, amwp2, amwp3
        real tlt, trid, vfull, vmax, vwnow, wleach, ws, wu, y, yyy
        real sareap, sareat, uo2rate
        integer i, ielem, j, jj, k, kountr, l, maxele, maxi, maxmem,
     &          maxnuc, maxnxm, maxste, nelem, nr
        integer ncon, kcon, icon, nchns, ni
        real sol, rd, rde, amall, halflife, curall, fggap
        integer mmi, mmj
        real fracn
        real fuewt, fueden, fuedif, fuepor, amassc
```

```
      real dissip, sum
      real dissipxx, rdpxx
      real rdp2, dissip2
      real oxwidth
      real ppor
      integer iflow
      real pi
      real r0z, rhouz, radu, radsg
cssss    REAL*8 alam, atoms, atall, am
      real alam, atoms, atall, am
      real xxx1,xxx2,xxx3
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
      parameter (maxele=50, maxmem=10, maxnuc=50)
      parameter (maxnxm=maxnuc*maxmem)
      parameter (maxste=300)
      parameter (maxi=20)

      dimension y(200), dydx(200)
      dimension diffusion1(maxnuc, maxmem), diffusion2(maxnuc, maxmem)
      dimension amt1(maxnuc, maxmem), dam(maxnuc, maxmem),
     &          amt2(maxnuc, maxmem), adflux(maxnuc, maxmem),
     &          rf(maxnuc, maxmem)

c     COMMON /parameters2/ rf
      common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc
      common /damvalues/ rdpxx, dissipxx, adflux, diffusion1,
     &                   diffusion2
      common /rcarbon1/ r0z, rhouz, radu, radsg
      common /oxidized/ oxwidth

      common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
     &                amall(maxnuc, maxmem), halflife(maxnuc, maxmem),
     &                curall(maxnuc, maxmem), fggap(maxnuc, maxmem),
     &                kcon(maxele, maxnuc), icon(maxele, maxnuc),
     &                rd(maxnuc, maxmem), ni(maxnuc), nchns,
     &                ci1000(maxnuc, maxmem)
      common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                ccfr(maxnuc, maxmem), tleach, nelem,
     &                amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                amassl(maxnuc), tlt, tftc
      common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi, 4),
     &                rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                ppor(maxi)
      common /array1/ sumre1(maxnuc, maxmem, maxste),
     &                sumre2(maxnuc, maxmem, maxste),
     &                sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                rlrate1(maxnuc, maxmem, maxste),
     &                rlrate2(maxnuc, maxmem, maxste),
     &                rlrate3(maxnuc, maxmem, maxste),
     &                amwp1(maxnuc, maxmem, maxste),
     &                amwp2(maxnuc, maxmem, maxste),
     &                amwp3(maxnuc, maxmem, maxste)

      data fut/1.0/
C-----------------------------------------------------------------------

c     Nomenclature:
```

```
c       vwnow:          volume of water in the wp at time t (same as y(1))
C       vmax:           maximum water volume in wp before overflow [l]
C       qout:           flow rate out of wp [l/y]
C       con1:           weir coefficent used for wp water overflow model
C       qin:            inflow of water to canister, [l/y]
c       dvdt:           time rate of change of water in the wp
c       dydx:           array containing derivatives for all equn. used in odeint
c       nchns:          number of chains
c       amt1:           amount of each r.n. in the wp water at time t
c       ni(nchns):      elements in the chain
C       nelem:          element of the chain (ni(ichns) assigned)
c       amt2:           amount of each r.n. outside the wp at time t(for mass balance)
c       tlt:            absolute time until which leaching takes place (tleach+tftc)
c       wu:             a multiplier for keeping leaching zero before time tlt
c       t:              time [yr]
c       atall:          inventory of radionuclides [atoms];
c                       obtained by converting curall(k,i) in ci
c       atoms:          number of atoms of radionuclides at time t
c       alam:           coefficient of decay for each radionuclide
c       srate:          the rate of dissolution of the uo2 matrix
C       amass(k, i):    solid mass of each radionuclide in fuel matrix [kg]
c       fggap:          gap fraction of each radionuclide
c       amall:          molecular weight of radionuclides
c       fut:            correction factor for present mass of fuel still left
C                       unconverted - presently, assume that mass or area of
C                       fuel doesn't change
C       fueden:         fuel density
c       fuepor:         porosity in between SF particles
c       sareap:         specific internal surface area per unit bulk vol. of sf
c       sareat:         total internal surface area in the wetted portion of sf
c       uo2rate:        leaching rate of sf matrix radionuclide [kg/yr]
c       wleach:         leaching rate of radionuclide congruent w/ sf leaching
C       amass0:         mass of fuel [kg]; amassc assigned to amass0
c       ncon(ielem):
c       amassl(ielem):  mass of element ielem in water
c       concn:          conc. given element in the wp water at a specified time
c       sol():          solubility limit of an element (input data)
c       kcon(ielem,l):  chain identifier among all chains in which element ielem
c                       occurs; l is the index for all chains with ielem
c       icon(ielem,l):  position of ielem in the chain kcon(ielem,l)
c       fracn:          elemental fraction of radionuclide in the wp water (mass/mass)
c       ccfr:           radionuclide conc. in the wp water at a specified time
c       vfull:          volume of water in the wp just before water overflows
C       ccfrd:          conc. scaled to vfull[m3]
c       dtd:            time interval [yr]
c       diffflux:       mass rate of r.n. production due to diffusive flux out
c       diffusion:      diffflux values stored in the array diffusion
c       rdp:            mass rate of production of r.n. from parent in the wp water
c       adflux(k,ii):   mass rate of r.n. release due to advective flux out of wp
c       dissip:         decay loss rate of the radionuclide from the wp water
c       dam(k,i):       rate of change of mass in wp water
c       rdp2:           mass rate of production of r.n. from parent outside
c                       the wp (for mass balance calculation)
c       rf(k,i):        total outflux from the wp with time
c       iflow:          a flag indicating whether water from the wp is overflowing

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
```

```
      pi = 4.*atan(1.)
C-->  use weir coefficent con1 in overflow model to smoothly
C     converge volume to steady state

csss  print*, 'xvol=',xvol
      vwnow = y(1)
      if ( vwnow.le.vmax ) then
        qout = 0.0
        iflow = 0
      else
        iflow = 1
        con1 = 0.8
        yyy = (vwnow/vmax)**2
        qout = qin*con1*yyy
      end if

      dvdt = qin - qout
      dydx(1) = dvdt

      j = 1
      do 100 k = 1, nchns
        do 50 i = 1, ni(k)
          j = j + 1
          amt1(k, i) = y(j)
 50     continue
100   continue

      do 200 k = 1, nchns
        do 150 i = 1, ni(k)
          j = j + 1
          amt2(k, i) = y(j)
150     continue
200   continue

c     print*, 'amt1(5,4)=',amt1(5,4)
C-->  calculate mass transfer from fuel to water

C     leaching period multiplier

      if ( t.lt.tlt ) then
        wu = 1.0
      else
        wu = 0.0
      end if

C     rate of release of contained radionuclides

      call decay(t, atall, atoms, alam)

C     congruent UO2 leach rate

      call leachrt(tavg, srate)

cssss
c        print*,'fueden,fuepor,rOz,amassO=',
c    &                fueden,fuepor,rOz,amassO

      do 300 k = 1, nchns
        do 250 i = 1, ni(k)
```

```
C          solid mass of each radionuclide in fuel matrix [kg]

            amass(k, i) = (1. - fggap(k,i))*(atoms(k,i)/6.02E23)
     &                   *amall(k, i)*0.001

c-->        waste matrix surface area and leach rate/unit mass UO2

cssss       sareap = 4.*pi*((rOz-oxwidth)**2+(3.*rOz**2*oxwidth-3.
cssss     &                   *rOz*oxwidth**2+oxwidth**3)/radu)
            sareap = 4.*pi*(radu - oxwidth)
     &              **2 + (3.*radu**2*oxwidth - 3.*radu*oxwidth**2 +
     &              oxwidth**3)/radu**3*(4.*pi*radu**2)

c-->        waste matrix leach rate from total wet mass UO2/wp

cssss       sareat = (amass0*xfrac)*sareap/(4./3.*pi*rOz**3*fueden)
            sareat = sareap*(amass0*xfrac)/(4./3.*pi*radu**3*fueden)
            uo2rate = srate*sareat

C          leach rate of daughter i of chain k [kg/y]

C          in this version, wu is only a 1 and 0 switch.

c          congruent release implementation

            wleach(k, i) = (amass(k,i)/amass0)*uo2rate*wu*fut
c           if(k.eq.5.and.i.eq.4) then
c            print*, 'amass,amass0,wleach',amass(k,i),amass0,wleach(k,i)
c           endif

  250     continue
  300   continue

C-->    collect all radionuclides by element in wp water

C-->    mass of element ielem in the wp water

        do 400 ielem = 1, nelem
          sum = 0.0
          do 350 l = 1, ncon(ielem)
            mmi = kcon(ielem, l)
            mmj = icon(ielem, l)
            sum = sum + amt1(mmi, mmj)
  350     continue
          amassl(ielem) = sum
  400   continue

C-->    fraction of nuclide w.r.to its element

        do 500 ielem = 1, nelem
cssss         IF ( vwnow.GT.0. ) THEN
          if ( vwnow.ge.1.E-20 ) then
            concn = amassl(ielem)/vwnow
            if ( concn.gt.sol(ielem) ) concn = sol(ielem)
          else
            concn = 0.0
          end if

C-->     mass of radionuclide per unit volume  of wp water
```

```
          do 450 l = 1, ncon(ielem)
            mmi = kcon(ielem, l)
            mmj = icon(ielem, l)
csss            IF ( amassl(ielem).GT.0.0 ) THEN
            if ( amassl(ielem).gt.1.E-20 ) then
              fracn = amt1(mmi, mmj)/amassl(ielem)
              ccfr(mmi, mmj) = concn*fracn
c              if (mmi.eq.5.and.mmj.eq.4)
c     &                print*,'concn,fracn',concn,fracn
c               ccfr(kcon(ielem,l), icon(ielem,l))
c     &            =concn*amt1(kcon(ielem,l), icon(ielem,l))
c     &            /amassl(ielem)
            else
cssss               ccfr(mmi,mmj) = 0.0
              ccfr(mmi, mmj) = 1.E-20
            end if
  450     continue

  500   continue

C-->    correction for diffusive flux

        kountr = 0

        do 600 k = 1, nchns
          do 550 i = 1, ni(k)
            kountr = kountr + 1
            vfull = xvol
            ccfrd = ccfr(k, i)*vwnow/vfull
cssss
c       if(it.eq.165) print*,'ccfrd (same as c0),vwnow=',
c     &                ccfrd,vwnow

cssss            IF ( ccfrd.GT.0.0 ) THEN
            if ( ccfrd.gt.1E-20 .and. iflow.eq.1 ) then

Csm      see the next constraint again...
              dt = dtd

              call dflux(ccfrd, rd(k,i), alam(k,i), kountr, difflux1,
     &                   difflux2, dt, it)
            else
              difflux1 = 0.0
              difflux2 = 0.0
            end if

            diffusion1(k, i) = difflux1
            diffusion2(k, i) = difflux2

  550     continue
  600   continue

        jj = 1

        do 700 k = 1, nchns
          do 650 i = 1, ni(k)

c       if (k.eq.5.and.i.eq.4) print*, 'dtd=',dtd
c-->        rate of production of am(k,i) from parent
```

```
            if ( i.gt.1 ) then
               xxx1 = amt1(k,i-1)*6.02E23/amall(k,i-1)/0.001
               rdp=xxx1*alam(k, i - 1)
cssss              rdp = amt1(k, i - 1)*alam(k, i - 1)
            else
              rdp = 0.0
            end if

c-->        decay loss rate of the radionuclide from the wp water
            xxx2 = amt1(k,i)*6.02E23/amall(k,i)/0.001
            dissip = xxx2*alam(k, i)
cssss              dissip = amt1(k, i)*alam(k, i)

c-->       radionuclide outflux  from the wp: advective
ccc        if (k.eq.5.and.i.eq.4) print*,'ccfr,qout',ccfr(k,i),qout

            adflux(k, i) = ccfr(k, i)*qout

C-->       total outflux  from the  wp

            rf(k, i) = adflux(k, i) + diffusion1(k, i)
cssss       rf(k,i) = 0.0

C==>       rate of change of mass in wp water

            xxx3 = (rdp-dissip)
c           from atoms --> kg
            xxx3 = (xxx3/6.02E23)*amall(k,i)*0.001
            dam(k,i) = wleach(k,i) + xxx3 - rf(k,i)

cssss            dam(k, i) = wleach(k, i) + rdp - dissip - rf(k, i)

cssss       if(k.eq.5.and.i.eq.4) write(*,99001) t,wleach(k,i)
c       print*,'it=',it
c           if(it.eq.165) write(*,99001) t,wleach(k,i)
c     &         ,rdp,dissip,adflux(k,i),diffusion(k,i),dam(k,i)
            jj = jj + 1
cccc        if (k.eq.5.and.i.eq.4) print*,'jj=',jj
            dydx(jj) = dam(k, i)
            if ( k.eq.5 .and. i.eq.4 ) dissipxx = dissip
            if ( k.eq.5 .and. i.eq.4 ) rdpxx = rdp

  650     continue
  700   continue
        do 800 k = 1, nchns
          do 750 i = 1, ni(k)
            jj = jj + 1
            if ( i.gt.1 ) then
               xxx1 = amt2(k,i-1)*6.02E23/amall(k,i-1)/0.001
               rdp2=xxx1*alam(k, i - 1)
cssss              rdp2 = amt2(k, i - 1)*alam(k, i - 1)
            else
               rdp2 = 0.0
            endif
            xxx2 = amt2(k,i)*6.02E23/amall(k,i)/0.001
            dissip2 = xxx2*alam(k, i)
cssss              dissip2 = amt2(k, i)*alam(k, i)
            xxx3 = (rdp2-dissip2)
c           from atoms --> kg
```

```
            xxx3 = (xxx3/6.02E23)*amall(k)*0.001
            dydx(jj) = xxx3 + adflux(k, i) + diffusion1(k, i)
c           if(k.eq.5.and.i.eq.4) write(*,99003)
c     &                 jj,t,dt,dydx(jj),y(jj)
  750     continue
  800   continue

        do 900 k = 1, nchns
          do 850 i = 1, ni(k)
            jj = jj + 1
            dydx(jj) = adflux(k, i) + diffusion2(k, i)
  850     continue
  900   continue

        return

 9001   format ('t,lch,rdp,dsp,adflux,diffn,dam==', 12(e10.4,2x))
 9002   format ('t,rdp,dissip,rdp-dissip,adflux,diffusion=', 12E10.2)
 9003   format ('from derivs: ', i5, 4x, 12(e10.4,2x))
        end
**==DECAY.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine decay(t, xni0, xnij, alam)
        implicit none
cssss      IMPLICIT NONE
C-----------------------------------------------------------------------
C       chain decay by bateman equation to calculate contribution of the
c       ith chain member to the jth chain member where j is a daughter
c       member
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
        real an, ci1000, p1, p2, sum, t, xxx
        integer i, j, k, kchn, l, m, maxele, maxi, maxmem, maxnuc,
     &          maxnxm, maxste, memb
        integer ncon, kcon, icon, nchns, ni
        real sol, rd, rde, amall, halflife, curall, fggap
cssss      REAL*8 xni0,xnij,alam
        real xni0, xnij, alam
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------

        parameter (maxele=50, maxmem=10, maxnuc=50)
        parameter (maxnxm=maxnuc*maxmem)
        parameter (maxste=300)
        parameter (maxi=20)

        dimension an(maxmem)
        dimension xni0(maxnuc, maxmem), xnij(maxnuc, maxmem),
     &            alam(maxnuc, maxmem)
        common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
     &                  amall(maxnuc, maxmem), halflife(maxnuc, maxmem),
     &                  curall(maxnuc, maxmem), fggap(maxnuc, maxmem),
     &                  kcon(maxele, maxnuc), icon(maxele, maxnuc),
     &                  rd(maxnuc, maxmem), ni(maxnuc), nchns,
     &                  ci1000(maxnuc, maxmem)
```

```
C-----------------------------------------------------------------------

c       Nomenclature:

C       maxele:         max number of elements (radionuclides)
C       maxnuc:         max number of isotopes
C       maxmem:         max number of enteries in table: age, prob of failure
C       maxste:         max number of time steps
C       maxi:           max number of x- or r-dir nodes
c       nchns:          number of chains
c       ni(nchns)       elements in the chain
C       nelem:          element of the chain (ni(ichns) assigned)
C       kchn:           index for chain number
C       xnij:           nventory of the jth element of kchn chain at time t
c       p1:             first product in the Bateman equation
c       p2:             second product in the Bateman equation
c       alam:           coefficient of decay for each radionuclide
c       t:              time [yr]
c       an(i):          mass contribution of the ith element to the jth element
c       xni0:           initial inventory of the jath elemnt of the kchn chain

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

        do 200 kchn = 1, nchns
          memb = ni(kchn)
          do 100 j = 1, memb
            xnij(kchn, j) = 0.0
            do 40 i = 1, j
C                first product in bateman equation
              p1 = 1.0
              if ( j.gt.1 ) then

                do 5 k = i, j - 1
                  p1 = p1*alam(kchn, k)
    5           continue

              end if

              sum = 0.0

              do 20 l = i, j
C                   second product in the bateman equation
                p2 = 1.0
                do 10 m = i, j
                  if ( m.ne.l ) p2 = p2*(alam(kchn,m) - alam(kchn,l))
   10           continue

C                   the sum in bateman equation
Csm     next line added
                xxx = alam(kchn, l)*t
                if ( xxx.gt.65.0 ) xxx = 65.0
                sum = sum + exp( - xxx)/p2
   20         continue

C               the contribution of the ith element to the jth element
              an(i) = p1*xni0(kchn, i)*sum
```

