Appendix H: Command Files and ASCII Files that Execute NUTS on the WIPP Alpha-VAX Cluster

This Appendix includes examples of three general cases encountered in the CCA calculation using the NUTS_CC executable and one general case of NUTS_SA executable. For further details, see explanations of inputs in Chapter 6.

Example (1): Single-porosity, matrix, tracer test conducted by implementing Dirichlet boundary conditions in the waste region with concentration equal 1 and infinite solubility. There are two input files: Binary input for the flux field from BRAGFLO (BF3_CCA_R1_S1_V23.CDB) and an ASCII file provided by the user (NUT_CCA_SCN_R1_S1.INP). The material map is read from BRAGFLO ASCII input (BF2_CCA_R1_S1_V23.INP). In this example two output files are required, they are: ASCII debug file (NUT_CCA_SCN_R1_S1_V023.OUT) and NUTS' CDB binary file (NUT_CCA_SCN_R1_S1_V023.CDB). The constituent properties are provided by NUTS and Liquid phase transport is conducted.

Interactive Input Command File (TRACER.COM)

```
$ SET DEFAULT DISK$TINA_CCA3:[BF.AASHINT.CCA3.INPUT]
$ NUTS:==$N1:[NOBACK.AASHINT.NMVP.NMVP96.CCASRC.TEMP]NUTS.EXE        ! NUTS EXECUTABLE
PATH.
$ NUTS -
  DISK$TINA_CCA3:[BF.DATA.R1S1]BF3_CCA_R1_S1_V23.CDB -               ! BRAGFLO CDB
INPUT.
  N -
       ! TEST (Y/N)?.
  BIN -
       ! ASC/BIN (CDB) OUTPUT.
  NUT_CCA_SCN_R1_S1.INP -
! NUTS ASCII INPUT.
  NUT_CCA_SCN_R1_S1_V023.CDB -
NUTS CDB OUTPUT.
  NUT_CCA_SCN_R1_S1_V023.OUT -
NUTS DEBUG FILE.
  L -
       ! LIQUID/GAS TRANSPORT.
  DISK$TINA_CCA3:[BF.AASHINT.CCA3.INPUT]BF2_CCA_R1_S1_V23.INP -      ! BRAGFLO ASC
INPUT.
  N -                                          ! NUCLIDE INPUT DATA (CDB (C)/NUTS (N)) .
  CANCEL -                                                ! PROPERTY CDB (SOLUBILITY DATA).
  CANCEL                                        ! NUTS UNDISTRUBED CDB OF THE SAME
VECTOR.
$ EXIT
```

