Decay Heat (DCH) Package
Users' Guide

The MELCOR decay heat package models the decay heat power resulting from the radioactive decay of fission products. Decay heat is evaluated for reactor core material and for suspended or deposited aerosols and gases. MELCOR couples thermal-hydraulic processes and fission product behavior during the calculation.

Both the radionuclides present in the reactor at the time of the accident and the radionuclide daughter products contribute to the decay heat. In the calculation of decay heat, MELCOR does not explicitly treat each decay chain, since detailed tracking of radionuclide decay chains would be too costly. When the radionuclide package is active, the decay heat is calculated for each radionuclide class by using pre-calculated tables from ORIGEN program runs. If the radionuclide package is not active, the whole-core decay heat is computed from one of several possible user-specified calculations.

This Users' Guide describes the input to the DCH package, including a brief description of the models employed, the input format, sample input, discussion of the output, sensitivity coefficients, plot variables, and control variables. Details on the models can be found in the DCH Package Reference Manual.

Contents

1. Introduction

The MELCOR Decay Heat (DCH) package models the heating from the radioactive decay of fission products. Decay heat power is evaluated for the fission products assumed to reside in reactor core materials, cavity materials, and in suspended or deposited aerosols and vapors. Decay heat power levels as a function of time are supplied as a utility function within MELCOR that may be called by other phenomenological packages. The DCH package is not involved in the calculation of fission product transport or chemical interactions. These processes are calculated by the RadioNuclide (RN) package (see the RN Package Reference Manual).

Both the radionuclides present in the reactor core and/or cavity from the time of reactor shutdown and the radionuclide daughters from decay contribute to the total decay heat power. In the calculation of decay heat power, the DCH package does not explicitly treat decay chains. Detailed tracking of radionuclide decay chains was seen as computationally costly and too detailed for MELCOR. Instead, when the RN package is active, elemental decay heat power information based on ORIGEN calculations is summed into the RN class structure, as described in the DCH Package Reference Manual.

There are also several options for calculating decay heat power when the RN package is not active (that is, when tracking of fission products is not desired). These are called *whole-core calculations* in the DCH package, although they may be applied to cavity inventories of melt debris as well.

2. User Input

2.1 MELGEN Input

2.1.1 General Input

These input records describe data used by both the whole-core and class decay heat calculations.

DCHREACTOR – Reactor type
Optional

This record enables the user to specify the type of reactor. This will affect the default power levels and, for the radionuclide class calculation, the radionuclide mass inventories. The valid options and the default are core-model specific; values given here are for the LWR COR package. Users of an alternate core package

should consult the documentation for that package. Note that the default type of 'PWR' is inconsistent with the default reactor type in the Core package on record COR00002; one or the other should be changed by the user.

(1) REACTP - Character string selecting reactor type:
(1) 'PWR', use PWR mass inventories for radionuclide class calculation and set default power to 3412 MW.
(2) 'BWR', use BWR mass inventories for radionuclide class calculation and set default power to 3578 MW.
(type = character * 3, default = 'PWR')

DCHSHUT – Reactor Shutdown Time
Optional

This record defines the problem time at which reactor shutdown occurs for purposes of decay heat computation.

(1) ISHTCF - Reactor shutdown trip control function number. If less than or equal to zero no reactor trip function is used. If positive, then a logical valued control function ISHTCF is used to determine the reactor shutdown time. During computation the reactor shutdown time is set to the current problem time whenever the control function value changes from .FALSE. to .TRUE.
(type = integer, default = 0, units = none)

(2) TMSHUT - Reactor shutdown time. If DCHSHUT record is input and ISHTCF field does not contain a positive integer then the TMSHUT field is required.
(type = real, default = 0.0, units = s)

2.1.2 Whole-Core Input

These input records describe data used by the whole-core decay heat calculations.

DCHDECPOW – Decay Power of Nuclides
Optional

This record enables the user to specify the calculation to be used for the whole-core decay heat calculation.

(1) WCTYPE - Character string of four possible forms:
(1) 'ORIGEN', use summation of default ORIGEN radionuclide decay heats
(2) 'ANS', use ANS standard calculation

(3) 'CF-nnn', use control function nnn for decay heat (W)
(4) 'TF-nnn', use tabular function nnn as table of whole-core decay heat (W) as function of time since shutdown in seconds
(type = character * 6, default = 'ORIGEN')

DCHFPOW – Fission Power of Nuclides
Optional

This record defines the total thermal operating power due to the nuclides U-235, Pu-239, and U-238 (from both fission and decay heat). These data are used only if WCTYPE on card DCHDECPOW is 'ORIGEN' or 'ANS.' The defaults are core-model specific; values given here are for the LWR COR package. These defaults are taken from a SANDIA-ORIGEN run giving the powers averaged over an equilibrium fuel cycle. The defaults for total power are 3412 MW (PWR) and 3578 MW (BWR). Users of an alternate core package should consult the documentation for that package.

(1) U235P - Power due to thermal fission of U-235.
(type = real, default = 2.2086E9 (PWR), 2.316E9 (BWR), units = W)

(2) PU239P - Power due to thermal fission of Pu-239.
(type = real, default = 1.0598E9 (PWR), 1.1114E9 (BWR), units = W)

(3) U238P - Power due to fast fission of U-238.
(type = real, default = 1.436E8 (PWR), 1.506E8 (BWR), units = W)

DCHOPRTIME – Reactor Operating Time
Optional

This record defines the irradiation time, the length of time the reactor fuel has been undergoing fission. A constant fission rate is assumed during this time. The default value is 0.8 x 2 years, or 584 days, chosen to match the ORIGEN run with an average in-core time of 2 years for the fuel at the end of the equilibrium cycle with an 80% capacity factor. These data are used only if WCTYPE on card DCHDECPOW is 'ANS.'

OPRTIM - Reactor operating time.
(type = real, default = 5.05E7, units = s)

DCHNCPSI – Number of fissions per Initial Fissile Atom
Optional

This factor is used as in the calculation of the neutron capture correction factor *G(t)* (see Section 3.2 of the DCH Package Reference Manual). The default is computed from SANDIA-ORIGEN data for a representative fissile material inventory. These data are used only if WCTYPE on card DCHDECPOW is 'ANS.'

(1) PSINC - Number of Fissions per initial fissile atom.
(type = real, default = 0.713, units = fissions/atom)

2.1.3 Radionuclide Class Input

These input records describe data used for the radionuclide class decay heat calculations. The grouping of elements into RN classes is described in detail in Section 2.2 of the DCH Package Reference Manual. The valid names for default elements input on records DCHNEMnn00 and DCHCLSnnnm are listed below. Only those listed without parentheses in Table 2.1 of the DCH Package Reference Manual have decay heat tables in MELCOR.

```
'H',   'HE',  'LI',  'BE',  'B',   'C',   'N',   'O',   'F',   'NE',
'NA',  'MG',  'AL',  'SI',  'P',   'S',   'CL',  'AR',  'K',   'CA',
'SC',  'TI',  'V',   'CR',  'MN',  'FE',  'CO',  'NI',  'CU',  'ZN',
'GA',  'GE',  'AS',  'SE',  'BR',  'KR',  'RB',  'SR',  'Y',   'ZR',
'NB',  'MO',  'TC',  'RU',  'RH',  'PD',  'AG',  'CD',  'IN',  'SN',
'SB',  'TE',  'I',   'XE',  'CS',  'BA',  'LA',  'CE',  'PR',  'ND',
'PM',  'SM',  'EU',  'GD',  'TB',  'DY',  'HO',  'ER',  'TM',  'YB',
'LU',  'HF',  'TA',  'W',   'RE',  'OS',  'IR',  'PT',  'AU',  'HG',
'TL',  'PB',  'BI',  'PO',  'AT',  'RN',  'FR',  'RA',  'AC',  'TH',
'PA',  'U',   'NP',  'PU',  'AM',  'CM',  'BK',  'CF',  'ES',  'FM',
'WT' (water)          'CC' (concrete)
```

DCHNEMnn00 – Element Name
$0 \leq nn \leq 99$, nn is the user-defined element number
Optional

This record, in conjunction with the DCHNEMnnmm records, allows the user to define a new element or to redefine a default element for purposes of decay heat calculation. If the user inputs a default element, the user-defined element decay

heat data are used instead of the default data. If the same element is input more than once, the first definition is used and a warning message is printed.

(1) ELMNAM - User-input element name. May be a default element or a new name.
(type = character * 2)

(2) ELMMAS - Mass inventory of element ELMNAM in reactor at shutdown.
(type = real, default = none, units = kg)

DCHNEMnnmm – Time, Decay Heat Data
$0 \leq nn \leq 99$, nn is the user-defined element number
$1 \leq mm \leq 99$, mm is used for ordering the input
Optional

These records define the pairs of decay heat data for element ELMNAM. The first field in a pair is the time after shutdown, and the second field is the decay heat power per unit mass at that time. There may be an arbitrary number of pairs on a record, but a pair may not be split across a record. The decay heat times do not have to be in ascending order.

(1) TIME - Time after shutdown.
(type = real, default = none, units = s)

(2) DCHEAT - Decay heat power per unit mass for this element at time TIME.
(type = real, default = none, units = W/kg)

DCHCLSnnn0 – Radionuclide Class Name
$0 \leq nnn \leq 999$, nnn is the class ID number
Optional

This record, in conjunction with the DCHCLSnnnm records, allows the user to define a new class or to redefine a default class for purposes of decay heat calculation. If the user inputs a default class ID number (1 through 15), the user-defined class is used instead of the default class listed in Table 2.1 of the DCH Package Reference Manual.

(1) RDCNAM - User-input class name
(type = character * 32)

DCHCLSnnnm – Elements in class

$0 \leq nnn \leq 999$, nnn is the class ID number
$1 \leq mm \leq 9$, m is used for ordering the input
Optional

These records define the elements in the class with ID nnn and name RDCNAM. The element names may be user-defined elements or default elements. There may be an arbitrary number of elements on a record.

(1) CLSELM - Name of element in class.
(type = character * 2)

DCHDEFCLSm – Default Classes

$0 \leq m \leq 9$, m is used for ordering the input
Optional (if not input, no default radionuclide classes are defined)

This record selects the default classes to be used in the radionuclide calculation. The default classes, numbered 1 through 15, are given in Table 2.1 of the DCH Package Reference Manual. A default class with a given ID may be input only once.

(1) DEFCLS - This field can be of two types:

integer - default class ID number. Numbers must be in the range from 1 through 15, and can be in any order. This field may be repeated on a record as often as necessary.
(default = none, units = none)

character - 'ALL' indicates that all default classes listed in Table 2.1 of the DCH Package Reference Manual are to be used in the calculation.
(type = character *3)

DCHCLSNORM – Class Decay Heat Normalization Flag

Optional

This record allows the user to have the radionuclide class decay heat power normalized to the whole-core decay heat power. If the normalization flag is set to 'YES', the calculated decay heat for each class (whether default or user-defined) will be multiplied by the ratio of the sum of all the class decay heats and the whole-core decay heat. Thus, the sum of all the class decay powers will be equal to the whole-core decay power.

If the whole-core power is 'ORIGEN', the sum of class powers including the effects of sensitivity coefficients 3210 and 3211 will be renormalized to the sum of class powers before these sensitivity coefficients are considered.

(1) CLSNRM - Class Normalization Flag
'YES' - Normalize class decay heats to whole-core decay heat
'NO' - No normalization
(type = character* 3, default = 'YES')

2.2 MELCOR Input

There is at present no MELCOR input to the decay heat package.

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters in the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the MELCOR EXEC Users' Guide.

3.1 DCH Sensitivity Coefficients

The sensitivity coefficients for the DCH package have identifier numbers from 3200 through 3299.

3200 – Multiplier for ANS decay heat curve

This sensitivity coefficient is the multiplier M_{user} given in the ANS decay heat equation (see Section 3.2 of the DCH Package Reference Manual).

(1) - Multiplier for ANS decay heat curve.
(default = 1.0, units = none, equiv = ANSMUL)

3201 – Energy per Fission for Nuclides

These sensitivity coefficients are the Q factors in the ANS decay heat equation (see Section 3.2 of the DCH Package Reference Manual). The defaults are computed from SANDIA-ORIGEN data giving the fissioning rates for each nuclide. The energies include both fission and decay energies.

(1) - Energy per thermal fission of U-235
(default = 199.0 units = MeV/fission, equiv = FEU235)

(2) - Energy per thermal fission of Pu-239
(default = 210.2, units = MeV/fission, equiv = FEP239)

(3) - Energy per fast fission of U-238
(default = 199.3, units = MeV/fission, equiv = FEU238)

3202 – Times for ANS decay heat power tables

These sensitivity coefficients provide the times at which the ANS decay heat powers for the nuclides and the neutron capture correction factors are available. The defaults, taken from the 56 tabulated times in the ANS standard (see Section 3.2 of the DCH Package Reference Manual), run from 0.0 s to 10^9 s.

(1–56)
- Times after shutdown for decay heat tables (sensitivity coefficient 3203) and neutron capture factors (sensitivity coefficient 3204).
(default = tabulated times from ANS standard, units = s, equiv = TIMDCH(1:56))

3203 – Decay heat powers for ANS decay heat curve

These sensitivity coefficients are the factors $F(t,\infty)$ needed to compute $F(t,T)$ used in the ANS decay heat equation (see Section 3.2 of the DCH Package Reference Manual). The calculation is $F(t,T)=F(t,\infty)-F(t+T,\infty)$.

(1–56,
1–3) - Decay heat powers DCHPOW (I, J), corresponding to times TIMDCH(I) in sensitivity coefficient 3202, resulting from decay of products fissioning of nuclide J, where J indicates nuclide:
J = 1, U-235
J = 2, Pu-239
J = 3, U-238
(default = values from Tables 4, 5, and 6 of the ANS standard, units = MeV/fission, equiv = DCHPOW (1:56,1:3))

3204 – Neutron capture correction factors for ANS decay heat curve

These sensitivity coefficients are the factors $G_{max}(t)$ that are used for $G(t)$ for shutdown times greater than 10^4 seconds. $G(t)$ is used in the ANS decay heat equation (see Section 3.2 of the DCH Package Reference Manual).

(1–56)
- Neutron capture correction factors CAPNEU(I), corresponding to times TIMDCH(I) in sensitivity coefficient 3202.

(default = values from Table 10 of the ANS standard, units = none, equiv = CAPNEU (1:56))

3205 – Parameters for actinide decay heat calculation

These sensitivity coefficients are the parameters in the ANS decay heat equation for the decay power from U-239 and Np-239 (see Section 3.2 of the DCH Package Reference Manual). The default for the first parameter is computed so that Equation 16 of the ANS standard matches the ORIGEN results for decay power from U-239 and Np-239. The other defaults are taken from the discussion of the equation on page 5 of the ANS standard.

(1) - Number of atoms of U-239 produced per second per fission per second at time of shutdown.
(default = 0.526, units = 1/fission, equiv = R)

(2) - Average energy from decay of U-239 atom.
(default = 0.474, units = MeV, equiv = E239U)

(3) - Average energy from decay of Np-239 atom.
(default = 0.419, units = MeV, equiv = E239NP)

(4) - Decay constant for U-239.
(default = 4.91E-4, units = s^{-1}, equiv = DCU)

(5) - Decay constant for Np-239.
(default = 3.41E-6, units = s^{-1}, equiv = DCNP)

3210 – Multiplier for all ORIGEN elemental decay heat curves

This sensitivity coefficient is a multiplier that will be applied to all elemental decay heat power curves stored as default data in MELCOR.

(1) - Multiplier for ORIGEN elemental decay heat power.
(default = 1.0, units = none, equiv = ORGMUL)

3211 – Multipliers for individual ORIGEN elemental decay heat curves

These sensitivity coefficients are multipliers for individual elemental decay heat power curves stored as default data in MELCOR. These multipliers will be applied in addition to the general multiplier ORGMUL. The list of relevant elements is core-model specific; the list given here is for the LWR COR package. Users of an alternate core package should consult the documentation for that package.

(1-29)

- Multiplier for individual elemental decay power. The indices for each element are:

1.	AS	2.	SE	3.	BR	4.	KR	5.	RB	6.	SR	7.	Y
8.	ZR	9.	NB	10.	MO	11.	TC	12.	RU	13.	RH	14.	PD
15.	AG	16.	SN	17.	SB	18.	TE	19.	I	20.	XE	21.	CS
22.	BA	23.	LA	24.	CE	25.	PR	26.	ND	27.	PM	28.	U
29.	NP												

(default = 1.0, units = none, equiv = ELMMUL(1:29))

3212 – Fraction of fuel equilibrium cycle elapsed

This sensitivity coefficient, which must have a value between 0.0 and 1.0, is used in determining the fission product mass inventory. 0.0 corresponds to the beginning of the fuel cycle (1/3 fresh fuel, 1/3 with one year in core, 1/3 with two years in core). 1.0 corresponds to the end of the fuel cycle (1/3 of fuel with one year in core, 1/3 with two years in core, 1/3 with three years in core). These data are used only if WCTYPE on card DCHDECPOW is 'ORIGEN.'

(1) - Fraction of fuel equilibrium cycle that has elapsed at beginning of problem (default = 1.0, units = none, equiv = TFLCYC)

4. Plot Variables and Control Function Arguments

The decay heat package's variables that may be used for plot variables and control function arguments are described below. The control function arguments are denoted by a 'c.' The plot variable arguments are denoted by 'p.' The 'c' or 'p' characters are inside slashes '/' following the variable name.

