

WM DOCKET CONTROL
CENTER

'83 DEC -5 P2:10



BATTELLE Project Management Division
505 King Avenue
Columbus, Ohio 43201

November 28, 1983

WM Record File

106

WM Project 16

Docket No. _____

PDR ✓

LPDR ✓

Mr. John T. Buckley
U.S. Nuclear Regulatory Commission
Mail Stop 623-SS
Washington, D.C. 20555

Distribution:

SBuckley

(Return to WM, 623-SS)

15

Dear Mr. Buckley:

TRANSMITTAL OF WAPPA CODE TO NRC

In response to the letter received on October 14, 1983 from Hubert J. Miller to J. O. Neff of the NWTs Program Office and in accordance with established DOE code distribution procedures, we at ONWI are sending you a magnetic tape containing the WAPPA source code, its data base, sample inputs, and sample outputs. We do not have access to a CDC-7600 computer or to the SCOPE 2.1 system so that we cannot comply with your specifications for loading the tape. We have used the standardized blocking specifications described on the code transfer form, which has been adequate for transfers between ONWI and its subcontractors who have various types of computer systems including yours.

The WAPPA code was developed under the National Waste Terminal Storage (NWTs) Program of the United States Department of Energy (DOE). A verification, validation, and peer review plan for these codes and models which will be used in licensing a nuclear waste repository is being prepared. DOE encourages other parties to use the codes and share their experiences for improving the document and computer codes.

A copy of the WAPPA code technical manual is also enclosed. INTERA Environmental Consultants, Inc., 1983. WAPPA: A Waste Package Performance Assessment Code, ONWI-452, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, OH. Shortly after this manual was written, a number of changes were made in the code by INTERA to correct fatal logic flaws and obvious output formatting errors. These changes were also made at ONWI and were incorporated in the baseline version used on the CYBER 74 and CDC-855 computers at ONWI and documented by Code Revision #1.

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PDR WASTE
WM-16

PDR

In addition we found it necessary to increase the time dimensions to larger values than our small CDC computers can handle without mapping. WAPPA is a rapidly running system-level code for which computer times and costs are relatively small. We have transferred the code to our DEC VAX/VMS 11/780 virtual memory computer and increased the time dimensions to allow small enough time steps to get reasonably accurate results with Euler's method, which is used for all integrations in the code.

We have included one complete listing of the code on paper for the baseline version including Code Revision #1 but with time dimensions reduced to 30 to run on CDC-855. We have also included a printed output of one sample run of the code on our CDC-855 computer with representative input values and the data base used by INTERA for verification.

To show the differences between the VAX and CDC versions, we have included a DIFFERENCE run between the two source versions and a DIFFERENCE run between the current VAX version with Code Revision #1 and the version described in ONWI-452. Please pay close attention to these differences because all future upgrades of the code will be on the VAX 11/780 computer and will be referenced to the VAX version with Code Revision #1.

The supplied code is suitable without modification for the verifications described in ONWI-452 and for illustrative package failure calculations. However, we have found it necessary to make additional changes to allow the radiation field to change with time, to distinguish chemical behavior such as leaching, mass transport and solubility limits from radionuclide specific behavior radioactive decay. We have tailored the code for salt repositories e.g., allowing consumption of part of the limited amount of water available to be consumed by stoichiometric reactions with metal barriers. These changes will be complete and documented by May 1984. The development of a validated data base is an additional task which will depend on much site specific information.

The enclosures were prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, any agency thereof, Battelle Project Management Division, nor any of their employees, makes any warranty, express or implied, or assumes any liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference to specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed do not necessarily state or reflect those of the United States Government, any agency thereof, or BPMD.