```
   40       continue

            do 60 i = 1, j
C                sum the contributions of all previous elements in chain
              xnij(kchn, j) = xnij(kchn, j) + an(i)
   60       continue
  100     continue
  200   continue

        return
        end
**==DFLUX.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine dflux(c0, rdi, al, kount, difflux1, difflux2, dt, it)
        implicit none
cssss       IMPLICIT NONE
C-----------------------------------------------------------------------
C       module for calculating diffusion flux with finite difference scheme
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
        integer it
        real al, amass, amassl, c0, ccfr, con3, con4, cp, cstore,
     &       dcoefm, difflux1, difflux2, dr, dt, rdi, rr, sumre1,
     &       sumre2, sumre3, rlrate1, rlrate2, rlrate3, tftc, time1
        real amwp1, amwp2, amwp3
        real tleach, tlt, trid, wleach, ws
        real marker
        real ppor
        integer i, kount, maxi, maxmem, maxnuc, maxnxm, maxste, nelem,
     &          nr, nrs
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------

        parameter (maxmem=10, maxnuc=50)
        parameter (maxnxm=maxnuc*maxmem)
        parameter (maxste=300)
        parameter (maxi=20)
        parameter (nrs=maxi)

cssss       REAL*8 alam, atoms, atall, am
        real alam, atoms, atall, am
        dimension cp(nrs)
        common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                  atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                  ccfr(maxnuc, maxmem), tleach, nelem,
     &                  amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                  amassl(maxnuc), tlt, tftc
        common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi, 4),
     &                  rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                  ppor(maxi)
        common /array1/ sumre1(maxnuc, maxmem, maxste),
     &                  sumre2(maxnuc, maxmem, maxste),
     &                  sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                  rlrate1(maxnuc, maxmem, maxste),
     &                  rlrate2(maxnuc, maxmem, maxste),
     &                  rlrate3(maxnuc, maxmem, maxste),
     &                  amwp1(maxnuc, maxmem, maxste),
```

```
     &                amwp2(maxnuc, maxmem, maxste),
     &                amwp3(maxnuc, maxmem, maxste)
      common /driftwall/ marker
C-----------------------------------------------------------------------

c       Nomenclature:

C       maxele:         max number of elements (radionuclides)
C       maxnuc:         max number of isotopes
C       maxmem:         max number of enteries in table: age, prob of failure
C       maxste:         max number of time steps
C       maxi:           max number of x- or r-dir nodes
c       c0:             concentration inside the wp (inner b.c.)
c       trid:           array containing coefficients for the tridiagonal matrix
c                       in the diffusion calculation
c       ws:
c       rdi:            retardation coefficient R
c       dt:             time interval
C       cstore:         concentration in cell, gm/l
c       nr:             number of node points
c       cp(i):          concentration at nide point i
c       con3:           coefficient for diffusion calculation
c:      difflux1:       diffusive flux at the inner sphere radius[gm mol/yr]

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

        trid(1, 4) = c0

C -->   set middle points for radionuclide in question

        do 100 i = 2, nr - 1
          trid(i, 2) = ws(i) + rdi*(al + 1.0/(dt))
          trid(i, 4) = rdi*cstore(kount, i)/(dt)
cssss      print*,'trid=',trid(i,1),trid(i,2),trid(i,3),trid(i,4)
  100   continue

cssss
c       if (it.eq.165) then
c          print*,'trid(i,1)=',(trid(i,1),i=1,nr-1)
c          print*,'trid(i,2)=',(trid(i,2),i=1,nr-1)
c          print*,'trid(i,3)=',(trid(i,3),i=1,nr-1)
c          print*,'trid(i,4)=',(trid(i,4),i=1,nr-1)
c          print*
c          print*,'1111111 dt,nr=',dt,nr
c          print*
c       endif

C-->    solve the tridiagonal matrix

        call diag3(trid, nr, cp)

        do 200 i = 1, nr
          cstore(kount, i) = cp(i)
cssss
          if ( cstore(kount,i).lt.1.E-20 ) cstore(kount, i) = 1.E-20
  200   continue
cssss
```

```
c       if (it.eq.165) then
c           print*,'cp(i)=',(cp(i),i=1,nr)
c           print*
c       endif

C-->    diffusive flux at the inner sphere radius, gm mol/yr

        difflux1 = con3*(cp(1) - cp(2))
        difflux2 = con4*(cp(marker) - cp(marker+1))

        return
        end
**==DIAG3.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine diag3(a, n, x)
        implicit none
cssss      IMPLICIT NONE
C-----------------------------------------------------------------------
c       module for implementing Thomas Algorithm
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
        real a, b, g, w, x
        integer i, j, maxi, n, np1
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
        parameter (maxi=20)

        dimension a(maxi, 4), w(maxi), b(maxi), g(maxi), x(maxi)
C-----------------------------------------------------------------------

c       Nomenclature:

C       maxi:           max number of x- or r-dir nodes
c       n:              same as nr in module dflux
c       x:              same as cp in module  dflux

C-----------------------------------------------------------------------
cccccc
C     Start here.
cccccc

        w(1) = a(1, 2)
        g(1) = a(1, 4)/w(1)
        if ( n.le.1 ) then
          x(1) = g(1)
        else

          do 50 i = 2, n
cssss         print*,'trid=',a(i,1),a(i,2),a(i,3),a(i,4)
            b(i - 1) = a(i - 1, 3)/w(i - 1)
            w(i) = a(i, 2) - a(i, 1)*b(i - 1)
            g(i) = (a(i,4) - a(i,1)*g(i-1))/w(i)
   50     continue

          x(n) = g(n)
          np1 = n + 1
```

```
          do 100 i = 2, n
            j = np1 - i
            x(j) = g(j) - b(j)*x(j + 1)
  100     continue

        end if

        return
        end
**==GASREL.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine gasrel(rhouz, r0z, radu, radsg, tfail, thclad, tcan,
     &                    ttemp, cfuel, czmetal, czoxide, cgap, sc14,
     &                    rrtfuel, rrtzirc, maxtim, oxwidth)
        implicit none
cssss       IMPLICIT NONE
C-----------------------------------------------------------------------
C       gaseous releases from a single waste package
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
        real al, cfuel, cgap, rrtfuel, rrtzirc, czmetal, czoxide, fclad,
     &       r0z, radu, radsg, rc14lb, rxe133, rc14la, rhouz, sc14,
     &       tcan, temp, tfail, thclad, time
        real timef, ttemp
        integer ifflag, itime, maxbin, ntemp, maxtim
        real dtt1
        real gapfrac
        real xxx, oxwidth
        real sum1, iflaguo24
        real rc14lapr, rc14lbpr, rxe133pr, fcladpr
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
        external derivgas

        parameter (maxbin=500)

        common /cther0/ ntemp
        common /uo24width/ sum1, iflaguo24

        dimension tcan(maxtim), ttemp(maxtim)
        dimension sc14(maxbin)

        data al/1.21E-4/
C-----------------------------------------------------------------------
c
c       Nomenclature:

C       al:             radioactive decay coefficient for c14
c       rrtfuel:        release rate of c-14 from the sf
c       rrtzirc:        release rate of c-14 from the cladding
C       ntemp:          num of entries in time versus temp table
C       ttemp(time):    times in table at which temperatures are given
C       tcan(time):     wp surface temp at above times
c       dtt1:           time interval [yr]
C       rc14la:         output fraction of oxidized clad [dimensionless]
```

```
C       rc14lb:         output fraction of sf matrix that oxidized
c       rxe133:         release rate of Xe-133
C       fclad:          output fraction of cladding that oxidized [dim.less]
c       r0z:            radius of sf particle [m]
C       radu:           radius of outer grain boundary layer[m]
c       radsg:          subgrain radius after transgranular fracture [m]
C       thclad:         thickness of cladding, meters
C       czoxide:        curies of c14 in cladding and other metal oxide / kg sf
C       cgap:           curies of c14 in gap and grain boundary / kg sf
C       tfail:          time of canister failure, years
C       sc14:           output array of c14 release rate, curies
C       cfuel:          curies of c14 per kg of fuel
C       czmetal:        curies of c14 per kg of metal
c       gapfrac:        c14 release from  cgap in dtt1 years
C       maxbin:         max number of c14 bins

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

C       convert to variables that can be used in the common

        ifflag = 0
        rrtfuel = 0.
        rrtzirc = 0.
        rc14la = 0.
        rc14lb = 0.
        rxe133 = 0.
        fclad = 0.
        timef = 0.
        rc14lapr = 0.0
        rc14lbpr = 0.0
        rxe133pr = 0.0
        fcladpr = 0.0

        do 100 itime = 2, ntemp
          temp = tcan(itime - 1)
          time = ttemp(itime)
          dtt1 = ttemp(itime) - ttemp(itime - 1)

C        normalized  release of c-14 and xe-133 and
c        differential normalized release from cladding oxidation

          if ( time.gt.tfail ) then
            timef = tfail
            call uo24oxd(rc14la, radu, dtt1, temp, oxwidth)
            call u3o8oxd(rc14lb, rxe133, radu, radsg, dtt1, temp, timef)
            call zircoxd(thclad, fclad, dtt1, temp)
            write (1, *) 'ttemp,rc14la,rc14lb,rxe133', ttemp(itime),
     &                   rc14la, rc14lb, rxe133
          end if

cdbg      print*
cdbg      print*,'++++ rc14la,c14lapr:',rc14la,rc14lapr
cdbg      print*,'rc14lb,c14lbpr:',rc14lb,rc14lbpr
cdbg      print*,'rxe133,rxe133pr:',rxe133,rxe133pr
cdbg      print*,'fclad,fcladpr:',fclad,fcladpr

C--> normalized release of c-14 by diffusion from outer layer
```

```
          rrtfuel = ((rc14la-rc14lapr) + (rc14lb-rc14lbpr)
     &              + (rxe133-rxe133pr))/dtt1
          rc14lapr = rc14la
          rc14lbpr = rc14lb
          rxe133pr = rxe133
          fcladpr = fclad

C--> release of c-14 by oxidation of cladding

          rrtzirc = (fclad - fcladpr)/dtt1

c        cfuel, czmetal etc. are in ci/kg sf

          if ( ttemp(itime).gt.tfail ) then
            if ( ifflag.eq.0 ) then
              xxx = -tfail*al
              if ( xxx.lt. - 65. ) xxx = -65.
              gapfrac = (czoxide + cgap)*exp(xxx)/dtt1
cdbg           print*, 'gapfrac, sc14(itime):', gapfrac, sc14(itime)
              sc14(itime) = rrtfuel*cfuel + rrtzirc*czmetal + gapfrac
              ifflag = 1
            else
              sc14(itime) = rrtfuel*cfuel + rrtzirc*czmetal
              gapfrac = 0.0
            end if
          end if

  100   continue

        return
        end
**==ODEINT.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine odeint(ystart, nvar, x1, x2, eps, h1, hmin, hmax,
     &                    nok, nbad, tiny, derivs, rkqc, xfrac, xvol,
     &                    tfail, qin, vmax, amass0, r0z, tavg, qout,
     &                    dydx, it)
        implicit none
cssss       IMPLICIT NONE
C-----------------------------------------------------------------------
        integer it
C*** Start of declarations inserted by SPAG
        real amass0, dydx, eps, errc, xfrac, xvol, h, h1, hdid, hmax,
     &       hmin, hnext, qin, qout, tavg, tfail, tiny, vmax, x, x1, x2
        real y, yscal, ystart, zero
        real xsav, r0z, two
        integer kmax, kount
        real dxsav, xp, yp
        real fuewt, fueden, fuedif, fuepor, amassc
        integer i, ieq, ifudge, maxstp, nbad, nok, nstp, nvar
C*** End of declarations inserted by SPAG
C  *********************************************************************
        external derivs, rkqc
        parameter (maxstp=50000, two=2.0, zero=0.0)
        dimension ystart(200), yscal(200), y(200), dydx(200)
```

```
      common /cwast1/ fuewt, fueden, f[illegible]f, fuepor, amassc
      common /path  / kmax, kount, dxsav, xp(200), yp(100, 200)
C  *********************************************************************
c       x:      independent variable
c       h1:     guessed first step size
c       nok:    number of good/okay steps taken
c       nbad:   number of steps taken but retried and fixed
c       y(i):   dependent variables
c       ystart(i):      starting values for integration
c       dydx:   derivative of the dependent variable
c       nvar:   number of starting values
c       tiny:   a small real number
c       dxsav:  intermediate integration results are stored at intervals > dxsav
c       yscal:  the vector against which the error is scaled
c       hdid:   the step size which was actually accomplished
c       hnext:  the estimated next step size
c       derivs: user supplied subroutine for calculating the right hand side
c                       of the derivative
c       x1:     lower limit of the integration
c       x2:     upper limit of the integration
c       eps:    integration to be done with required accuracy eps
c       hmin:   minimum allowed step size
c       r0z:    radius of sf particle
C       xfrac:  fraction of fuel exposed
C       tfail:  time of canister failure, years
C       qin:    inflow of water to canister, liters per year
C       vmax:   maximum water volume in canister before it overflows, liters
C       amass0: mass of fuel[kg]; amassc assigned to amass0
c       tavg:   same as tcan (wp surface temperature)
c       qout:   water outfloe rate from the wp
C       ieq:    equation controlling step size,
C       errc:   the critical error
C----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
C----------------------------------------------------------------------
      x = x1
      h = sign(h1, x2 - x1)
      nok = 0
      nbad = 0
      kount = 0

      do 100 i = 1, nvar
        y(i) = ystart(i)
  100 continue

ccc      print*,'from odeint at the beginning  y(15)=',y(15)

      if ( kmax.gt.0 ) xsav = x - dxsav*two

  200 continue
      do 400 nstp = 1, maxstp

c     print*, 'nstp, h, hmax=',nstp,h,hmax

        call derivs(x, y, dydx, xfrac, xvol, tfail, qin, vmax, amass0,
     &              tavg, qout, h, it)
        do 250 i = 1, nvar
          yscal(i) = abs(y(i)) + abs(h*dydx(i)) + tiny
```

```
  250     continue

ccc      print*,'from odeint after first derivs y(15)=',y(15)

          if ( kmax.gt.0 ) then
            if ( abs(x-xsav).gt.abs(dxsav) ) then
              kount = kount + 1
              xp(kount) = x
              do 260 i = 1, nvar
                yp(i, kount) = y(i)
  260         continue
              xsav = x
            end if
          end if

          if ( (x+h-x2)*(x+h-x1).gt.zero ) h = x2 - x
csm pay attention to this extra constraint
          if ( h.gt.hmax ) h = hmax
          call rkqc(y, dydx, nvar, x, h, eps, yscal, hdid, hnext, ieq,
     &              errc, derivs, xfrac, xvol, tfail, qin, vmax, amass0,
     &              r0z, tavg, qout, it)
          if ( hdid.eq.h ) then
            nok = nok + 1
          else
            nbad = nbad + 1
          end if

ccc      print*,'from odeint after rkqc h and y(15)=',h,y(15)

          if ( (x-x2)*(x2-x1).ge.zero ) then
            do 280 i = 1, nvar
              ystart(i) = y(i)
cssss
c         if (it.gt.164) then
c           prinT*, '##### x,x2,x1=',x,x2,x1
c         endif
  280       continue
            if ( kmax.ne.0 ) then
              kount = kount + 1
              xp(kount) = x
              do 290 i = 1, nvar
                yp(i, kount) = y(i)
  290         continue
            end if
c  pay close attention to the next two lines
cssss           eps=eps/(10.**ifudge)
cssss           tiny=tiny/(10.**ifudge)
            go to 600
csm       RETURN
          end if

          if ( abs(hnext).lt.hmin ) then
            write (*, *) 'runge-kutta error messages,',
     &                   ' step size too small'
            write (*, *) 'i,y,dydx,yscal'
            do 300 i = 1, nvar
              write (*, *) i, y(i), dydx(i), yscal(i)
  300       continue

            write (*, *) 'equation controlling step size is:  ', ieq
```

```
            write (*, *) 'controlling equation error is: ', errc
            write (*, *) 'step size is: ', hdid

C jcw   note: if it does not make it then we increase the allowable
C       error and try again

csm     pay close attention to the next three lines
cssss             ifudge=ifudge + 1
cssss             eps=eps*10.
cssss             tiny=tiny*10.
          end if

          h = hnext
  400   continue

        write (*, *) 'runge-kutta error messages'
        write (*, *) 'i, y(i), dydx(i), yscal(i)'
        write (*, *) 'time = ', x

        do 500 i = 1, nvar
          write (*, *) i, y(i), dydx(i), yscal(i)
  500   continue

        write (*, *) 'equation controlling step size is:  ', ieq
        write (*, *) 'controlling equation error is: ', errc
        write (*, *) 'step size is: ', hdid

C note: if it does not make it then we increase the allowable
C      error and try again

cssss             ifudge=ifudge + 1
cssss             eps=eps*10.
cssss             tiny=tiny*10.
        go to 200
C       pause 'too many steps.'