DCH-COREPOW.0	/cp/	Whole-core decay heat power. (units = W)
DCH-CLSPOW.n	/cp/	Decay heat power per unit mass for radionuclide class n. (units = W/kg)
DCH-TOTCLSPOW.0	/cp/	Total decay heat power for all radionuclide classes. (units = W)

5. Example Input

The following example input to MELCOR will input the default decay heat data set in MELCOR. The input will be in three sections; general, whole-core, and radionuclide class.

5.1 General Input

```
*
*          REQUEST PWR DEFAULT REACTOR POWER AND
*               RADIONUCLIDE INVENTORIES
*
DCHREACTOR PWR
*
*     SET REACTOR SHUTDOWN TIME TO DEFAULT - 0.0 S, NO SHUTDOWN FUNCTION.

*
DCHSHUT    0      0.0
*
```

5.2 Whole-Core Input

```
*     SELECT ANS DECAY CURVE FOR WHOLE-CORE DECAY HEAT
*
DCHDECPOW  ANS
*
*     SET REACTOR OPERATING TIME TO DEFAULT - 0.8 * 2 YEARS
*
DCHOPRTIME 5.05E7
*
*     SET TOTAL REACTOR FISSION POWER DUE TO:
*          U-235       2208.6 MW   (DEFAULT FOR PWR)
*          PU-239      1059.8 MW   (DEFAULT FOR PWR)
*          U-238       143.6 MW    (DEFAULT FOR PWR)
*
DCHFPOW    2.2086E9    1.0598E9    1.436E8
*
*
*     SET PSI IN NEUTRON CAPTURE CORRECTION EQUATION TO DEFAULT
*
DCHNCPSI   0.713
*
*
*     ANS DECAY HEAT SENSITIVITY COEFFICIENTS
*
*          SET ANS MULTIPLIER TO DEFAULT
SC00001    3200  1.00        1
*     SET ENERGY PER FISSION FOR U-235       DEFAULT - 199 MEV/FISSION
SC00002    3201  199.0       1
```

```
*     SET ENERGY PER FISSION FOR PU-239      DEFAULT - 210.2 MEV/FISSION
SC00003     3201  210.2       2
*     SET ENERGY PER FISSION FOR U-238       DEFAULT - 199.3 MEV/FISSION
SC0004      3201  199.3       3
*     SET TIME AT WHICH DECAY HEAT POWER AND NEUTRON
*     CAPTURE CORRECTION FACTOR GIVEN - FIRST POINT ONLY
*     TIME = 0.0 S AFTER SHUTDOWN
SC0005      3202  0.0         1
*     SET DECAY HEAT POWER FOR U-235 AT FIRST TIME POINT -
*     DEFAULT = 13.18 MEV/FISSION
SC0006      3203  13.18       1 1
*     SET DECAY HEAT POWER FOR PU-239 AT FIRST TIME POINT -
*     DEFAULT = 10.93  MEV/FISSION
SC0007      3203  10.93       1 2
*     SET DECAY HEAT POWER FOR U-238 AT FIRST TIME POINT -
*     DEFAULT = 16.23 MEV/FISSION
SC0008      3203  16.23       1 3
*     SET NEUTRON CAPTURE CORRECTION FACTOR GMAX AT FIRST TIME POINT
*     DEFAULT = 1.02
SC0009      3204  1.02        1
*
*     SET PARAMETERS FOR ACTINIDE DECAY HEATS
*
* ATOMS OF U-239 PRODUCED PER SECOND PER FISSION PER SECOND, DEFAULT
SC00010     3205  0.54        1
*     ENERGY FROM DECAY OF U-239 ATOM - MEV
SC00011     3205  0.474       2
*     ENERGY FROM DECAY OF NP-239 ATOM - MEV
SC00012     3205  0.419       3
*     DECAY CONSTANT FOR U-239 - INVERSE SECONDS
SC00013     3205  4.91E-4     4
*     DECAY CONSTANT FOR NP-239 - INVERSE SECONDS
SC00014     3205  3.41E-6     5
*
```

5.3 Radionuclide Class Input

```
*           DEFINE NEW ELEMENTS
*              NEW ELEMENT XX
*
*           NAME  MASS (KG)
DCHNEM0100 XX     0.100
*           TIME (S)    DECAY HEAT (W/KG)
DCHNEM0101 0.0          10.0
DCHNEM0102 5.0          0.01
*
*                 NEW ELMENT YY
*
DCHNEM0200        YY            9.900
DCHNEM0201        0.0           0.1
DCHNEM0202        10.0          0.01
```

```
DCHNEM0203       100.0      0.001
*
*     ********** DEFINE CLASSES **********
*
*          DEFINE CLASS 16 - NEW ELEMENT XX
*
DCHCLS0160 'FIRST NEW CLASS'
DCHCLS0161 XX
*
*          DEFINE CLASS 17 - NEW ELEMENTS YY AND XX
*
DCHCLS0170 'SECOND NEW CLASS'
DCHCLS0171 YY    XX
*
*          DEFINE CLASS 18 - NEW ELEMENT YY + DEFAULT ELEMENT PM
*
DCHCLS0180 'THIRD NEW CLASS'
DCHCLS0181 YY    PM
*
*     SELECT ALL DEFAULT CLASSES
*
DCHDEFCLS0 ALL
*
*     SET ORIGEN SENSITIVITY COEFFICIENTS
*
*     SET MULTIPLIER FOR ALL ORIGEN DATA TO 1.0
SC00015     3210  1.0   1
*           SET MULTIPLIER FOR BROMINE TO 1.0
SC00016     3211  1.0   3
*
* SET FRACTION OF FUEL EQUILIBRIUM ELAPSED - DEFAULT = END OF CYCLE
*
SC00017 3212     1.0   1
*     TO NORMALIZE CLASS DECAY HEATS TO WHOLE-CORE DECAY HEAT,
*           INPUT NEXT CARD
*DCHCLSNORM      YES
```

Note that the fact that XX, YY, and PM each appear in two classes (PM is also in default class 9) does not mean that their decay heat will be double counted. Any mass that appears in any of the classes as a result of initialization or calculations in the RN package will have the specific power (W/kg) of a mixture of the elements it contains in proportion to their inventories at shutdown. Thus, any mass in class 16 will have the specific power of element XX, while mass in class 17 will have a specific power corresponding to a mixture of 0.1/(0.1+9.9) parts by mass of XX and 9.9/(0.1+9.9) parts of YY. Finally, any mass in class 18 will be treated as a mixture of YY and PM, in the proportions of 9.9 kg of YY to 9.8948 kg (the initial inventory) of PM. If the RN package calculates these masses in a way that conserves XX, YY, and PM, no double counting will occur.

6. Example Output

6.1 MELGEN Output

```
***** DECAY HEAT SETUP EDIT *****

For a PWR reactor with an operating power of 0.34120 x 10^10 watts, and
with an elapsed fraction of the equilibrium fuel cycle of 1.0, the
following default elements are defined for use in forming radionuclide
classes.

ELEMENT  MASS (KG)         DECAY HEAT AT SHUTDOWN (W/KG)
AS       0.78476D-02       0.14783D+9
SE       0.37532D+01       0.61818D+06
BR       0.14330D+01       0.47619D+07
KR       0.24908D+02       0.32877D+06
RB       0.23543D+02       0.63768D+06
SR       0.64828D+02       0.17895D+06
Y        0.32755D+02       0.55208D+06
ZR       0.22860D+03       0.34328D+05
NB       0.34120D+01       0.50000D+07
MO       0.19448D+03       0.33333D+05
TC       0.51180D+02       0.15333D+06
RU       0.12966D+03       0.13947D+05
RH       0.23543D+02       0.89855D+05
PD       0.58004D+02       0.22353D+04
AG       0.30026D+01       0.67045D+05
SN       0.26614D+01       0.56410D+06
SB       0.98948D+00       0.62069D+07
TE       0.26272D+02       0.27273D+06
I        0.13307D+02       0.12051D+07
XE       0.31732D+03       0.25806D+05
CS       0.16719D+03       0.89796D+05
BA       0.85300D+02       0.10400D+06
LA       0.75064D+02       0.20000D+06
CE       0.18084D+03       0.18868D+05
PR       0.68240D+02       0.70000D+05
ND       0.22178D+03       0.26154D+04
PM       0.98948D+01       0.41379D+05
U        0.85300D+05       0.48000D+02
NP       0.30026D+02       0.82955D+05

TIME-DECAY HEAT POWER DATA FOR USER-DEFINED ELEMENT XX WITH MASS = 0.1
KG

TIME (S)      DECAY HEAT POWER (W/KG)
0.00000D+00   0.10000D+02
0.50000D+01   0.10000D-01
```

```
TIME-DECAY HEAT POWER DATA FOR USER-DEFINED ELEMENT YY WITH MASS =
0.990D+01 KG
TIME (S)      DECAY HEAT POWER (W/KG)
0.00000D+00   0.10000D+00
0.10000D+02   0.10000D-01
0.10000D+03   0.10000D-02

TOTAL NUMBER OF DECAY HEAT F.P. CLASSES     =      18
TOTAL NUMBER OF DECAY HEAT ELEMENTS    =     107
TOTAL NUMBER OF DECAY HEAT CLASS TIMES=     456

EDIT OF ANS DECAY HEAT DATA
TYPE OF REACTOR = PWR
REACTOR OPERATING PERIOD = 0.50500D+08 SECONDS
REACTOR SHUTDOWN TIME = 0.00000D+00 SECONDS
NUMBER OF FISSIONING NUCLIDES = 3
NUMBER OF TIMES AT WHICH ANS DATA AVAILABLE = 56
OPERATING POWER FROM FISSIONING OF U235 = 0.22086D+10 WATTS
OPERATING POWER FROM FISSIONING OF PU239 = 0.10598D+10 WATTS
OPERATING POWER FROM FISSIONING OF U238 = 0.14360D+09 WATTS
TOTAL OPERATING POWER = 0.34120D+10 WATTS

TOTAL REACTOR DECAY HEAT POWER COMPUTED FROM ANS STANDARD
```

(The "TOTAL NUMBER OF DECAY HEAT ELEMENTS" counts each appearance of an element. Thus, there are two appearances of XX, two of YY, and an additional appearance of PM in addition to the default list of 102 elements, for a total of 107. The "POINTER TO FIRST ELEMENT IN CLASS" in the class edits on the following pages is the position of the first element in that class in a packed list of elements.)

```
** EDIT OF 18 FISSION PRODUCT CLASSES **

* 3 USER-DEFINED CLASSES *

EDIT OF DECAY HEAT FISSION PRODUCT CLASS - FIRST NEW CLASS
CLASS NUMBER = 16
CLASS MASS = 0.10000D+00 KG
NUMBER OF ELEMENTS IN CLASS = 1
POINTER TO FIRST ELEMENT IN CLASS = 1
ELEMENTS IN CLASS =
XX

TIME (S)      DECAY HEAT POWER (W/KG)

0.0000D+00    0.10000D+02
0.5000D+01    0.10000D-01

EDIT OF DECAY HEAT FISSION PRODUCT CLASS - SECOND NEW CLASS
CLASS NUMBER = 17
CLASS MASS = 0.10000D+02 KG
NUMBER OF ELEMENTS IN CLASS = 2
```

```
POINTER TO FIRST ELEMENT IN CLASS = 2
ELEMENTS IN CLASS =
YY
XX

TIME (S)      DECAY HEAT POWER (W/KG)

0.00000D+00   0.19900D+00
0.50000D+01   0.31407D-01
0.10000D+02   0.99001D-02
0.10000D+03   0.99000D-03

EDIT OF DECAY HEAT FISSION PRODUCT CLASS - THIRD NEW CLASS
CLASS MEMBER = 18
CLASS MASS = 0.19795D+02 KG
NUMBER OF ELEMENTS IN CLASS = 2
POINTER TO FIRST ELEMENT IN CLASS = 4
ELEMENTS IN CLASS =
YY
PM

TIME (S)      DECAY HEAT POWER (W/KG)

0.00000D+00   0.20684D+05
0.61200D+01   0.20684D+05
0.10000D+02   0.19507D+05
0.11880D+02   0.18961D+05
0.18000D+02   0.18961D+05
0.29880D+02   0.18961D+05
0.61200D+02   0.16720D+05
0.10000D+03   0.15297D+05
0.11880D+03   0.14651D+05
0.24120D+03   0.12583D+05
0.61200D+03   0.91355D+04
0.11880D+04   0.75842D+04
0.36000D+04   0.70671D+04
0.54000D+04   0.70671D+04
0.72000D+04   0.70671D+04
0.14400D+05   0.65500D+04
0.21600D+05   0.65500D+04
0.28800D+05   0.60329D+04
0.36000D+05   0.60329D+04
0.43200D+05   0.55158D+04
0.54000D+05   0.55158D+04
0.72000D+05   0.49987D+04
0.86400D+05   0.46539D+04
0.12960D+06   0.37921D+04
0.17280D+06   0.31026D+04
0.25920D+06   0.22408D+04
0.34560D+06   0.15686D+04
0.51840D+06   0.86184D+03
0.69120D+06   0.49987D+03
```

```
0.86400D+06  0.34474D+03
* 15 DEFAULT CLASSES *

EDIT OF DECAY HEAT FISSION PRODUCT CLASS - NOBLE GASES
CLASS NUMBER =  1
CLASS MASS = 0.34222d+03 KG
NUMBER OF ELEMENTS IN CLASS =  8
POINTER TO FIRST ELEMENT IN CLASS = 6
ELEMENTS IN CLASS =
XE
KR
RN
HE
NE
AR
H
N

TIME (S)      DECAY HEAT POWER (W/KG)

0.00000D+00  0.47856D+05
0.61200D+01  0.39880D+05
0.11880D+02  0.35892D+05
0.18000D+02  0.33898D+05
0.29880D+02  0.31904D+05
0.61200D+02  0.27916D+05
0.11880D+03  0.22931D+05
0.24120D+03  0.19043D+05
0.61200D+03  0.14855D+05
0.11880D+04  0.12861D+05
0.36000D+04  0.98704D+04
0.54000D+04  0.81755D+04
0.72000D+04  0.67797D+04
0.14400D+05  0.40977D+04
0.21600D+05  0.26122D+04
0.28800D+05  0.18544D+04
0.36000D+05  0.13958D+04
0.43200D+05  0.11067D+04
0.54000D+05  0.87737D+03
0.72000D+05  0.68495D+03
0.86400D+05  0.61615D+03
0.12960D+06  0.53340D+03
0.17280D+06  0.47178D+03
0.25920D+06  0.41167D+03
0.34560D+06  0.35184D+03
0.51840D+06  0.28205D+03
0.69120D+06  0.21226D+03
0.86400D+06  0.16241D+03
```

(Similar tables for the remaining default classes – 2 through 15 – follow.)

6.2 MELCOR Output

```
Edit for Decay Heat Package

POWER FROM FISSION PRODUCT CLASSES

CLASS                                          POWER/MASS    POWER
NUMBER    CLASS NAME                           W/KG          W

16        FIRST NEW CLASS                      0.10000D+02   0.10000D+01
17        SECOND NEW CLASS                     0.19900D+00   0.19900D+01
18        THIRD NEW CLASS                      0.20684D+05   0.40944D+06
1         NOBLE GASES                          0.47856D+05   0.16378D+08
2         ALKALI METALS                        0.15742D+06   0.30026D+08
3         ALKALINE EARTHS                      0.13636D+06   0.20472D+08
4         HALOGENS                             0.15509D+07   0.22860D+08
5         CHALCOGENS                           0.31591D+06   0.94854D+07
6         PLATINOIDS                           0.19192D+05   0.40535D+07
7         TRANSITION METALS                    0.12603D+06   0.31390D+08
8         TETRAVALENTS                         0.31289D+05   0.13750D+08
9         TRIVALENTS                           0.95314D+05   0.38863D+08
10        URANIUM                              0.48000D+02   0.40944D+07
11        MORE VOLATILE MAIN GRP ELEMENTS      0.73212D+07   0.73017D+07
12        LESS VOLATILE MAIN GRP ELEMENTS      0.30060D+06   0.17026D+07
13        BORON                                0.00000D+00   0.00000D+00
14        WATER                                0.00000D+00   0.00000D+00
15        CONCRETE                             0.00000D+00   0.00000D+00

TOTAL POWER FROM FISSION PRODUCT CLASSES = 0.20079D+09 WATTS
WHOLE REACTOR CORE DECAY HEAT POWER COMPUTED FROM ANS STANDARD WHOLE
REACTOR
CORE DECAY HEAT POWER AT TIME = 0.00000D+00 IS 0.21981D+09 WATTS
```

7. Diagnostics and Error Messages

An error message is printed if the decay heat package is asked to compute the decay heat for an invalid class ID number. The class number and calling package name are printed.

If the problem time is off the range of the decay heat tables, an error message is printed.

External Data File (EDF) Package
Users' Guide

The External Data File (EDF) package serves as a utility in MELCOR to allow a general means of communication with external data files containing time history data. In any MELCOR run, one or more such files may be defined. Each file contains values of time and the corresponding values of one or more dependent variables, and therefore defines each dependent variable as a function of time. Data can be either read from or written to each file; the permitted direction is defined in MELGEN. All characteristics of each file are also defined by EDF input. The EDF package assumes all responsibility for opening and positioning the files, and for reading from each file or writing to it, as appropriate.

Data that have been read in by the EDF package may be accessed and used by other packages in MELCOR. Data to be written out are obtained from the databases of other MELCOR packages. The interface may be either through the Control Function package or—in cases where appropriate coding has been provided—through utility-level entries in the EDF package.

The primary use of the EDF package is to facilitate input of data that define sources and/or boundary conditions as a function of time, particularly in cases where the volume of data is so great that the generation of tabular function input would be extremely tedious and error prone, or completely impractical. The ability to write files allows these input data to be generated directly by another MELCOR calculation; files written by other codes (or even by hand) may also be used. In addition, data files written by MELCOR could be used as input to another simulation code or to an output processor.