NUTS' ASCII Input (NUT_CCA_SCN_R1_S1.INP)

```
** NUTS TITLE **
'NUTS TRACER SCREENING TEST FOR CCA R1S1 (UNDISTURBED SCENARIO)'
** 1.# OF SITES,# OF MATERIAL,(2.SITE NAME,# COMP. TO BE MODELED)1,..,NSITES **
1,46
'WIPP_SITE'    1
**(1. SITE, 2.COMP., DAUGHTER, PARENT, GROUP NAMES)1,..,NSITES **
'WIPP_SITE'
'TWASTE'   'NONE'   'NONE'   'WASTE'
** 1.# OF ELEMENT,(2.ELEM. NAME, TEMP. DEPEND., TABLE LOOK-UP)1,..,NELEMENT **
1
'WASTE'    .FALSE.   .FALSE.
```

```
** COLLOIDAL TRANSPORT FLAG (T/F) **
.FALSE.
** PH DEPENDENT SOLUBILITY(IS PH REQUIRED (Y/N)) **
'N'
** ORDER OF THE METHOD **
1
** DEGREE OF IMPLICITNESS **
1.D0
** IS MATRIX SORPTION REQUIRED (Y/N) **
'N'
** DO YOU HAVE DISPERSION IN THE MATRIX (Y/N) **
'N'
** DOES MATRIX HAVE SYMMETRIC DISPERSION (T/F): ANSWER IF DISPERSION IS Y **
** DO YOU HAVE INJECTION/PRODUCTION IN THE MATRIX (Y/N) **
'N'
** DO YOU HAVE DIRICHLET B.CS. IN THE MATRIX (F/T) **
.TRUE.
** IS CONCENTRATION INITIALIZED MANUALLY IN THE MATRIX (F/T) **
.FALSE.
** OPEN NUTS UNDISTURBED CDB FOR INTRUSION TIME OTHER THAN 350,1000 YRS **
.FALSE.
** PRINT FLAGS OF MATRIX VARIABLES IN A BINARY FILE **
0,0,0,0,0,0,1,0,0,0,0,0,0,0
** TEMP. DEPEND. OF Kd (ENTER DATA IF ADSORP. IS (Y) AND TEMP. DEPEND.) **
** PRINTING FREQUENCY IN A BINARY FILE **
1,1.D14
** DO YOU HAVE EXTERNAL NUCLIDE SOURCE? (T/F) **
.FALSE.
** MINIMUM LIMIT OF TIME TO BE SET IF ZERO ENCOUNTERED **
1.D-18
** INTRUSION TIME, ITERPOLATED INTRUSION TIME, TOLERANCE **
*** END MATERIAL MAP AND START NUCLIDES PROPERTIES ***
** IF NOT TEMP. DEPEND. (ELEMENT NAME, SOLUBILITY LIMIT) 1,..,NELEMENT **
'WASTE'      -2.D0
** (COMP. NAME, MOL.(ATOMIC) WT., INITIAL INVENTS., HALF LIFE)1,..,NUCLIDE **
'TWASTE'     .1D0    0.D0    0.D0    0.D0
** GROUND WATER PH INPUT **
** STANDARD BR. DENS. IF NOT BRAGFLO RUN (READ ASCII FILE FOR FLUX FIELD) **
** MOLECULAR DIFFUSION OF EACH COMPONENT **
** ROCK GRAIN DENSITY INPUT (REQUIRED ONLY IF SORPTION OR SOIL BASE CONC.) **
** WASTE MATRIX INPUT (1.# OF ISO,2.NAME, LOC. IN THE INPUT, WASTE SITE #) **
1
'TWASTE'  1   1
*** (1.SITE NAME, NUMBER OF GRIDS IN THE SITE 2.INDECES)1...NSITES ***
'WIPP_SITE' 30
  9,8,1    10,8,1    11,8,1    12,8,1    13,8,1    14,8,1    15,8,1
 17,8,1    18,8,1    19,8,1
  9,9,1    10,9,1    11,9,1    12,9,1    13,9,1    14,9,1    15,9,1
 17,9,1    18,9,1    19,9,1
 9,10,1   10,10,1   11,10,1   12,10,1   13,10,1   14,10,1   15,10,1
17,10,1   18,10,1   19,10,1
** MATRIX SORPTION INPUT **
** MATRIX DISPERSION INPUT **
** MATRIX SOURCE INPUT (INJECTED NUCLIDES IF ANY) **
** MATRIX DIR. B.CS. INPUT (REP.='GENERAL',ANYWHERE= 'NOT_GENERAL') **
1  'NOT_GENERAL'
'TWASTE'     1     30
  9,8,1    10,8,1    11,8,1    12,8,1    13,8,1    14,8,1    15,8,1
 17,8,1    18,8,1    19,8,1
  9,9,1    10,9,1    11,9,1    12,9,1    13,9,1    14,9,1    15,9,1
 17,9,1    18,9,1    19,9,1
 9,10,1   10,10,1   11,10,1   12,10,1   13,10,1   14,10,1   15,10,1
17,10,1   18,10,1   19,10,1
'TWASTE'
 1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0
 1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0
 1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0  1.D0
** TIME DEPENDENT SOURCE IN THE MATRIX **
** MATRIX CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE MATRIX **
```

Example (2): Single-porosity, matrix, radiological transport with five isotopes. Three single isotopes and one chain of two members are used. The repository location is described by the waste matrix input. The inventories, atomic weights, half-life, and solubilities are provided by the properties CDB. There are three input files: CDB Binary input file for the flux field from BRAGFLO (BF3_CCA_R1_S4_V23.CDB) and an ASCII file provided by the user (NUT_CCA_ISO_R1_S4.INP). The material map is read from BRAGFLO ASCII input (BF2_CCA_R1_S4_V23.INP), whereas the radioactive material properties are read from the CDB binary input file NUT_CCA_PROP_R1_S4_V023.INP.

In this example, liquid transport is conducted and two output files are required, they are: ASCII debug file (NUT_CCA_ISO_R1_S4_V023.OUT) and NUTS' CDB binary file (NUT_CCA_ISO_R1_S4_V023.CDB).