  600   continue
        return
        end
**==RKQC.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine rkqc(y, dydx, n, x, htry, eps, yscal, hdid, hnext,
     &                  ieq, errc, derivs, xfrac, xvol, tfail, qin,
     &                  vmax, amass0, r0z, tavg, qout, it)
        implicit none
cssss      IMPLICIT NONE
C-----------------------------------------------------------------------
C       quality controlled runge kutta integration routine
C       from numerical recipes
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
        integer it
        real r0z, xvol
        real fuewt, fueden, fuedif, fuepor, amassc
        real amass0, dydx, dysav, eps, errc, errcon, errmax, fcor,
```

```
     &       xfrac, h, hdid, hh, hnext, h[illegible], one, pgrow, pshrnk, qin,
     &       qout, safety
        real tavg, tfail, vmax, x, xsav, y, ysav, yscal, ytemp
        integer i, ieq, n, nmax
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
        parameter (nmax=1000, pgrow= - 0.20, pshrnk= - 0.25,
     &             fcor=1.D0/15.D0, one=1.D0, safety=0.9, errcon=6.D-4)

        dimension y(200), dydx(200), yscal(200), ytemp(nmax), ysav(nmax)
     &            , dysav(nmax)

        common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc

        external derivs
C-----------------------------------------------------------------------

c       Nomenclature:

c       x:      independent variable
c       htry:   step size to be attempted
c       n:      length of the dependent variable vector y
c       ytemp:  an array containing error estimates
c       derivs: name of the subroutine with the derivative of the eq.
c               to be integrated
c       y(i):   dependent variable vector
c       dydx:   derivative of the dependent variable
c       eps:    integration to be done with required overall tolerance eps
c       hdid:   step size which was actually accomplished
c       hnext:  estimated next stepsize
C       xfrac:  fraction of fuel exposed
C       tfail:  time of canister failure, years
C       qin:    inflow of water to canister, liters per year
C       vmax:   maximum water volume in canister before it overflows, liters
C       amass0: mass of fuel[kg]; amassc assigned to amass0
c       r0z:    radius of sf particle
c       tavg:   same as tcan (wp surface temperature)
c       qout:   water outfloe rate from the wp
C-----------------------------------------------------------------------

        xsav = x

        do 100 i = 1, n
          ysav(i) = y(i)
          dysav(i) = dydx(i)
  100   continue

        h = htry
  200   continue
        hh = 0.5*h
ccc     print*, 'before first rk4 call y(15),dydx(15)=',
ccc     &               y(15),dydx(15)

        call rk4(ysav, dysav, n, xsav, hh, ytemp, derivs, xfrac, xvol,
     &          tfail, qin, vmax, amass0, r0z, tavg, qout, it)
        x = xsav + hh

        call derivs(x, ytemp, dydx, xfrac, xvol, tfail, qin, vmax,
     &             amass0, tavg, qout, hh, it)
```

```
ccc     print*, 'before 2nd rk4 call y(15),dydx(15)=',
ccc  &         y(15),dydx(15)
        call rk4(ytemp, dydx, n, x, hh, y, derivs, xfrac, xvol, tfail,
     &          qin, vmax, amass0, r0z, tavg, qout, it)
        x = xsav + h
        if ( x.eq.xsav ) then
          write (*, *) 'x,xsav=&&&&&&&&&&=', x, xsav
          write (*, *) 'stepsize not significant in rkqc'
          write (*, *) 'The code is forcibly stopped'
          stop
        end if

ccc     print*, 'before 3rd rk4 call y(15),dydx(15)=',
ccc     &               y(15),dydx(15)
        call rk4(ysav, dysav, n, xsav, h, ytemp, derivs, xfrac, xvol,
     &          tfail, qin, vmax, amass0, r0z, tavg, qout, it)
        errmax = 0.
        errc = 0.
        ieq = 0

ccc     stop

        do 300 i = 1, n
          ytemp(i) = y(i) - ytemp(i)
csss
c       print*,'eps,yscal(i)',eps,yscal(i)

          if ( abs(ytemp(i)/yscal(i)).gt.errmax ) then
            ieq = i
            errc = ytemp(i)
          end if
          errmax = max(errmax, abs(ytemp(i)/yscal(i)))
  300   continue

        errmax = errmax/eps
        if ( errmax.gt.one ) then
          h = safety*h*(errmax**pshrnk)
          go to 200
        else
          hdid = h
          if ( errmax.gt.errcon ) then
            hnext = safety*h*(errmax**pgrow)
          else
            hnext = 4.*h
          end if
        end if

        do 400 i = 1, n
          y(i) = y(i) + ytemp(i)*fcor
  400   continue
cssss
c       if (it.eq.165) then
c          print*,'it,ieq in rkqc is=',it,ieq
c          stop
c       endif

        return
        end
**==RK4.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996
```

```
      subroutine rk4(y, dydx, n, x, h, yout, derivs, xfrac, xvol,
     &                tfail, qin, vmax, amass0, r0z, tavg, qout, it)
      implicit none
cssss      IMPLICIT NONE
C-----------------------------------------------------------------------
C     runge kutta routine from numerical recipes
C-----------------------------------------------------------------------

C*** Start of declarations inserted by SPAG
      integer it
      real r0z, xvol
      real amass0, dydx, dym, dyt, xfrac, h, h6, hh, qin, qout, tavg,
     &     tfail, vmax, x, xh, y, yout, yt
      integer i, n, nmax
      real fuewt, fueden, fuedif, fuepor, amassc
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
      external derivs
      parameter (nmax=1000)
      dimension y(200), dydx(200), yout(200), yt(nmax), dyt(nmax),
     &          dym(nmax)
      common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc
C-----------------------------------------------------------------------
c     n:              number of variables
c     h:              r-k to advance the solution over an interval h
c     xh:
c     y(i):           dependent variables
c     dydx(i):        derivatives of dependent variables
c     yout(i):        an array containing the incremented y values
c     r0z:            radius of the sf particle [m]
C     xfrac:          fraction of fuel exposed
C     tfail:          time of canister failure, years
C     qin:            inflow of water to canister, liters per year
C     vmax:           maximum water volume in canister before it overflows, liters
C     amass0:         mass of fuel[kg]; amassc assigned to amass0
c     tavg:           isame as tcan (wp surface temperature)
c     qout:           water flow rate out of the wp
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
C-----------------------------------------------------------------------
      hh = h*0.5
      h6 = h/6.
      xh = x + hh

      do 100 i = 1, n
        yt(i) = y(i) + hh*dydx(i)
  100 continue

      call derivs(xh, yt, dyt, xfrac, xvol, tfail, qin, vmax, amass0,
     &            tavg, qout, hh, it)

      do 200 i = 1, n
        yt(i) = y(i) + hh*dyt(i)
  200 continue
```

```
        call derivs(xh, yt, dym, xfrac, xvol, tfail, qin, vmax, amass0,
     &              tavg, qout, hh, it)

        do 300 i = 1, n
          yt(i) = y(i) + h*dym(i)
          dym(i) = dyt(i) + dym(i)
  300   continue

        call derivs(x + h, yt, dyt, xfrac, xvol, tfail, qin, vmax,
     &              amass0, tavg, qout, hh, it)

        do 400 i = 1, n
          yout(i) = y(i) + h6*(dydx(i) + dyt(i) + 2.*dym(i))
  400   continue

        return
        end
**==U3O8OXD.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine u3o8oxd(rc14lb, rxe133, radu, radsg, dtime, t, timef)
        implicit none
cssss       IMPLICIT NONE
C-----------------------------------------------------------------------
C       cumulative release from dry oxidation of SF matrix to U3O8
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
        real dfsvty133, dfsvty14, grainr, pi, ratio, rc14lb, rxe133,
     &       sum, t, temp, dtime, timef, timehr, xxx1, xxx2
        integer n, nseries
        real radu, radsg
        real sgrainr
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
c       nseries:        number of terms to be used in the infinite series
c       pi:             the constant pi
c       radsg:          subgrain radius after transgranular fracture [m]
c       grainr:         grain radius [micrometer]
c       radu:           grainr [m]
c       sgrainr:        subgrain radius after transgranular fracture[micrometer]
c       temp:           temperature [K]
c       t               temperature [C]
c       timehr:         time [hr]
C       dtime:          time [y]
c       dfsvty14:       diffusion coefficient for c-14 releases
c       n:
C       rc14lb:         output fraction of SF matrix that oxidized
c       dfsvty133:      diffusion coefficient  for xe-133 release
c       rxe133:         release rate of Xe-133
c
c  example values:
c       grainr=10./2.   ! [micrometer]
C
C       note: gas phase release in U3O8 (spherical model, Crank,1975)
C       the Dmatrix used in the following applies to
```

```
C       Xe-133, Cl-36, Tc-99, I-129 relea
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

        nseries = 25
        pi = 4.*atan(1.)
        grainr = radu*1E6
        sgrainr = radsg*1E6

        temp = t + 273.
        timehr = dtime*365.*24.

        if ( temp.ge.250. + 273. ) then

C          group 1:  c-14 release ..............................

          sum = 0.
          xxx1 = 26.6E3/1.987/temp
          dfsvty14 = 0.6*grainr**2/(2.6E-9*exp(xxx1))

          do 50 n = 1, nseries
            xxx2 = dfsvty14*n**2*pi**2*timehr/sgrainr**2
            if ( xxx2.gt.35 ) go to 100
            sum = sum + (1./n**2)*exp( - xxx2)
   50     continue

  100     continue
          ratio = 1. - 6./pi**2*sum
          rc14lb = ratio

C          group 2: xe-133 release .............................

C          at this point, treated as c-14.

          sum = 0.
          xxx1 = -18.6E3/(1.987*temp)
          dfsvty133 = 1.5E-10*exp(xxx1)
          dfsvty133 = dfsvty133*1.E-4*1.E12*60*60

          do 150 n = 1, nseries
            xxx2 = dfsvty133*n**2*pi**2*timehr/(sgrainr)**2
            if ( xxx2.le.35 ) sum = sum + (1./n**2)*exp( - xxx2)
  150     continue

          ratio = 1. - (6./pi**2)*sum
          rxe133 = ratio
        else
          rc14lb = 0.
          rxe133 = 0.
        end if

        return
        end
**==U024OXD.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996
```

```
      subroutine uo24oxd(c14lc, radu, dtime, t, oxwidth)
      implicit none
C*** Start of declarations inserted by SPAG
      integer iflaguo24
C*** End of declarations inserted by SPAG
cssss      IMPLICIT NONE
C-----------------------------------------------------------------------
C       normalized release rate from dry oxidation of
C       spent fuel uo2 to uo2.4
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real c14invf, c14lc, oxwidth, ratek, sfpr, t, temp, dtime,
     &       timehr
      real radu
      real sum1, oxwidth1
      common /uo24width/ sum1, iflaguo24
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------

c       Nomenclature:

C       rc14la:         output fraction of oxidized clad [dimensionless]
C       dtime:          time [y]
C       timehr:         time  in hr
C       t:              temperature of fuel [c]
c       temp:           temperature of fuel [K]
C       radu:           radius of SF grain [m]
c       sfpr:           radu in micrometer
c       oxwidth:        oxidized zone width in a spherical particle[micrometer]
c       c14invf:        fractional initial inventory of c-14 in a WP
c       ratek:          rate constant [micrometer/hr]
c       c14lc:          c14 release in unoxidized SF and UO2.4

c      note:  sfpr=0.2/100.*1.E6        ! convert to micrometer
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

      sfpr = radu*1.E6
      c14invf = 1.
      temp = t + 273.
      timehr = dtime*365.*24.
      ratek = 1.04E8*exp( - 24.E3/1.987/temp)
      oxwidth1 = sqrt(2.*ratek*timehr)
      sum1 = sum1 + oxwidth1
      if ( sum1.gt.sfpr ) then
        sum1 = 1.0
        iflaguo24 = 1
      end if
      write (1, *) , 'oxd. width and grain rad. [micrometer]=', sum1,
     &              sfpr

      if ( iflaguo24.eq.0 ) c14lc = (1./sfpr**3)
     &      *(3.*sfpr**2*sum1 - 3.*sfpr*sum1**2 + sum1**3)*c14invf

      oxwidth = sum1*1.E-6
```

```
      write (1, *) 'oxwidth [m]=,temp-2[redacted] oxwidth, temp - 273

      return
      end
**==ZIRCOXD.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




      subroutine zircoxd(thclad, fclad, dtime, t)
      implicit none
cssss     IMPLICIT NONE
C-----------------------------------------------------------------------
C     release from zirconium metal upon oxidation model
c     of dalgaard ref einziger 1991
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real dweight, fclad, t, temp, thclad, dtime, timedays, zdensity,
     &     zdensity1
      real xxx1
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
c
c     nomenclature:
c
c     zdensity:       zircalloy density [gm/cc]
c     zdensity1:      zircalloy density [mg/dm3]
C     thclad:         thickness of cladding [dm]
C     dtime:          time [y]
c     timedays:       time in days
C     t:              temperature of the cladding [c]
c     dweight:        weight gain of the oxidizing zircalloy layer [mg/dm2]
C     fclad:          output fraction of cladding that oxidized [dim.less]
c
c     note:  the weight gain is assumed to be proportional to the cladding
c     oxidized layer thickness. Therefore, the oxidation stops
c     when the thickness of the oxidized layer equals that of
c     the cladding

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
      zdensity = 6.56
      zdensity1 = (zdensity*1000.)*1000.
      thclad = 0.6*1.E-2
      temp = t
      timedays = dtime*365
cccc     dweight=75.3*exp( - 556./temp) + 1.12E8*exp( - 12529./temp)
cccc    &       *timedays
      xxx1 = -12529./temp
      if ( xxx1.lt. - 65. ) xxx1 = -65.
      dweight = 1.12E8*exp(xxx1)*timedays
      fclad = dweight/(zdensity1*thclad)

      return
      end
```

```
      subroutine leachrt(temp, srate)
      implicit none
cssss     IMPLICIT NONE
C-----------------------------------------------------------------------
C     spent fuel matrix dissolution [Stewart and gray, 1994,
C     Gray and Wilson, 1995]
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real cco3, oxgnovpr, phvalue, rate1, rate2, xfrac, srate, temp,
     &     tempk, xxx
      integer imodel
C*** End of declarations inserted by SPAG
      common /leach / imodel, phvalue, oxgnovpr, cco3, xfrac
      real srate1, srate2
      real aaa
C-----------------------------------------------------------------------

c     Nomenclature:

C     model 1###
C     cco3:          carbonate concentration [moles/liter]
C     oxgnovpr:      dissolved oxygen (0.002-0.2 atm overpressure)
c     phvalue:       pH
C     time:          time [days]
C     temp:          temperature [C]
c     tempk:         temp in K
C     rate1:         spent fuel matrix dissolution rate from
c                    model 1 [mg/m2/day]
C     srate1:        rate1 in kg/m2/yr
C     model 2###
c     rate2:         spent fluel matrix dissolution rate from model 2
c                    [gm/day/205 cm2 surface area]
c     srate2:        rate2 in kg/yr/m2
c
C     srate:         spent fuel matrix dissolution rate [kg/m2/yr]

C-----------------------------------------------------------------------
C     example values:
C             phvalue:       9.
C             oxgnovpr:      0.2 ppm
C             cco3:          2.e-3 mol/liter
c
C     note:  ph = -log(h)
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
      tempk = temp + 273.

C-->  model 1:  in the absence of Ca and Si

      if ( imodel.eq.1 ) then
        xxx = 9.310 + 0.142*log10(cco3) - 16.7*log10(oxgnovpr)
```

```
     &          - 0.14*phvalue - 2130./tempk + 6.811*log10(tempk)
     &          *log10(oxgnovpr)
           rate1 = 10**xxx
           srate1 = rate1*1.E-6*365.
           srate = srate1
         end if

C-->     model 2: dissolution in the presence of Ca and Si

         if ( imodel.eq.2 ) then
c         a rate equation to introduc experimental data
c         obtained at 25 C and 85 C
           aaa = 3.45
           rate2 = aaa*1.E4*exp( - 34.3/8.314E-3/tempk)
           srate2 = rate2*1.E-6*365.
           srate = srate2
         end if

         return
         end
**==OPNFIL.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996
C




         subroutine opnfil(unit, filnam, status, lplain, errnum, errmsg)
         implicit none
cssss       IMPLICIT NONE
C-----------------------------------------------------------------------
C        name: opnfil - open file
C
C        purpose:
C        this module opens a formatted file on the unit specified with the
C        attributes provided in the argument list.
C
C        method:
C        a check is first made to determine the availablility of the
C        requested unit and file.  if either is already in use, then
C        precessing is terminated and control is returned to the
C        calling routine.  otherwise, 'status' is checked for the
C        desired operation.
C
C        status       operation
C        ------       ---------
C        read         open an existing file for input. the file must
C                     exist in a closed state for a successful completion.
C        new          open a new file for output.  the file must not
C                     exist for a successful completion.
C        replace      open a new file for output.  the file may or may not
C                     exist.  if it does exist it is deleted before
C                     opening the new file.
C        append       open a new or existing file for output.  the file
C                     may or may not exist.  if it does exist it is
C                     opened and positioned at the end of the file so
C                     any new information is appended to the old file.
C                     if it does not exist it is opened as a new file.
C
```

```
C       the fourth argument controls the record attibute of vms type
C       file systems.  a value of .false. will enable the use of
C       fortran carriage control characters as the file is written.
C       these files are not conveinient for bufferring dat between
C       programs since the first column will have extraneous data.
C       for this purpose a value of .true. should be used to provide
C       a plain vanilla file without carriage control characters.
C
C       an error number and message are returned to give the status
C       of the requested operation.  the message string is defined
C       in the calling module and should be of length 64 for complete
C       messages to be returned.
C
C       error number    meaning
C       ------------    -------
C              0          no error, successful open.
C              1          requested unit is in use by another file.
C              2          requested file is in use by another unit or
C                         user.
C              3          requested input file was not found.
C              4          requested new file is not new, it already
C                         exists.
C              5          an unknown or invlid open request was provided
C                         in the argument list.
C              -1         system failure.  the system has not acted in
C                         a manner consistent with the assumptions used in
C                         the module design.
C
C       arguments:
C       input:
C       unit   = integer, fortran unit number.
C       filnam = character, file name of file to be opened.
C       status = character, file disposition and relation to
C                any existing files with the same name.
C       lplain = logical, flag for the file system attribute to be
C                associated with this file.  this is only useful with
C                vms type file systems where fortran carriage control
C                causes different handling characteristics when used
C                with system utilities.  true = no fortran carriage
C                control characters in column 1.
C
C       output:
C       errnum = integer, error number indicating the success or
C                the conflict of the request with the file system.
C       errmsg = character, error message text.
C
C       history:
C       04-23-92  original text.          ron janetzke
Ccccc
        integer errnum
        integer unit
        logical lplain
        character*(*) filnam
        character*(*) status
        character*(*) errmsg
Ccccc
C       lexist = file exist flag.
C       lfopen = file open flag.
C       luopen = unit open flag.
C       attrib = carriagecontrol attribute (vms type file systems only).
```

```
Ccccccc
        logical lexist
        logical lfopen
        logical luopen
C-------------------------------------------------------------------
Ccccccc
C     start here.
Ccccccc
C     the error variables are initialized.  with proper operation of
C     the 'opnfil' subroutine they should be reset to other values
C     before returning.  if they are not reset, that would indicate
C     a problem with assumptions made about how the operating system
C     handles the inquire or open statements.
Ccccccc
        errnum = -1
        errmsg = 'open operation incomplete.  check opnfil source code.'
Ccccccc
C     check the availabilty of the unit.
Ccccccc
        inquire (unit=unit, opened=luopen)
        if ( luopen ) then
          errnum = 1
          errmsg =
     &           'unit is open.  use of opnfil requires a closed unit.'

          return
        end if

Ccccccc
C     check the availability of the file.
Ccccccc
        inquire (file=filnam, exist=lexist, opened=lfopen)
        if ( lfopen ) then
          errnum = 2
          errmsg = 'file is in use, probably on another unit or '//
     &             'by another user.'