This document gives an introduction to the package, describes input requirements, lists sensitivity coefficients, plot variables and control function arguments, and describes output. Sample input is provided and discussed.

Contents

1. Introduction

The External Data File (EDF) package serves as a utility in MELCOR to allow other packages to communicate with external data files. One or more such files may be defined in any MELCOR calculation. Each file is identified by a user-assigned number and a user-defined name in addition to the name by which the operating system recognizes the file, and contains values of time and of one or more dependent variables. It therefore defines a function of time, referred to as a "data channel", for each dependent variable in the file. Data can be either read from or written to each file; the permitted direction is defined in MELGEN. A file may not be both read from and written to in a single calculation.

A file from which data are read is termed a *READ* file; the data that have been read in may be accessed by other packages in MELCOR, either as control function arguments through the Control Function (CF) package or directly through utility-level calls to the EDF package. In the former case, only "old" values, appropriate to the start of the current timestep, are defined. (This is the case for *any* control function value.) In the latter case, only values for times within the current timestep are available, since only that portion of the external file is required to be in the EDF database. Simple linear interpolation is used between tabulated points read from the file. Direct access requires specific coding that must be provided by the code developer. This capability is currently used only by the Control Function Hydrodynamics (CVH) and Transfer Process (TP) packages.

As suggested above, the EDF database provides storage for only a limited number of records to be read in from each file. The requirement that these records must span the entire MELCOR timestep may imply a limitation on that timestep in cases where very small time increments are used in portions of a data file. Therefore, the size of each record buffer may be changed (enlarged) by user input if desired.

Data to be written out are obtained from the databases of other MELCOR packages. Time is accessed directly and automatically by EDF; dependent variables may be obtained in either of two ways. For a *WRITE* file, the value of any variable accessible as a control function argument may be "pulled" into the EDF database using methods that exactly parallel those used for arguments in the CF package. For a *PUSH* file, values must be "pushed" into the EDF database by another package through utility-level entries in the EDF package. Such direct access again requires specific coding in the controlling routine, and the option is currently used only by the Transfer Process package. The frequency with which records are written is controlled by the user.

With the current coding of EDF, the values of variables which are to be written to a file are also available as control function arguments. However, use of these control function arguments should be avoided because the values available in EDF at the time the CF package is called are one timestep out of date. (If the order of execution were reversed, the values of any Control Functions written to an external file would be out of date.) In

essentially all cases, up-to-date information may be obtained by direct reference to a control function argument in the package from which EDF is obtaining the data.

If data are pushed into the EDF database by other packages, EDF has no way of identifying (for edit purposes) what they represent. Therefore, a path is provided to allow the other package to also define character labels for the data channels it pushes. A check is made in the EDF package to verify that values are actually pushed for every channel on every timestep.

The primary use of the EDF package is to facilitate input of data which define sources and/or boundary conditions as functions of time. The most obvious use is to communicate data from one MELCOR run to another. For example, ex-vessel sources can be calculated with a detailed nodalization of the primary system and a very simple containment model. These sources can be stored in a file, and then input to a later calculation with detailed containment nodalization but little or no representation of the primary.

In cases where an external data file specifies a source or sink of mass or energy, it is generally preferable that the file record cumulative (integral) sources rather than rates. This assures that, regardless of the actual timesteps taken by MELCOR, the total source in the calculation will match that in the data file. Construction of an integral source may involve use of the INTEGRAL control function in the MELCOR run which writes the file. If the receiving package does not accept cumulative sources, data read from this file in a later run can be converted to rates using the forward difference (DER-F) control function.

The EDF package can also be used to communicate data to or from another code. An input file need not have been generated by MELCOR; it might be the output of another code, or might even have been constructed by hand. A file written by MELCOR can be used as input to another simulation code or to an output processor such as a special-purpose plot program. To facilitate these uses, the format of records in each file may be specified in MELGEN; the default is for the file to be unformatted.

EDF files have also been used to generate tabular data, in prescribed standard formats, for code comparison exercises. In such cases, the required files can be written directly by MELCOR in the specified format, with no code modifications required, if all desired quantities are available (or can be constructed) as control function arguments.

On each restart, including the initial execution of MELCOR from the restart file generated by MELGEN, a limited check is made of the data in each file to be read in. It is required that the last record before the current time match *some* record read during the previous execution; a warning is issued if the position of this record in the file has been altered. This is intended to detect obvious errors without preventing the user from performing some editing of the file if he so desires.

2. User Input Requirements

A full description of all external data files must be provided as part of MELGEN input. Certain elements of the description may be changed on restart through input to MELCOR.

2.1 MELGEN User Input

The user input for the External Data File package is described below. One set of records is required for each external data file; the actual records required differ for the different types of files. Although the input formats would permit 1000 different files to be defined, current coding limits the total number to 20 for any single calculation.

EDFnnn00 – External Data File Definition Record

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
Required

This record defines a user name for the data file, the number of data channels (dependent variables), and the direction and mode of information transfer.

(1) EDFNAM - User defined external data file name.
(type = character*16, default = none)

(2) NCHAN - Number of channels (dependent variables) in each record of the file.
(type = integer, default = none, units = dimensionless)

(3) MODE - Direction and mode of information transfer. May be 'READ', 'WRITE', or 'PUSH', see Section 1.
(type = character, default = none)

EDFnnn01 – File Specification

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
Required

This record defines the name by which the file is known to the operating system. It is the character string which will be used in the FILE-FILNAM parameter when the file is opened. If FILNAM contains lower case characters which must be preserved, enclose it in single quotes (').

(1) FILNAM - Name of file on the operating system, such as 'input47.dat'.
(type = character*80, default = none)

EDFnnn02 – External Data File Format

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
Optional

A format may be defined for each external data file; the default is for the file to be unformatted. The field specifier for TIME in WRITE or PUSH files should provide sufficient significant digits to allow the written time values to be distinguished. The format may specify that a logical record contain more than one physical record ("line" in the file). A physical record length in excess of 133 characters may cause problems on many systems.

(1) IFMT - Format of records in the external file. If the record is omitted or blank, the file is assumed to be unformatted. If the format contains one or more commas, it must be enclosed in single quotes. The enclosing parentheses may be included '(4E12.4)' or omitted '4E12.4'; in the latter case, the input string is limited to character*22.
(type = character*24, default = " ")

EDFnnn03 – Time Offset for External Data File

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
Optional

To simplify communications between different codes, the zero of time in a data file need not coincide with that in the MELCOR run. The relationship is $t_{file} = t_{MELCOR} + t_{off}$. The offset may be positive or negative.

(1) TIMOFF - Offset of time in the external data file relative to time in MELCOR.
(type = real, default = 0.0, units = s)

EDFnnn04 – Buffer Length for READ File

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
Optional

Only a portion of the data in a READ file is stored in the EDF database. The buffer employed must contain enough records to cover the range of time from the beginning to the end of the current MELCOR timestep; the buffer size may therefore impose a limit on the permissible timestep. The minimum practical number of records in the buffer is 3; the default is 5. If the READ file contains closely spaced records, it may be desirable to increase this number to avoid unnecessarily slowing the calculation.

(1) NBUFF - Size of READ file data buffer, in records. Must be ≥ 3.
(type = integer, default = 5, units = dimensionless)

EDFnnn1k – Write Increment Control for WRITE or PUSH File

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
0 ≤ k ≤ Z is used for sequencing
Required

The output of records to a WRITE or PUSH file is controlled by the user. The control consists of (start time, time increment) pairs. It is similar to that for MELCOR output as described in the MELCOR/MELGEN EXEC Users' Guide, but *no* output is generated until the first time value has been passed. The "k" character in the record identifier is used only to distinguish records; the (start time, time increment) pairs input will be sorted by the code. At least one such pair must be input. No more than 10 pairs are permitted under current coding.

(1) TWEDF - Time at which the following output increment takes effect.
(type = real, default = none, units = s)

(2) DTWEDF - Time increment between output records.
(type = real, default = none, units = s)

Several pairs of (TWEDF, DTWEDF) may be entered on a single record; elements of a pair may not be split between two records.

EDFnnnkk – Channel Variables for WRITE File

001 ≤ nnn ≤ 999, nnn is the user-assigned number of the data file.
A0 ≤ kk ≤ ZZ is used for sequencing
Required

Values for each channel (dependent variable) of a WRITE data file are obtained by reference to control function arguments. The varaibles available in this way are listed in the Users' Guides for the various packages. Exactly NCHAN arguments are required; they are assigned to channels in the order of appearance on records sequenced according to the fields kk. Note that the independent variable, TIME, is automatically written as the first datum in each record.

(1) CHARG - Control function argument to identify an element of the database. Refer to the Users' Guides for the various packages for permitted values.
(type = character*24, default = none)

More than one control function argument may be entered on a single record.

2.2 MELCOR User Input

Certain elements of the input for an external data file may be changed at a restart (this includes the first execution of MELCOR). This is intended to allow the user to replace or rename files, or to alter the frequency with which records are written to WRITE or PUSH files.

The input to MELCOR is a subset of that described for MELGEN; the permitted records are described below (the presence of any others will be treated as a fatal input error, and the calculation will not be run).

EDFnnn01 – File Specification

The name of the file on the operating system may be changed.

EDFnnn02 – External Data File Format

The format of the file may be changed. The user should be aware that for a WRITE or PUSH file an attempt will be made to open and read the old file under the new format in order to position it correctly. This could result in a read error if the old file exists and the old and new formats are incompatible.

EDFnnn03 – Time Offset for External Data File

EDFnnn1k – Write Increment Control for WRITE or PUSH File

Note that on any restart, a limited check is made for changes in a READ file. An error is assumed if the last record found on the newly connected file before the time of the restart does not match *any* record already in the buffer (read from the file previously connected). If there is a matching record but the record number is different, a warning message is issued to the output and diagnostic files.

3. Sensitivity Coefficients

There are no sensitivity coefficients associated with the External Data File package.

4. Plot Variables and Control Function Arguments

The variables in the External Data File package which may be used for plot variables and control function arguments are listed and described below. The control function arguments are denoted by a "c", the plot variables by a "p", within slashes ("/") following the variable name

EDF.n.m	/cp/	Value of the m^{th} data channel in external data file n. If the data are plotted, the units will be given (by default) as "UNK" because they are not—and cannot be—known by EDF. The user may, of course, specify the correct units by defining a nondefault axis label as part of the input to the plot program.

The use of channels in WRITE of PUSH files as control function arguments should be avoided because the values available at the time the CF package is called are one timestep out of date. In most cases, up-to-date values of the underlying variables may be obtained by direct reference to control function arguments in the packages from which EDF is obtaining the data.

5. Example Input

An example of input for a READ file is:

```
EDF00700  MELT-SOURCE     4     READ
EDF00701  RUN27.DAT
EDF00702  5E12.5      *Time and four dependent variables
EDF00703  2600.       *Melcor time 0 corresponds to 2600 s on file
EDF00704  10          *Expand buffer to 10 data points
```

This defines an external data file with the user-specified number 7, and will cause data, consisting of time and four dependent variables, to be read from the file RUN27.DAT under FORMAT 5E12.5. The (interpolated) values of the dependent variables are available as control function arguments with the names EDF.7.1 through EDF.7.4. Space is reserved in the data buffer for 10 time points (for each dependent variable). This allows a MELCOR advancement to "step over" as many as 8 tabulated points while retaining a point before the start of the step and one after its end.

The data from a READ file may always be accessed as Control Function arguments; in general, this is the *only* method available to the user. However, in a few cases specific coding has been included in a package to access EDF data directly. At present only two packages make use of this capability:

(1) The Control Volume Hydrodynamics (CVH) package allows a property of a time-specified (boundary) volume to be specified by direct reference to the contents of an external data file. The field 'EDF.n.m' on a CVHnnAk record (as described in the CVH Users' Guide) will result in the value of the corresponding property being extracted directly from channel m of external data file n.

(2) The Transfer Process (TP) package can be instructed to actively construct "parcels" of debris (or of radionuclides) from data contained in a READ file specified on a

TPINnnn01 record. These parcels are treated exactly as if they had been received from another package (e.g., from Core); they are held until called for by some other package (e.g., by CAV). This allows debris and/or radionuclides to be added to a MELCOR calculation at a rate determined by some other calculation performed by MELCOR, by another code, or by hand. The user has relatively few options in defining such a file. See the Cavity, Core, Radionuclide, and Transfer Process Users' Guides for more information.

An example of input for a WRITE file is:

```
EDF11100  SPECIAL-DATA    3     WRITE
EDF11101  'specdat.dat'
EDF11110   500.        100.
EDF11111  1000.         10.
EDF11112  5000.       1000.
EDF111AA  CVH-P.200
EDF111AB  CFVALU.4
EDF111AC  CAV-MEX-H2.3
```

This defines an external data file with the user-specified number 111, and will cause unformatted records to be written to a file specdat.dat. A record will be written every 100 s starting at 500 s, every 10 s starting at 1000 s, and every 1000 s starting at 5000 s. Each record will contain the time, the pressure in volume 200, the value of control function 4, and the total mass of hydrogen released in control volume 3.

The difference between a WRITE file and a PUSH file is that in the latter the values of NCHAN data channels must be defined *by some other package*. MELGEN will terminate with an error message unless *some* package defines all of the data channels for a PUSH file during initialization. Similarly, MELCOR will terminate without completing the timestep on any step during which a new value for one or more channels fails to be defined before the end of the advancement. Thus, specific coding must be included in some package to transmit data directly to EDF. At this time, only the Transfer Process package has the capability to push data to EDF. It can record data about material parcels transferred to TP by some "IN" process in a file for later use.

An example of input for such a PUSH file is:

```
EDF00500  MELT-EJECTION  16    PUSH
EDF00501  MELTEJ.DAT
EDF00502  5E15.7     *Each logical EDF record requires 4 lines
EDF00510  3000.      10.
```

This defines an external data file with the user-specified number 5 and, in conjunction with the record

```
TPINnnn01 WRITE 5
```

will cause formatted records to be written to a file MELTEJ.DAT every 10 s, starting at 3000 s. (This file may be used as input to define debris sources in a later MELCOR run. A second, similar file would be required to record the associated radionuclide transfers and define sources in the second run.) See the description of input record TPINnnn01 in the Transfer Process Users' Guide for more information.

6. Discussion of Output

The output from the EDF package will be self-explanatory. For each file, it includes a user-defined name, the transfer mode, and the values of all data channels. The channels for WRITE files are labeled by the control function argument involved; those for PUSH channels by names defined by the PUSHing package, or by the label "UNDEFINED*PUSHED*DATA" if no other was defined. The channels for READ files are not labeled, as there is no way of knowing their contents.

Additional output provided for the first edit of each run gives the system name of the file, buffer information for READ files, and write increment control information for WRITE and PUSH files.

Fan Cooler (FCL) Package
Users' Guide

The MELCOR ESF Package models the phenomena for the various Engineered Safety Features (ESFs) in a nuclear power plant. The Fan Cooler (FCL) package constitutes a subpackage within the ESF Package, and calculates the heat and mass transfer associated with operation of the fan coolers. This Users' Guide provides basic information needed to run the FCL model with the rest of MELCOR, including a detailed explanation of the user input and package output for MELGEN, MELCOR, and HISPLT. Required and optional input, sensitivity coefficients, control function arguments, plot variables, and error messages are all covered.

More detailed information on the phenomenological modeling and numerical solution schemes implemented in the FCL package can be found in the FCL Package Reference Manual.

Contents

1. Introduction

The MELCOR fan cooler model is based on the fan cooler model in the MARCH 2.0 code. An effective heat transfer area is calculated in MELGEN from the rated primary and secondary flows and temperatures, and from the heat transfer coefficient and cooler capacity at those conditions. The actual heat transfer rate during a transient is calculated based on the effective area, the heat transfer coefficient for the current steam mole fraction, and the average temperatures of the primary gas and secondary coolant, which are themselves implicit functions of the heat transfer rate. Details of the model can be found in the FCL Package Reference Manual.

Several extensions to the model have been made. The user may optionally specify a separate discharge control volume for the fan cooler outlet air flow. The user may also specify a control function to control operation of the cooler by turning it on or off. Finally, the MELCOR implementation roughly partitions the total heat transfer coefficient into separate convection and condensation components to try to account for the effects of noncondensible gases and superheated atmosphere. The user can control how this partitioning is made by adjusting the sensitivity coefficients used in the heat transfer correlation.

2. Input Requirements

This section gives the input requirements for the MELCOR FCL package, including a short description of the input quantities and their units and default values, if any. Further description of the input variables and their meaning in the models can be found in the FCL Package Reference Manual.

Input record identifiers for the FCL model all begin with the character string "ESFFCL". Multiple fan coolers can be specified, and input is grouped into sets for each fan cooler modeled, identified by the three digits "nnn".

2.1 MELGEN Input

ESFFCLnnn00 - Fan Cooler Name
$1 \leq nnn \leq 999$, where nnn is the fan cooler number
Required

This record specifies a user-supplied name for the fan cooler for purposes of easy identification and is required. The following character field (limited to 16 characters) must be present:

(1) FCNAME - Fan cooler name.
(type = character*16, default = none)

ESFFCLnnn01 - Fan Cooler Interface and Control Integers
$1 \leq nnn \leq 999$, where nnn is the fan cooler number
Required

This record specifies the control volumes to which the fan cooler is interfaced, a control function to turn the cooler on or off, and a flag to control the phenomenological model that is used (currently, only the MARCH-based model is available). This record is required, but only the first field must be present; the remaining three fields are optional.