Interactive Input Command File (ISO.COM)

```
$ SET DEFAULT DISK$TINA_CCA3:[BF.AASHINT.CCA3.INPUT]
$ NUTS:==$N1:[NOBACK.AASHINT.NMVP.NMVP96.CCASRC.TEMP]NUTS.EXE        ! NUTS EXECUTABLE
PATH.
$ NUTS -
  DISK$TINA_CCA3:[BF.DATA.R1S4]BF3_CCA_R1_S4_V23.CDB -               ! BRAGFLO CDB
INPUT.
  N -
        ! TEST (Y/N)?.
  BIN -
        ! ASC/BIN (CDB) OUTPUT.
  NUT_CCA_ISO_R1_S4.INP -
! NUTS ASCII INPUT.
  NUT_CCA_ISO_R1_S4_V023.CDB -
NUTS CDB OUTPUT.
  NUT_CCA_ISO_R1_S4_V023.OUT -
NUTS DEBUG FILE.
  L -
        ! LIQUID/GAS TRANSPORT.
  DISK$TINA_CCA3:[BF.AASHINT.CCA3.INPUT]BF2_CCA_R1_S4_V23.INP -      ! BRAGFLO ASC
INPUT.
  CDB -                                          ! NUCLIDE INPUT DATA (CDB (C)/NUTS (N))
.
  NUT_CCA_PROP_R1_S4_V023.INP -                        ! PROPERTY CDB (SOLUBILITY DATA).
  CANCEL                                                ! NUTS UNDISTRUBED CDB OF THE
SAMEVECTOR.
$ EXIT
```

NUTS' ASCII Input (NUT_CCA_ISO_R1_S4.INP)

```
** NUTS TITLE **
'NUTS RADIOLOGICAL TRANSPORT FOR CCA R1S4 (E2 SCENARIO, 350 YRS INTRUSION)'
** 1.# OF SITES,# OF MATERIAL,(2.SITE NAME,# COMP. TO BE MODELED)1,..,NSITES **
1,49
'WIPP_SITE'    5
**(1. SITE, 2.COMP., DAUGHTER, PARENT, GROUP NAMES)1,..,NSITES **
'WIPP_SITE'
'AM241L'   'NONE'     'NONE'   'AML'
'PU239L'   'NONE'     'NONE'   'PUL'
'PU238L'   'NONE'     'NONE'   'PUL'
'U234L'    'TH230L'   'NONE'   'UL'
'TH230L'   'TH230D'   'NONE'   'THL'
** 1.# OF ELEMENT,(2.ELEM. NAME, TEMP. DEPEND., TABLE LOOK-UP)1,..,NELEMENT **
4
'AML'    .FALSE.   .FALSE.
```

```
'PUL'    .FALSE.   .FALSE.
'UL'     .FALSE.   .FALSE.
'THL'    .FALSE.   .FALSE.
** COLLOIDAL TRANSPORT FLAG (T/F) **
.FALSE.
** PH DEPENDENT SOLUBILITY(IS PH REQUIRED (Y/N)) **
'N'
** ORDER OF THE METHOD **
1
** DEGREE OF IMPLICITNESS **
1.D0
** IS MATRIX SORPTION REQUIRED (Y/N) **
'N'
** DO YOU HAVE DISPERSION IN THE MATRIX (Y/N) **
'N'
** DOES MATRIX HAVE SYMMETRIC DISPERSION (T/F): ANSWER IF DISPERSION IS Y **
** DO YOU HAVE INJECTION/PRODUCTION IN THE MATRIX (Y/N) **
'N'
** DO YOU HAVE DIRICHLET B.CS. IN THE MATRIX (F/T) **
.FALSE.
** IS CONCENTRATION INITIALIZED MANUALLY IN THE MATRIX (F/T) **
.FALSE.
** OPEN NUTS UNDISTURBED CDB FOR INTRUSION TIME OTHER THAN 350,1000 YRS **
.FALSE.
** PRINT FLAGS OF MATRIX VARIABLES IN A BINARY FILE **
0,0,0,0,0,0,1,1,1,0,0,0,0,1
** TEMP. DEPEND. OF Kd (ENTER DATA IF ADSORP. IS (Y) AND TEMP. DEPEND.) **
** PRINTING FREQUENCY IN A BINARY FILE **
1,1.D12
** DO YOU HAVE EXTERNAL NUCLIDE SOURCE? (T/F) **
.FALSE.
** MINIMUM LIMITS OF TIME TO BE SET IF ZERO ENCOUNTERED **
1.D-18
** INTRUSION TIME, ITERPOLATED INTRUSION TIME, TOLERANCE **
*** END MATERIAL MAP AND START NUCLIDES PROPERTIES ***
** IF NOT TEMP. DEPEND. (ELEMENT NAME, SOLUBILITY LIMIT) 1,..,NELEMENT **
** (COMP. NAME, MOL.(ATOMIC) WT., INITIAL INVENTS., HALF LIFE)1,..,NUCLIDE **
** GROUND WATER PH INPUT **
** STANDARD BR. DENS. IF NOT BRAGFLO RUN (READ ASCII FILE FOR FLUX FIELD) **
** MOLECULAR DIFFUSION INPUT **
** ROCK DENSITY INPUT **
** WASTE MATRIX INPUT (LOCATION OF THE WASTE) **
5
'AM241L'    1    1
'PU239L'    2    1
'PU238L'    3    1
'U234L'     4    1
'TH230L'    5    1
*** (1.SITE NAME, NUMBER OF GRIDS IN THE SITE 2.INDECES)1...NSITES ***
'WIPP_SITE' 30
  9,8,1   10,8,1    11,8,1    12,8,1    13,8,1   14,8,1   15,8,1
 17,8,1   18,8,1    19,8,1
  9,9,1   10,9,1    11,9,1    12,9,1    13,9,1   14,9,1   15,9,1
 17,9,1   18,9,1    19,9,1
 9,10,1  10,10,1   11,10,1   12,10,1   13,10,1  14,10,1  15,10,1
17,10,1  18,10,1   19,10,1
** MATRIX SORPTION INPUT **
** MATRIX DISPERSION INPUT **
** MATRIX SOURCE INPUT (INJECTED NUCLIDES IF ANY) **
** MATRIX DIR. B.CS. INPUT (REP.='GENERAL',ANYWHERE= 'NOT_GENERAL') **
** TIME DEPENDENT SOURCE IN THE MATRIX **
** MATRIX CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE MATRIX **
```