          return
        end if

Ccccccc
C     input file read.
C
C     it is suggested that this status be used only for opening pre-
C     existing files for input.
Ccccccc
        if ( status.eq.'read' .or. status.eq.'read' ) then
          if ( lexist ) then
            open (unit=unit, file=filnam, status='old')
            errnum = 0
            errmsg = 'opnfil successful.'
          else
            errnum = 3
            errmsg = 'requested read file was not found.'
          end if

Ccccccc
C     output file new.
C
C     it is suggested that this status be used only for opening
```

```
C     files for output.
Ccccc
        else if ( status.eq.'new' .or. status.eq.'new' ) then
          if ( lexist ) then
            errnum = 4
            errmsg = 'new file creation blocked by existing file.'
          else
            open (unit=unit, file=filnam, status='new')
            errnum = 0
            errmsg = 'opnfil successful.'
          end if

Ccccc
C     output file replace.
C
C     it is suggested that this status be used only for opening
C     files for output.
Ccccc
        else if ( status.eq.'replace' .or. status.eq.'replace' ) then
          if ( lexist ) then
            open (unit=unit, file=filnam, status='old')
            close (unit=unit, status='delete')
          end if

          open (unit=unit, file=filnam, status='new')
          errnum = 0
          errmsg = 'opnfil successful.'
Ccccc
C     output file append.
C
C     it is suggested that this status be used only for opening
C     files for output.
Ccccc
        else if ( status.eq.'append' .or. status.eq.'append' ) then
          if ( lexist ) then
            open (unit=unit, file=filnam, status='old', access='append')
          else
            open (unit=unit, file=filnam, status='new')
          end if

          errnum = 0
          errmsg = 'opnfil successful.'
Ccccc
C     unknown file status request.
Ccccc
        else
          errnum = 5
          errmsg = 'file status request is not valid.'
        end if
Ccccc

        return
        end
**==SETDIF.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996




        subroutine setdif(r0)
```

```
      implicit none
cssss      IMPLICIT NONE
C-----------------------------------------------------------------------
C     set coefficient matrix for the diffusive flow out of wp.
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real a1, a2, a3, amass, amassl, ccfr, con3, con4, cstore,
     &     dcoefm, dr, dr12, dr32, r0, r12, r32, rr, sumre1, sumre2,
     &     sumre3, rlrate1, rlrate2, rlrate3, tftc
      real amwp1, amwp2, amwp3
      real time1, tleach, tlt, trid, wleach, ws
      real ppor
      integer i, j, maxi, maxmem, maxnuc, maxnxm, maxste, nelem, nr

C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
      parameter (maxmem=10)
      parameter (maxnuc=50)
      parameter (maxste=300)
      parameter (maxnxm=maxnuc*maxmem)
      parameter (maxi=20)
cssss      REAL*8 alam, atoms, atall, am
      real alam, atoms, atall, am
      common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                ccfr(maxnuc, maxmem), tleach, nelem,
     &                amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                amassl(maxnuc), tlt, tftc
      common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi, 4),
     &                rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                ppor(maxi)
      common /array1/ sumre1(maxnuc, maxmem, maxste),
     &                sumre2(maxnuc, maxmem, maxste),
     &                sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                rlrate1(maxnuc, maxmem, maxste),
     &                rlrate2(maxnuc, maxmem, maxste),
     &                rlrate3(maxnuc, maxmem, maxste),
     &                amwp1(maxnuc, maxmem, maxste),
     &                amwp2(maxnuc, maxmem, maxste),
     &                amwp3(maxnuc, maxmem, maxste)
C-----------------------------------------------------------------------
c     Nomenclature:

C     a1,2,3:         transformed radial coordinate
C     cstore:         concentration in cell, gm/l
C     dcoefm:         molecular diffusion coefficient of pack and rock (m2/yr)
C     dr:             delta x
c     dr12,dr32:      distance betwe. the center and left & right distance, resp.
C     r0:             outer radius of sphere
c     r12,r32:        position of the cenetrs of the left and right blocks
C     rr:             zone distances from the edge of teh wp [m]
c     trid:           array containing coefficients for the tridiagonal matrix
c                     in the diffusion calculation
c     ws:
C     maxi:           max number of x- or r-dir nodes
C     maxmem:         max number of enteries in table: age, prob of failure
C     maxnuc:         max number of isotopes
C     maxste:         max number of time steps
C     nr:             number of zones for diffusion calculation (same as imax)
C
```

```
C       Note:  assumes a spherical shell surrounding spherical source term.
c       advection considered seperately, and results of advection and
c       diffusion added assumes molecular diffusion only in the sphere
C       accounts for decay of parent, but no generation of daughters
C       in the sphere.
C       inner boundary at r.n. concentrations inside the wp;
c       outer boundary at r.n. conccentration=0.0

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

        do 100 i = 1, maxnxm
          do 50 j = 1, maxi
            cstore(i, j) = 1.E-20
   50     continue
  100   continue

        rr(1) = r0

        write (1, *) 'nr in setdif =', nr

        do 200 i = 2, nr
          rr(i) = rr(i - 1) + dr(i - 1)
  200   continue

C       set up some of the coefficients for the tridiagonal matrix

        trid(1, 1) = 0.0
        trid(1, 2) = 1.0
        trid(1, 3) = 0.0

        do 300 i = 2, nr - 1
          dr32 = (dr(i) + dr(i+1))/2
          dr12 = (dr(i-1) + dr(i))/2
          r12 = (rr(i-1) + rr(i))/2
          r32 = (rr(i) + rr(i+1))/2
          a1 = dcoefm(i - 1)*r12**2/(rr(i)**2*dr(i-1)*dr12)
          a3 = dcoefm(i + 1)*r32**2/(dr(i)*rr(i)**2*dr32)
          a2 = a1 + a3
          trid(i, 1) = -a1
          trid(i, 3) = -a3
          ws(i) = a2
  300   continue

C       zero concentration at outer boundary

        trid(nr, 1) = 0.0
        trid(nr, 2) = 1.0
        trid(nr, 3) = 0.0
        trid(nr, 4) = 0.0

        return
        end
**==INIT.spg  processed by SPAG 4.00Aa at 19:34 on  9 Dec 1996
```

```
      subroutine init
      implicit none
cssss     IMPLICIT NONE
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real amassc, cftime, ctemp, cvol, floref, flowfactr, flow,
     &     fueden, fuedif, fuewt, funnel, rpor, sftime, simtimex,
     &     tcaqu, tflo, deffrac
      real xco, xcon
      integer i, imax, iscon, izone, j, jmax, maxi, maxj, maxtim,
     &        mtot, icfcon, ntemp, nzones
      real wplen, wpdia, driftdia
      real xvol, dintl, xlintl
      real fuepor
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
Ccccc
      parameter (maxtim=500)
      parameter (maxi=20, maxj=30)

      common /ccont2/ deffrac
      common /ccont5/ sftime, iscon
      common /ccoro1/ cftime, tcaqu, icfcon
      common /cgeom / cvol, xcon, funnel, mtot
      common /cnume1/ simtimex, imax, jmax
      common /cnume2/ xco(maxi), nzones, izone(maxi, maxj)
      common /crhyd1/ rpor(maxi), flowfactr, flow, tflo(maxtim),
     &                floref(maxtim)
      common /cther2/ ctemp
      common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc
      common /wpvol / wplen, wpdia, driftdia, xvol, dintl, xlintl
      common /cther0/ ntemp
C-----------------------------------------------------------------------
c
c     Nomenclature:
c
C     cvol:          cell volume
C     xcon:          num of packages in a cell
C     wplen:         length of package
C     wpdia:         diameter of waste package
C     ctemp:         crit. temp.[C] for the onset of liquid flow  around wp
C     ntemp:         num of entries in time versus temp table
C     rpor:          porosity:: three layers damaged, disturbed, host rock
C     flow:          flow rate into the container
C     floref:        reference flow at tflo
C     icfcon:        number failed containers in the cell due to corrosion
C     tcaqu:         time at which aqueous conditions begin in cell i
C     cftime:        corrosion failure time [y]
C     sftime:        time at which scenario causes container failures in a cell
C     fuewt:         formula wt for spent fuel
C     fueden:        fuel density
C     fuedif:        fuel diffusion coefficient
C     imax:          nodes in x (or r) direction
C     jmax:          nodes in y (or theta) direction
c     simtimex::     maximum simulation time [y]
C     xco:           x (or r) coordinates
C     izone(i,j):    zone number of node (i,j)

C-----------------------------------------------------------------------
```

```
c       Notes:
C               1 cal=4.186 joule
C               gas constant, r = 8.134 joules/mol-k
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

C-->    geometric elements: length,width,height for wp and drift

        cvol = 1.
        xcon = 1.
        wplen = 1.
        wpdia = 1.

C-->    thermal parameters

        ctemp = 97.
        ntemp = 0

C-->    hydrologic parameters

        do 100 i = 1, maxi
          rpor(i) = 0.1
  100   continue

        flow = 0.

        do 200 i = 1, maxtim
          floref(i) = 0.
  200   continue

C-->    container data

        icfcon = 0
        tcaqu = 0.
        cftime = 1.E30
        sftime = 1.E20

C-->    radionuclide properties

        fuewt = 0.
        fueden = 1.
        fuedif = 1.

C-->    grid and time step information

        imax = 1
        jmax = 1
        simtimex = 0.

        do 300 i = 1, maxi
          xco(i) = 1.
  300   continue

        do 400 i = 1, maxi
          do 350 j = 1, maxj
            izone(i, j) = 1
  350     continue
  400   continue
```

```
      return
      end
**==INPUT.spg  processed by SPAG 4.00Aa at 19:35 on  9 Dec 1996



      subroutine input
      implicit none
cssss     IMPLICIT NONE
C-----------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real amass, amassc, amassl, ccfr, cco3, cftime, cfuel, cgap,
     &     con3, con4, cstore, ctemp, cvol, czmetal, czoxide, deffrac,
     &     dcoefm, dr
      real diff
      real fuepor
      real xfrac
      real floref, flowfactr, flow, fueden, fuedif, fuewt, funnel,
     &     oxgnovpr, phvalue, ppor, r0z, radu, radsg, rhouz, rpor, rr
      real wetfrac, simtimex, sumre1, sumre2, sumre3, rlrate1,
     &     rlrate2, rlrate3, tcan, tcaqu, tflo, tftc, thclad, time1,
     &     tleach, tlt, trid, ttemp
      real amwp1, amwp2, amwp3
      real wleach, ws, xco, xcon, yco, sftime
      integer nbt
      integer i, ib, ie, imax, imodel, it, iz, izone, j, jb, je, jmax,
     &        m, maxi, maxj, maxmem, maxnuc, maxnxm, maxste, maxtim
      integer mtot, icfcon, nelem, nr, ntemp, ntflo, nzones,
     &        iscon
      real dtinit, dtmax, dtmin, eps, tiny
      real wplen, wpdia, driftdia, xvol, dintl, xlintl
cssss     REAL*8 alam, atoms, atall, am
      real alam, atoms, atall, am
C*** End of declarations inserted by SPAG
C-----------------------------------------------------------------------
      parameter (maxmem=10)
      parameter (maxnuc=50)
      parameter (maxste=300)
      parameter (maxtim=500)
      parameter (maxnxm=maxnuc*maxmem)
      parameter (maxi=20, maxj=30)

      common /ccont2/ deffrac
      common /ccont5/ sftime, iscon
      common /ccoro1/ cftime, tcaqu, icfcon
      common /cgeom / cvol, xcon, funnel, mtot
      common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                ccfr(maxnuc, maxmem), tleach, nelem,
     &                amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                amassl(maxnuc), tlt, tftc
      common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi, 4),
     &                rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                ppor(maxi)
      common /array1/ sumre1(maxnuc, maxmem, maxste),
     &                sumre2(maxnuc, maxmem, maxste),
     &                sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                rlrate1(maxnuc, maxmem, maxste),
```

```
     &                 rlrate2(maxnuc, maxmem, maxste),
     &                 rlrate3(maxnuc, maxmem, maxste),
     &                 amwp1(maxnuc, maxmem, maxste),
     &                 amwp2(maxnuc, maxmem, maxste),
     &                 amwp3(maxnuc, maxmem, maxste)
      common /cnume1/ simtimex, imax, jmax
      common /cnume2/ xco(maxi), nzones, izone(maxi, maxj)
      common /cnum3 / diff(maxi)
      common /ctherO/ ntemp
      common /crhyd1/ rpor(maxi), flowfactr, flow, tflo(maxtim),
     &                 floref(maxtim)
      common /cther1/ ttemp(maxtim), tcan(maxtim)
      common /cther2/ ctemp
      common /cwast1/ fuewt, fueden, fuedif, fuepor, amassc
      common /rcarbon1/ rOz, rhouz, radu, radsg
      common /rcarbon2/ cfuel, czmetal, czoxide, cgap
      character*32 , temfil, elefil, hydfil
      common /leach / imodel, phvalue, oxgnovpr, cco3, xfrac
      common /leach1/ wetfrac
      common /rkutta/ eps, tiny, dtinit, dtmin, dtmax
      common /outpt / nbt
      common /wpvol / wplen, wpdia, driftdia, xvol, dintl, xlintl
      real tave(maxtim)
      integer nunit(9)
C-----------------------------------------------------------------------

c     Nomenclature:

C     amassc:         initial mass of uranium oxide fuel, kg
C     cco3:           carbonate concentration [moles/liter]
C     cftime:         corrosion failure time [y]
C     cfuel:          ci of c14 / kg of fuel in fuel
C     cgap:           ci of c14 / kg of fuel in grain boundary and gap
C     ctemp:          crit. temp.[C] for the onset of liquid flow  around wp
C     cvol:           cell volume
C     czmetal:        ci of c14 / kg of fuel in zirconium cladding
C     czoxide:        ci of c14 / kg of fuel in initial zirc. oxide and crud
C     deffrac:        fraction of initially failed packages
C     dcoefm:         mol. diffusion coeficient for pack and rock [m^2/yr]
C     dr:             delta x
c     fuepor:         porosity in between SF particles
C     floref:         reference flow at tflo
C     flowfactr:      flow loading in a cell
c     flow:           same as floref(1)
C     fueden:         fuel density
C     fuedif:         fuel diffusion coefficient
C     fuewt:          formula wt for spent fuel
C     funnel:         area above wp where water is assumed to funnel
C     oxgnovpr:       dissolved oxygen (0.002-0.2 atm overpressure)
c     phvalue:        pH
C     ppor:           porosity of packing
C     rOz:            initial radius of uo2 grain, m
C     radu:           radius of uo2 fragment, m
C     radsg:          subgrain radius after transgranular fracture [m]
C     rhouz:          density of uo2 kg mole/m^3
C     rpor:           porosity:: three layers damaged, disturbed, host rock
C     wetfrac:        the fractional liuid level in the wp below which
c                     the waste matrix is wet
C     simtimex:       maximum simulation time [y]
C     sumre(1,2,3):   release history:1=defective,2=scenario,3=normal
```

```
C                       failure in the cell, the results are overwritten in
C                       sumrel(maxnuc,maxmem,time step)
C       rlrate(1,2,3):  release rate history:1=defective,2=scenario,3=normal
C                       failure in the cell, the results are overwritten in
C                       rlrate(maxnuc,maxmem,time step)
C       tcan(time,cell):wp surface temp at above times
C       tcaqu:          time at which aqueous condition begins in  the cell
C       tflo:           time of table entry i for floref
C       thclad:         thickness of cladding, m
C       time1,2,3:      times corresponding to releases for each type of
C                       container failure
C       ttemp(time):    times in table at which temperatures are given
C       xco:            x (or r) coordinates
C       xcon:           num of packages in a cell
C       yco:            y (or theta) coordinates
C       sftime:         time at which scenario causes wp failures in a cell
c       nbt:            output time interval
C       imax:           nodes in x (or r) direction
c       imodel:         an index for identifying leaching rate model
C       izone(i,j):     zone number of node (i,j)
c       iz:             zone identifier
c       ib:             beginning x-node for a zone
c       jb:             beginning y-node for a zone
c       ie:             ending x-node for a zone
c       je:             ending y-coordinate for a zone
C       jmax:           nodes in y (or theta) direction
C       maxi:           max number of x- or r-dir nodes
C       maxj:           max number of y- or theta dir nodes
C       maxmem:         max number of enteries in table: age, prob of failure
C       maxnuc:         max number of isotopes
C       maxste:         max number of time steps
C       maxtim:         max (time-data set) values
C       mtot:           total number of containers in the cell
C       icfcon:         number failed containers in the cell due to corrosion
C       nr:             number of zones for diffusion cal. (same as imax)
C       ntemp:          num of entries in time versus temp table
C       ntflo:          num of entries in flow table
C       nzones:         number of material zones
C       iscon:          integer variable of the same thing
c       dtinit:         initial time step used in the R-K algorithm
c       dtmax:          maximum allowed timestep
c       dtmin:          minimum allowed timestep
C       eps:            integration accuracy for runge kutta integration
c       tiny:           a small number needed for odeint subroutine
c       wplen:          wp length [m]
C       wpdia:          diameter of waste package [m]
c       xvol:           interior volume of the wp [m^3]
c       dintl:          internal diameter of the wp [m]
c       xlintl:         internal length of the wp [m]

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

C-->    unit numbers for i/o

        nunit(1) = 5
        nunit(2) = 6
        nunit(3) = 10
```

```
        nunit(4) = 11
        nunit(5) = 12
        nunit(6) = 13
        nunit(7) = 14
        nunit(8) = 16
        nunit(9) = 17
        open (unit=4, file='release.inp', status='old')
C-----------------------------------------------------------------------

C==>    cell parameters

C-->    read # of waste packages/cell,  scenario failure WPs,
c       time of scenario failure, and # of defective (pre-failed) WPs
        read (4, *)
        read (4, *)
        read (4, *)
        read (4, *) xcon
        read (4, *) iscon
        read (4, *) sftime
        read (4, *) deffrac
        write (1, *) 'xcon,deffrac=', xcon, deffrac

        mtot = int(xcon + 0.05)

C==>    waste package size

C-->    read radius of the sphere with equivalent surface area as that
c       of the WP and the maximum volume before WP water overflows

        read (4, *)
        read (4, *)
        read (4, *) dintl, xlintl
        read (4, *) xvol
        write (1, *)
        write (1, *) 'xvol, dintl, xlintl=', xvol, dintl, xlintl