(1) ICVI - Fan cooler inlet control volume number.
(type = integer, default = none, units = none)

(2) ICVD - Fan cooler discharge control volume number. If this field is omitted, the discharge volume is the same as the inlet volume, i.e., the fan coolers sits entirely within a control volume. If this field is different from the inlet volume, the fan cooler operates somewhat like a flow path with a constant volumetric flow (that is cooled or dehumidified) from the inlet volume to the discharge volume.
(type = integer, default = ICVI, units = none)

(3) ICF - The number of the fan cooler logical control function that determines whether the fan cooler is on or off. This control function should return a value of .TRUE. whenever the fan cooler should be on. If this field is omitted, the fan cooler is always on.
(type = integer, default = none, units = none)

(4) IOPT - Fan cooler model flag. Currently, only IOPT=0, designating the MARCH-based model, is allowed.
(type = integer, default = 0, units = none)

ESFFCLnnn02 - Fan Cooler Rated Flows and Temperatures
$1 \leq nnn \leq 999$, where nnn is the fan cooler number
Required

This record specifies the rated primary and secondary flow rates and inlet temperatures. This record is required. NOTE: Care must be exercised to ensure that rated flows and temperatures are consistent with the rated cooler capacity.

(1) XVFGSR - Rated fan cooler gas volumetric flow rate.
(type = real, default = none, units = m^3/s)

(2) XMFSER - Rated fan cooler secondary coolant mass flow rate.
(type = real, default = none, units = kg/s)

(3) TSECIR - Rated fan cooler secondary coolant inlet temperature.
(type = real, default = none, units = K)

(4) TPR - Rated fan cooler inlet gas temperature.
(type = real, default = none, units = K)

ESFFCLnnn03 - Additional Fan Cooler Rated Conditions
$1 \leq nnn \leq 999$, where nnn is the fan cooler number
Required

This record specifies additional fan cooler rated conditions. This record is required. NOTE: Care must be exercised to ensure that rated flows and temperatures are consistent with the rated cooler capacity.

(1) QRAT - Rated fan cooler capacity.
(type = real, default = none, units = W)

(2) FMLSTR - Steam mole fraction at rated conditions.
(type = real, default = none, units = none)

ESFFCLnnn04 - Fan Cooler Actual Flows and Temperatures
$1 \leq nnn \leq 999$, where nnn is the fan cooler number
Optional

This record specifies the actual primary volumetric flow rate and secondary mass flow rate and inlet temperature during the transient if different from the rated values. If zero or a negative number is input for a field, it defaults to the rated value.

(1) XVFGSI - Actual fan cooler gas volumetric flow rate.
(type = real, default = XVFGSR, units = m^3/s)

(2) XMFSEC - Actual fan cooler secondary coolant mass flow rate.
(type = real, default = XMFSER, units = kg/s)

(3) TSECIN - Actual fan cooler secondary coolant inlet temperature.
(type = real, default = TSECIR, units = K)

2.2 MELCOR Input

No input for the fan cooler model is processed during MELCOR execution.

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters in the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the MELCOR EXEC Users' Guide.

3.1 FCL Sensitivity Coefficients

This section lists the sensitivity coefficients in the FCL model that are accessible to the user, along with a brief description, and gives their default values, units, and EQUIVALENCE names.

9001 - Coefficients for MARCH Fan Cooler Heat Transfer Correlation

These coefficients are used to calculate the effective heat transfer coefficient (W/m^2-K), as a function of the steam mole fraction X_{H2O}. The total heat (energy) transferred results from sensible and latent heat transfers. The sensible heat portion of the heat transfer coefficient, h_H is calculated by:

$$h_H = C9001(1) \cdot C9001(2)$$

The latent heat portion of the heat transfer coefficient, h_M, is calculated by:

$$h_M = h_L + C9001(1) \cdot [1 - C9001(2)]$$

where

$$h_L = C9001(4) \cdot X_{H2O},\ X_{H2O} \le C9001(3)$$

$$h_L = C9001(3) \cdot C9001(4) + C9001(5)[X_{H2O} - C9001(3)],\ X_{H2O} > C9001(3)$$

The default values are taken from the MARCH correlation.

(1) - sensible heat transfer coefficient
(default = 590.54, units = W/m^2-K, equiv = HSEN)

(2) - sensible heat transfer multiplier
(default = 1.0, units = none, equiv = FSEN)

(3) - steam mole fraction (boundary) in latent heat transfer coefficient correlation
(default = 0.26, units = none, equiv = FMLSCR)

(4) - coefficient in latent heat transfer coefficient correlation for low steam mole fractions
(default = 3603.4, units = W/m^2-K, equiv = DHLAT1)

(5) - coefficient in latent heat transfer coefficient correlation for high steam mole fractions
(default = 2325.25, units = W/m^2-K, equiv = DHLAT2)

4. Plot Variables and Control Function Arguments

The plot variables and control function arguments currently included in the FCL model are listed below, along with a brief description. Within slashes (/ /) a 'p' indicates a plot variable and a 'c' indicates a control function argument.

ESF-QFC-RAT.n	/pc/	Heat transfer rate for fan cooler n. (units = W)
ESF-QFC-TOT-n.	/pc/	Total energy transfer for fan cooler n. (units = J)
ESF-MFC-RAT.n	/pc/	Condensation rate for fan cooler n. (units = kg/s)
ESF-MFC-TOT.n	/pc/	Total steam condensed for fan cooler n. (units = kg)

5. Example Input

The following are sample MELGEN input records for the FCL model for a fan cooler treated by the MARCH-based model. No MELCOR input records are necessary to run the FCL model.

```
*     FAN COOLER INPUT
*
ESFFCL10100     'MARCH1'
*
```

```
*                ICVI      ICVD      ICF       IOPT
ESFFCL10101      100       100       20        0
*
*                XVFGSR    XMFSER    TSECIR    TPR
ESFFCL10102      100.0     65.0      294.0     339.0
*
*                QRAT      FMLSTR
ESFFCL10103      1.9E6     0.693
*
*                XVFGSI    XMFSEC    TSECIN
ESFFCL10104      -1.       -1.       314.0
**
*
*           CONTROL FUNCTION FOR FAN COOLER
*
*           TURN FAN COOLER ON WHEN TIME GT 100.
*
CF02000       'ON100'  L-GT 2  1.0
CF02001       .FALSE.
CF02010       1.0   0.0  TIME
CF02011       0.0 100.0  TIME
*
```

6. FCL Model Output

In general, the FCL model output is self-explanatory. The heat transfer and condensation rates and the total cumulative energy transferred and steam condensed are output for each fan cooler.

7. Diagnostics and Error Messages

Diagnostics and error messages generated during MELGEN are concerned with input processing and are generally self-explanatory. Currently, no messages are generated during MELCOR execution.

Fuel Dispersal Interactions (FDI) Package Users' Guide

The FDI (Fuel Dispersal Interactions) package models both low-pressure molten fuel ejection from the RPV into the reactor cavity and high-pressure molten fuel ejection from the RPV with the possibility of dispersion of the debris over multiple containment volumes and surfaces. The possibility of steam explosions from fuel-coolant interactions is not considered. New in MELCOR 1.8.5 is a FDI sensitivity coefficient used to control the numerical order in which oxygen or steam is used to oxidize DCH metals. This parameter affects the amount of hydrogen that results from burning DCH materials in steam/oxygen atmospheres.

This document includes a brief description of the models employed, the input format, sample input, sensitivity coefficients, plot variables and control functions. Details on the models can be found in the FDI Reference Manual.

Contents

1. Model Description

The capabilities of the FDI package are briefly summarized in this section. More details will be provided in the FDI package reference manual.

Two types of phenomena are treated in the FDI package:

(1) low-pressure molten fuel ejection from the reactor vessel, LPME, and

(2) high-pressure molten fuel ejection from the reactor vessel, HPME, (direct containment heating).

There is currently no plan to model steam explosions within or outside the FDI package in MELCOR.

During low-pressure ejection, heat is transferred from the molten fuel to the water pool (if present in the associated control volume) as it breaks up and falls to the cavity floor. The heat transfer normally occurs by radiation, but a convective lower bound is also included. All of the energy transfer from the molten fuel is used to boil the pool water (sensible heating is assumed to be unimportant). If no pool is present, material passes through FDI without any energy removal.

If the velocity of the molten debris ejected from the reactor vessel exceeds a critical value, prescribed by an adjustable sensitivity coefficient, or if the user has invoked the stand-alone option for high pressure melt ejection modeling, then the FDI will be treated by the high-pressure model instead of the low-pressure model. The parametric high-pressure model requires user input to control both the distribution of debris throughout the containment and the interaction of the hot debris with the containment atmosphere and heat structure (deposition) surfaces. The processes modeled include oxidation of the metallic components of the debris (Zircaloy, aluminum and steel are considered) in both steam and oxygen, surface deposition of the airborne debris by trapping or settling and heat transfer to the atmosphere and deposition surfaces. First-order rate equations with user-specified time constants for oxidation, heat transfer and settling are used to determine the rate of each process. Heat transfer to structure surfaces is limited by a heat transfer coefficient specified by a sensitivity coefficient. Debris entering the CAV package, either by direct deposition or settling from the atmosphere, is not treated by the FDI package; hence, the oxidation and heat transfer on deposition surfaces refers only to heat structure deposition surfaces. If a pool of water exists in the reactor cavity at the time of debris ejection, then the model ejects the water into the droplet field (fog) of the atmosphere at a rate proportional to the rate of injection of the debris into the pool.

If HPME model user input is absent, the HPME model will be disabled and all FDI events will be treated by the LPME model irrespective of ejection conditions. No direct

containment heating will occur if the user has not included the necessary input on records FDInn04 and FDInnmm.

2. User Input

The user input for the FDI package is described in this section. MELGEN input is described first, followed by MELCOR input, which is a subset of MELGEN input. The FDI model may be applied at several melt ejection locations within a problem; however, in the vast majority of problems the model is applied at only one location. An FDI location is basically a location at which debris may be ejected from a reactor vessel upon failure or a location at which debris is introduced from a source external to the problem domain. In most full-scale reactor calculations the model is applied in the CVH control volume beneath the reactor vessel lower head (specified by entry ICVCAV on COR record CORLHDii). In stand-alone HPME analyses of direct containment heating issues, the model is applied in the volume immediately downstream of the debris source.

For reactor plant calculations that may lead to vessel failure at relatively high pressure, users should provide input for both the LPME and HPME models. The LPME model input designates the FDI location, which is normally the reactor cavity CVH volume number as discussed above, the transfer process number associated with debris transfer from the COR package to the FDI package, the CAV cavity number and the associated transfer process number for debris transferred from the FDI package to the CAV package. The HPME model input specifies volumes into which the debris may be injected and parameters for controlling the interaction between the debris and its surroundings. If HPME input is not provided, then the LPME model will be invoked irrespective of the differential pressure between the reactor vessel and the reactor cavity during the melt ejection.

The FDI model may also be used to explore direct containment heating issues and experiments which do not involve actual modeling of the reactor (the COR package). In such cases, the HPME model is used in stand-alone mode, and the high-pressure debris source to the model is provided by the user. In stand-alone HPME calculations, the LPME model is inactive, and the LPME model input that normally controls the LPME model is used as follows to control the stand-alone HPME model. The stand-alone HPME model is invoked by setting NFDCAV = -1 on record FDInn00. For the stand-alone HPME model, there are two options for entering the debris source. The first option is to enter the debris source via the EDF package (see EDF package documentation) making normal use of NFDTPO on record FDInn00. The second option is to enter the debris source via tabular function input (see TF package documentation). The second option is invoked by setting NFDTPO = -N on record FDInn00, where N is the number of materials sourced in with separate tabular functions identified by records FDInnII. For the second option, the debris source temperature is entered via a tabular function, and the tabular function number is entered in NFDTPI on record FDInn00. The COR package must not be active when using the stand-alone HPME model.

Only the parameters that control the distribution of HPME debris throughout containment and the parameters that control the interaction of HPME debris with the containment atmosphere can be changed on restart in the MELCOR input. Therefore, it is important for users to determine which control volumes and deposition surfaces will be included in the data base at the time MELGEN is executed because volumes and surfaces cannot be added later.

2.1 MELGEN User Input

One set of the following records is required for each FDI location. (Up to 100 locations may be defined.) Input records FDInn00 and FDInn02 are required to activate either the LPME or HPME model, and, in addition, the FDInn04 and FDInnmm records are required to activate the HPME model.

Low-Pressure Model Input:

FDInn00 – FDI Location and Transfer Process Numbers
$00 \leq nn \leq 99$, nn is the FDI location number
Required

This record identifies the control volume, cavity, "in" transfer process number (for transfers to CORCON) and "out" transfer process number (for transfers from core) for each FDI location. NOTE: For stand-alone HPME model applications, NFDCAV, NFDTPI and NFDTPO have special meanings described below.

(1) NFDICV - User number of associated control volume
(type = integer, default = none, units = none)

(2) NFDCAV - User number of associated cavity
(type = integer, default = none, units = none)

NOTE: The stand-alone HPME model is invoked by setting NFDCAV = -1.

(3) NFDTPI - "In" transfer process number ('nnn' on the TPINnnn00 RECORD), for transfers to CORCON. For more details, see below. If NFDCAV = -1, set NFDTPI = N, where N is the tabular function number for the table of source temperature versus time. If an external data file (EDF) is used for the stand-alone HPME source, then set NFDTPI = -1.
(type = integer, default = none, units = none)

(4) NFDTPO - "Out" transfer process number ('nnn' on the TPOTnnn00 RECORD), for transfers from the core or EDF. For more details,

see below. If NFDCAV = -1, set NFDTPO = -N, where N is the number of source materials entered with separate tabular functions. If the EDF option is invoked, this entry has its normal definition.
(type = integer, default = none, units = none)

Material is transferred from the COR package (or an EDF file in the stand-alone HPME application) to the FDI package and from the FDI package to the CAV package through the Transfer Process (TP) package. The user must define transfer processes (in the TP package input) to perform the transfers. For transferring material from COR to FDI, an "in" transfer process must be defined to transfer material into the TP package from the COR package, and entered (as NTPCOR) on the COR00004 record in the COR package input. A corresponding "out" transfer process, with number NFDTPO (above), must be defined to take material out of the TP package and transfer it into the FDI package. Transfers between FDI and CAV are performed similarly. They involve the "in" process NFDTPI (above) and an "out" process entered as NTPOT on the CAVnnTP record in the CAV package input. If desired, material may be transferred directly from the COR package to the CAV package, bypassing the FDI package.

For transfers from FDI to CAV, the number of masses and the number of thermodynamic variables on the TPINnnn00 record (where nnn is NFDTPI) must be NMSIN = 5 and NTHRM = 9. Also, on the corresponding TPMnnn0000 record, the input must be NCOL = 5. The order of masses ejected from the FDI package (to be used when generating the translation matrix in the corresponding TPMnnnkkkk records) is:

(1) UO_2,

(2) Zr,

(3) steel,

(4) ZrO_2, and

(5) steel oxide.

Additional discussion of FDI-CAV transfers is included in the CAV Users' Guide.

IMPORTANT NOTE

In order to transfer the radionuclides along with the fuel and metal masses, additional transfer process numbers must be defined. Currently, these radionuclide TP numbers must be exactly 500 greater than the corresponding TP numbers defined for mass and energy transfers among the COR, FDI and CAV packages. The TP input should set the number of masses equal to the total number of radionuclide classes, NTHERM equal to 1, and should specify a unity translation matrix (DEF.1 on the TPOTnnn00 record).

FDInn01 – FDI Name
00 ≤ nn ≤ 99, nn is the FDI Location number
Optional

(1) FDINAM - Name of FDI Location.
(type = Character*16, default = ' ', units = none)

FDInn02 – Elevations
00 ≤ nn ≤ 99, nn is the FDI location number
Required

This record specifies the elevation at which material begins undergoing the FDI (usually, this will be the elevation of the bottom head penetration) and the elevation of the floor on which the material is deposited after the FDI is completed.

(1) ZBOTTM - Floor elevation. Must lie within the control volume identified by NFDICV on record FDInnn00. If not coincident with the bottom of that volume, a warning message will be issued.
(type = real, default = none, units = m)

(2) ZTOP - Top elevation of interaction region. Must be greater than ZBOTTM. If above the top of the associated control volume, a warning message will be issued.
(type = real, default = none, units = m)

High-Pressure Model Input:

FDInn04 – HPME Model Information
00 ≤ nn ≤ 99, nn is the FDI location number
Optional

The inclusion of this record activates the HPME model. This record is required if NFDCAV = -1 on record FDInn00. The sum of FATM and FDEP over all the volumes and surfaces associated with each FDI location must equal one or an error message will be issued.

(1) NATM - Number of control volumes HPME debris enters for this FDI location.
(type = integer, default = none, units = none)

(2) NDEP - Number of deposition surfaces associated with this FDI location by either settling or direct deposition from the HPME source.
(type = integer, default = none, units = none)

FDInnII – HPME Source Information

00 ≤ nn ≤ 99, nn is the FDI location number

10 ≤ II ≤ 10+|*NFDTPO*|-1, one card for each of the |*NFDTPO*| material sources

Required if NFDTPO < 0 on record FDInn00

These records describe the materials sourced into the stand-alone HPME model by tabular function input. The tabular function should be the total mass of the specified material sourced in to the specified table time (integral of the mass source rate).

(1) MATNAM - Source material name.
(type = character, default = none, units = none)

(2) ITABLE - Tabular function number for material source MATNAM.
(type = integer, default = none, units = none)

Valid Entries for MATNAM:

(NOTE: Entries are case insensitive.)