Example (3): Single-porosity, matrix, radiological transport with five isotopes. Three single isotopes and one chain of two members are used. The repository location is described by the waste matrix input. The inventories, atomic weights, half-life, and solubilities are provided by the properties CDB. There are four input files: CDB Binary input file for the flux field from BRAGFLO (BF3_CCA_R1_S5_V23.CDB) and an ASCII file provided by the user (NUT_CCA_INT3_R1_S5_V023.INP). The material map is read from BRAGFLO ASCII input (BF2_CCA_R1_S5_V23.INP), whereas the radioactive material properties are read from the CDB binary input file NUT_CCA_PROP_R1_S5_V023.INP. There is an additional CDB input file required to initialization the intrusion time calaculation at 3000 years. This file is the output of NUTS for the undisturbed scenario of vector 23 (NUT_CCA_ISO_R1_S1_V023.INP).

In this example, liquid transport is conducted and two output files are required, they are: ASCII debug file (NUT_CCA_INT3_R1_S5_V023.OUT) and NUTS' CDB binary file (NUT_CCA_INT3_R1_S5_V023.CDB).

Interactive Input Command File (INT3.COM)

```
$ SET DEFAULT DISK$TINA_CCA3:[BF.AASHINT.CCA3.INPUT]
$ NUTS:==$N1:[NOBACK.AASHINT.NMVP.NMVP96.CCASRC.TEMP]NUTS.EXE        ! NUTS EXECUTABLE
PATH.
$ NUTS -
  DISK$TINA_CCA3:[BF.DATA.R1S5]BF3_CCA_R1_S5_V23.CDB -               ! BRAGFLO CDB
INPUT.
  N -
        ! TEST (Y/N)?.
  BIN -
        ! ASC/BIN (CDB) OUTPUT.
  NUT_CCA_INT3_R1_S5_V023.INP -
! NUTS ASCII INPUT.
  NUT_CCA_INT3_R1_S5_V023.CDB -
! NUTS CDB OUTPUT.
  NUT_CCA_INT3_R1_S5_V023.OUT -
! NUTS DEBUG FILE.
  L -
        ! LIQUID/GAS TRANSPORT.
  DISK$TINA_CCA3:[BF.AASHINT.CCA3.INPUT]BF2_CCA_R1_S5_V23.INP -      ! BRAGFLO ASC
INPUT.
  CDB -                                          ! NUCLIDE INPUT DATA (CDB (C)/NUTS (N))
.
  NUT_CCA_PROP_R1_S5_V023.INP -                        ! PROPERTY CDB (SOLUBILITY DATA).
 NUT_CCA_ISO_R1_S5_V023.CDB                      ! NUTS UNDISTRUBED CDB OF THE SAME
VECTOR.
$ EXIT
```