C==>    environmental parameters

C-->    thermal

C       temperature and rel humidity data as a function of time
C       ttemp: time;  tcan: ave temp
C       filename is temphumd.dat:- four values per row
C       (time, wp surface temp, drift wall temp, relative humidity)
        read (4, *)
        read (4, *)
        read (4, *) temfil
        write (1, *) 'name of temeprature file- ', temfil
        open (nunit(3), file=temfil, status='old')
        read (nunit(3), *) simtimex
        read (nunit(3), *) ntemp
        read (nunit(3), *)
        write (1, *) 'ntemp=', ntemp
        write (1, *) 'it    ttemp       tcan      tave         humd'

        do 100 it = 1, ntemp
          read (nunit(3), *) it, ttemp(it), tcan(it), tave(it)
          write (1, *) it, ttemp(it), tcan(it), tave(it)
  100   continue
```

```
      read (nunit(3), *) cftime
      write(1,*) 'corrosion failure time cftime[yr]=', cftime

c     passing wp dimensions (for this version)

      read (nunit(3), *) wplen, wpdia
      write (1, *) 'wp dia and length [m]=', wplen, wpdia

C-->  read ctemp: crit. temp.[C] for the onset of liquid flow  around wp

      read (4, *) ctemp
      write (1, *) 'ctemp=', ctemp

C==>  liquid flow rate

      read (4, *)
      read (4, *)
      read (4, *) hydfil
      read (4, *) funnel

C-->  read infiltration and load factors from 'floebs.dat'
c     ntflo is hardwired until future development

      ntflo = 2
      open (nunit(5), file=hydfil, status='old')
      read (nunit(5), *) flowfactr

      do 200 i = 1, ntflo
        read (nunit(5), *) tflo(i), floref(i)
        write (1, *) 'i,tflo,floref=', i, tflo(i), floref(i)
  200 continue

c     assigned the flow rate at time =0 as the steady state flow rate
c     in this version of EBSPAC
      flow = floref(1)

      write (1, *) 'ntflo=', ntflo
      write (1, *) 'flow=', flow
      write (1, *) 'flowfactr=', flowfactr

C==>  waste material

C-->  spent fuel properties

C     read amount of SF in a WP [kg], SF mol. wt, SF density, SF diffusion
c      coefficient??, SF porosity
      read (4, *)
      read (4, *)
      read (4, *)
      read (4, *) amassc
      read (4, *) fuewt, fueden, fuedif, fuepor
      write (1, *) 'amassc=', amassc
      write (1, *) 'fuewt=', fuewt
      write (1, *) 'fueden=', fueden
      write (1, *) 'fuedif=', fuedif
      write (1, *) 'fuepor=', fuepor

C==>  SF leaching parameters

      read (4, *)
```

```
      read (4, *)
      read (4, *) imodel, phvalue, oxgnovpr, cco3, wetfrac
      write (1, *) 'imodel,phvalue,oxgnovpr,cco3,wetfrac=', imodel,
     &             phvalue, oxgnovpr, cco3, wetfrac

C-->  nuclide inventory

C     read nuclide inventory from 'ebspac.nuc' file.
C     nuclide names from the file 'ebspac.nuc'

      read (4, *)
      read (4, *)
      read (4, *) elefil
      write (1, *) elefil

C-->  read properties of radionuclides from a table with four
C     columns: nuclide name, half life,specific activity,
C     and parent-daughter relationship.parent=1,daughter=11,111,1111 etc.
C     these are independent of time and cell numbers

      call rdelem(nunit(9), elefil)

C==>  Parameters for C-14 gas release

C     data provided for r0,rhou,dref1,e,oxz,
C     radu,thclad,cfuel,czmetal,czoxide,cgap

      read (4, *)
      read (4, *)
      read (4, *) r0z
      read (4, *) rhouz
      read (4, *) radu
      read (4, *) radsg
      read (4, *) thclad
      read (4, *) cfuel
      read (4, *) czmetal
      read (4, *) czoxide
      read (4, *) cgap
      write (1, *) 'r0z, rhouz, radu,radsg', r0z, rhouz, radu, radsg
      write (1, *) 'thclad, cfuel, czmetal, czoxide, cgap', thclad,
     &             cfuel, czmetal, czoxide, cgap

C==>  grid and time step info

C-->  spatial grid

      read (4, *)
      read (4, *)
      read (4, *)
      read (4, *)
      read (4, *) imax, jmax
      write (1, *) 'imax=', imax
      write (1, *) 'jmax=', jmax

      nr = imax

C-->  read x-coordinates

      read (4, *)
      read (4, *) (xco(i), i=1, imax)
```

```
      dr(1) = xco(1)

      do 300 i = 2, nr
        dr(i) = xco(i) - xco(i - 1)
  300 continue

C-->  read y-coordinates

      read (4, *)
      read (4, *) (yco, i=1, jmax)

C-->  set zones (material types)
C     syntax: zone  1 from (2,2) to (5,5)

      read (4, *)
      read (4, *)
      read (4, *) nzones

      do 400 m = 1, nzones
        read (4, *) iz, ib, jb, ie, je
        do 350 j = jb, je
          do 320 i = ib, ie
            izone(i, j) = iz
  320     continue
  350   continue
  400 continue

C====  rock and backfill hydrological parameters

c     rpor(zone): porosity is assumed to be constant in time
c     zone 1 is teh backfill zone
C     porosity is assumed to be constant in time
C     porosity = 1 means air gap between wp and drift

      read (4, *)
      read (4, *)
      read (4, *) (rpor(i), i=1, nzones)
      write (1, *) 'rpor(i):', (rpor(i), i=1, nzones)


C==>  Radionuclide transport properties

C-->  diffusion coefficients in rock

      read (4, *)
      read (4, *)
      read (4, *) (diff(i), i=1, 4)

c-->  drift diameter

      read (4, *) driftdia

C==>  parameters to control solution algorithm

      read (4, *)
      read (4, *)
      read (4, *) dtinit, dtmin, dtmax
      read (4, *) eps, tiny

c-->  parameters for results output
```

```
      read (4, *)
      read (4, *)
      read (4, *) nbt

      return
      end
**==RDELEM.spg  processed by SPAG 4.00Aa at 19:35 on  9 Dec 1996




      subroutine rdelem(unit, elefil)
      implicit none
cssss     IMPLICIT NONE
C*--------------------------------------------------------------------
c       module to input the radionuclide inventory and properties
C*--------------------------------------------------------------------
C*** Start of declarations inserted by SPAG
      real amass, amassl, ccfr, ci1000, con3, con4, cstore, dcoefm,
     &      dr, rr, sumre1, sumre2, sumre3, rlrate1, rlrate2, rlrate3,
     &      tftc, time1, tleach, tlt, trid, wleach
      real amwp1, amwp2, amwp3
      real ws
      real ppor
      integer i, ielem, inuc, k, l, maxele, maxi, maxmem, maxnuc,
     &        maxnxm, maxste, nelem, nn, nr
      integer unit
      integer ncon, kcon, icon, nchns, ni
      real sol, rd, rde, amall, halflife, curall, fggap
cssss     REAL*8 alam, atoms, atall, am
      real alam, atoms, atall, am
C*** End of declarations inserted by SPAG
C*--------------------------------------------------------------------
      parameter (maxele=50)
      parameter (maxmem=10)
      parameter (maxnuc=50)
      parameter (maxste=300)
      parameter (maxnxm=maxnuc*maxmem)
      parameter (maxi=20)
      character*(*) elefil
      character*3 elem
      character*6 namall
      common /cnucl1/ elem(maxele), namall(maxnuc, maxmem)
      common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
     &                amall(maxnuc, maxmem), halflife(maxnuc, maxmem),
     &                curall(maxnuc, maxmem), fggap(maxnuc, maxmem),
     &                kcon(maxele, maxnuc), icon(maxele, maxnuc),
     &                rd(maxnuc, maxmem), ni(maxnuc), nchns,
     &                ci1000(maxnuc, maxmem)
      common /cnucl3/ atall(maxnuc, maxmem), alam(maxnuc, maxmem),
     &                atoms(maxnuc, maxmem), am(maxnuc, maxmem),
     &                ccfr(maxnuc, maxmem), tleach, nelem,
     &                amass(maxnuc, maxmem), wleach(maxnuc, maxmem),
     &                amassl(maxnuc), tlt, tftc
      common /difrel1/con3, con4, cstore(maxnxm, maxi), trid(maxi,4),
     &                rr(maxi), dr(maxi), ws(maxi), nr, dcoefm(maxi),
     &                ppor(maxi)
      common /array1/ sumre1(maxnuc, maxmem, maxste),
```

```
     &                 sumre2(maxnuc, maxmem, maxste),
     &                 sumre3(maxnuc, maxmem, maxste), time1(maxste),
     &                 rlrate1(maxnuc, maxmem, maxste),
     &                 rlrate2(maxnuc, maxmem, maxste),
     &                 rlrate3(maxnuc, maxmem, maxste),
     &                 amwp1(maxnuc, maxmem, maxste),
     &                 amwp2(maxnuc, maxmem, maxste),
     &                 amwp3(maxnuc, maxmem, maxste)
C-----------------------------------------------------------------------
c
c       Nomenclature:
c
C       maxi:           max number of x- or r-dir nodes
C       namall:         the radionuclide name
C       maxele:         max number of elements (radionuclides)
C       maxnuc:         max number of isotopes
C       maxmem:         max number of enteries in table: age, prob of failure
C       maxste:         max number of time steps
C       maxtim:         max (time-data set) values
c       nelem:          number of elements
c       elefil:         parameter to read radionuclide inventory file
c       elem(ielem):    name of all element (different from namall)
c       ielem:          element identifier
c       ncon(ielem):    number of chains in which isotopes of element ielem occurs
c       sol(ielem):     solubility limit of elemets
c       rde(ielem):     retardation factor for elements
c       kcon(ielem,l):  chain identifier among all chains in which element ielem
c                       occurs; l is the index for all chains with ielem
c       icon(ielem,l):  position of ielem in the chain kcon(ielem,l)
c       rd:             retardation factor for nuclides (same as elements)
c       nchns:          number of chains
c       ni(i):          size of chains
c       namall(k,i):    name of all radionuclides
c       amall:          molecular weight of radionuclides
c       halflife:       half life of radionuclides [yr]
c       curall          radionuclide inventory per WP in curies
c       fggap:          gap fraction of each radionuclide
c       inuc:           a counter for counting the number of nuclides

C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC
c-->    open file for radionuclide inventory, elefil is the
c       file name parameter

        open (unit=unit, file=elefil, status='old')

c       read number of elements

        read (unit, *) nelem

        do 100 ielem = 1, nelem

c          read element name, num.chains in which it appears, and
c          solubility gram moles/liter,and retardation coefficient

           read (unit, 9001) elem(ielem), ncon(ielem), sol(ielem),
     &                       rde(ielem)
          write (1, *) 'ielem,elem,ncon,sol,rde', ielem, elem(ielem),
```

```
     &                ncon(ielem), sol(ielem), rde(ielem)

c          read l and ielem locations in chains of all same elements

           do 50 l = 1, ncon(ielem)

             read (unit, *) kcon(ielem, l), icon(ielem, l)
             write (1, *) 'ielem,l,kcon(ielem,l),icon(ielem,l)=', ielem,
     &                    l, kcon(ielem, l), icon(ielem, l)

c               fill in the radionuclide retardation from the element

             rd(kcon(ielem,l), icon(ielem,l)) = rde(ielem)

   50      continue
  100    continue

c-->     isotope data

c        read number and size of chains
c
         read (unit, *) nchns, (ni(i), i=1, nchns)

         inuc = 0

c        read atomic wt, name, halflife [yr], inventory [ci], gap fraction

         do 200 k = 1, nchns
           nn = ni(k)
           do 150 i = 1, nn
             read (unit, 9002) amall(k, i), namall(k, i), halflife(k, i),
     &                         curall(k, i), fggap(k, i)
             inuc = inuc + 1
  150      continue
  200    continue

         return
 9001    format (a3, 2x, i5, 2F10.0)
 9002    format (e10.0, 4x, a6, 4E10.0)
         end
**==LINT.spg  processed by SPAG 4.00Aa at 19:35 on  9 Dec 1996




         subroutine lint(xa, ya, n1, n, x, y)
         implicit none
C*** Start of declarations inserted by SPAG
         real h, x, xa, y, ya
         integer k, khi, klo, n, n1
C*** End of declarations inserted by SPAG
c-----------------------------------------------------------------------
c        module for linear interpolation between two specified limits
c-----------------------------------------------------------------------
         dimension xa(n1), ya(n1)
c-----------------------------------------------------------------------
c
c  Nomenclature:
c
c        xa:     vector of length n of x values (independent variable)
```

```
c       ya:     vector of length n of y values
c       n:      length of xa and ya vectors
c       x:      x value at which interpolation is required
c       y:      returned value of dependent variable corresponding to x value
c
c-----------------------------------------------------------------------
        if ( xa(1).lt.xa(n) ) then
c  increasing order list
          if ( x.le.xa(1) ) then
            y = ya(1)
          else if ( x.ge.xa(n) ) then
            y = ya(n)
          else
            klo = 1
            khi = n
   20       continue
            if ( khi - klo.gt.1 ) then
              k = (khi + klo)/2
              if ( xa(k).gt.x ) then
                khi = k
              else
                klo = k
              end if
              go to 20
            end if
            h = xa(khi) - xa(klo)
            if ( h.eq.0. ) pause 'bad xa input.'
            y = ya(klo) + (x - xa(klo))/h*(ya(khi) - ya(klo))
          end if
c  decreasing order list
        else if ( x.ge.xa(1) ) then
          y = ya(1)
        else if ( x.le.xa(n) ) then
          y = ya(n)
        else
          klo = 1
          khi = n
   50     continue
          if ( khi - klo.gt.1 ) then
            k = (khi + klo)/2
            if ( xa(k).lt.x ) then
              khi = k
            else
              klo = k
            end if
            go to 50
          end if
          h = xa(khi) - xa(klo)
          if ( h.eq.0. ) pause 'bad xa input.'
          y = ya(klo) + (x - xa(klo))/h*(ya(khi) - ya(klo))
        end if

        return
        end
```

pcl5

JOB 1786

example_release.inp

For: **scratchy1!mohanty**
Date: **Mon Jan 6 18:09:24 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:41:44 1991
Started: Wed Nov 13 10:41:44 1991

QMS 3825 Print System

```
\input data file for ebspac release code: ebspac_release.f
|
\Cell information
2335.                          ! xcon: number of WP
1000                           ! iscon: # of WP in scenario failure
4500.                          ! sftime: time of  scenario failure [y]
0.00                           ! deffrac: defective fraction of WPs/cell
|
\WP information
1.421, 4.572                   ! dintl: wp ID, xintl: internal length [m]
4.83                           ! xvol: wp internal vol[m3]
|
\Thermal data
'temphumd.dat'                 ! temfil: temp. file (output from ebspac_fail.f)
97.                            ! ctemp: BP of water at atm. condition [C]
|
\Flow parameters
'floebs.dat'                   ! hydfil: flow parameters file
7.                             ! funnel: funnel factor
|
\SF  materials
\
2800.                          ! amassc: SF mass [kg]
250., 10000., 1.0E-08, 0.5     ! fuewt,fueden,fuedif,fuepor
\
\Fuel leaching
2, 9.0, 0.2, 2.e-3, 5.e-1      ! imodel,phvalue,oxgnovpr [atm],cco3 [mol/L],wetfrac
|
\ Radionuclide inventory
'ebspac.nuc'                   ! elefil: nuclide names, halflife,inventory
|
\C-14 generation
0.5e-3                         ! r0z: initial radius of SF particle [m]
37.                            ! rhou: density of SF [kg mole/m^3]
1.e-5                          ! r1z: radius of the SF grain [m]
1.e-6                          ! r2z: subgrain fragment radius after trans. frac. [m]
6.1e-4                         ! thclad: thickness of cladding [m]
7.2e-4                         ! cfuel: c-14 [ci] /kg SF
4.89e-4                        ! czmetal: c-14 [ci] /kg SF in Zry clad & other metals
2.48e-5                        ! czoxide: c-14/kg SF in initial Zry oxide & crud
6.2e-6                         ! cgap: c-14/kg SF in grain and gap
|
\NUMERICAL
\
\Grids
10, 10                         ! imax,jmax: # of grid nodes in i,j directions
\X-COOR of grid nodes
.1, .5, 1.0, 2.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0
\Y-COOR of grid nodes
.1, .5, 1.0, 2.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0
\ Note: zones apply to the above grid, zones are the same for all cell
\ZONES
4                              ! nzones: no. of zones for material types
1    1  1    1  1              ! iz,ib,jb,ie,je: for zone 1
2    2  1    2  1              ! iz,ib,jb,ie,je: for zone 2
3    3  1    3  1              ! iz,ib,jb,ie,je: for zone 3
4    4  1    10 1              ! iz,ib,jb,ie,je: for zone 4
|
\Rock parameters
0.14, 0.34, 0.34, 0.34         ! rpor(1..nzones): rock porosity
```

```
|
\ Radionuclide transport
5.6e-5, 5.6e-5, 5.6e-5, 5.6e-5  ! rdiff(1..nzones):diffusion coef. [m2/yr]
5.0                             ! driftdia [m]
|
\ Solution algorithm control parameters (Runge-Kutta)
25., 0.0, 10.                   ! dtinit [yr], dtmin [yr], dtmax [yr]
1.0e-2, 1.0e-10                 ! eps, tiny
|
\output parameters
200                             ! nbt: number of time intervals for output
|
\END
```

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pcl5

JOB 1774

ebspacrun

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:53:37 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:25:46 1991
Started: Wed Nov 13 10:25:46 1991

QMS
QMS 3825 Print System

QMS 3825 Print System

```
f77 fail.f -o fail.x
f77 -r8 release4.f -o release4.x
rm echo1.out
rm echo2.out
time fail.x > echo1.out
time release4.x > echo2.out
```

pcl5

JOB 1771

example_fail.inp

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:43:02 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:15:11 1991
Started: Wed Nov 13 10:15:11 1991

QMS 3825 Print System