Zircaloy
zirconium-oxide
uranium-dioxide
stainless-steel
stainless-steel-oxide
boron carbide
silver-indium-cadmium
uranium-metal
aluminum
aluminum-oxide
cadmium

FDInnmm – HPME Control Volume Parameters

00 ≤ nn ≤ 99, nn is the FDI location number

50 ≤ mm ≤ 50+NATM-1, one card for each of the NATM volumes

Required if FDInn04 record entered

(1) IDATM - User number of CVH volume receiving debris.
(type = integer, default = none, units = none)

(2) IFLR - User number of HS surface or CAV cavity debris will settle onto from volume IDATM.
(type = integer, default = none, units = none)

(3) ITYP - Character string which indicates what type of surface IFLR is.

'CAV' for CORCON cavity
'LHS' for left-hand side of HS structure
'RHS' for right-hand side of HS structure
(type = character, default = none, units = none)

(4) FATM - Fraction of debris ejected from location nn that enters atmosphere of control volume IDATM.
(type = real, default = none, units = none)

(5) TOXV - Time constant for oxidation reactions in the atmosphere of control volume IDATM. The time constant will have a value equal to the absolute value of TOXV. A positive value for TOXV indicates that a hierarchical scheme will be used in which the order of oxidation is Zr, Al then steel. A negative value of TOXV indicates that oxidation of all metals will occur simultaneously.
(type = real, default = none, units = s)

(6) THT - Time constant for heat transfer to the atmosphere of control volume IDATM.
(type = real, default = none, units = s)

(7) TST - Time constant for settling onto surface IFLR from control volume IDATM.
(type = real, default = none, units = s)

NOTE: Time constants with absolute values smaller than 10^{-6} s will be reset to 10^{-6} s to avoid numerical problems.

FDInnkk – HPME Deposition Surface Parameters
$00 \leq nn \leq 99$, nn is the FDI location number
$50+NATM \leq kk \leq 50+NATM+NDEP-1$, one card for each NDEP surface
NOTE: kk continues where mm finished from preceding records.
Required if FDInn04 record entered.

These records describe the surfaces that debris is deposited onto from both settling (from control volumes) and/or direct deposition from the HPME source.

(1) IDDEP - User number of HS surface or CAV cavity that receives debris from settling and/or direct deposition from the HPME source.
(type = integer, default = none, units = none)

(2) ITYP - Character string which indicates what type of surface IDDEP is.
'CAV' for CORCON cavity
'LHS' for left-hand side of HS structure

'RHS' for right-hand side of HS structure
(type = character, default = none, units = none)

(3) FDEP - Fraction of debris ejected from location nn which is deposited directly on surface IDDEP (independent of settling from control volumes).
(type = real, default = none, units = none)

If ITYP = 'LHS' or 'RHS', then

(4) TOXS - Time constant for oxidation reactions on surface IDDEP. The time constant will have a value equal to the absolute value of TOXS. A positive value of TOXS indicates that a hierarchical scheme will be used in which the order of oxidation is Zr, Al then steel. A negative value of TOXS indicates that oxidation of all metals will occur simultaneously.
(type = real, default = none, units = s)

Otherwise, if ITYP = 'CAV', then

(4) NFDITP - "In" transfer process number associated with the deposition process to a CORCON cavity.
This record is only read if ITYP = 'CAV'.
(type = integer, default = none, units = none)

2.2 MELCOR User Input

The FDInn04, FDInnmm, and FDInnkk records may be modified on restart.

FDInn04 – HPME Model Information
$00 \leq nn \leq 99$, nn is the FDI location number
Optional

Only control volumes and deposition surfaces that were initially defined in the data base may be modified, so that the values of NATM and NDEP must not exceed their MELGEN values. The sum of FATM and FDEP over all volumes and surfaces associated with FDI location nn must be equal to one or an error message will be issued.

(1) NATM - Number of control volumes to be modified.
(type = integer, default = none, units = none)

(2) NDEP - Number of deposition surfaces to be modified.
(type = integer, default = none, units = none)

FDInnmm – HPME Control Volume Parameters
00 ≤ nn ≤99, nn is the FDI location number
50 ≤ mm ≤ 50+NATM-1, one card for each modified volume
Required if FDInn04 record entered

(1) IDATM - User number of modified CVH volume.
(type = integer, default = none, units = none)

(2) IFLR - User number of HS surface or CAV cavity debris will settle onto from volume IDATM.
(type = integer, default = none, units = none)

(3) ITYP - Character string which indicates what type of surface IFLR is.
'CAV' for CORCON cavity
'LHS' for left-hand side of HS structure
'RHS' for right-hand side of HS structure
(type = character, default = none, units = none)

(4) FATM - Fraction of ejected debris that enters atmosphere of control volume IDATM.
(type = real, default = none, units = none)

(5) TOXV - Time constant for oxidation reactions in the atmosphere of control volume IDATM. The time constant will have a value equal to the absolute value of TOXV. A positive value for TOXV indicates that a hierarchical scheme will be used in which the order of oxidation is Zr, Al then steel. A negative value of TOXV indicates that oxidation of all metals will occur simultaneously.
(type = real, default = none, units = s)

(6) THT Time constant for heat transfer to the atmosphere of control volume IDATM.
(type = real, default = none, units = s)

(7) TST - Time constant for settling onto surface IFLR from control volume IDATM.
(type = real, default = none, units = s)

NOTE: Time constants with absolute values smaller than 10^{-6} s will be reset to 10^{-6} s to avoid numerical problems.

FDInnkk – HPME Deposition Surface Parameters
00 ≤nn ≤ 99, nn is the FDI location number
50+NATM ≤ kk ≤ 50+NATM+NDEP-1, one card for each modified surface

NOTE: kk continues where mm finished from preceding records.
Required if FDINN04 record entered.

These records are used to modify the values of FDEP.
NFDIP cannot be modified on restart and does not appear.

(1) IDDEP - User number of modified surface.
(type = integer, default = none, units = none)

(2) ITYP - Character string which indicates what type of surface IDDEP is.
'CAV' for CORCON cavity
'LHS' for left-hand side of HS structure
'RHS' for right-hand side of HS structure
(type = character, default = none, units = none)

(3) FDEP - Fraction of ejected debris which is deposited directly on surface IDDEP (independent of settling from control volumes).
(type = real, default = none, units = none)

If ITYP = 'LHS' or 'RHS', then

(4) TOXS - Time constant for oxidation reactions on surface IDDEP. The time constant will have a value equal to the absolute value of TOXS. A positive value of TOXS indicates that a hierarchical scheme will be used in which the order of oxidation is Zr, Al then steel. A negative value of TOXS indicates that oxidation of all metals will occur simultaneously.
(type = real, default = none, units = s)

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the the MELCOR EXEC Users' Guide.

3.1 FDI Sensitivity Coefficients

4602 – High/Low Ejection Velocity Transition

Vessel ejection velocity at transition between high and low pressure ejection modeling. The ejection velocity calculated in the COR package is compared to this coefficient to determine whether to invoke the high- or low-pressure model.
(default = 10., units = m/s, equiv = none)

4603 – Airborne Debris Temperature Limit

If the airborne debris temperature exceeds this value, then any oxidation energy is deposited directly into the atmosphere to simulate the effect of a rapid increase in debris-to-gas heat transfer caused by debris fragmentation associated with rapidly escalating internal vapor pressure above the debris boiling point.
(default = 3700., units = K, equiv = none)

4604 – Maximum Change in CVH Atmosphere Temperature per Timestep

If direct containment heating will change the CVH atmosphere temperature by more than this value in a single timestep, then the FDI package will request a timestep fallback.
(default = 500., units = K, equiv = none)

4605 – Pool Water Ejection Ratio

Proportionality constant between the mass of water ejected from the cavity pool and the mass of debris injected into the pool from the HPME source. If X kg of debris is ejected from the COR package in a timestep, then X*C4605(1) kg of pool water is transferred to the fog component of the reactor cavity atmosphere during that timestep.
(default = 10., units = none, equiv = none)

4606 – Minimum Airborne Mass Ratio

The ratio of the current airborne mass to the integrated airborne debris mass source in a control volume below which the mass will be deposited onto the settling surface associated with the control volume – deactivates direct containment heating when the airborne mass remaining in a control volume becomes negligible.
(default = 0.001, units = none, equiv = none)

4607 – Initial Timestep Size for HPME initiation

If the current timestep size exceeds this value, at HPME model initiation, then the FDI package will request a timestep fallback.
(default = 0.0001, units = s, equiv = DTHPME)

4608 – Maximum Debris-to-Wall Heat Transfer Coefficient

The rate of heat transfer from deposited debris to the deposition surface is determined by a heat transfer time constant which is equal to MIN(0.5*TOXS,.001). The intention is to establish equilibrium between the debris temperature and the surface temperature on a reasonably short time scale. However, as the amount of

deposited debris accumulates, this can result in a very large heat flux to the surface. This sensitivity coefficient limits the rate of heat transfer if that value exceeds $HTC_{MAX} * A_{SRF}(T_{OLD} - T_{SRF})$, where HTC_{MAX} is the value of sensitivity coefficient 4608, A_{SRF} is the surface area of the deposition surface, T_{OLD} is the temperature of the deposited debris at the beginning of the timestep and T_{SRF} is the deposition surface temperature (from the Heat Structures package data base).
(default = 1000., units = W/m^2-K, equiv = HTCMAX)

4609 – Minimum Debris Temperature for Oxidation

The temperature of the debris (either airborne or deposited) must exceed this value, or oxidation of the metallic components of the debris is not permitted.
(default = 600., units = K, equiv = TOXMIN)

4610 – Oxygen/Steam Oxidation Weighting Factor

Weighting factor to control relative oxidation of debris by oxygen versus steam. The default value of 0.5 will give equal weighting proportional to their relative mole fractions in the atmosphere. A value of 0.0 will result in oxidation using all available steam in preference to oxygen, and a value of 1.0 will result in oxidation by available oxygen in preference to steam.
(default = 0.5, units = none, equiv = none)

4. Plot Variables and Control Function Arguments

The FDI package variables that may be used for plot variables and control function arguments are listed and described below. The control function arguments are denoted by a 'c'. The plot variable arguments are denoted by a 'p'. The 'c' or 'p' characters are inside slashes '/' following the variable name. In the following list n refers to the FDI location number and m refers to the CVH user volume numbers associated through MELGEN input with FDI location n.

FDI-FMREL.n	/cp/	Mass of material released to CORCON from FDI location n for this timestep. (kg)
FDI-FMRELT.n	/cp/	Integrated mass released to CORCON from FDI location n for entire calculation. (kg)
FDI-ETRAN.n	/cp/	Energy transferred to water from FDI location n for this timestep. (J)

FDI-ETRANT.n	/cp/	Integrated energy transferred to water from FDI location n for entire calculation. (J)
FDI-STGEN.n	/cp/	Mass of steam generated in FDI location n for this timestep. (kg)
FDI-STGENT.n	/cp/	Integrated steam mass generation for FDI location n for entire calculation. (kg)
FDI-ZR-OXRAT.n.m	/cp/	Zircaloy oxidation rate in CVH volume m for FDI location n. (kg/s)
FDI-ZR-OXTOT.n.m	/cp/	Integral over time of the Zircaloy oxidation rate in CVH volume m for FDI location n. (kg)
FDI-AL-OXRAT.n.m	/cp/	Aluminum oxidation rate in CVH volume m for FDI location n. (kg/s)
FDI-AL-OXTOT.n.m	/cp/	Integral over time of the aluminum oxidation rate in CVH volume m for FDI location n. (kg)
FDI-SS-OXRAT.n.m	/cp/	Steel oxidation rate in CVH volume m for FDI location n. (kg/s)
FDI-SS-OXTOT.n.m	/cp/	Integral over time of the steel oxidation rate in CVH volume m for FDI location n. (kg)
FD-O2-OXRAT.n.m	/cp/	Oxygen consumption rate in CVH volume m for FDI location n. (kg/s)
FDI-O2-OXTOT.n.m	/cp/	Integral over time of the oxygen consumption rate in CVH volume m for FDI location n. (kg)
FDI-ST-OXRAT.n.m	/cp/	Steam consumption rate in CVH volume m for FDI location n. (kg/s)
FDI-ST-OXTOT.n.m	/cp/	Integral over time of the steam consumption rate in CVH volume m for FDI location n. (kg)

FDI-H2-OXRAT.n.m	/cp/	Hydrogen generation rate in CVH volume m for FDI location n. (kg/s)
FDI-H2-OXTOT.n.m	/cp/	Integral over time of the hydrogen generation rate in CVH volume m for FDI location n. (kg)
FDI-ATM-POWR.n.m	/cp/	Heat transfer rate to atmosphere in CVH volume m for FDI location n. (W)
FDI-ATM-HEAT.n.m	/cp/	Heat transferred to atmosphere in CVH volume m for FDI location n. (J)
FDI-DEBRIS-T.n.m	/cp/	Airborne debris temperature in CVH volume m for FDI location n. (k)
FDI-OX-ENRGY.n.m	/cp/	Energy generated by the oxidation of Zircaloy and steel in CVH volume m for FDI location n. (J)
FDI-MASS-ADD.n.m	/cp/	Mass transferred from TP package to CVH volume m for FDI location n. (kg)
FDI-ENTH-ADD.n.m	/cp/	Enthalpy transferred from TP package to CVH volume m for FDI location n. (J)
FDI-ATM-ZRM.n.m	/cp/	Airborne mass of Zircaloy in CVH volume m for FDI location n. (kg)
FDI-ATM-ZRX.n.m	/cp/	Airborne mass of ZrO_2 in CVH volume m for FDI location n. (kg)
FDI-ATM-UO2.n.m	/cp/	Airborne mass of UO_2 in CVH volume m for FDI location n. (kg)
FDU-ATM-SSM.n.m	/cp/	Airborne mass of steel in CVH volume m for FDI location n. (kg)
FDI-ATM-SSX.n.m	/cp/	Airborne mass of steel oxide in CVH volume m for FDI location n. (kg)

FDI-ATM-ALM.n.m	/cp/	Airborne mass of aluminum in CVH volume m for FDI location n. (kg)
FDI-ATM-ALX.n.m	/cp/	Airborne mass of Al_2O_3 in CVH volume m for FDI location n. (kg)
FDI-ATM-UMT.n.m	/cp/	Airborne mass of uranium metal in CVH volume m for FDI location n. (kg)
FDI-ATM-CDM.n.m	/cp/	Airborne mass of cadmium in CVH volume m for FDI location n. (kg)
FDI-ATM-B4C.n.m	/cp/	Airborne mass of boron carbide in CVH volume m for FDI location n. (kg)
FDI-ATM-AIC.n.m	/cp/	Airborne mass of Ag-In-Cd in CVH volume m for FDI location n. (kg)
FDI-ATM-ALL.n.m	/p/	Airborne mass of all components in CVH volume m for FDI location n. (kg)
FDI-ZR-SXRAT.s.n.k	/cp/	Zircaloy oxidation rate on the s side of HS structure k for FDI location n. (kg/s)
FDI-ZR-SXTOT.s.n.k	/cp/	Integral over time of the Zircaloy oxidation rate on the s side of HS structure k for FDI location n. (kg)
FDI-AL-SXRAT.s.n.k	/cp/	Aluminum oxidation rate on the s side of HS structure k for FDI location n. (kg/s)
FDI-AL-SXTOT.s.n.k	/cp/	Integral over time of the aluminum oxidation rate on the s side of HS structure k for FDI location n. (kg)
FDI-SS-SXRAT.s.n.k	/cp/	Steel oxidation rate on the s side of HS structure k for FDI location n. (kg/s)
FDI-SS-SXTOT.s.n.k	/cp/	Integral over time of the steel oxidation rate on the s side of HS structure k for FDI location n. (kg)

FDI-O2-SXRAT.s.n.k	/cp/	Oxygen consumption rate on the s side of HS structure k for FDI location n. (kg/s)
FDI-O2-SXTOT.s.n.k	/cp/	Integral over time of the oxygen consumption rate on the s side of HS structure k for FDI location n. (kg)
FDI-ST-SXRAT.s.n.k	/cp/	Steam consumption rate on the s side of HS structure k for FDI location n. (kg/s)
FDI-ST-SXTOT.s.n.k	/cp/	Integral over time of the steam consumption rate on the s side of HS structure k for FDI location n. (kg)
FDI-H2-SXRAT.s.n.k	/cp/	Hydrogen generation rate on the s side of HS structure k for FDI location n. (kg/s)
FDI-H2-SXTOT.s.n.k	/cp/	Integral over time of the hydrogen generation rate on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-POWR.s.n.k	/cp/	Heat transfer rate to the s side of HS structure k for FDI location n. (W)
FDI-SRF-HEAT.s.n.k	/cp/	Heat transferred to the s side of HS structure k for FDI location n. (J)
FDI-TBD-SURF.s.n.k	/cp/	Temperature of deposited debris on the s side of HS structure k for FDI location n. (K)
FDI-SX-ENRGY.s.n.k	/cp/	Energy generated by the oxidation of metals on the s side of HS structure k for FDI location n. (J)
FDI-MASS-SET.s.n.k	/cp/	Total mass that has settled out of the atmosphere onto the s side of HS structure k for FDI location n. (kg)
FDI-ENTH-SET.s.n.k	/cp/	Total enthalpy that has settled out of the atmosphere onto the s side of HS structure k for FDI location n. (J)
FDI-SRF-ZRM.s.n.k	/cp/	Mass of Zircaloy on the s side of HS structure k for FDI location n. (kg)