Any questions regarding underlying models, code documentation or running of the code should be addressed to Leslie A. Scott, Code Custodian, Performance Assessment Department, ONWI. (FTS 976-4326)

Sincerely,



George Jansen, Jr.
Analytical Engineer
Performance Assessment
Department

GJ:rb

Attachments:

1. Code Transfer Form
2. Table of Contents of Tape
3. Job Control Language from CDC-855 Computer to Tape #445
4. Tape #4451
5. Code Revision #1 Notice
6. Listing of version of WAPPA Code used on CDC-855 includes:
 1. Sample User Input File (LU #1)
 2. Sample Output
 3. Code Listing.
7. DIFFERENCE Run between source codes on VAX-11/780:
8. DIFFERENCE Run between source codes:
9. ONWI-452, WAPPA Code Manual

cc: JO Neff (3) (NPO)
R. Wu (NPO)
H Miller (NRC)
W. Bennett (DOE-HQ)
L. Olsen (DOE-RL)
D. Vieth (DOE-NV)
L. Casey (NPO)

To: John T. McKley Date: _____
U.S. Nuclear Regulatory Comm
Mail STOP 623-55
Washington, D.C. 20555

From: ONWI
Battelle Project Management Division
505 King Avenue
Columbus, Ohio 43201
Attention: Leslie Scott (614) 424-4326/7806

Subject: Computer Modeling Technology Transfer
Model Name WaPPa QA Number _____
Reference: Request for Transfer ACTION TEAM
Intended Application _____

Enclosed are the items as described below. Please report to us your acceptance of the materials, any problem encountered during your installation of the model and execution of the benchmark test problem on your computer, and any problems you may encounter or modifications you made which either correct problems or might be of general utility.

Model Tape File Index ☒

Documentation ☐; Title _____

Model Tape Listing (Optional) ☒

Magnetic Tape (9-Track) ☒

Unlabeled ☒; Other ☐ _____

1600 bpi ☒; Other ☐ _____

EBCDIC ☒; Other ☐ _____

Files 1-15, 19, Blocksize 1360, Record Length 80

Files 16-18, Blocksize 1360, Record Length 136

Model Tape generated and files verified by P. J. McKley
Transmittal Package reviewed and approved by Leslie Scott (CC)
Transfer approved by DAW to JF Kuch 11/28/83 (MGR)

For Use by Recipient: (Please complete and return this original copy to ONWI)

Above items accepted ☐: Acceptance contingent ☐ upon receipt of the following:

Comments: _____

Signed: _____

Date: _____

FILES	CHARACTERS/RECORD	CHARACTERS/BLOCK
1-15	80	1360
16-18	136	1360
19	80	1360

#2

FILE NAME	FILE	UNIT	FILE DESCRIPTION
WPINDX	1		420--20C-02:SEQUENCE OF WASTE PACKAGE (WAPPA) FILES ON TAPE
MCODES	2		(7)-(LOCAT2)-SYSTEM-COMPREHENSIVE LIST OF DATABASE MATERIALS
GAMMA	3		(10)-(RPROP2)-RADIATION-GAMMA BUILD-UP FACTORS,CROSS-SECTION
ORIGEN2	4		(11)-(RADDAT3)-RADIATION-SOURCE TERM=F(TIME) ETC.FROM ORIGEN
THERMAL	5		(12)-(TPROP3)-THERMAL- TEMP. DEP. PROPS. QUADRATIC COEFFS.
RBT	6		(21)-(REPOST2)-THERMAL-REPOSITORY BOUNDARY TEMPS = F(TIME)
MEK	7		(30)-(FPROP2)-MECHANICAL- MECHANICAL PROPERTIRS DATA
FICP	8		(40)-(CTEMP2)-CORROSION-FLUID-INDEPENDENT CORR. PROPERTIES
FDCP	9		(41)-(CTMPFL3)-CORROSION-FLUID-DEPENDENT CORROSION PROPS.
CED	10		(42)-(CORENC2)-RADIATION- CORROSION ENHANCEMENT DATA
WFLP	11		(20)-(WFPROP3)-LEACH-WASTE-FORM LEACHING PROPERTIES
BFP	12		(51)-(WBPROP2)-LEACH-- BACKFILL POROSITY AND DENSITY
NTP	13		(52)-(WSOLUT3)-LEACH- NUCLIDE TRANSPORT PROPERTIES
IS1	14		(1)-INPUT FOR SAMPLE (SIMPLIFIED) PROBLEM
WAPPA	15		420--20C-02B: SINGLE FILE WAPPA SOURCE PROGRAM
OS1	16		OUTPUT FOR SAMPLE (SIMPLIFIED) WESTINGHOUSE PROBLEM
WAPPA	17		DIFFERENCE FILE CDC VERSION ,VS. VAX VERSION
WAPPA	18		DIFFERENCE FILE OLD INTERA VERSION ,VS. NEW INTERA VERSION VAX
CDC JCL	19		JOB STREAM FOR THE CDC COMPUTER