NUTS' ASCII Input (NUT_CCA_INT3_R1_S5_V023.INP)

```
** NUTS TITLE **
'NUTS RADIOLOGICAL TRANSPORT FOR CCA R1S5V023 (E2 SCENARIO, 3000 YRS INTRUSION)'
** 1.# OF SITES,# OF MATERIAL,(2.SITE NAME,# COMP. TO BE MODELED)1,..,NSITES **
1,49
'WIPP_SITE'    5
**(1. SITE, 2.COMP., DAUGHTER, PARENT, GROUP NAMES)1,..,NSITES **
'WIPP_SITE'
'AM241L'   'NONE'     'NONE'   'AML'
'PU239L'   'NONE'     'NONE'   'PUL'
'PU238L'   'NONE'     'NONE'   'PUL'
'U234L'    'TH230L'   'NONE'   'UL'
'TH230L'   'TH230D'   'NONE'   'THL'
** 1.# OF ELEMENT,(2.ELEM. NAME, TEMP. DEPEND., TABLE LOOK-UP)1,..,NELEMENT **
```

```
4
'AML'    .FALSE.   .FALSE.
'PUL'    .FALSE.   .FALSE.
'UL'     .FALSE.   .FALSE.
'THL'    .FALSE.   .FALSE.
** COLLOIDAL TRANSPORT FLAG (T/F) **
.FALSE.
** PH DEPENDENT SOLUBILITY(IS PH REQUIRED (Y/N)) **
'N'
** ORDER OF THE METHOD **
1
** DEGREE OF IMPLICITNESS **
1.D0
** IS MATRIX SORPTION REQUIRED (Y/N) **
'N'
** DO YOU HAVE DISPERSION IN THE MATRIX (Y/N) **
'N'
** DOES MATRIX HAVE SYMMETRIC DISPERSION (T/F): ANSWER IF DISPERSION IS Y **
** DO YOU HAVE INJECTION/PRODUCTION IN THE MATRIX (Y/N) **
'N'
** DO YOU HAVE DIRICHLET B.CS. IN THE MATRIX (F/T) **
.FALSE.
** IS CONCENTRATION INITIALIZED MANUALLY IN THE MATRIX (F/T) **
.FALSE.
** OPEN NUTS UNDISTURBED CDB FOR INTRUSION TIME OTHER THAN 350,1000 YRS **
.TRUE.
** PRINT FLAGS OF MATRIX VARIABLES IN A BINARY FILE **
0,0,0,0,0,0,1,1,1,0,0,0,0,1
** TEMP. DEPEND. OF Kd (ENTER DATA IF ADSORP. IS (Y) AND TEMP. DEPEND.) **
** PRINTING FREQUENCY IN A BINARY FILE **
1,1.D12
** DO YOU HAVE EXTERNAL NUCLIDE SOURCE? (T/F) **
.FALSE.
** MINIMUM LIMITS OF TIME TO BE SET IF ZERO ENCOUNTERED **
1.D-18
** INTRUSION TIME, ITERPOLATED INTRUSION TIME, TOLERANCE **
0.3155693D11    0.946708D11    0.D0
*** END MATERIAL MAP AND START NUCLIDES PROPERTIES ***
** IF NOT TEMP. DEPEND. (ELEMENT NAME, SOLUBILITY LIMIT) 1,..,NELEMENT **
** (COMP. NAME, MOL.(ATOMIC) WT., INITIAL INVENTS., HALF LIFE)1,..,NUCLIDE **
** GROUND WATER PH INPUT **
** STANDARD BR. DENS. IF NOT BRAGFLO RUN (READ ASCII FILE FOR FLUX FIELD) **
** MOLECULAR DIFFUSION INPUT **
** ROCK DENSITY INPUT **
** WASTE MATRIX INPUT (LOCATION OF THE WASTE) **
5
'AM241L'   1    1
'PU239L'   2    1
'PU238L'   3    1
'U234L'    4    1
'TH230L'   5    1
*** (1.SITE NAME, NUMBER OF GRIDS IN THE SITE 2.INDECES)1...NSITES ***
'WIPP_SITE' 30
  9,8,1   10,8,1    11,8,1    12,8,1    13,8,1   14,8,1   15,8,1
 17,8,1   18,8,1    19,8,1
  9,9,1   10,9,1    11,9,1    12,9,1    13,9,1   14,9,1   15,9,1
 17,9,1   18,9,1    19,9,1
 9,10,1  10,10,1   11,10,1   12,10,1   13,10,1  14,10,1  15,10,1
17,10,1  18,10,1   19,10,1
** MATRIX SORPTION INPUT **
** MATRIX DISPERSION INPUT **
** MATRIX SOURCE INPUT (INJECTED NUCLIDES IF ANY) **
** MATRIX DIR. B.CS. INPUT (REP.='GENERAL',ANYWHERE= 'NOT_GENERAL') **
** TIME DEPENDENT SOURCE IN THE MATRIX **
** MATRIX CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE MATRIX **
```

Example (4): Dual-permeability, One Site, Eleven Component, No Temperature Dependency, No waste emplacement, Injection in the Matrix only, No Dirichlet B.Cs., No External Dynamic Source, Material-map from Input, and writing in an ASCII output.