FDI-SRF-ZRX.s.n.k	/cp/	Mass of ZrO_2 on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-UO2.s.n.k	/cp/	Mass of UO_2 on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-SSM.s.n.k	/cp/	Mass of steel on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-SSX.s.n.k	/cp/	Mass of steel oxide on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-ALM.sn.k	/cp/	Mass of aluminum on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-ALX.s.n.k	/cp/	Mass of Al_2O_3 on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-UMT.s.n.k	/cp/	Mass of uranium metal on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-CDM.s.n.k	/cp/	Mass of cadmium on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-B4C.s.n.k	/cp/	Mass of boron carbide on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-AIC.s.n.k	/cp/	Mass of Ag-In-Cd on the s side of HS structure k for FDI location n. (kg)
FDI-SRF-ALL.s.n.k	/p/	Mass of all components on the s side of HS structure k for FDI location n. (kg)

5. Example Input

The following input records define a single FDI location. In this example, the FDI location is labeled 15. It interfaces with control volume 210 and cavity 50. The corresponding transfer process input is also shown to help clarify the required input. Material is

transferred from the core to FDI through "in" transfer process 101 and "out" transfer process 101. Material is transferred from FDI to CORCON through "in" transfer process 102 and "out" transfer process 102. Note that any control poison (material 6) that is transferred from COR to TP is eliminated by Transfer Matrix 103 before reaching FDI. See the CPR, CAV, and TP Users' Guides for more information. The radionuclides are transferred through transfer processes 601 and 602 (INFDTPO+500 and NFDTPI+500, respectively). NOTE: Because the FDI1504 and FDI15NN records are absent, this input invokes the LPME model only.

```
***** FDI PACKAGE INPUT *****
* NFDICV NFDCAV NFDTPI NFDTPO
FDI1500 210 50 102 101
* ZBOTTM ZTOP
FDI1502  -5.  0.

***** COR AND CAV PACKAGE INPUT *****
* NTPCOR
COR00004 101
* NTPOT
CAV50TP 102
***** TP INPUT *****
* NMSIN NTHRM
TPIN10100  6  9
TPIN10200  5  9
* NMSOT NPOTOI IOTMTX
TPOT10100  5  101  UIN.103
TPOT10200  5  102  DEF.1
* NROW NCOL
TPM10300  5  6
* NROW/NCOL VALUE
TPM1030001  1/1  1.0
TPM1030002  2/2  1.0
TPM1030003  3/3  1.0
TPM1030004  4/4  1.0
TPM1030005  5/5  1.0
*             RADIONUCLIDE TRANSFER PROCESSES
TPIN60100  16  1
TPIN60200  16  1
*
TPOT60100  16  601  DEF.1
TPOT60200  16  602  DEF.1
```

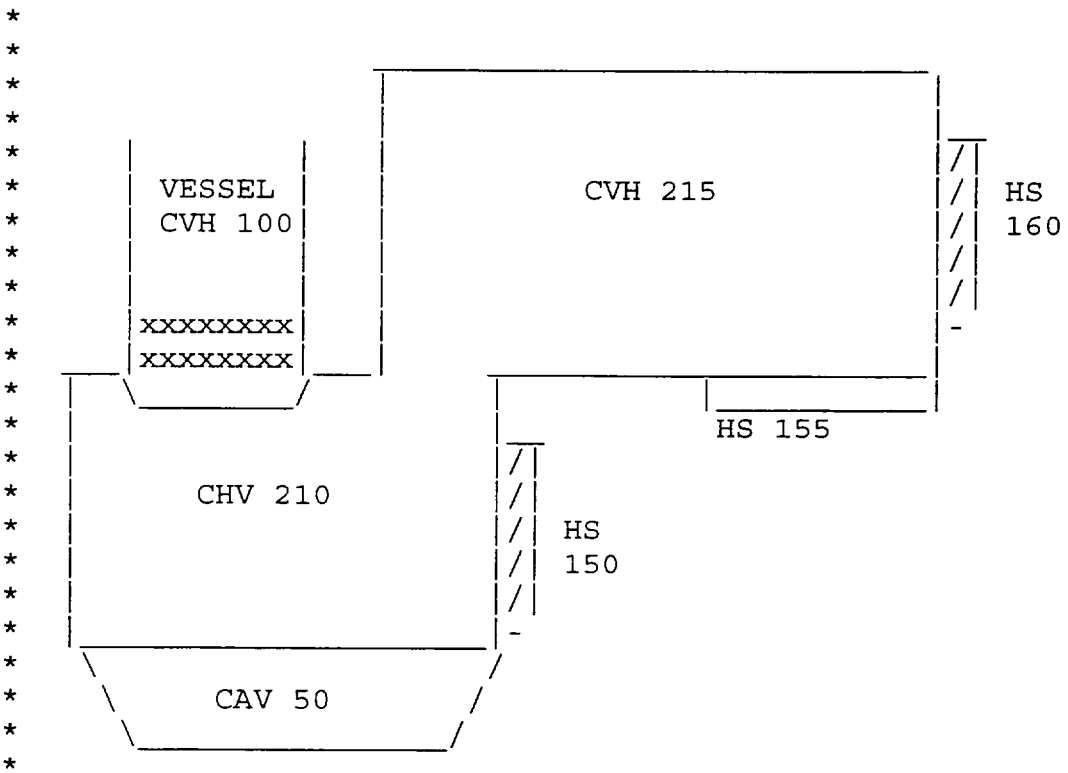
The next example shows how to invoke the stand-alone HPME model. Note the use of the EDF input for the debris source and the MP input to define the composition of the steel.

```
*****EXTERNAL DATA FILE PACKAGE INPUT *****
*
```

```
EDF00100 DCH-DATA 15 READ  *  READ FROM EXTERNAL DATA FILE
EDF00101 DCHDATA
     *  EDF FILE IS NAMED DCHDATA
EDF00102  '(8E9.3)'           * FORMAT OF DATA IN DCHDATA
*
***** TP INPUT *****
*
* 'IN'  TRANSFER PROCESS FROM EDF PACKAGE
TPIN10100  5  9      *  5 MATERIALS,  9 AUX.  VARIABLES
TPIN10101 READ 1  *  READ DCH SOURCE FROM EDF FILE 1
* 'OUT' TRANSFER PROCESS TO FDI PACKAGE
TPOT10200  5  101  DEF.1  *  USE MATRIX DEF.1 ON TP101
*
***** FDI INPUT *****
*
* NFDICV NFDCAV NFDTPI  NFDTPO
FDI0100  300  -1  -1  102  * INVOKE STAND-ALONE
* NAME
FDI0101  CVH300/HS20001    * MAKEUP A NAME
* ZBOTTM ZTOP
FDI0102  0.0  5.0          * ANY TWO REAL VALUES OK
* NATM NDEP
FDI0104  1  1
*IDATM IFLR  ITYP FATM TOXV  THT  TST
FDI0150  300  20001  LHS 1.0  3.E-1  2.E-1  1.E20
* IDDEP ITYP  FDEP  TOXS
FDI0151  20001 LHS  0.0  1.E1
*
*****  MP INPUT  *****
*
MPMAT00600 'STEEL'
*
MPMAT00699  1.0  0.0  0.0  0.0     * 100% FE, no CR, NI, or C
```

The final example shows how the FDI input from the first example can be expanded to activate the normal HPME model. If CVH 210 represents the reactor cavity volume with associated CORCON cavity 50, the LPME model input in the first example is perfectly reasonable. However, if the reactor vessel were to fail at high pressure there is a possibility that some of the ejected debris could be blown out of the reactor cavity into the upper containment, in which case HPME model input must be included to treat the situation reasonably. Assume that the nuclear power plant under investigation has been nodalized as depicted in the diagram below. Furthermore, assume that 60% of the ejected debris is deposited directly in the molten pool that forms at the bottom of the rector cavity (CAV 50), 30% splashes into the atmosphere but remains within the reactor cavity (CVH 210), 1% is deposited on the walls of the reactor cavity (HS 150) and of the 9% that escapes from the reactor cavity 4% is deposited directly on the walls of the upper

containment (HS 160) while the remaining 5% is dispersed throughout the upper containment atmosphere. Appropriate values for the time constants for oxidation, heat transfer and settling in CVH 210 and CVH 215 can be obtained in basically two ways—through analysis of the results of an independent DCH calculation of the problem or through simple hand calculations based upon reasonable assumptions concerning containment geometry dimensions, particle size and transfer coefficients (see FDI package Reference Manual). Assume values of 0.1 s have been obtained for the oxidation and heat transfer time constants, while a value of 1 s was obtained for the settling time constant. Then the appropriate LPME and HPME input would appear as follows:




```
***** FDI PACKAGE INPUT  *****
* NFDICV NFDCAV NFDTPI NFDTPO
FDI1500  210  50  102  101
* ZBOTTM ZTOP
FDI1502  -5.  0.
* NATM NDEP
FDI1504  2  4
*          IDATM     IFLR  ITYP  FATM   TOXV    THT    TST
FDI1550    210         50   CAV  .30    1.E-1   1.E-1  1.E-0
*          IDATM     IFLR  ITYP FATM   TOXV    THT    TST
FDI1551    215       155   LHS  .05    1.E-1   1.E-1  1.E-0
*          IDDEP     ITYP  FDEP NFDITP
```

```
FDI1552     50        CAV     0.60 102    * DIRECT DEP. AND SETTLING
*           IDDEP     ITYP    FDEP TOXS
FDI1553     150       LHS     .01  1.E1
*           IDDEP     ITYP    FDEP TOXS
FDI1554     155       LHS     0.0  1.E1
*           IDDEP     ITYP    FDEP TOXS
FDI1555     160       LHS     .04  1.E1
```

As might be expected the "in" transfer process number for the HPME model (NFDITP) is the same as the number associated with the LPME model (NFDTPI) since they transfer material to the same CORCON cavity. Notice that the left-hand side of heat structures 150, 155 and 160 do not and cannot have values of NFDITP associated with them. It is assumed that HS input will be included to properly orient the left hand sides of structures 150, 155 and 160 with respect to volumes 210 and 215.

In the absence of better information for deriving appropriate time constants for oxidation, heat transfer and settling for airborne debris, values for these parameters may be estimated as discussed in the following sections.

5.1 Settling time constant

The settling time constant in volume *i*, *TST(i)*, may be approximated as

$$TST(i) = L(i)/V(i)$$

where

L(i) = settling height in volume i (m)

V(i) = settling velocity in volume i (m/s)

The settling height is limited to the maximum ceiling height in volume i but may be less if the injected debris is not expected to reach that height for some reason. The settling velocity may be estimated from the lesser of the value from an appropriate correlation for the terminal velocity of falling bodies and

$$[2\,L(i)/g]^{0.5}\ ,$$

where g is the acceleration of gravity. Typical values of *L(i)* and *V(i)* would be on the order of 1 to 10 m and 1 to 10 m/s, respectively. Consequently, *TST(i)* is expected to be on the order of 1 s.

5.2 Heat transfer time constant

The heat transfer time constant in volume *i*, *THT(i)*, may be approximated as

$$THT(i) = RHOD \times CPD \times D / (6 \times H)$$

where

RHOD = density of debris (kg/m^3)

CPD = specific heat capacity of debris (J/kg-K)

D = equivalent spherical diameter of debris particles (m)

H = debris-to-gas heat transfer coefficient (W/m^2-K)

Typically, *RHOD* is on the order of 10,000 kg/m^3, *CPD* is on the order of 500 J/kg-K, *D* is on the order of 0.001 m and *H* is on the order of 1000 W/m^2-K. Hence, *THT(i)* is expected to be on the order of 0.5 s.

5.3 Oxidation time constant

Assuming the oxidation rate is limited primarily by mass transfer in the gas phase and applying the analogy between heat and mass transfer rates in turbulent flow, it is expected that the oxidation time constant in volume *i*, *TOX(i)*, will be approximately equal to *THT(i)*.

NOTE: Because of the uncertainties associated with the values of *TST(i)*, *THT(i)*, *TOX(i)* and most of the phenomena affecting direct containment heating, it is recommended that users conduct sensitivity studies by varying the assumed values of the HPME model input, if the results of a calculation concerning DCH do not conclusively resolve the issues of primary importance.

6. Diagnostic and Error Messages

The FDI package prints a message if any of the following occur:

(1) an error is detected during MELGEN input processing

(2) an error is detected during MELCOR input processing

(3) the HPME model becomes active

(4) direct containment heating begins in a volume

(5) the ejection velocity drops sufficiently to switch from the HPME model to the LPME model

(6) direct containment heating ceases in a volume due to settling

(7) FDI requests repeating a MELCOR cycle with a smaller timestep due to excessive predicted CVH atmosphere temperature change

The following examples were extracted from MELCOR files:

(from MELGEN diagnostics file)

*** ERROR IN SUBROUTINE FDIP2 ***

SUM OF ALL FATM AND FDEP NOT EQUAL ONE FOR FDI LOCATION 1

This message informs the user that there is an inconsistency in the specified debris distribution input on records FDInnmm (values of FATM) and FDInnkk (values of FDEP). As stated in the description of record FDInn04, the user is required to ensure that the sum of FATM and FDEP over all the volumes and surfaces associated with each FDI location is equal to one.

(from MELCOR message file)

/SMESSAGE/ CYCLE = 1011 TIME(S) = 9.14114E+03

COR0001: MESSAGE FROM CORE PACKAGE

LOWER HEAD PENETRATION 1 IN RADIAL RING 1 HAS FAILED

INITIAL DIAMETER OF HOLE IS 3.400E-02 M

COR0002: MEASSAGE FROM CORE PACKAGE

BEGINNING OF DEBRIS INJECTION TO CAVITY

***** FDI PACKAGE HPME MESSAGE *****

HIGH PRESSURE MELT EJECTION HAS BEGUN IN VOLUME 300

***** FDI PACKAGE HPME MESSAGE *****

DIRECT CONTAINMENT HEATING HAS BEGUN IN VOLUME 300

CAV0002 – MESSAGE FROM CAVITY PACKAGE

CAVITY 7 WAKING UP

/SMESSAGE/ CYCLE = 1061 TIME(S) = 9.14471E+03

***** FDI PACKAGE HPME MESSAGE *****

HPME HAS SWITCHED TO LPME IN VOLUME 300

/SMESSAGE/ CYCLE = 1078 TIME(S) = 9.14551E+03

CF0403 – MESSAGE FROM CONTROL FUNCTION PACCKAGE

CONTROL FUNCTION 403 – FAILURE MESSAGE BECAME .TRUE.

THE CONTAINMENT HAS FAILED FROM OVERPRESSURE

/SMESSAGE/ CYCLE = 1131 TIME(S) = 9.15098E+03

***** FDI PACKAGE HPME MESSAGE *****

DIRECT CONTAINMENT HEATING HAS CEASED IN VOLUME 300

These messages inform the user that:

(1) HPME began in control volume 300 immediately after lower head penetration 1 in radial ring 1 of the reactor vessel failed at cycle 1011 of the calculation,

(2) as a result of the HPME, direct containment heating began in control volume 300 at the same time,

(3) that approximately 4.6 seconds later the pressure in the reactor vessel was no longer sufficient to drive HPME, so that after that time all additional debris ejected from the vessel was treated by the LPME model, and

(4) by about 10 seconds after HPME began, most of the airborne debris ejected into the atmosphere of control volume 300 had settled onto deposition surfaces, so that direct containment heating had effectively ceased.

(from MELCOR diagnostics file)

***** FDI PACKAGE TIMESTEP CUT *****

CYCLE = 1026 TIME = 9.14131E+03 DT = 9.998E-02

This message informs the user that the FDI package cut the timestep at cycle 1026 (because of the rapid rate of heat transfer from direct containment heating) to avoid causing excessive change in the CVH atmosphere temperature.

Flow Path (FL) Package
Users' Guide

The Control Volume Hydrodynamics (CVH) and Flow Path (FL) packages are responsible for modeling the thermal-hydraulic behavior of liquid water, water vapor, and gases in MELCOR. Modeling is based on a control volume/flow path formulation and is described in detail in the Thermal Hydraulic (CVH and FL) Packages Reference Manual.

This Users' Guide describes input to the FL package, which is concerned with the geometry and characteristics of connections between control volumes, through which the control volume contents may be transported. FL input describes these connections, and defines the network through which hydrodynamic materials (water, its vapor, and noncondensible gases, residing in control volumes) may flow. No material resides in flow paths. When a flow of atmospheric materials (water vapor and noncondensible gases) enters a control volume below the surface of a water pool in that volume, the resulting mass and heat transfer will be calculated if requested by user input to the FL package. The phenomena of thermal equilibration and condensation of evaporation are treated as occurring within the flow path, using models from the SPARC90 code.

In addition to geometry, FL input includes all definition of flow resistance, including any frictional losses associated with the walls of control volumes and blockages calculated by the COR package. Special models including externally controlled flow areas (valves), forced flows, and momentum sources (pumps) are also defined by FL input in conjunction with functions defined by the Tabular Function (TF) and Control Function (CF) packages.

The geometry and contents of control volumes are defined by input to the CVH package, as described in the Control Volume Hydrodynamics (CVH) Package Users' Guide.

Contents

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1. Flow Path Models

The Users' Guide presents only an overview of the modeling in the MELCOR Flow Path (FL) package. More detailed descriptions, with appropriate references, may be found in the Thermal Hydraulic (CVH and FL) Packages Reference Manual.

1.1 Flow Path Definition

Each *flow path* connects two control volumes. Each connection is referred to as a *junction*; the two junctions associated with a flow path may be at different elevations. One volume is referred to as the *from* volume and the other as the *to* volume, thus defining the direction of positive flow.