```
\example input file for ebspac_fail
|
\simulation time
10000.                          ! tend: simulation time length [yr]
\                               ! when iflag=1 (defined later)
\
5.682, 1.802                    ! wplen,wpdia: wp length and diameter [m]
0.1, 0.02                       ! cthick1,cthick2: wp layers 1&2 thicknesses [m]
|
\choose source of temperature data
2                               ! iflag 1: emp. equation, 2: tab.data
1                               ! nset (temp.-rel hum. relationship to use
49.9999999                      ! timintv (used when iflag=2)
|
\other temperature parameters
0.                              ! age of fuel (not used in this version)
|
\Dry oxidation of wp outer overpack
5.                              ! grainr: metal grain radius [micrometer]
25                              ! nseries (terms in the infinite series)
0.7e-3                          ! gbthick [micrometer]
1.e-2                           ! constant: used in the dry oxidation equn.
|
\evaporation-condensation
0.65                            ! humdc: critical relative humidity
2.e-3                           ! filmthk: thickness of water film [m]
97.                             ! ctemp: boiling point of water [C]
|
\Corrosion Parameters(Ep: pitting potential [mV]; Erp: repassivation potential [mV])
-584.8                          ! xipto: outer overpack Ep intercept
3.92                            ! pttemo: temp. coef. of outer overpack Ep intercept
-24.5                           ! slpto: outer overpack Ep slope
-1.1                            ! slpttemo: temp. coef. of outer overpack Ep slope
-620.3                          ! xirpo: outer overpack Erp intercept
0.47                            ! rptemo: temp. coef. of outer overpack Erp intercept
-95.2                           ! slrpo: outer overpack Erp slope
0.88                            ! slrptemo: temp. coef. of outer overpack Erp slope
200.                            ! xipti: inner overpack Ep intercept
0.                              ! pttemi: temp. coef. of inner overpack Ep intercept
-240.                           ! slpti: inner overpack Ep slope
0.                              ! slpttemi: temp. coef. of inner overpack Ep slope
422.8                           ! xirpi: inner overpack Erp intercept
-4.1                            ! rptemi: temp. coef. of inner overpack Erp intercept
-64.                            ! slrpi: inner overpack Erp slope
-0.80                           ! slrptemi: temp. coef. of inner overpack Erp slope
0.75, 0.5                       ! betaox1, betahy1: beta kinetics parameters
\                                 for oxygen and water for WP outer overpack
0.75, 0.5                       ! betaox2, betahy2: beta kinetics parameters for
\                                 oxygen and water for WP inner overpack
3.80e12, 1.6e-1                 ! rkox1 [c*m/y/mol], rkhy1 [c/m2/yr]
37300., 25000.                  ! gox1 [J/mol], ghy1 [J/mol]
3.0e10, 3.2                     ! rkox2 [c*m/y/m], rkhy2 [c/m2/yr]
40000., 25000.                  ! gox2 [J/mol], ghy2 [J/mol]
3.15e5, 0.0, 0.0                ! aa(1,1) [C/m2/yr], aa(1,2), aa(1,3)
6.30e4, 0.0, 0.0                ! aa(2,1) [C/m2/yr], aa(2,2), aa(2,3)
-0.46                           ! eexpt: in Vshe
8.66e-3                         ! rcoef:
0.45                            ! rexpont:
2.05e-4                         ! crate2: m/yr corrosion rate
0.0                             ! xcouple, a fractional coupling strength
```

```
0.0                             ! xread
3.e-1                           ! clconc: chloride concentration [mol/L]
3.e-4                           ! clcrit1: crit. chloride conc. for 1st layer [mol/L]
2.e-3                           ! clcrit2: crit. chloride conc. for 2nd layer [mol/L]
100.                            ! cfactor: chloride dilution factor
9.0                             ! refph: reference pH
1.0, 1.0                        ! taus:deposit tortuosity,spor:deposit porosity
|
\Runge-kutta control parameters
1.e-3, 1.e0                     ! dtini, dtmax
1.e-2, 1.e-30                   ! errrel (same as eps), errabs (same as tiny)
|
\end
////2000                               ! nhista (used when iflag=1)
```

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pcl5

JOB 1767

echo1.out

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:39:45 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:11:54 1991
Started: Wed Nov 13 10:11:54 1991

QMS
QMS 3825 Print System

QMS 3825 Print System

EBSPAC (Engineering Barrier System Performance Assessment Code)
This is the part of the code that computes WP Failure Time
Version= 1.0
Mon Jan 6 17:36:57 1997

CALCULATION OF WASTE PACKAGE FAILURE TIME

end of simulation time [yr]: 10000.
No. of rows of data to pass to release.f: 196

ilayer	tstop [yr]	tcan [C]	ecrit [Vshe]	ecorr [Vshe]	chloride flag	rthick [m]	mode
1	50.42	161.90	0.0000	0.0000	0	1.1999993E-01	dry oxd
1	100.50	155.60	0.0000	0.0000	0	1.1999986E-01	dry oxd
1	152.40	150.70	0.0000	0.0000	0	1.1999980E-01	dry oxd
1	206.00	147.40	0.0000	0.0000	0	1.1999974E-01	dry oxd
1	259.40	145.80	0.0000	0.0000	0	1.1999968E-01	dry oxd
1	312.80	144.70	0.0000	0.0000	0	1.1999962E-01	dry oxd
1	366.20	143.90	0.0000	0.0000	0	1.1999956E-01	dry oxd
1	419.70	143.00	0.0000	0.0000	0	1.1999950E-01	dry oxd
1	473.10	142.30	0.0000	0.0000	0	1.1999944E-01	dry oxd
1	533.80	141.00	0.0000	0.0000	0	1.1999938E-01	dry oxd
1	585.70	139.90	0.0000	0.0000	0	1.1999932E-01	dry oxd
1	637.50	138.80	0.0000	0.0000	0	1.1999926E-01	dry oxd
1	689.30	137.70	0.0000	0.0000	0	1.1999920E-01	dry oxd
1	741.10	136.60	0.0000	0.0000	0	1.1999914E-01	dry oxd
1	793.00	135.60	0.0000	0.0000	0	1.1999908E-01	dry oxd
1	844.80	134.60	0.0000	0.0000	0	1.1999902E-01	dry oxd
1	896.60	133.70	0.0000	0.0000	0	1.1999896E-01	dry oxd
1	948.40	132.70	0.0000	0.0000	0	1.1999890E-01	dry oxd
1	1000.00	131.80	0.0000	0.0000	0	1.1999884E-01	dry oxd
1	1065.00	130.50	0.0000	0.0000	0	1.1999878E-01	dry oxd
1	1129.00	129.30	0.0000	0.0000	0	1.1999872E-01	dry oxd
1	1194.00	128.00	0.0000	0.0000	0	1.1999866E-01	dry oxd
1	1258.00	126.80	0.0000	0.0000	0	1.1999860E-01	dry oxd
1	1323.00	125.60	0.0000	0.0000	0	1.1999854E-01	dry oxd
1	1388.00	124.40	0.0000	0.0000	0	1.1999848E-01	dry oxd
1	1452.00	123.30	0.0000	0.0000	0	1.1999842E-01	dry oxd
1	1517.00	122.10	0.0000	0.0000	0	1.1999836E-01	dry oxd
1	1581.00	121.00	0.0000	0.0000	0	1.1999830E-01	dry oxd
1	1646.00	119.90	0.0000	0.0000	0	1.1999824E-01	dry oxd
1	1710.00	118.80	0.0000	0.0000	0	1.1999818E-01	dry oxd
1	1775.00	117.70	0.0000	0.0000	0	1.1999813E-01	dry oxd
1	1839.00	116.70	0.0000	0.0000	0	1.1999807E-01	dry oxd
1	1904.00	115.60	0.0000	0.0000	0	1.1999801E-01	dry oxd
1	1986.00	114.40	0.0000	0.0000	0	1.1999795E-01	dry oxd
1	2036.00	113.60	0.0000	0.0000	0	1.1999789E-01	dry oxd
1	2086.00	112.90	0.0000	0.0000	0	1.1999783E-01	dry oxd
1	2136.00	112.30	0.0000	0.0000	0	1.1999777E-01	dry oxd
1	2186.00	111.60	0.0000	0.0000	0	1.1999771E-01	dry oxd
1	2236.00	111.00	0.0000	0.0000	0	1.1999765E-01	dry oxd
1	2286.00	110.30	0.0000	0.0000	0	1.1999759E-01	dry oxd
1	2336.00	109.70	0.0000	0.0000	0	1.1999753E-01	dry oxd
1	2386.00	109.10	-0.5694	0.1950	1	6.8837903E-02	local
1	2436.00	108.50	-0.5695	0.1945	1	5.0405446E-02	local
1	2486.00	107.90	-0.5695	0.1940	1	3.6636310E-02	local
1	2536.00	107.30	-0.5695	0.1935	1	2.5225966E-02	local
2	2586.00	106.80	0.0631	0.1932	1	1.4995669E-02	local
2	2636.00	106.20	0.0653	0.1932	1	4.7456686E-03	local
2	2686.00	105.70	0.0671	0.1932	1	-5.5043314E-03	local