Interactive Input Command File (DUAL.COM)

```
$ RUN N1:[NOBACK.AASHINT.NMVP.NMVP96.CCASRC.TEMP]NUTS_STANDALONE
N
N
DUALNUTS.IN
Y
N
Y
DUALTEST.IN
ASC
DPM
1
L
VAX
ALPHA
```

DUALNUTS.IN

```
** NUTS TITLE **
'NUTS TEST RUN EXAMPLE'
** 1.# OF SITES,# OF MATERIAL,(2.SITE NAME,# OF COMP. TO BE MODELED)1,..,NSITES **
1   7
'TEST_SITE'     11
**(1.SITE NAME,2.COMP.,DAUGHTER,PARENT,GROUP NAMES)1,..,NSITES **
'TEST_SITE'
'PU239'       'U235'        'NONE'        'PU'
'U235'        'PA231'       'PU239'       'U '
'PA231'       'NONE'        'U235'        'PA'
'NP237'       'U233'        'NONE'        'NP'
'U233'        'NONE'        'NP237'       'U '
'U238'        'U234'        'NONE'        'U '
'U234'        'NONE'        'U238'        'U '
'I129'        'NONE'        'NONE'        'I '
'TC99'        'NONE'        'NONE'        'TC'
'SE79'        'NONE'        'NONE'        'SE'
'U235'        'NONE'        'NONE'        'U '
** 1.# OF ELEMENT,(2.ELEMENT NAME, TEMP. DEPENDENCY, TABLE LOOK-UP)1,..,NELEMENT **
7
'U     .FALSE.       .FALSE.
'PU'   .FALSE.       .FALSE.
'PA'   .FALSE.       .FALSE.
'NP'   .FALSE.       .FALSE.
'I     .FALSE.       .FALSE.
'TC'   .FALSE.       .FALSE.
'SE'   .FALSE.       .FALSE.
** COLLOIDAL TRANSPORT FLAG (T/F) **
.FALSE.
** pH DEPENDENT SOLUBILITY(IS pH REQUIRED (Y/N)) **
'N'
** ORDER OF THE METHOD **
1
** DEGREE OF IMPLICITNESS **
1.
** IS FRACTURE SORPTION REQUIRED (Y/N) **
'N'
** DO YOU HAVE DISPERSION IN THE FRACTURE (Y/N) **
'Y'
*FRACTURE DISPERSION IS SYMMETRIC AND DATA PROVIDED BY NUTS(T/F):ANSWER IF DISP IS Y*
.TRUE.       .TRUE.
```

```
** DO YOU HAVE INJECTION/PRODUCTION IN THE FRACTURE (Y/N) **
'N'
** DO YOU HAVE DIRICLET B.CS. IN THE FRACTURE (F/T) **
.FALSE.
** IS CONCENTRATION INITIALIZED MANUALLY IN THE FRACTURE (T/F) **
.FALSE.
** PRINT FLAGS OF FRACTURE VARIABLES IN ASCII FILE **
0,0,0,0,0,0,1,0,0,0,0,0,0,0,0
** DO YOU HAVE DATA TO BE PRINTED IN FRACTURE SPECIFIED GRID BLOCK RANGE **
'N'
** IS MATRIX SORPTION REQUIRED (Y/N) **
'Y'
'L'
'PU239'              'ADSORP'      .FALSE.
'U235 '              'ADSORP'      .FALSE.
'PA231'              'ADSORP'      .FALSE.
'NP237'              'ADSORP'      .FALSE.
'U233 '              'ADSORP'      .FALSE.
'U238 '              'ADSORP'      .FALSE.
'U234 '              'ADSORP'      .FALSE.
'I129 '              'ADSORP'      .FALSE.
'TC99 '              'ADSORP'      .FALSE.
'SE79 '              'ADSORP'      .FALSE.
'U236 '              'ADSORP'      .FALSE.
** DO YOU HAVE DISPERSION IN THE MATRIX (Y/N) **
'Y'
*MATRIX DISPERSION IS SYMMETRIC AND DATA PROVIDED BY NUTS(T/F):ANSWER IF DISP IS Y*
.TRUE.       .TRUE.
** DO YOU HAVE MATRIX/FRACTURE DISPERSION (Y/N) **
'Y'
** DO YOU HAVE INJECTION/PRODUCTION IN THE MATRIX (Y/N) **
'Y'
** DO YOU HAVE DIRICLET B.CS. IN THE MATRIX (F/T) **
.FALSE.
** IS CONCENTRATION INITIALIZED MANUALLY IN THE MATRIX (T/F) **
.FALSE.
** MATRIX INITIAL. IN THE CDB FOR INTERPOLATED INTRUSION TIME IN E1 SCENARIO(T/F) **
.FALSE.
** PRINT FLAGS OF MATRIX VARIABLES IN ASCII FILE**
0,0,0,0,0,0,1,0,0,0,0,0,0,0,0
** DO YOU HAVE DATA TO BE PRINTED IN MATRIX SPECIFIED GRID BLOCK RANGE **
'N'