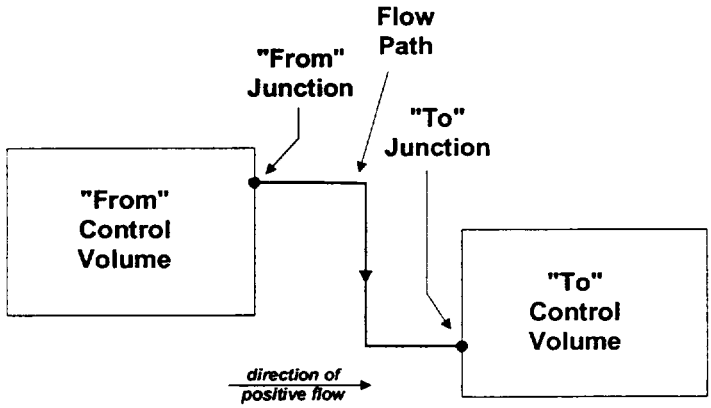

Figure 1.1 Flow Path Definition

There is no residence time for material flowing through a flow path. Therefore, there is no mass or energy associated with a flow path; all mass and energy reside in the control volumes. There is no heat or mass transfer between the pool and atmosphere materials flowing through the flow paths, nor is there heat transfer to or from structures since heat structures are not allowed to interact with flow paths.

A flow path may represent a pipe-like connection in a tank-and-tube model, or the open area of a separating surface (cell boundary) in a finite-difference-like model. The former case represents the limit of a control volume when residence effects are not important. In the interest of computational speed, MELCOR nodalizations are typically made relatively coarse, with only a modest number of control volumes. Therefore, it is common to reduce volumes of intermediate size but potentially high flow—such as relief valve discharge lines, pressurizer spray lines in a PWR, and jet pumps in a BWR—to simple flow paths in a MELCOR nodalization. The associated volume is typically included in one of the connected control volumes.

The same input parameters, differently chosen, are used to represent the two limiting types of flow paths (pipe-like and cell boundary), and a variety of intermediate cases. The primary difference is in the definition of the junctions of control volumes. The *junction elevations* represent the elevations of the central points of the connections to the respective control volumes; the *junction opening heights* represent the range of elevations over which material can be drawn *out of* the corresponding volume into the flow path.

For a pipe-like flow path, the junction elevations are typically unequal and the opening heights should be characteristic of the dimensions of the pipe. For a cell-boundary flow path, the junction elevations should be chosen to be equal, defined by the elevation of the mid-point of the cell boundary, and each opening height should be characteristic of the dimensions of the associated control volume.

1.1.1 Area and Length

Among the fundamental properties of a flow path are its area and its length. In many cases a flow path represents a geometry with varying flow area. In most cases, the area input as FLARA on the FLnnn01 record in FL input should be chosen as the minimum area along the path.

A flow path need not be fully open. The fraction F $(0.0 \le F \le 1.0)$ that is initially open may be defined by the variable FLOPO on the FLnnn01 record. F may also be modified as a function of time by a valve model in the flow path, as described in Section 1.6.1.

The CVH package calculates a velocity for each phase, pool and atmosphere, in each flow path. Only the open area, $F \bullet FLARA$, is used in the models: the volume flow $J \equiv F \bullet FLARA \bullet v$ is used in the advection of materials and in definition of wall friction (Section 1.2.2), and the mass flux based on the open area is the one compared with the critical mass flux in the choking model (Section 1.4). The individual variables F and FLARA may clearly be chosen in several ways. It is common—but not universal—in constructing FL package input to choose FLARA as the *maximum* area that will *ever* be open in the flow path. FLOPO will then be 1.0 for all flow paths not containing valves, and a fully open valve will correspond to an open fraction of 1.0.

The length specified as FLLEN on the FLnnn01 record in the FL input will be used as an *inertial length*. The inertia of a flow path is a measure of the average mass per unit area along its length. If the area is not constant, a rigorous approach is to chose the length input as FLLEN in conjunction with the flow path area, FLARA, to match this average:

$$\frac{FLLEN}{FLARA} = \int_{"fm"}^{"to"} \frac{dx}{A(x)} \qquad (1.1)$$

Here x measures distance along a path from the center of the "from" volume to the center of the "to" volume, and $A(x)$ is the flow area at x. In practice, this is rarely necessary.

FLLEN may also be used as the default length over which the force between pool and atmosphere acts. See Section 1.3.2 for details. It is *not* used in friction calculations; *segment lengths* are used instead, as discussed in Section 1.2.2.

1.1.2 Horizontal and Vertical Paths, Junction Openings

Flow paths are designated as *horizontal* or *vertical*, depending on the dominant direction of flow in the path, by user input on record FLnnn02; the default is *vertical*. The designation affects the definition of junction geometry and the default definition of the momentum exchange length in two-phase flow (Section 1.3.2).

The *nominal elevation* of each junction, defined by ZFM or ZTO on input record FLnnn00, represents the midpoint of the connection, and must lie within the range of elevations contained in the volume. The *junction opening height*, defines the range of elevations, H, over which material may be drawn *out of* a control volume through a flow path. By default, as discussed below, this range is calculated from a total junction height based on the flow path area and orientation; this total height may be over-ridden by user input of FLHGTF or FLHGTT on record FLnnn01. In either case, if the top and/or bottom of the junction opening, at elevation $Z \pm H/2$, lies outside of the control volume, the junction opening for a horizontal flow path will be truncated; for a vertical flow path, it will first be translated to preserve as much as possible of the original height H.

In MELCOR, the user may elect to specify the elevations of the top and bottom of the junction opening to either or both control volumes directly on FLnnn0F and/or FLnnn0T records. (These records may also be used to modify the junction opening on restart.) If these records are used, no adjustments will be made. The bottom of the opening must lie between the bottom of the control volume and the nominal junction elevation (inclusive), while the top must lie between the nominal junction elevation and the top of the control volume (inclusive).

The default values of junction opening heights (H in Figure 1.2) are the diameter of a circle of area FLARA for a horizontal path, and the radius of such a circle for a vertical path. These values are appropriate for a tank-and-tube model, as shown in Figure 1.2. For a horizontal flow path, the default represents the range of altitudes seen by a circular pipe; for a vertical flow path, the default represents a rough estimate of the extent to which the pool surface may be drawn down by flow through a vertical drain.

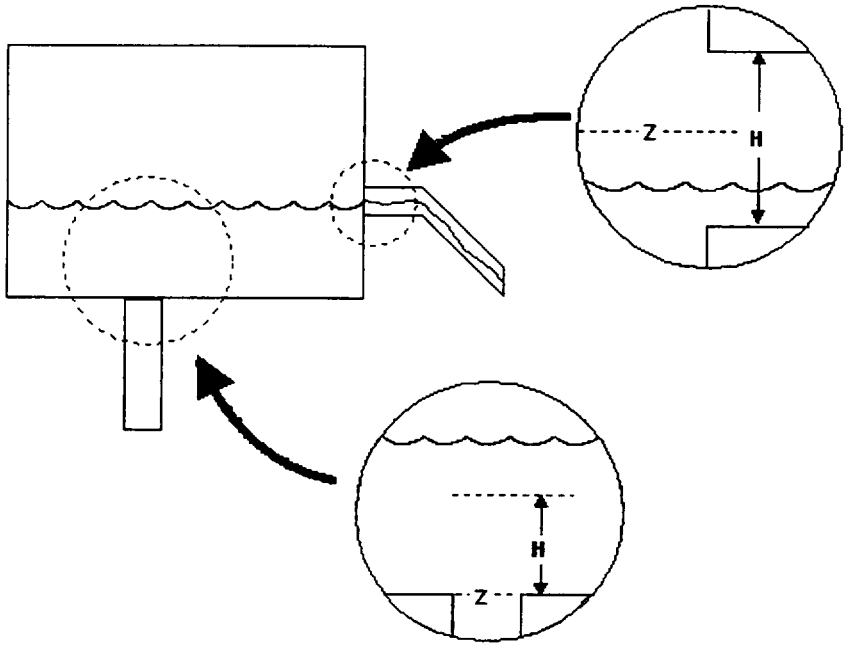

Figure 1.2 Junction Geometry in Tank-and-Tube Limit

The elevations of the top and bottom of each flow path, whether directly input or calculated, are included in the "FLOW PATH TIME INDEPENDENT EDIT" generated by MELGEN and reproduced at the beginning of each MELCOR run.

A flow path may also represent an open surface separating two control volumes. For a horizontal flow path, corresponding to a vertical surface, the opening height should be taken to include the entire open area. The elevation of the center of the opening should be used for *both* junction elevations, as shown in Figure 1.3. It is generally necessary to override the default opening height to ensure that the entire open area—and only that area—lies within the junction opening. For vertical flow through a horizontal separating surface, the junction elevations should again be chosen to be equal as shown in Figure 1.3. The opening height has no rigorous interpretation; it serves only to define the range of elevations from which material may be drawn, and some significant fraction of the volume height is appropriate. Because the flow equations include both gravitational (buoyancy) and momentum exchange (entrainment) forces, slip between the phases will tend to create and preserve stratification unless velocities are great enough to cause entrainment. Thus, extremely small junction openings are not necessary to preserve the stratification of pool and atmosphere in cases where it would be expected to occur. This is discussed further, in the context of the two-phase flow, in Section 1.3.1.

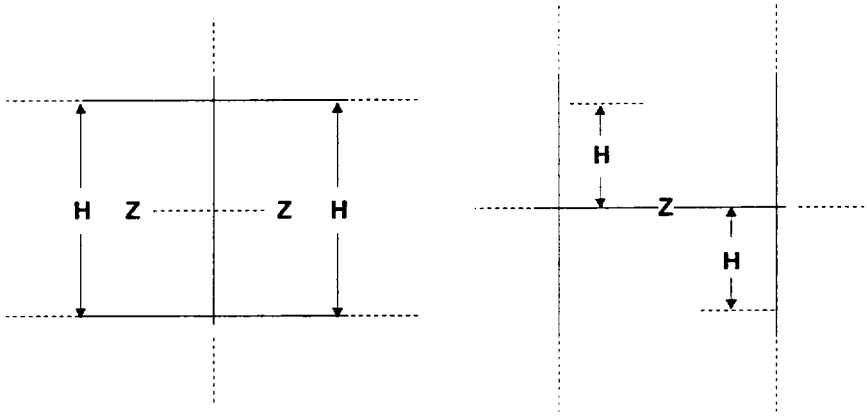

Figure 1.3 Junction Geometry in Separating-Surface Limit

1.1.3 Gravitational Head Terms

The equation for each flow includes a gravitational head term, calculated as the sum of three contributions:

(1) the head difference between the reference point for pressure in the *from* volume and the junction in that volume;

(2) the head difference associated with the change of elevation within the flow path; and

(3) the head difference from the junction in the *to* volume and the reference point in that volume.

The pressure in a MELCOR control volume is defined at the pool/atmosphere interface, taken as the bottom of the volume if there is no pool and the top of the volume if there is no atmosphere.

For a pipe-like flow path with junctions at different elevations, the second, within-path contribution is particularly significant. There is a basic limitation in its evaluation: the flow path has no contents and therefore no density or temperature of its own. A control volume density (or an average) must therefore be used for the within-path contribution to the head. This is adequate for those purposes where the net head results from the difference between pool and atmosphere density. In particular, it properly accounts for the additional head which must be overcome to depress a liquid surface and clear sparger vents or to raise a liquid surface to initiate overflow of a standpipe. It is *not* adequate for calculation of natural convection where the net head results from the change in density of one phase as a function of temperature.

Therefore, if a natural convection loop involving a number of control volumes is expected to be an important part of a MELCOR calculation, flow paths connecting points with

different elevations should *not* be used to represent connections through which the circulating flow will pass.

1.2 Frictional Losses

All dissipative pressure drops between volumes are assumed to take place within the flow paths connecting them. Contributions from both form loss and wall friction are included. An additional frictional term calculated by the COR package may be included where appropriate to model the effect of blockage by core debris, as described in Section 1.6.6.

1.2.1 Form Loss Coefficients

The form loss calculation is based on user-input loss coefficients (K in Equation (1.2)), which may be different for forward and reverse flow. These coefficients are input on the FLnnn03 record, and are applied directly to the velocities calculated by the CVH and FL packages. The resulting pressure differential (in the direction of positive flow) is

$$\Delta P_\varphi = -\frac{1}{2} K \rho_\varphi |v_\varphi| v_\varphi \tag{1.2}$$

for phase ϕ, where $\phi = P$ or A to denote pool or atmosphere.

For a complicated pipe network, the individual contributions from multiple changes of area must be combined into a single loss coefficient, to be used in Equation (1.2).

1.2.2 Flow Path Segments and Wall Friction

A wall friction contribution is added to the form loss term. In evaluating this contribution, the flow path is treated as consisting of one or more segments in series; this allows an accurate representation of wall friction in complicated, pipe-like geometries.

The flow path velocity and open area are used with the segment area to calculate a distinct velocity within each segment, based on the assumption of incompressible flow. The segment velocity is then given by

$$v_s = FAv/A_s \tag{1.3}$$

(F is again the fraction of the nominal area that is open), so that the segment velocity depends only on the volumetric flow through the flow path, $J \equiv FAv$. The frictional pressure differential is evaluated as

$$\Delta P_\varphi = -\sum_s (2f_s L_s / D_s)\rho_\varphi |v_{\varphi,s}| v_{\varphi,s} \qquad (1.4)$$

where L_s and D_s are the length and hydraulic diameter of the segment. The Fanning friction coefficient, f_s, is calculated according to the method of Beattie and Whalley, using a mixture Reynolds number based on the segment velocity.

The segments should represent all important aspects of the flow path, from volume center to volume center. If wall losses within a volume are important, the geometry of the appropriate parts of the volume should therefore be included as segments in the flow path, because all frictional losses are assumed to occur within the flow paths.

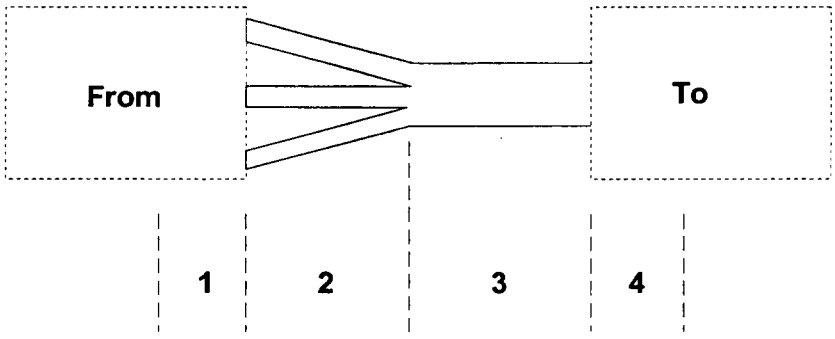

Figure 1.4 Flow Path Segments

Figure 1.4 illustrates the use of flow path segments. Volumes *from* and *to* are connected by a pipe manifold, which will be represented as a flow path. For the situation depicted, input for segment 1 should be based on the flow area, hydraulic diameter, and half length of volume *from* and input for segment 4 on the same properties for the *to* volume. Input for segment 2 should use the length and hydraulic diameter of a single tube and the total area, which is three times the area of a single tube. Appropriate tube properties should be used for segment 3. Note that no material resides in the flow path; if the volume of the manifold is significant, it should be accounted for by increasing the volumes of *from* and/or *to*.

The segmentation of a flow path affects frictional losses only; the segment lengths and areas are not used by any other models.

1.3 Two-Phase Flow

The cross-sectional area of a flow path may be shared by flows of pool and atmosphere materials. If both are present, their velocities will not, in general be equal, and countercurrent flow is possible. The open flow area is partitioned between them in accordance with a calculated void fraction, α, which should, strictly speaking, be referred to as an "atmosphere fraction."

Separate equations are solved for the two velocities. A *momentum exchange* term is included to model the forces acting between the two flows. A balance among this term, gravitational terms, and friction terms is responsible for the prediction of unequal velocities in quasi-steady flow.

1.3.1 Void Fraction

The void fraction in a MELCOR flow path is defined as the fraction of the open area of that path that is occupied by atmosphere flow. For concurrent flow of pool and atmosphere, it is taken as the fraction of the upstream junction opening that is occupied by atmosphere. For countercurrent flow, a weighted average of the area fractions at the two junctions is used.

This effectively prevents flow of pool *out of* a control volume unless the pool surface is above the bottom of the junction opening in that volume. Similarly, atmosphere is prevented from flowing unless the pool surface is below the top of the opening. Junction opening heights must be specified to ensure that such trapping of pool or atmosphere will occur only where it is physically appropriate.

MELCOR calculations sometimes show a small water pool in the upper of a pair of vertically stacked control volumes, with an atmosphere in the volume below. Users sometimes specify extremely small opening heights for the vertical flow path that defines a separating surface between them in an attempt to produce near-perfect separation of the phases. We have not found this approach to be particularly effective, and have seen evidence that it contributes to numerical problems and slow running of MELCOR. Use of somewhat larger opening heights frequently leads to a more orderly draining of the pool into the lower control volume.

1.3.2 Momentum Exchange Length

As noted above, the flow equations include both gravitational separation (buoyancy) and momentum exchange (entrainment) forces. A simple model is used for the momentum exchange; it was chosen to reproduce the Wallis flooding curve in the appropriate limit, and is described in the CVH/FL Reference Manual. The extent of coupling or separation between the flows is strongly influenced by the relative magnitudes of these forces, which

are proportional to the distances over which they act. For horizontal flow paths, the default length over which momentum exchange occurs is taken as the inertial length of the flow path. For vertical flow paths, it is taken as the difference in elevation between the lowest point (including the junction opening) and the highest point in the flow path. The different treatment of vertical paths is intended to make the two forces act over the same distance for vertical paths which represent the boundaries of vertically stacked control volumes.