```
                wp wetting time [yr]:       2336.
                wp failure time [yr]:       2636.
      penetration by dry oxidation [m]:     2.467E-06
                echoed inpot data in:       echo_fail.dat
              output data are in files:     temphumd.dat and corrode.out
```

14/6/95

pcl5

JOB 1768

temphumd.dat

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:40:03 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:12:11 1991
Started: Wed Nov 13 10:12:11 1991

QMS 3825 Print System

10000.0000000000
196

i	timr	tcan	tavg	humd
1	0.0002	21.8700	21.0000	0.9480
2	50.4200	161.9000	147.6000	0.1399
3	100.5000	155.6000	146.4000	0.1645
4	152.4000	150.7000	143.8000	0.1872
5	206.0000	147.4000	141.6000	0.2046
6	259.4000	145.8000	140.7000	0.2138
7	312.8000	144.7000	140.0000	0.2203
8	366.2000	143.9000	139.6000	0.2253
9	419.7000	143.0000	139.1000	0.2310
10	473.1000	142.3000	138.6000	0.2355
11	533.8000	141.0000	137.6000	0.2443
12	585.7000	139.9000	136.7000	0.2520
13	637.5000	138.8000	135.8000	0.2600
14	689.3000	137.7000	134.9000	0.2683
15	741.1000	136.6000	133.9000	0.2770
16	793.0000	135.6000	133.0000	0.2851
17	844.8000	134.6000	132.2000	0.2935
18	896.6000	133.7000	131.3000	0.3014
19	948.4000	132.7000	130.5000	0.3104
20	1000.0000	131.8000	129.6000	0.3187
21	1065.0000	130.5000	128.5000	0.3313
22	1129.0000	129.3000	127.3000	0.3434
23	1194.0000	128.0000	126.2000	0.3572
24	1258.0000	126.8000	125.0000	0.3705
25	1323.0000	125.6000	123.9000	0.3843
26	1388.0000	124.4000	122.8000	0.3988
27	1452.0000	123.3000	121.7000	0.4126
28	1517.0000	122.1000	120.6000	0.4284
29	1581.0000	121.0000	119.5000	0.4435
30	1646.0000	119.9000	118.5000	0.4592
31	1710.0000	118.8000	117.4000	0.4755
32	1775.0000	117.7000	116.4000	0.4926
33	1839.0000	116.7000	115.4000	0.5087
34	1904.0000	115.6000	114.4000	0.5272
35	1986.0000	114.4000	113.1000	0.5483
36	2036.0000	113.6000	112.4000	0.5629
37	2086.0000	112.9000	111.7000	0.5760
38	2136.0000	112.3000	111.1000	0.5876
39	2186.0000	111.6000	110.4000	0.6014
40	2236.0000	111.0000	109.8000	0.6136
41	2286.0000	110.3000	109.2000	0.6282
42	2336.0000	109.7000	108.6000	0.6410
43	2386.0000	109.1000	108.0000	0.6541
44	2436.0000	108.5000	107.4000	0.6675
45	2486.0000	107.9000	106.8000	0.6813
46	2536.0000	107.3000	106.3000	0.6954
47	2586.0000	106.8000	105.7000	0.7074
48	2636.0000	106.2000	105.1000	0.7221
49	2686.0000	105.7000	104.6000	0.7347
50	2736.0000	105.1000	104.1000	0.7501
51	2786.0000	104.6000	103.5000	0.7632
52	2836.0000	104.0000	103.0000	0.7793
53	2886.0000	103.5000	102.5000	0.7930
54	2936.0000	103.0000	102.0000	0.8070
55	2986.0000	102.5000	101.5000	0.8213
56	3036.0000	102.0000	101.0000	0.8359
57	3086.0000	101.6000	100.6000	0.8478

58	3136.0000	101.1000	100.1000	0.8630
59	3186.0000	100.7000	99.6900	0.8753
60	3236.0000	100.3000	99.2700	0.8879
61	3286.0000	99.8400	98.8500	0.9026
62	3336.0000	99.4300	98.4500	0.9160
63	3386.0000	99.0300	98.0500	0.9292
64	3436.0000	98.6300	97.6600	0.9427
65	3486.0000	98.2500	97.2800	0.9557
66	3536.0000	97.8700	96.9000	0.9654
67	3586.0000	97.5000	96.5300	0.9653
68	3636.0000	97.1300	96.1700	0.9656
69	3686.0000	96.7700	95.8200	0.9659
70	3736.0000	96.4200	95.4700	0.9658
71	3786.0000	96.0800	95.1200	0.9654
72	3836.0000	95.7400	94.7900	0.9657
73	3886.0000	95.4000	94.4500	0.9656
74	3936.0000	95.0700	94.1300	0.9659
75	3986.0000	94.7500	93.8100	0.9658
76	4036.0000	94.4300	93.4900	0.9657
77	4086.0000	94.1100	93.1800	0.9660
78	4136.0000	93.8000	92.8700	0.9660
79	4186.0000	93.5000	92.5700	0.9659
80	4236.0000	93.2000	92.2700	0.9658
81	4286.0000	92.9000	91.9800	0.9661
82	4336.0000	92.6100	91.6900	0.9661
83	4386.0000	92.3300	91.4100	0.9660
84	4436.0000	92.0400	91.1300	0.9663
85	4486.0000	91.7600	90.8500	0.9663
86	4536.0000	91.4900	90.5800	0.9662
87	4586.0000	91.2200	90.3100	0.9662
88	4636.0000	90.9500	90.0500	0.9665
89	4686.0000	90.6900	89.7900	0.9664
90	4736.0000	90.4300	89.5300	0.9664
91	4786.0000	90.1700	89.2700	0.9663
92	4836.0000	89.9200	89.0200	0.9662
93	4886.0000	89.6700	88.7800	0.9666
94	4936.0000	89.4300	88.5300	0.9661
95	4986.0000	89.1800	88.2900	0.9665
96	5036.0000	88.9400	88.0500	0.9664
97	5086.0000	88.7000	87.8100	0.9664
98	5136.0000	88.4600	87.5700	0.9663
99	5186.0000	88.2200	87.3400	0.9666
100	5236.0000	87.9800	87.1100	0.9670
101	5286.0000	87.7500	86.8800	0.9669
102	5336.0000	87.5200	86.6500	0.9669
103	5386.0000	87.2900	86.4200	0.9668
104	5436.0000	87.0600	86.2000	0.9672
105	5486.0000	86.8400	85.9800	0.9671
106	5536.0000	86.6200	85.7600	0.9671
107	5586.0000	86.4000	85.5400	0.9670
108	5636.0000	86.1800	85.3200	0.9670
109	5686.0000	85.9600	85.1100	0.9673
110	5736.0000	85.7500	84.9000	0.9673
111	5786.0000	85.5400	84.6900	0.9672
112	5836.0000	85.3300	84.4800	0.9672
113	5886.0000	85.1200	84.2800	0.9675
114	5936.0000	84.9200	84.0700	0.9671
115	5986.0000	84.7100	83.8700	0.9674
116	6036.0000	84.5100	83.6700	0.9674
117	6086.0000	84.3100	83.4800	0.9677

118	6136.0000	84.1100	83.2800	0.9677
119	6186.0000	83.9200	83.0900	0.9676
120	6236.0000	83.7200	82.9000	0.9680
121	6286.0000	83.5300	82.7100	0.9680
122	6336.0000	83.3400	82.5200	0.9679
123	6386.0000	83.1500	82.3300	0.9679
124	6436.0000	82.9700	82.1500	0.9678
125	6486.0000	82.7800	81.9600	0.9678
126	6536.0000	82.6000	81.7800	0.9678
127	6586.0000	82.4200	81.6000	0.9677
128	6636.0000	82.2400	81.4300	0.9681
129	6686.0000	82.0600	81.2500	0.9680
130	6736.0000	81.8800	81.0700	0.9680
131	6786.0000	81.7100	80.9000	0.9680
132	6836.0000	81.5300	80.7300	0.9683
133	6886.0000	81.3600	80.5600	0.9683
134	6936.0000	81.1900	80.3900	0.9683
135	6986.0000	81.0200	80.2200	0.9682
136	7036.0000	80.8500	80.0600	0.9686
137	7086.0000	80.6900	79.8900	0.9682
138	7136.0000	80.5200	79.7300	0.9685
139	7186.0000	80.3600	79.5700	0.9685
140	7236.0000	80.1900	79.4100	0.9688
141	7286.0000	80.0300	79.2500	0.9688
142	7336.0000	79.8700	79.0900	0.9688
143	7386.0000	79.7200	78.9300	0.9684
144	7436.0000	79.5600	78.7800	0.9687
145	7486.0000	79.4000	78.6200	0.9687
146	7536.0000	79.2500	78.4700	0.9687
147	7586.0000	79.1000	78.3200	0.9686
148	7636.0000	78.9400	78.1700	0.9690
149	7686.0000	78.7900	78.0200	0.9690
150	7736.0000	78.6400	77.8700	0.9689
151	7786.0000	78.4900	77.7200	0.9689
152	7836.0000	78.3500	77.5800	0.9689
153	7886.0000	78.2000	77.4300	0.9688
154	7936.0000	78.0600	77.2900	0.9688
155	7986.0000	77.9100	77.1500	0.9692
156	8036.0000	77.7700	77.0100	0.9692
157	8086.0000	77.6300	76.8700	0.9691
158	8136.0000	77.4900	76.7300	0.9691
159	8186.0000	77.3500	76.5900	0.9691
160	8236.0000	77.2100	76.4500	0.9690
161	8286.0000	77.0700	76.3200	0.9694
162	8336.0000	76.9400	76.1800	0.9690
163	8386.0000	76.8000	76.0500	0.9694
164	8436.0000	76.6700	75.9100	0.9689
165	8486.0000	76.5300	75.7800	0.9693
166	8536.0000	76.4000	75.6500	0.9693
167	8586.0000	76.2700	75.5200	0.9693
168	8636.0000	76.1400	75.3900	0.9692
169	8686.0000	76.0100	75.2600	0.9692
170	8736.0000	75.8800	75.1400	0.9696
171	8786.0000	75.7500	75.0100	0.9696
172	8836.0000	75.6200	74.8800	0.9695
173	8886.0000	75.5000	74.7600	0.9695
174	8936.0000	75.3700	74.6400	0.9699
175	8986.0000	75.2500	74.5100	0.9695
176	9036.0000	75.1200	74.3900	0.9698
177	9086.0000	75.0000	74.2700	0.9698

178	9136.0000	74.8800	74.1500	0.9698
179	9186.0000	74.7600	74.0300	0.9698
180	9236.0000	74.6400	73.9100	0.9698
181	9286.0000	74.5200	73.7900	0.9697
182	9336.0000	74.4000	73.6700	0.9697
183	9386.0000	74.2800	73.5600	0.9701
184	9436.0000	74.1600	73.4400	0.9701
185	9486.0000	74.0500	73.3200	0.9696
186	9536.0000	73.9300	73.2100	0.9700
187	9586.0000	73.8200	73.1000	0.9700
188	9636.0000	73.7000	72.9800	0.9700
189	9686.0000	73.5900	72.8700	0.9700
190	9736.0000	73.4800	72.7600	0.9699
191	9786.0000	73.3600	72.6500	0.9703
192	9836.0000	73.2500	72.5400	0.9703
193	9886.0000	73.1400	72.4300	0.9703
194	9936.0000	73.0300	72.3200	0.9703
195	9986.0000	72.9200	72.2100	0.9702
196	10000.0000	72.8900	72.1800	0.9702

2636.0000000000

5.6820000000000

1.8020000000000

151/195

pcl5

JOB 1769

corrode.out

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:40:15 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:12:34 1991
Started: Wed Nov 13 10:12:34 1991

QMS 3825 Print System

ilayer	tstop [yr]	tcan [C]	ecrit [Vshe]	ecorr [Vshe]	chloride flag	rthick [m]	mode
1	50.42	161.90	0.0000	0.0000	0	1.1999993E-01	
1	100.50	155.60	0.0000	0.0000	0	1.1999986E-01	
1	152.40	150.70	0.0000	0.0000	0	1.1999980E-01	
1	206.00	147.40	0.0000	0.0000	0	1.1999974E-01	
1	259.40	145.80	0.0000	0.0000	0	1.1999968E-01	
1	312.80	144.70	0.0000	0.0000	0	1.1999962E-01	
1	366.20	143.90	0.0000	0.0000	0	1.1999956E-01	
1	419.70	143.00	0.0000	0.0000	0	1.1999950E-01	
1	473.10	142.30	0.0000	0.0000	0	1.1999944E-01	
1	533.80	141.00	0.0000	0.0000	0	1.1999938E-01	
1	585.70	139.90	0.0000	0.0000	0	1.1999932E-01	
1	637.50	138.80	0.0000	0.0000	0	1.1999926E-01	
1	689.30	137.70	0.0000	0.0000	0	1.1999920E-01	
1	741.10	136.60	0.0000	0.0000	0	1.1999914E-01	
1	793.00	135.60	0.0000	0.0000	0	1.1999908E-01	
1	844.80	134.60	0.0000	0.0000	0	1.1999902E-01	
1	896.60	133.70	0.0000	0.0000	0	1.1999896E-01	
1	948.40	132.70	0.0000	0.0000	0	1.1999890E-01	
1	1000.00	131.80	0.0000	0.0000	0	1.1999884E-01	
1	1065.00	130.50	0.0000	0.0000	0	1.1999878E-01	
1	1129.00	129.30	0.0000	0.0000	0	1.1999872E-01	
1	1194.00	128.00	0.0000	0.0000	0	1.1999866E-01	
1	1258.00	126.80	0.0000	0.0000	0	1.1999860E-01	
1	1323.00	125.60	0.0000	0.0000	0	1.1999854E-01	
1	1388.00	124.40	0.0000	0.0000	0	1.1999848E-01	
1	1452.00	123.30	0.0000	0.0000	0	1.1999842E-01	
1	1517.00	122.10	0.0000	0.0000	0	1.1999836E-01	
1	1581.00	121.00	0.0000	0.0000	0	1.1999830E-01	
1	1646.00	119.90	0.0000	0.0000	0	1.1999824E-01	
1	1710.00	118.80	0.0000	0.0000	0	1.1999818E-01	
1	1775.00	117.70	0.0000	0.0000	0	1.1999813E-01	
1	1839.00	116.70	0.0000	0.0000	0	1.1999807E-01	
1	1904.00	115.60	0.0000	0.0000	0	1.1999801E-01	
1	1986.00	114.40	0.0000	0.0000	0	1.1999795E-01	
1	2036.00	113.60	0.0000	0.0000	0	1.1999789E-01	
1	2086.00	112.90	0.0000	0.0000	0	1.1999783E-01	
1	2136.00	112.30	0.0000	0.0000	0	1.1999777E-01	
1	2186.00	111.60	0.0000	0.0000	0	1.1999771E-01	
1	2236.00	111.00	0.0000	0.0000	0	1.1999765E-01	
1	2286.00	110.30	0.0000	0.0000	0	1.1999759E-01	
1	2336.00	109.70	0.0000	0.0000	0	1.1999753E-01	
1	2386.00	109.10	-0.5694	0.1950	1	6.8837903E-02	
1	2436.00	108.50	-0.5695	0.1945	1	5.0405446E-02	
1	2486.00	107.90	-0.5695	0.1940	1	3.6636310E-02	
1	2536.00	107.30	-0.5695	0.1935	1	2.5225966E-02	
2	2586.00	106.80	0.0631	0.1932	1	1.4995669E-02	
2	2636.00	106.20	0.0653	0.1932	1	4.7456686E-03	
2	2686.00	105.70	0.0671	0.1932	1	-5.5043314E-03	

Rows originally identified 153/155

pcl5

JOB 1770

echo2.out

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:40:34 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:12:43 1991
Started: Wed Nov 13 10:12:43 1991

QMS 3825 Print System

EBSPAC (Engineering Barrier System Performance Assessment Code)
This is the release part of the EBSPAC code
Mon Jan 6 17:36:59 1997

154/155

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failure type: 1
number of failed wp: 0
wp failure time [yr]: 0.
onset of flow [yr]: 3686.

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failure type: 2
number of failed wp: 0
wp failure time [yr]: 4500.
onset of flow [yr]: 3686.

no release due to scenario failure because it occurred after corrosion failure

---

failure type: 3
number of failed wp: 2335
wp failure time [yr]: 2636.
onset of flow [yr]: 3686.
sf leaching time span [yr]: 186.
sf leaching onset time [yr]: 3686.
sf leaching will end at [yr]: 3872.

---

time [yr]	cwpwater [kg]	rgenerate [kg/yr]	rdecay [kg/yr]	rconv [kg/yr]	rdiff_r0 [kg/yr]	rdiff_ebs [kg/yr]
3736.0	1.397E-07	1.581E+15	1.560E+15	3.132E-09	1.118E-11	2.373E-21
3786.0	3.017E-07	1.598E+15	1.577E+15	3.165E-09	1.130E-11	2.494E-21
3836.0	4.686E-07	1.614E+15	1.593E+15	3.198E-09	1.141E-11	2.521E-21
3886.0	6.128E-07	1.290E+14	1.270E+14	2.550E-10	8.997E-13	1.806E-21
3936.0	6.268E-07	3.244E+11	6.328E+10	1.270E-13	4.438E-16	1.519E-25
3986.0	6.393E-07	2.622E+11	3.916E+10	7.861E-14	2.805E-16	1.333E-27
4036.0	6.518E-07	2.243E+11	3.351E+10	6.727E-14	2.400E-16	1.499E-27
4086.0	6.644E-07	1.915E+11	2.865E+10	5.752E-14	2.053E-16	2.477E-27
4136.0	6.771E-07	1.633E+11	2.451E+10	4.921E-14	1.756E-16	2.990E-27
4186.0	6.898E-07	1.444E+11	2.167E+10	4.350E-14	1.552E-16	2.286E-27
4236.0	7.026E-07	1.277E+11	1.913E+10	3.841E-14	1.370E-16	1.713E-27
4286.0	7.154E-07	1.128E+11	1.688E+10	3.390E-14	1.210E-16	1.214E-27
4336.0	7.282E-07	9.961E+10	1.490E+10	2.991E-14	1.067E-16	8.299E-28
4386.0	7.411E-07	8.792E+10	1.314E+10	2.637E-14	9.412E-17	5.205E-28
4436.0	7.540E-07	7.757E+10	1.158E+10	2.325E-14	8.295E-17	2.435E-28
4486.0	7.670E-07	6.842E+10	1.020E+10	2.047E-14	7.305E-17	1.731E-29
4536.0	7.800E-07	5.903E+10	9.118E+09	1.830E-14	6.532E-17	1.439E-27
4586.0	7.931E-07	5.217E+10	8.062E+09	1.618E-14	5.776E-17	1.205E-27
4636.0	8.062E-07	4.610E+10	7.126E+09	1.431E-14	5.105E-17	9.981E-28
4686.0	8.193E-07	4.072E+10	6.296E+09	1.264E-14	4.511E-17	8.150E-28
4736.0	8.325E-07	3.595E+10	5.562E+09	1.117E-14	3.985E-17	6.528E-28
4786.0	8.457E-07	3.174E+10	4.912E+09	9.861E-15	3.519E-17	5.093E-28

time [yr]	cwpwater [kg]	rgenerate [kg/yr]	rdecay [kg/yr]	rconv [kg/yr]	rdiff_r0 [kg/yr]	rdiff_ebs [kg/yr]

4836.0	8.589E-07	2.802E+10	4.337E+09	8.706E-15	3.107E-17	3.824E-28
4886.0	8.722E-07	2.472E+10	3.828E+09	7.685E-15	2.743E-17	2.703E-28
4936.0	8.855E-07	2.182E+10	3.379E+09	6.783E-15	2.421E-17	1.712E-28
4986.0	8.989E-07	1.925E+10	2.982E+09	5.987E-15	2.137E-17	8.697E-29
5036.0	9.123E-07	1.700E+10	2.633E+09	5.285E-15	1.886E-17	7.676E-29
5086.0	9.257E-07	1.501E+10	2.325E+09	4.667E-15	1.665E-17	6.777E-29
5136.0	9.391E-07	1.326E+10	2.053E+09	4.122E-15	1.471E-17	5.986E-29
5186.0	9.526E-07	1.172E+10	1.814E+09	3.643E-15	1.300E-17	5.289E-29
5236.0	9.661E-07	1.036E+10	1.604E+09	3.220E-15	1.149E-17	4.675E-29
5286.0	9.796E-07	9.166E+09	1.419E+09	2.849E-15	1.017E-17	4.134E-29
5336.0	9.931E-07	8.115E+09	1.256E+09	2.521E-15	8.997E-18	3.659E-29
5386.0	1.007E-06	7.189E+09	1.112E+09	2.233E-15	7.969E-18	3.240E-29
5436.0	1.020E-06	6.375E+09	9.860E+08	1.979E-15	7.064E-18	2.872E-29
5486.0	1.034E-06	5.658E+09	8.748E+08	1.756E-15	6.268E-18	2.547E-29
5536.0	1.048E-06	5.028E+09	7.770E+08	1.560E-15	5.567E-18	2.262E-29
5586.0	1.061E-06	4.473E+09	6.909E+08	1.387E-15	4.950E-18	2.011E-29
5636.0	1.075E-06	3.985E+09	6.152E+08	1.235E-15	4.408E-18	1.790E-29
5686.0	1.089E-06	3.557E+09	5.486E+08	1.101E-15	3.931E-18	1.596E-29
5736.0	1.102E-06	3.180E+09	4.901E+08	9.840E-16	3.512E-18	1.426E-29
5786.0	1.116E-06	2.849E+09	4.387E+08	8.808E-16	3.143E-18	1.276E-29
5836.0	1.130E-06	2.558E+09	3.935E+08	7.900E-16	2.819E-18	1.144E-29
5886.0	1.144E-06	2.302E+09	3.537E+08	7.102E-16	2.534E-18	1.028E-29

time [yr]	cwpwater [kg]	rgenerate [kg/yr]	rdecay [kg/yr]	rconv [kg/yr]	rdiff_r0 [kg/yr]	rdiff_ebs [kg/yr]
5936.0	1.158E-06	2.076E+09	3.188E+08	6.400E-16	2.284E-18	9.261E-30
5986.0	1.171E-06	1.878E+09	2.880E+08	5.782E-16	2.063E-18	8.364E-30
6036.0	1.185E-06	1.704E+09	2.609E+08	5.238E-16	1.869E-18	7.575E-30
6086.0	1.199E-06	1.550E+09	2.371E+08	4.759E-16	1.698E-18	6.880E-30
6136.0	1.213E-06	1.415E+09	2.161E+08	4.338E-16	1.548E-18	6.267E-30
6186.0	1.227E-06	1.295E+09	1.976E+08	3.966E-16	1.415E-18	5.728E-30
6236.0	1.241E-06	1.190E+09	1.812E+08	3.639E-16	1.299E-18	5.252E-30
6286.0	1.255E-06	1.097E+09	1.669E+08	3.350E-16	1.195E-18	4.833E-30
6336.0	1.269E-06	1.015E+09	1.542E+08	3.095E-16	1.104E-18	4.463E-30
6386.0	1.283E-06	9.431E+08	1.430E+08	2.870E-16	1.024E-18	4.136E-30
6436.0	1.297E-06	8.792E+08	1.330E+08	2.671E-16	9.532E-19	3.847E-30
6486.0	1.311E-06	8.226E+08	1.243E+08	2.495E-16	8.904E-19	3.592E-30
6536.0	1.325E-06	7.725E+08	1.165E+08	2.339E-16	8.348E-19	3.366E-30
6586.0	1.339E-06	7.281E+08	1.097E+08	2.201E-16	7.856E-19	3.166E-30
6636.0	1.353E-06	6.887E+08	1.036E+08	2.079E-16	7.419E-19	2.988E-30
6686.0	1.367E-06	6.536E+08	9.814E+07	1.970E-16	7.031E-19	2.830E-30
6736.0	1.381E-06	6.225E+08	9.333E+07	1.874E-16	6.686E-19	2.690E-30
6786.0	1.395E-06	5.947E+08	8.904E+07	1.788E-16	6.379E-19	2.565E-30
6836.0	1.409E-06	5.699E+08	8.521E+07	1.711E-16	6.105E-19	2.453E-30
6886.0	1.423E-06	5.477E+08	8.179E+07	1.642E-16	5.860E-19	2.353E-30
6936.0	1.437E-06	5.278E+08	7.873E+07	1.581E-16	5.641E-19	2.264E-30
6986.0	1.451E-06	5.100E+08	7.599E+07	1.525E-16	5.444E-19	2.184E-30

time [yr]	cwpwater [kg]	rgenerate [kg/yr]	rdecay [kg/yr]	rconv [kg/yr]	rdiff_r0 [kg/yr]	rdiff_ebs [kg/yr]
7036.0	1.465E-06	4.939E+08	7.352E+07	1.476E-16	5.267E-19	2.112E-30
7086.0	1.479E-06	4.794E+08	7.129E+07	1.431E-16	5.107E-19	2.047E-30
7136.0	1.493E-06	4.662E+08	6.928E+07	1.391E-16	4.963E-19	1.988E-30
7186.0	1.508E-06	4.543E+08	6.745E+07	1.354E-16	4.832E-19	1.935E-30
7236.0	1.522E-06	4.435E+08	6.579E+07	1.321E-16	4.714E-19	1.887E-30
7286.0	1.536E-06	4.336E+08	6.428E+07	1.291E-16	4.605E-19	1.843E-30
7336.0	1.550E-06	4.245E+08	6.290E+07	1.263E-16	4.506E-19	1.803E-30

7386.0	1.564E-06	4.162E+08	6.1[illegible]07	1.237E-16	4.415E-19	1.766E-30
7436.0	1.578E-06	4.085E+08	6.046E+07	1.214E-16	4.331E-19	1.731E-30
7486.0	1.592E-06	4.014E+08	5.938E+07	1.192E-16	4.254E-19	1.700E-30
7536.0	1.607E-06	3.947E+08	5.837E+07	1.172E-16	4.182E-19	1.671E-30
7586.0	1.621E-06	3.886E+08	5.744E+07	1.153E-16	4.115E-19	1.643E-30
7636.0	1.635E-06	3.828E+08	5.657E+07	1.136E-16	4.053E-19	1.618E-30
7686.0	1.649E-06	3.774E+08	5.575E+07	1.119E-16	3.994E-19	1.594E-30
7736.0	1.663E-06	3.722E+08	5.498E+07	1.104E-16	3.939E-19	1.572E-30
7786.0	1.677E-06	3.674E+08	5.425E+07	1.089E-16	3.887E-19	1.550E-30
7836.0	1.692E-06	3.628E+08	5.356E+07	1.075E-16	3.837E-19	1.530E-30
7886.0	1.706E-06	3.584E+08	5.290E+07	1.062E-16	3.790E-19	1.511E-30
7936.0	1.720E-06	3.542E+08	5.227E+07	1.049E-16	3.745E-19	1.493E-30
7986.0	1.734E-06	3.502E+08	5.167E+07	1.037E-16	3.702E-19	1.475E-30
8036.0	1.748E-06	3.463E+08	5.110E+07	1.026E-16	3.661E-19	1.458E-30
8086.0	1.763E-06	3.426E+08	5.054E+07	1.015E-16	3.621E-19	1.442E-30

time [yr]	cwpwater [kg]	rgenerate [kg/yr]	rdecay [kg/yr]	rconv [kg/yr]	rdiff_r0 [kg/yr]	rdiff_ebs [kg/yr]
8136.0	1.777E-06	3.390E+08	5.001E+07	1.004E-16	3.583E-19	1.427E-30
8186.0	1.791E-06	3.355E+08	4.949E+07	9.935E-17	3.545E-19	1.412E-30
8236.0	1.805E-06	3.322E+08	4.898E+07	9.834E-17	3.509E-19	1.397E-30
8286.0	1.819E-06	3.289E+08	4.849E+07	9.736E-17	3.474E-19	1.383E-30
8336.0	1.834E-06	3.256E+08	4.802E+07	9.640E-17	3.440E-19	1.369E-30
8386.0	1.848E-06	3.225E+08	4.755E+07	9.547E-17	3.407E-19	1.355E-30
8436.0	1.862E-06	3.194E+08	4.710E+07	9.455E-17	3.374E-19	1.342E-30
8486.0	1.876E-06	3.164E+08	4.665E+07	9.366E-17	3.342E-19	1.329E-30
8536.0	1.891E-06	3.135E+08	4.622E+07	9.279E-17	3.311E-19	1.316E-30
8586.0	1.905E-06	3.106E+08	4.579E+07	9.193E-17	3.281E-19	1.304E-30
8636.0	1.919E-06	3.078E+08	4.537E+07	9.108E-17	3.250E-19	1.291E-30
8686.0	1.933E-06	3.050E+08	4.496E+07	9.026E-17	3.221E-19	1.279E-30
8736.0	1.947E-06	3.022E+08	4.455E+07	8.944E-17	3.192E-19	1.268E-30
8786.0	1.962E-06	2.995E+08	4.415E+07	8.864E-17	3.163E-19	1.256E-30
8836.0	1.976E-06	2.969E+08	4.376E+07	8.785E-17	3.135E-19	1.244E-30
8886.0	1.990E-06	2.942E+08	4.337E+07	8.707E-17	3.107E-19	1.233E-30
8936.0	2.004E-06	2.916E+08	4.298E+07	8.630E-17	3.080E-19	1.222E-30
8986.0	2.018E-06	2.891E+08	4.261E+07	8.554E-17	3.052E-19	1.211E-30
9036.0	2.033E-06	2.865E+08	4.223E+07	8.479E-17	3.026E-19	1.200E-30
9086.0	2.047E-06	2.840E+08	4.186E+07	8.404E-17	2.999E-19	1.189E-30
9136.0	2.061E-06	2.816E+08	4.150E+07	8.331E-17	2.973E-19	1.179E-30
9186.0	2.075E-06	2.791E+08	4.114E+07	8.259E-17	2.947E-19	1.168E-30

time [yr]	cwpwater [kg]	rgenerate [kg/yr]	rdecay [kg/yr]	rconv [kg/yr]	rdiff_r0 [kg/yr]	rdiff_ebs [kg/yr]
9236.0	2.089E-06	2.767E+08	4.078E+07	8.187E-17	2.922E-19	1.158E-30
9286.0	2.104E-06	2.743E+08	4.043E+07	8.116E-17	2.896E-19	1.147E-30
9336.0	2.118E-06	2.719E+08	4.008E+07	8.046E-17	2.871E-19	1.137E-30
9386.0	2.132E-06	2.696E+08	3.973E+07	7.976E-17	2.846E-19	1.127E-30
9436.0	2.146E-06	2.673E+08	3.939E+07	7.908E-17	2.822E-19	1.117E-30
9486.0	2.160E-06	2.650E+08	3.905E+07	7.840E-17	2.798E-19	1.107E-30
9536.0	2.174E-06	2.627E+08	3.871E+07	7.772E-17	2.774E-19	1.097E-30
9586.0	2.189E-06	2.604E+08	3.838E+07	7.705E-17	2.750E-19	1.088E-30
9636.0	2.203E-06	2.582E+08	3.805E+07	7.639E-17	2.726E-19	1.078E-30
9686.0	2.217E-06	2.560E+08	3.773E+07	7.574E-17	2.703E-19	1.068E-30
9736.0	2.231E-06	2.538E+08	3.740E+07	7.509E-17	2.680E-19	1.059E-30
9786.0	2.245E-06	2.516E+08	3.708E+07	7.445E-17	2.657E-19	1.050E-30
9836.0	2.259E-06	2.495E+08	3.676E+07	7.381E-17	2.634E-19	1.040E-30
9886.0	2.274E-06	2.473E+08	3.645E+07	7.318E-17	2.611E-19	1.031E-30
9936.0	2.288E-06	2.452E+08	3.614E+07	7.255E-17	2.589E-19	1.022E-30

9986.0	2.302E-06	2.431E+08	3.58[illegible]07	7.193E-17	2.567E-19	1.013E-30
10000.0	2.306E-06	2.423E+08	3.578E+07	7.184E-17	2.564E-19	1.908E-31

cumulative release [ci/cell] by 10000.0 years

namall	halflife(yr)	xnoloss(ci)	amwp(ci)	xmass(ci)	fracleft
CM246	0.473E+04	0.195E+02	0.587E-06	0.197E+02	-0.01
PU242	0.386E+06	0.514E+04	0.636E-02	0.519E+04	-0.01
U238	0.447E+10	0.104E+04	0.113E-03	0.105E+04	-0.01
CM245	0.850E+04	0.182E+03	0.291E-04	0.184E+03	-0.01
AM241	0.432E+03	0.193E+03	0.259E-06	0.195E+03	-0.01
NP237	0.214E+07	0.202E+04	0.240E-02	0.204E+04	-0.01
AM243	0.738E+04	0.198E+05	0.171E-02	0.200E+05	-0.01
PU239	0.241E+05	0.763E+06	0.470E+00	0.771E+06	-0.01
PU240	0.654E+04	0.575E+06	0.491E-01	0.581E+06	-0.01
U236	0.234E+08	0.109E+04	0.102E-03	0.110E+04	-0.01
U234	0.245E+06	0.600E+04	0.608E-03	0.606E+04	-0.01
TH230	0.770E+05	0.524E+03	0.201E-03	0.529E+03	-0.01
RA226	0.160E+04	0.409E+03	0.485E-06	0.413E+03	-0.01
PB210	0.223E+02	0.407E+03	0.716E-07	0.411E+03	-0.01
CS135	0.230E+07	0.114E+04	0.109E-02	0.115E+04	-0.01
I129	0.157E+08	0.969E+02	0.653E-05	0.979E+02	-0.01
TC99	0.213E+06	0.389E+05	0.241E-02	0.393E+05	-0.01
NI59	0.800E+05	0.107E+05	0.931E-03	0.108E+05	-0.01
C14	0.573E+04	0.150E+04	0.453E-05	0.151E+04	-0.01
SE79	0.650E+05	0.112E+04	0.574E-04	0.113E+04	-0.01
NB94	0.203E+05	0.185E+04	0.316E-03	0.187E+04	-0.01

zeroth yr inventory for liquid releases: 10040.5
zeroth yr inventory for gaseous releases: 8107.1
1000-yr c14 inv. for liq. rel [ci/cell: 10036.7
1000-yr c14 inv. for gaseous rel. [ci/cell]: 8104.1
output files: release.out, ebsnef.dat, relcum.out, relfrac.out
maxrel.dat, ebs14.dat, maxc14.dat, ratec14.out, inv1000.out

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pcl5

JOB 1775

ebspac.nuc

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:53:55 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:26:03 1991
Started: Wed Nov 13 10:26:03 1991

QMS
QMS 3825 Print System

QMS 3825 Print System