** TEMP. DEPEND. OF Kd (ENTER DATA IF ADSORP. IS (Y) AND TEMP. DEPEN.) **
** TEMP. DEPEND.OF MOLECULAR DIFFUSION (ENTER DATA IF DISPER. IS (Y)) **
'PU239'              .FALSE.
'U235 '              .FALSE.
'PA231'              .FALSE.
'NP237'              .FALSE.
'U233 '              .FALSE.
'U238 '              .FALSE.
'U234 '              .FALSE.
'I129 '              .FALSE.
'TC99 '              .FALSE.
'SE79 '              .FALSE.
'U236 '              .FALSE.
** PRINTING FREQUENCY IN ASCII FILE **
1,1.E10
** DO YOU HAVE EXTERNAL NUCLIDE SOURCE? (T/F) **
.FALSE.
** MINIMUM LIMIT OF TIME TO BE SET IF ZERO ENCOUNTERED **
1.E-18
** IF CDB, INTRUSION TIME, INTERPOLATED TIME, TOLERANCE IN SECONDS **
  NUMBER OF TIMES FOR SPECIFING MATERIAL MAP
1
START TIME FOR MAP 1
0.E0
MATERIAL TYPE GRID MAP
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
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7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
#   NAME
1   FMN#1
2   FMN#2
3   FMN#3
4   FMN#4
5   FMN#5
6   FMN#6
7   FMN#7
NUMBER OF WASTE REGIONS
1
MAT_WASTEI
5
5
*** END OF MAT_MAP AND START NUCLIDE PROPERTIES ***
** IF NOT TEMP. DEPEND. (ELEMENT NAME,LOG SOLUBILITY LIMIT) 1,..,NELEMENT **
'U '   7
'PU'   7
'PA'   7
'NP'   7
'I '   7
'TC'   7
'SE'   7
** (COMP. NAME, MOL. WT., INITIAL INVENTORIES, HALF LIFE)1,..,NUCLIDE **
'PU239'       0.239        392.   0.     7.59E11
'U235 '       0.235        0.     0.     2.22E16
'PA231'       0.231        0.     0.     1.03E12
'NP237'       0.237        0.     0.     6.75E13
'U233 '       0.233        0.     0.     5.00E12
'U238 '       0.238        0.     0.     1.41E17
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'U234 '       0.234         0.     0.     7.72E12
'I129 '       0.129         110.   0.     4.95E14
'TC99 '       0.99          0.     0.     6.72E12
'SE79 '       0.79          0.     0.     2.05E12
'U236 '       0.236         1.45E4 0.     7.39E14
** GROUND WATER pH INPUT **
** STANDARD BRINE DENSITY IF NOT BRAGFLO RUN (ASCII FILE FOR FLUX FIELD) **
1000.
** MOLECULAR DIFFUSION OF EACH COMPONENT **
'PU239'             1.00E-9
'U235 '             1.00E-9
'PA231'             1.00E-9
'NP237'             1.00E-9
'U233 '             1.00E-9
'U238 '             1.00E-9
'U234 '             1.00E-9
'I129 '             1.00E-9
'TC99 '             1.00E-9
'SE79 '             1.00E-9
'U236 '             1.00E-9
** REFERENCE VISCOSITY AND TEMPERATURE **
** ROCK DENSITY INPUT **
1993    1746    1838    2021    2283    1714    2366
** WASTE MATRIX INPUT **
3
'PU239'             1      1
'I129 '             8      1
'U236 '             11     1
** (SITE NAME, NO. OF GRID IN THE SITE, 2. INDICES), 1,..., NSITES **
'TEST_SITE'    1
28  15  1
** FRACTURE SORPTION INPUT **
** FRACTURE DISPERSION INPUT **
** FRACTURE LONGITUDINAL MATERIAL DISPERSIVITIES **
7*1.D0
** FRACTURE TRANSVERSE MATERIAL DISPERSIVITIES **
7*1.D0
** FRACTURE MATERIAL TORTUOSITY **
7*1.D0
** FRACTURE SOURCE INPUT (INJECTION PRODUCTION) IF ANY **
** FRACTURE DIRICHLET BOUNDARY CONDITIONS, IF ANY **
** TIME DEPENDENT SOURCE IN THE FRACTURE **
** FRACTURE MANUAL CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE FRACTURE **
** MATRIX SORPTION **
'PU239'