\$

#3

PHIL,T270,CM300000,AC=A3287-2002
ATTACH,TAPE1,WCHLW3,ID=MOHL.
ATTACH,TAPE7,LOCAT2,ID=MOHL.
ATTACH,TAPE10,RPROP2,ID=MOHL.
ATTACH,TAPE52,WSOLUT3,ID=MOHL.
ATTACH,TAPE21,REPOST2,ID=MOHL.
ATTACH,TAPE30,FPROP2,ID=MOHL.
ATTACH,TAPE12,TPROP3,ID=MOHL.
ATTACH,TAPE42,CORENC2,ID=MOHL.
ATTACH,TAPE51,WBPROP2,ID=MOHL.
ATTACH,TAPE11,RADDAT3,ID=MOHL.
ATTACH,TAPE40,CTEKPS2,ID=MOHL.
ATTACH,TAPE41,CTMPFL3,ID=MOHL.
ATTACH,TAPE20,WFPROP3,ID=MOHL.
ATTACH,WAPEXE,ID=MOHL.
REQUEST,TAPE71,PF.
LDSET,PRESET=0.
WAPEXE.
CATALOG,TAPE71,RESTR, ID=MOHL,RP=999.
\$ T WAPPA1.IND

BATTELLE PROJECT MANAGEMENT DIVISION

PERFORMANCE ASSESSMENT DEPARTMENT

COMPUTER MODEL REVISION NOTICE

Model Title WAPPA - A Waste Package Performance Assessment Code
 ONWI Model Control Number _____ Revision Number #1
 Supplier QA Identification Number _____ Revision Number _____

☐ Addition of Part of Model ☐ Addition to Data Set(s) of Model
☒ Partial Change to Model ☐ Partial Change to Data Set(s) of Model
☒ Partial Change to Document

Purpose of Revision:

Correct fatal logic errors in barrier failure sequence and revise some words in output format. See details in attached list (memo by Phil Mohler). The need for these changes and a list of them was transmitted to ONWI by INTERA just after the document ONWI-452 was finalized. The changes have been necessary in order to run the code to packages failure with multiple barriers that fail in different time steps. Increase the dimensions of number of time steps from 30 to 400 so that more accurate integrations of time varying quantities can be made. Convert the reference version of the WAPPA code from the CYBER 74 to the VAX/VMS 11-80 computer.

Document Affected:

ONWI-452 WAPPA - A Waste Package Performance Assessment Code (1983)

Assessment of possible impact on results of analyses as compared to results obtained from the previous version of the model

No change in verification results, code also will now ~~also~~ run for typical modeling input data.

Originator		Signature (Code Custodian)		Date	
G. Jansen <i>G. Jansen</i>		L. A. Scott <i>L. A. Scott</i>		12/11/83	
Date		Signature (Dept Mgr)		Date	
11/23/83		JF Kircher <i>JF Kircher</i>		12/1/83	
Bldg. - Room		Phone			

CHANGES MADE BY *Phil Mohler* 11/29/83
VERIFIED BY *Leslie Scott* 11/29/83
APPROVED BY *DAW for J. Kucher* 11/29/83

PAGE 1 OF 6

The following additions, deletions, and replacements have been made to the WAPPA code documented in ONWI-452, entitled, 'WAPPA: A Waste Package Performance Assessment Code' (April 1983). All of the following changes have been referenced from the enclosed listings.

The following statements were replaced by Phil Mohler in January 1983 as a result of a telephone conversation with Clifford Noronha of INTERA. These changes were required to execute the waste package concept described by the data set.