```
 15
 CM       2 .24E-6     100.0
1 1
2 1
 PU       3 .01E-3     100.0
1 2
3 2
4 1
  U       3  0.95E-3   2.0
1 3
4 2
5 1
AM        2  .24E-6    200.0
2 2
3 1
NP        1  .237E-3   50.0
2 3
TH        1  2.3E-10   100.0
5 2
RA        1  6.8E-8    30.0
5 3
PB        1  1.        20.0
5 4
CS        1  1.        200.0
6 1
I         1  1.         1.0
7 1
TC        1  1.         1.0
8 1
NI        1  0.59E-3    2.0
9 1
C         1  1.         1.0
10 1
SE        1  7.9E-11    1.0
11 1
NB        1  1.         20.0
12 1
12 3 3 2 2 4 1 1 1 1 1 1 1
     246.0      CM246   4.73E03  0.07224     0.
     242.0      PU242   3.86E05  4.47857     0.
     238.0       U238   4.47E09  0.89038     0.
     245.0      CM245   8.50E03  0.35322     0.
     241.0      AM241   4.32E02  4590.53     0.
     237.0      NP237   2.14E06  0.8064      0.
     243.0      AM243   7.38E03  43.4528     0.
     239.0      PU239   2.41E04  862.391     0.
     240.0      PU240   6.54E03  1422.21     0.
     236.0       U236   2.34E07  0.67178     0.
     234.0       U234   2.45E05  5.283       0.
     230.0      TH230   7.70E04  3.61E-4     0.
     226.0      RA226   1.60E03  1.0E-6      0.
     210.0      PB210   2.23E01  1.3E-1      0.
     135.0      CS135   2.30E06  0.9796      0.000
     129.0       I129   1.57E07  0.083       0.000
      99.0      TC99    2.13E05  34.38       0.000
      59.0      NI59    8.00E04  9.97        0.
      14.0       C14    5.73E03  4.30        0.000
      79.0      SE79    6.50E04  1.0663      0.000
      94.0      NB94    2.03E04  2.2259      0.
12345678901234567890123456789012345678901234567890
```

\ Pu238 inventory is put into U234 inventory.

161 195

pcl5

JOB 1777

cumc14.out

For: **scratchy1!mohanty**
Date: **Mon Jan 6 17:57:24 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:29:33 1991
Started: Wed Nov 13 10:29:33 1991

QMS
QMS 3825 Print System

QMS 3825 Print System

time [yr]	cumulative c14 release [ci
2.00000000000000D-04	0.
50.420000000000	0.
100.500000000000	0.
152.40000000000	0.
206.00000000000	0.
259.40000000000	0.
312.80000000000	0.
366.20000000000	0.
419.70000000000	0.
473.10000000000	0.
533.80000000000	0.
585.70000000000	0.
637.50000000000	0.
689.30000000000	0.
741.10000000000	0.
793.00000000000	0.
844.80000000000	0.
896.60000000000	0.
948.40000000000	0.
1000.00000000000	0.
1065.0000000000	0.
1129.0000000000	0.
1194.0000000000	0.
1258.0000000000	0.
1323.0000000000	0.
1388.0000000000	0.
1452.0000000000	0.
1517.0000000000	0.
1581.0000000000	0.
1646.0000000000	0.
1710.0000000000	0.
1775.0000000000	0.
1839.0000000000	0.
1904.0000000000	0.
1986.0000000000	0.
2036.0000000000	0.
2086.0000000000	0.
2136.0000000000	0.
2186.0000000000	0.
2236.0000000000	0.
2286.0000000000	0.
2336.0000000000	0.
2386.0000000000	0.
2436.0000000000	0.
2486.0000000000	0.
2536.0000000000	0.
2586.0000000000	0.
2636.0000000000	0.
2686.0000000000	1598.7004081295
2736.0000000000	2695.9752127578
2786.0000000000	3496.6721938441
2836.0000000000	4060.0139550623
2886.0000000000	4433.3760243497
2936.0000000000	4662.7913577320
2986.0000000000	4786.9828967300
3036.0000000000	4840.5272322924
3086.0000000000	4854.1798480462
3136.0000000000	4854.1798480462
3186.0000000000	4854.1798480462

3236.0000000000	4854.1798480462
3286.0000000000	4854.1798480462
3336.0000000000	4854.1798480462
3386.0000000000	4854.1798480462
3436.0000000000	4854.1798480462
3486.0000000000	4854.1798480462
3536.0000000000	4854.1798480462
3586.0000000000	4854.1798480462
3636.0000000000	4854.1798480462
3686.0000000000	4854.1798480462
3736.0000000000	4854.1798480462
3786.0000000000	4854.1798480462
3836.0000000000	4854.1798480462
3886.0000000000	4854.1798480462
3936.0000000000	4854.1798480462
3986.0000000000	4854.1798480462
4036.0000000000	4854.1798480462
4086.0000000000	4854.1798480462
4136.0000000000	4854.1798480462
4186.0000000000	4854.1798480462
4236.0000000000	4854.1798480462
4286.0000000000	4854.1798480462
4336.0000000000	4854.1798480462
4386.0000000000	4854.1798480462
4436.0000000000	4854.1798480462
4486.0000000000	4854.1798480462
4536.0000000000	4854.1798480462
4586.0000000000	4854.1798480462
4636.0000000000	4854.1798480462
4686.0000000000	4854.1798480462
4736.0000000000	4854.1798480462
4786.0000000000	4854.1798480462
4836.0000000000	4854.1798480462
4886.0000000000	4854.1798480462
4936.0000000000	4854.1798480462
4986.0000000000	4854.1798480462
5036.0000000000	4854.1798480462
5086.0000000000	4854.1798480462
5136.0000000000	4854.1798480462
5186.0000000000	4854.1798480462
5236.0000000000	4854.1798480462
5286.0000000000	4854.1798480462
5336.0000000000	4854.1798480462
5386.0000000000	4854.1798480462
5436.0000000000	4854.1798480462
5486.0000000000	4854.1798480462
5536.0000000000	4854.1798480462
5586.0000000000	4854.1798480462
5636.0000000000	4854.1798480462
5686.0000000000	4854.1798480462
5736.0000000000	4854.1798480462
5786.0000000000	4854.1798480462
5836.0000000000	4854.1798480462
5886.0000000000	4854.1798480462
5936.0000000000	4854.1798480462
5986.0000000000	4854.1798480462
6036.0000000000	4854.1798480462
6086.0000000000	4854.1798480462
6136.0000000000	4854.1798480462
6186.0000000000	4854.1798480462

6236.0000000000	4854.1798480462
6286.0000000000	4854.1798480462
6336.0000000000	4854.1798480462
6386.0000000000	4854.1798480462
6436.0000000000	4854.1798480462
6486.0000000000	4854.1798480462
6536.0000000000	4854.1798480462
6586.0000000000	4854.1798480462
6636.0000000000	4854.1798480462
6686.0000000000	4854.1798480462
6736.0000000000	4854.1798480462
6786.0000000000	4854.1798480462
6836.0000000000	4854.1798480462
6886.0000000000	4854.1798480462
6936.0000000000	4854.1798480462
6986.0000000000	4854.1798480462
7036.0000000000	4854.1798480462
7086.0000000000	4854.1798480462
7136.0000000000	4854.1798480462
7186.0000000000	4854.1798480462
7236.0000000000	4854.1798480462
7286.0000000000	4854.1798480462
7336.0000000000	4854.1798480462
7386.0000000000	4854.1798480462
7436.0000000000	4854.1798480462
7486.0000000000	4854.1798480462
7536.0000000000	4854.1798480462
7586.0000000000	4854.1798480462
7636.0000000000	4854.1798480462
7686.0000000000	4854.1798480462
7736.0000000000	4854.1798480462
7786.0000000000	4854.1798480462
7836.0000000000	4854.1798480462
7886.0000000000	4854.1798480462
7936.0000000000	4854.1798480462
7986.0000000000	4854.1798480462
8036.0000000000	4854.1798480462
8086.0000000000	4854.1798480462
8136.0000000000	4854.1798480462
8186.0000000000	4854.1798480462
8236.0000000000	4854.1798480462
8286.0000000000	4854.1798480462
8336.0000000000	4854.1798480462
8386.0000000000	4854.1798480462
8436.0000000000	4854.1798480462
8486.0000000000	4854.1798480462
8536.0000000000	4854.1798480462
8586.0000000000	4854.1798480462
8636.0000000000	4854.1798480462
8686.0000000000	4854.1798480462
8736.0000000000	4854.1798480462
8786.0000000000	4854.1798480462
8836.0000000000	4854.1798480462
8886.0000000000	4854.1798480462
8936.0000000000	4854.1798480462
8986.0000000000	4854.1798480462
9036.0000000000	4854.1798480462
9086.0000000000	4854.1798480462
9136.0000000000	4854.1798480462
9186.0000000000	4854.1798480462

9236.0000000000	4854.1798480462
9286.0000000000	4854.1798480462
9336.0000000000	4854.1798480462
9386.0000000000	4854.1798480462
9436.0000000000	4854.1798480462
9486.0000000000	4854.1798480462
9536.0000000000	4854.1798480462
9586.0000000000	4854.1798480462
9636.0000000000	4854.1798480462
9686.0000000000	4854.1798480462
9736.0000000000	4854.1798480462
9786.0000000000	4854.1798480462
9836.0000000000	4854.1798480462
9886.0000000000	4854.1798480462
9936.0000000000	4854.1798480462
9986.0000000000	4854.1798480462
10000.0000000000	4854.1798480462

164/195

pcl5

JOB 1778

maxrel.dat

For: **scratchy1!mohanty**
Date: **Mon Jan 6 18:01:07 CST 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Wed Nov 13 10:33:16 1991
Started: Wed Nov 13 10:33:16 1991

QMS
QMS 3825 Print System

QMS 3825 Print System

title: maximum fractional release of c14

tmaxc14 [yr]	rmaxc14 [fraction]
2686.0000000000	1.7625492907432D-03

maximum fractional release of all nuclides

name	timrel (year)	maxrel (fraction)
CM246	3750.0000000000	1.5783522754812D-03
PU242	3750.0000000000	2.71414016623530-03
U238	3750.0000000000	2.73449003293380-03
CM245	3750.0000000000	2.01326964729120-03
AM241	3750.0000000000	6.88435406185510-06
NP237	3750.0000000000	5.82559110736700-03
AM243	3750.0000000000	1.92208190130920-03
PU239	3750.0000000000	2.46506943288100-03
PU240	3750.0000000000	1.83720857755380-03
U236	3750.0000000000	3.26388209372530-03
U234	3750.0000000000	2.70566656266860-03
TH230	3800.0000000000	0.93875542526128
RA226	3800.0000000000	154.56445111361
PB210	3800.0000000000	2.05042171527780-03
CS135	3750.0000000000	2.72911361888810-03
I129	3750.0000000000	2.73559037051350-03
TC99	3750.0000000000	2.70290321910840-03
NI59	3750.0000000000	2.64718685200120-03
C14	3750.0000000000	9.62338395638200-04
SE79	3750.0000000000	2.62893700739240-03
NB94	3750.0000000000	2.40448978681450-03