1.00E-1  4.00E-2  1.00E-1  4.00E-2  1.00E-1  4.00E-2  1.00E-1
'U235 '
2.50E-3  1.00E-2  2.00E-3  1.00E-2  2.25E-3  1.00E-2  2.50E-3
'PA231'
2.00E-3  4.00E-3  5.00E-4  4.00E-3  1.25E-3  4.00E-3  2.00E-3
'NP237'
2.00E-3  4.00E-3  5.00E-4  4.00E-3  1.25E-3  4.00E-3  2.00E-3
'U233 '
2.50E-3  1.00E-2  2.00E-3  1.00E-2  2.25E-3  1.00E-2  2.50E-3
'U238 '
2.50E-3  1.00E-2  2.00E-3  1.00E-2  2.25E-3  1.00E-2  2.50E-3
'U234 '
2.50E-3  1.00E-2  2.00E-3  1.00E-2  2.25E-3  1.00E-2  2.50E-3
'I129 '
0.00E0   0.00E0   0.00E0   0.00E0   0.00E0   0.00E0   0.00E0
'TC99 '
0.00E0   0.00E0   0.00E0   0.00E0   0.00E0   0.00E0   0.00E0
'SE79 '
2.50E-3  1.00E-2  2.00E-3  1.00E-2  2.25E-3  1.00E-2   2.50E-3
'U236 '
2.50E-3  1.00E-2  2.00E-3  1.00E-2  2.25E-3  1.00E-2  2.50E-3
** MATRIX DISPERSION INPUT **
** MATRIX LONGITUDINAL MATERIAL DISPERSIVITIES **
1.30E02  1.70E02  1.10E02
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```
1.70E02  1.20E02  1.70E02
1.30E02
** MATRIX TRANSVERSE MATERIAL DISPERSIVITIES **
1.30E01  1.70E01  1.10E01
1.70E01  1.20E01  1.70E01
1.30E01
** MATRIX MATERIAL TORTUOSITY **
10.  10.  10.
10.  10.  10.
10.
** MATRIX SOURCE INPUT (INJECTED NUCLIDES IF ANY) **
11
'PU239'              1      1
28           15      1
'U235 '              2      1
28           15      1
'PA231'              3      1
28           15      1
'NP237'              4      1
28           15      1
'U233 '              5      1
28           15      1
'U238 '              6      1
28           15      1
'U234 '              7      1
28           15      1
'I129 '              8      1
28           15      1
'TC99 '              9      1
28           15      1
'SE79 '              10     1
28           15      1
'U236 '              11     1
28           15      1
'PU239'
1.E-7
'U235 '
1.E-7
'PA231'
1.E-7
'NP237'
1.E-7
'U233 '
1.E-7
'U238 '
1.E-7
'U234 '
1.E-7
'I129 '
1.E-7
'TC99 '
1.E-7
'SE79 '
1.E-7
'U236 '
1.E-7
** INJECTION RATE IN THE MATRIX **
1      0.     1.E30
28     15     1      1.E0
** MATRIX DIRICHLET B.CS. INPUT, IF ANY **
** TIME DEPENDENT SOURCE IN THE MATRIX **
** MATRIX MANUAL CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE MATRIX **
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DUALTEST.IN

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** DO YOU HAVE HOMOGENEOUS PROPERTIES? (T/F) **
T
** TITLE OF THE TEST RUN  **
'FLUX FIELD TEST'
** TIME STEP SIZE AND NUMBER  **
3.1536E4       100
** # OF GRID BLOCKS IN X,Y,Z **
58     22     1
** DIMENSION OF GRID BLOCKS IN X,Y,Z **
100.   100.    100.
** POROSITY AND SATURATION OF THE FRACTURE **
0.01           0.6
** VELOCITIES IN X,Y,Z IN THE FRACTURE **
8.E-6        8.E-6        0.
** FRACTURE TEMPERATURE AND FLUID VISCOSITY **
298.15       1.E-3
** POROSITY AND SATURATION OF THE MATRIX **
0.3          .6
** VELOCITIES IN X,Y,Z IN THE MATRIX **
4.E-8        4.E-8        0.
** MATRIX TEMPERATURE AND FLUID VISCOSITY **
298.15       1.E-3
** SHAPE FACTOR, AND TRNSFER FUNCTION **
0.08      4.E-10
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