* Statement 238 in subroutine DRIVER has been replaced with
9009 FORMAT (' BARRIER RADII: ', (10E12.4))

* Statement 325 in subroutine DRIVER has been replaced with
IF(ISCWTM.GT.ISBARM) GO TO 140

* Statement 373 in subroutine DRIVER has been replaced with
IF(ISCWTM.LE.ISBARM) GO TO 160

* Statement 577 in subroutine DRIVER has been replaced with
IF(ISCWTM.GT.ISBARM) GO TO 320

* Statement 630 in subroutine DRIVER has been replaced with
IF(ISCWTM.LE.ISBARM) GO TO 340

* Statement 646 in subroutine DRIVER has been replaced with
7001 FORMAT (' ADF: ', 1P9E10.3)

* Statement 291 in subroutine CMODEL has been replaced with
2222 FORMAT (' CA,CB,CC: ', 1P8E12.5)

The following statements were changed by Phil Mohler as suggested by Clifford Noronha in February 1983 because 1) it was not possible to include more than one fluid in the database and select any one of the fluids for a particular problem, and 2) it was not possible to add or delete a wasteform or backfill in the database independently of each other. It should be noted that the user is still restricted to using consecutive integers between 300 and 399 to identify fluid materials in the database.

* Statement 2 in the main routine has been replaced with
+ TAPE20,TAPE21,TAPE30,TAPE12,TAPE40,TAPE41,TAPE42,TAPE50,TAPE51

* Statement 457 in the main routine has been replaced with
OPEN(UNIT=12,FILE='FILE5',STATUS='OLD')

* Statement 463 in the main routine has been replaced with
OPEN(UNIT=20,FILE='FILE11',STATUS='OLD')

* Statements 474, 475, 476, and 477 in the main routine have been replaced with

C IF(MATMOD(IMOD,MAT) .GT. 0) READ/SKIP DATA FOR MATERIALS CLASS,MAT,
C ON UNIT NUMBERS (IMOD*10) + IFILE - 1. MATMOD IS A (5,6) ARRAY.
DATA MATMOD/1,1,1,0,0,1,0,1,1,0,1,0,0,0,1,0,0,0,0,
+ 1,0,1,0,1,1,0,0,0,0/

* Statements 478, 479, and 480 in the main routine have been replaced with

C IF(IREC(IMOD,IFILE) .GT. 0) READ/SKIP IREC RECORDS ON UNIT NUMBERS
C (IMOD*10) + IFILE - 1. IREC IS A (5,5) ARRAY.
DATA IREC /1,1,1,4,0,0,0,0,32,1,5,0,0,4,0,0,0,0,0,0,0,0,0,0,0/

* Statement 481 in the main routine has been replaced with
DATA IRFILE/4/,ICFILE/3/,NFLUID/0/

* Statements 485 and 486 in the main routine have been replaced with
C UNIT NUMBERS CHANGED FROM = TO: 20=12 50=20
DATA IR4/13/,IT1/12/,IF1/30/,IC1/40/,IC2/41/,IW1/20/,IW2/51/

* Statements 97 through 111 in subroutine DATAIN have been inserted
C COUNT TOTAL NUMBER OF FLUIDS IN DATABASE AND SAVE FIRST(MINIMUM)
C FLUID CODE FOR LATER SKIPS ON UNITS IC2 AND IC3.
C

I1=0
5 CONTINUE
READ(IS2,1000,END=4) ICODE
IF(ICODE .LT. 300 .OR. ICODE .GE. 400) GO TO 3
IF(I1 .EQ. 0) IFLU1=ICODE
NFLUID=NFLUID+1
I1=1
3 CONTINUE
GO TO 5
4 CONTINUE
REWIND IS2

C

* Statements 211 through 221 in subroutine DATAIN have been inserted

```

C
C   ALLOW FOR ALL FLUIDS INCLUDED ON UNITS IC2 AND IS3.
C   IF(ITHIS .EQ. IC2 .OR. ITHIS .EQ. IS3) LSKIP=LSKIP+NFLUID
C
C   FLUID THERMAL PROPERTIES HAVE JUST BEEN READ FROM UNIT IT1.
C   DO NOT SKIP. SHOULD'NT THIS BE TRUE FOR UNIT IR1 ALSO. I COULD
C   NOT FIND AN ARRAY LOCATION IN RBLOOP AND RMUGAM TO READ FLUID
C   RADIATION PROPERTIES INTO. HENCE ALLOW A RECORD SKIP ON UNIT IR1.
C
C   IF(ICODE .EQ. ISFLU .AND. ITHIS .EQ. IT1) GO TO 110

```

* Statements 250 through 256 in subroutine DATAIN have been replaced with

```

C
C   IF MORE THAN ONE FLUID IS NINCLUDED IN THE DATABASE, THEIR
C   MATERIAL CODES MUST BE **CONSECUTIVE** INTEGERS BETWEEN 300,399
C
C   IGAP=ISFLU-IFLU1
C   SKIP TO FLUID OF INTEREST FOR THIS METAL
C   I4SKIP=IREC(4,2)*IGAP

```

* Statement 260 in subroutine DATAIN has been replaced with
I1SKIP=IREC(4,3)*IGAP

* Statements 266 and 267 in subroutine DATAIN have been replaced with
SKIP RECORDS FOR REMAINING FLUIDS FOR THIS METAL
I4SKIP=IREC(4,2)*(NFLUID-(IGAP+1))

* Statement 271 in subroutine DATAIN has been replaced with
I1SKIP=IREC(4,3)*(NFLUID-(IGAP+1))

```

C
C   * Statements 81 through 85 in subroutine DATRED have been replaced with
C   IT1 IS NOW 12(=1*10+2) NOT 20(=2*10). THEREFORE MODEL=1 NOT 2 FOR
C   UNIT 12
100 IPOS=ISPACK(IP,MODEL)
MODEL=MODEL+1

```

* Statement 90 in subroutine REPRED has been inserted
DATA (STIME(I),I=1,30) /30*0.0/

* Statement 8 in subroutine CINQA has been replaced with
DATA QACIN/4H420--,4H-20C,4H-02B/

* Statement 38 in subroutine CINQA has been replaced with
+T53,19HCIN = 420--20C--02B,T30,1H*,

The following statements were changed by Phil Mohler as suggested by Jeff Hockman of LLNL in February 1983 because 1) the Grashof number should be computed based on the full-gap width, and not the half-gap width, and 2) the limits of the Grashof number for determining which of the equivalent conductance expressions should be utilized, was not consistent with the original reference to Jakob in the documentation.

- * Statements 159 and 160 in subroutine TTEMP have been replaced with
C ----- GRASHOF NUMBER EXPRESSED IN TERMS OF GAP WIDTH
DRM=SRADII(J)-SRADII(K)
- * Statements 174 and 175 in subroutine TTEMP have been replaced with
IF(GR .LT. 2.E04) GO TO 130
DL=(SHTWP/DRM)**(-0.1111)
- * Statement 177 in subroutine TTEMP has been replaced with
IF(GR .GT. 2.E05) GO TO 120

The following statements were changed by Phil Mohler in February 1983 to increase the number of time steps in order to compute a more precise corrosion rate for the metal barriers, and to compute a more precise waste-form leaching rate.

NOTE: These changes have been made to the VAX 11/780 version of the WAPPA code. Due to the lack of memory allocated to us on the CDC 170/855, these changes have been omitted in the enclosed code. We suggest that you incorporate these changes upon receipt of the code in order to assure proper execution.

- * The dimension of STIM to 400 which is declared in all STIMES labeled commons (i.e. 14).
- * The dimension of SPWRT, SPWRTN, SWHMT, SRFLMT, SNWFF, SRADWF, SHWPT, SWFRMT, and WCNBMT to 400 which is declared in all SOUT labeled commons (i.e. 7).
- * The dimension of the second element of BADF, SBWIDF, SRADIT, SWPT, SWFRG, STNUCW, WCNCMT, SNUWPT, and WCNCBT to 400 which is declared in all SOUT labeled commons (i.e. 7).
- * The dimension of the third element of WCONCT to 400 which is declared in all SOUT labeled commons (i.e. 7).
- * Statement 516 in the main routine has been replaced with
IF(NST .LT. 400) STIM(NST+1)=0.0

The following changes were made by Phil Mohler in February 1983.

- * The variable array TITLE(8,5) in COMMON labeled STITL was changed to TITLE(20,5). This change was required in order for the code to be executed on the VAX 11/780.
- * Open statements were inserted in the main program. This was necessary for the code to be executed on the VAX 11/780 system.
- * Format 1003 in the main program was changed to FORMAT(20A4). This was necessary for the code to be executed on the VAX 11/780 system.
- * In FUNCTION SINTER(TAB,VNOW) TAB was dimensioned to 10. TAB was originally dimensioned to 1.
- * In subroutine DRIVER lines 226 and 227 were commented out.
- * In subroutine Driver line 265 was commented out.
- * In subroutine DRIVER lines 428 and 429 were commented out.
- * In subroutine HEADING line 52 was changed to read
WRITE(IO,2001) (TITLE(J,I),J=1,20)
- * In subroutine HEADING Format 2001 was changed to read
2001 FORMAT(30X,20A4)
- * In subroutine RADINT lines 86 and 113 were inserted. This was necessary to assure that variables ARRAY(J,K) and ANS(L) use the correct subscript value.

Changes for
WAPPA

A Waste Package Performance Assessment Code
2/15/83

<u>ONWI-452</u> <u>Page#</u>	<u>Draft</u> <u>Page#</u>	<u>Description</u>	<u>Date</u>	<u>QA ID</u>
229 (Done previously)	229	Used to be p. 329	2/15/83	-02B
230 (Done previously)	230	Used to be p. 330	2/15/83	-02B
Not done	298	Made blank since it is a repeat of p. 297.	2/15/83	-02B
299-300	---	Table 12.1 was put on two pages.	4/83	-02B
298	299	Insert at the end of paragraph 1: ...which must be modified. "Incidentally, if more than one fluid is included in the database, the record skipping logic for the corrosion data files (Subroutine DATAIN) requires that the fluid material codes be <u>consecutive</u> integers between 300 and 399."	2/15/83	-02B

Changes verified 11/29/83

H. Jensen

Changes checked 11/29/83

P. S. Maki

Revised: 2/15/83; 4/83

420--20G-02B

ONWI-452
Page

Page

Description

Date

QA ID

299, 300	300	Change Unit Numbers 20 to 12 and 50 to 20	2/15/83	-02B
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301	301	Section 12.3.2... (Unit No. 21)	2/15/83	-02B
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307	307	Section 12.5.1...(Unit No. 12)	2/15/83	-02B
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317	317	Section 12.8.1...(Unit No. 20)	2/15/83	-02B
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330 (Done previously)	330	Replace variable SRHOF with SRATIO	2/15/83	-02B
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		<u>Error Code</u>	<u>Type</u>	<u>Description</u>		
332	332	Section 13.3.2				
		1002	Fatal	Nuclide not in Database (Unit 11)	2/15/83	-02B
332		1005	Fatal	Nuclide not in Database (Unit 52)	2/15/83	-02B

335 (Done previously)	335	Section 13.3.6				
		1205	Fatal	Diffusion Co-efficient <0	2/15/83	-02B

335		1206	Fatal	Areal Degradation factor < 0 or > 1.	2/15/83	-02B
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339-340	339-340	Change TAPE20 to TAPE12 and TAPE50 to TAPE20 in Figures 14-1 and 14-1 cont'd	2/15/83 4/83	-02B -02B
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504-595 (Done previously)	504-585	Pages bound in reverse order were corrected.	2/15/83	-02B
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Changes verified 11/29/83

Changes checked 11/29/83

Revised: 2/15/83

420--20G-02B

SAMPLE PROBLEM INTEGRATED MODEL.
SIMPLIFIED CASE OF BARRIERS, 2 METALS, 9 NUCLIDES, 2 AIR GAPS,
1 WASTEFORM, 1 BACKFILL

1	1	0	0	0	0	0	0	0
24	0.		1.00E04	0.0		0		
0.0	100.0	200.0	300.0	400.0	500.0	700.0	900.0	
1000.0	1200.0	1400.0	1600.0	1800.0	2000.0	2500.0	3000.0	
3500.0	4000.0	5000.0	6000.0	7000.0	8000.0	9000.0	10000.0	
9	6	2	300					
96245	96244	38090	43099	93237	94239	88226	89227	90229
012	0.1555							
203	0.1555							
101	0.1619							
203	0.1683							
108	0.1746							
402	0.5080							
20.	600.	20.						
2.49	0.30	3.1	9.6	1.0				
1.E16								
\$								

6A