These defaults are appropriate for simple vertical pipes, and not unreasonable for horizontal pipes. However, they can lead to significant overprediction of coupling between the phases—and underprediction of countercurrent flow—in a number of cases where a flowpath includes a number of separated channels. Examples include the entrance or exit paths for a reactor core, and perhaps steam generator tube bundles, where the two phases may flow through distinct, noninteracting portions of the actual geometry.

The default length may be replaced by a user-input length XL2PF on the optional FLnnn05 input record. Increasing the length will tend to tighten coupling between the flows, reducing both the relative velocities and the limits on countercurrent flow; decreasing the length will have the opposite effect. Reducing the length for core flow paths will tend to reduce the "levitation" of water sometimes predicted by MELCOR in the upper plenum and core regions after lower regions have voided. A momentum exchange length of zero can be used to model a "perfect" separator in steam generator secondaries.

1.4 Choked Flow

The critical mass flux for pool flow in MELCOR is based on the RETRAN model; it uses the Moody model for saturated water and the Henry-Fauske model for subcooled water, with a small interpolation region between them. A further interpolation to simple orifice flow is imposed at large subcooling. The critical mass flux for atmosphere flow is based on sonic flow at the minimum section. An interpolation scheme motivated by the Moody model is used for mixed flows. The mass flux is evaluated based on the open area of the flow path (the fraction open times the nominal area).

The possibility of choked flow is automatically modeled in all flow paths. No user input is required, but the default forward and reverse discharge coefficients of 1.0 may be modified, if desired. The choking model restricts the mass flux, through a flow path (based on the open area) to be no greater than the critical value, multiplied by the discharge coefficient corresponding to the current flow direction. A discharge coefficient less than 1.0 may be used to account for *vena contracta* effects. The possibility of choking in a given flow path may be effectively eliminated by specifying a value substantially greater than 1.0 for the associated discharge coefficient.

If choking is detected, pool and atmosphere velocities are set equal. For more details, see the Thermal Hydraulics (CVH and FL) Packages Reference Manual.

1.5 Bubble (SPARC) Physics

If a flow of atmospheric material enters a control volume below the surface of the pool in that volume, it must pass through the pool to reach its final destination. By default, any interactions during this passage are ignored and the atmospheric material is simply added to the control volume atmosphere.

The user may specify that interactions between the pool and the rising gases be modeled by setting one or both of the flags IBUBF and/or IBUBBT on the FLnnn02 input record. Selection of the interaction model may be made independently for the two flow directions. If it is active, the RadioNuclide (RN) package will perform a pool scrubbing calculation using the SPARC90 model to evaluate the removal of fission products from rising gases for those flow paths and flow directions—*and only those paths and directions*—for which the model is activated on the FLnnn02 record. No additional input (other than activation of the RN package) is required, and RN cannot be made to perform a pool scrubbing calculation for a flow path where SPARC modeling was not selected in the FL package input.

The condition of the transmitted gases and the receiving pool is modified by mass and heat transfer processes. The interaction process is viewed as involving the breakup of the injected gas stream into a swarm of bubbles, thermal equilibration of the gases with the pool, and saturation of the bubbles with water vapor at local conditions. It is treated parametrically. If there are no noncondensible gases in the flow, the bubbles may be completely condensed. Details of the model are contained in Section 6.1 of the CVH/FL Reference Manual. The efficiency of the process is controlled by sensitivity coefficients in the array C4405.

The interaction is treated as occurring within the flow path. The bubbles are *not* considered to be resident in the pool for the purposes of calculating the pool composition and do *not* contribute to pool swelling.

1.6 Other Models

Several additional models are available for use in flow paths. These can be used to modify the fraction of the flow path area that is open, define momentum sources in the path, specify the velocity in the path, modify the treatment of two-phase flow, include the effects of momentum flux, or model blockage of the path by materials such as core debris.

1.6.1 Valves

The user may include a valve in a flow path to control the fraction of the area of the path that is open. The open area of the flow path is defined as the fully open area (FLARA)

multiplied by the fraction open. Valves do not modify the areas of flow path segments and therefore do not affect the dependence of wall friction on volumetric flow.

For the specific case of an ideal check valve that allows flow in one direction only, an alternate approach is available in MELCOR, where the definition of flow path types has been extended to include *one-way* flow paths. This approach avoids the limitations of the numerically explicit nature of the general valve model, including the numerical difficulties that may arise when a user specifies a very large reverse form loss coefficient in an attempt to restrict any calculated reverse flow through a check valve that was open at the start of an advancement. If, however, it is essential to model the differential pressure necessary to open a check valve, valve inertia, or hysteresis, the general approach described below must be used.

Control functions are used to define the fraction open; values returned will be bounded internally to lie between zero and one before they are used. When the fraction open is zero, the flow path is closed. When the fraction open is one, the flow path is fully open and the open area is equal to user input flow path area FLARA. Two approaches are permitted. In simple cases, the user can specify a single control function which defines the fraction of the area that is open. In particular, a relief valve is typically modeled in MELCOR by defining the open fraction as a hysteresis function of the pressure differential between the volume connected by the flow path. (See the example control function input in Section 6.3 of the CF Package Users' Guide.)

In more complicated situations, a trip control function can be specified that is used to switch among three definitions of that fraction as follows:

(1) If the trip control function is zero, the trip is "off" and the area fraction is unchanged from its last value;

(2) if the trip control function is positive, the trip is "on-forward" and the area fraction is that defined by an "on-forward" control function; and

(3) if the trip control function is negative, the trip is "on-reverse" and the area fraction is that defined by an "on-reverse" control function.

See the CF Package Users' Guide for more information on trip control functions.

1.6.2 Pumps and Fans

Pumps can be included in flow paths. They are modeled as introducing a pressure "boost" which is ordinarily a function of the volumetric flow through the path. In defining a pump, the flow should be thought of as the independent variable and the pressure head delivered by the pump as the dependent variable; the actual flow on any timestep is calculated from

the balance of this head (as a function of flow) against static, frictional, and acceleration pressure differentials in the rest of the flow circuit.

There are two types of pumps available in MELCOR. The first, referred to as "FANA," was originally intended to model a fan that impels the atmosphere through a flow path. It can also be used to represent a constant speed coolant pump, although in a very simple form. The second, called "QUICK-CF," simply uses a control function to define the pressure head, allowing the user complete freedom but also giving him complete responsibility for all details.

Both models are numerically explicit; that is, the pressure head is based on conditions at the start of the MELCOR system timestep, and remains unchanged throughout the step—even if the CVH package is subcyling.

The FANA model assumes that the fan can be adequately represented by a parabolic pressure head *vs* volumetric flow rate equation. The velocity of the pool is set equal to that of the atmosphere when the pump is on, so that the pump will move pool water through the flow path if the void fraction in the flow path is less than 1.0. The major limitation in the model is the absence of any direct dependence of the pressure head on the density of the flowing material.

The user must define the maximum pressure head, DPMAX, and the volumetric flow, VPZERO, at which the head is zero. The user may optionally define a non-zero volumetric flow, VPMAX, corresponding to the point of maximum head generation; otherwise, maximum head is assumed to occur at zero flow. If DPMAX and VPZERO are both positive, the fan produces a pressure boost in the direction of positive flow, corresponding to a fan blowing from the "from" volume to the "to" volume. The pressure head is then given by

$$\frac{DP}{DPMAX} = \begin{cases} 1.0 & VDOT \le VPMAX \\ \sqrt{\dfrac{VPZERO - VDOT}{VPZERO - VPMAX}} & VPMAX \le VDOT \le VPZERO \\ 0.0 & VPZERO \le VDOT \end{cases} \qquad (1.5)$$

where DP and VDOT are the pressure head and volumetric flow, respectively. A fan which is oriented in the opposite direction, producing its head in the direction of negative flow, can be modeled by simply defining DPMAX and VPZERO to be negative, and reversing the sign of VPMAX, if it is input. In this case, the effect of the pump is maximum for VDOT $\ge$ VPMAX, and is zero for VDOT $\le$ VPZERO $<$ 0.

There is no provision to control the speed of the fan, but it can be turned on and off, if desired, by defining either a control function or a tabular function of time which will be zero

when the fan is to be off, and non-zero when it is to be on. By default, the fan is always on; when it is, DP is simply set to zero.

Note that this model is not a reasonable representation of a real pump far outside the range of flows given by VPMAX ≤ VDOT ≤ VPZERO.

The QUICK-CF pump model relies on a user-defined control function to evaluate the pressure boost (in Pa) for the pump. All control logic must be included in the control function. Section 6.7 of the CF Package Users' Guide provides example input for a homologous pump similar to TRAC and RELAP.

1.6.3 Time Dependent Flow Paths

The velocities in a flow path can be specified by the user through control functions or tabular functions. The specified velocity is used for both the atmosphere and the pool. The void fraction is calculated using the standard model.

1.6.4 Pool-First and Other Flow Path Options

Several modifications may be made to the treatment of two-phase flow described in Section 1.3. These are activated by choice of the KFLGFL flag on input record FLnnn02, the same flag that defines the vertical or horizontal orientation of the path.

The velocities of the pool and of the atmosphere in a flow path may be forced to be equal rather than calculated independently.

The partition of the flow area between pool and atmosphere (defined by the flow path void fraction) is ordinarily based on current geometry. Alternatively, it may be defined such that either pool or atmosphere is preferentially transmitted. These options, referred to as *pool-first* and *atmosphere-first*, respectively, should be used with great care (if at all), as they often produce unexpected results. The preferential flow is accomplished by overriding the normal definition of the flow path void fraction if the preferred phase is available to flow through the flow path, setting it to 0.0 for a pool-first path and 1.0 for an atmosphere-first path. If the preferred phase is not available within the junction opening, the other phase is permitted to flow in the normal manner.

1.6.5 Momentum Flux Terms

Momentum flux terms can be included as an option in certain designated flow paths, using information supplied by the user to calculate them. These terms may be important in paths where large flow accelerations may occur, when multidimensional flow patterns occur, or where frictional and form loss terms are very small. In order to obtain a meaningful velocity difference for the momentum flux terms in the direction of flow, the user is required to

specify appropriate upstream and downstream flow areas. As currently implemented, the momentum flux terms are calculated in a numerically explicit manner, and are only one-dimensional in nature; i.e., they do not currently include the cross-derivative term $v_y (\partial v_x / \partial y)$, where y is perpendicular to x, the direction of flow. The current model treatment will therefore be incomplete in situations where velocity gradients transverse to the direction of flow are important.

Although the momentum flux terms can be included, other terms in the CVH equations on the order of the velocity squared (the kinetic energy terms) are still omitted.

1.6.6 Flow Blockage Controlled by Other Packages

Phenomena modeled by other packages in MELCOR can result in changes to the geometry—area and flow resistance—of flow paths modeled by the MELCOR hydrodynamic packages. Although such effects can be captured through use of control functions to define effective valves and friction coefficients, this approach places a large burden on the user. Among the most important of these for reactor safety calculations are changes resulting from degradation of the reactor core. In MELCOR, the blockage of flow by relocation of core debris and the opening of flow paths by failure of channel boxes in a Boiling Water Reactor (BWR) can be easily included in the modeling of a flow path. The user is required only to specify the flow orientation and the core cell or cells that contribute to the geometry of the path. When particulate debris is involved, the calculation is based on the Ergun equation for flow in a porous medium.

1.7 Flow Paths to and from Core Volumes

The core package employs a model, referred to as the "dT/dz" model, to infer an axial temperature variation in a control volume containing core cells. (The details of this model are presented in the COR Reference Manual.) It uses the mass flow into the bottom of the control volume as a boundary condition and, as currently coded, assumes that fluid flows up the core. It further assumes that this corresponds to the direction of positive flow, which places a constraint on the definition of flow path orientations: the user must define the "to" and "from" control volumes for core flow paths such that the sign of the velocity is positive when fluid flows up the core. This is illustrated in Figure 1.5.

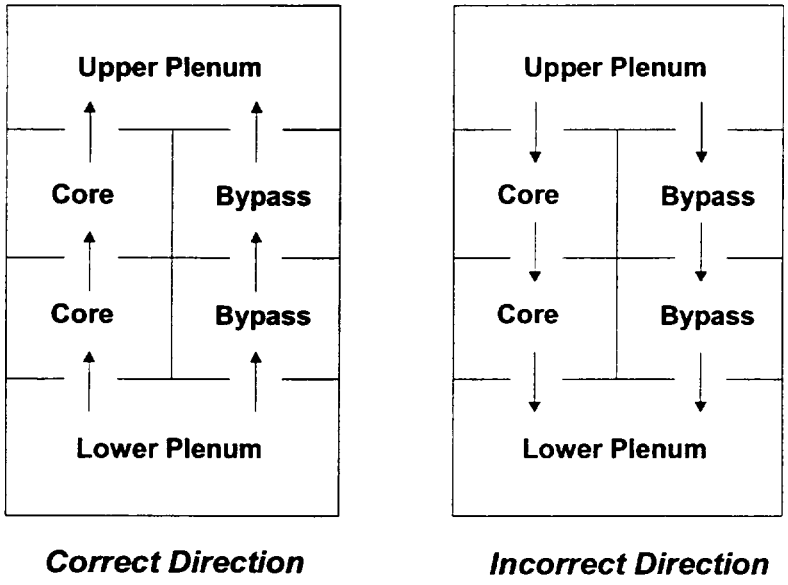

Figure 1.5 Flow Paths for To and From Core Volumes

1.8 Modeling Breaks and Failures

All types of failures which lead to the opening of additional paths for fluid flow are modeled by using flow paths containing valves which are defined to open when a failure criterion is reached. This includes pipe breaks, melt-through or catastrophic failure of the pressure vessel, failure of rupture disks and blowout panels, and failure of containment. Valve models are based on control functions, as described in Section 1.6.1. The flexibility of the MELCOR CF Package, described in the CF Package Users' Guide, makes it possible to define extremely general failure criteria through user input to the CF package in addition to simple pressure or temperature thresholds.

Input to the CF package includes user-specified bounds on the permitted values of the control functions. These limits may be changed on restart of MELCOR. This makes it possible to include in FL input *all* the failure paths and failure criteria that will be required to investigate a variety of scenarios. In any given MELCOR run, all but one can be inactivated by limiting the unwanted failure areas to zero through limits on the associated control functions.

For related scenarios, the transient response of the system will be identical until failures occur. If restart dumps are generated at the times when failures occur, the invariant portions of the calculation need not be repeated. Multiple branches may be followed by restarting MELCOR from the common point with one or another of the failure modes enabled by appropriate modification of control function bounds through CF package input.

2. User Input

FL input to MELGEN defines the geometry of flow paths connecting control volumes, any initial velocities in these flow paths, and various options in the modeling. It also defines momentum sources (pumps) and control logic (valves) through reference to tabular and control functions defined in the TF and CF packages.

FL input to MELCOR is limited to modification of the momentum exchange length for two-phase flow. However, control function data may be modified on a restart, giving the user significant access to control logic affecting pumps and valves. It is common to define input decks to include representations of several possible failures, with all but one disabled through limits imposed on values of control functions through CF package input. This allows several scenarios to be investigated by using modifications to CF input to branch calculations from intermediate restarts without rerunning the earlier, invariant portion of the transient.

2.1 MELGEN User Input

The user input for the flow path package is described below. One set of the following records is required for each flow path. Up to 999 flow paths may be defined. Practically, the number is limited only by the available memory on the computer. Unless otherwise stated, if the field variable starts with I through N, it is an integer. Unless otherwise stated, if the field variable starts with A through H or O through Z, it is a real number.

FLnnn00 – Flow path name, *to* and *from* control volume data
$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
Required

This record defines the flow path name. It defines the control volumes that the flow path connects. The flow is positive when it flows from the *from* volume to the *to* volume. The altitude of the connection with *from* and *to* control volumes is also defined.

(1) FLNAME - User defined flow path name
(type = character*16)

(2) KCVFM - *From* control volume number
(type = integer, default = none, units = dimensionless)

(3) KCVTO - *To* control volume number
(type = integer, default = none, units = dimensionless)

(4) ZFM - Altitude of *from* junction
(type = real, default = none, units = m)

(5) ZTO - Altitude of *to* junction
(type = real, default = none, units = m)

FLnnn01 – Flow path geometry
1 ≤ nnn ≤ 999, nnn is the user-assigned flow path number
Required

This record defines the flow path geometry. Only the first three fields need be present. If record FLnnn0F and/or FLnnn0T are present, data on those records will define the junction opening, and the values of FLHGTF and/or FLHGTT, whether input or default, will not be used.

(1) FLARA - Flow path area
(type = real, default = none, units = m^2)

(2) FLLEN - Flow path length
(type = real, default = none, units = m)

(3) FLOPO - Fraction of flow path open
(type = real, default = none, units = dimensionless)

(4) FLHGTF - *From* junction flow path opening height
(type = real, default = diameter of circle with area FLARA for a horizontal flow path = radius of circle with area FLARA for a vertical flow path, units = m)

(5) FLHGTT - *To* junction flow path opening height
(type = real, default = diameter of circle with area FLARA for a horizontal flow path, = radius of circle with area FLARA for a vertical flow path, units = m)

FLnnn02 – Flow path junction switches
1 ≤ nnn ≤ 999, nnn is the user-assigned flow path number
Optional

This record defines the type of flow path. A flow path may be horizontal or vertical. The algorithm used to define the equivalent opening height is different for the two cases. A pool-first flow path will only flow pool water until all available pool water is exhausted. When there is no pool available, it will flow atmosphere. The atmosphere-first flow path is equivalent with the pool and atmosphere roles

reversed. The normal horizontal or vertical flow paths will flow a mixture of pool and atmosphere consistent with the pool elevation, velocities and flow path opening elevation and height. It is also possible to specify that the pool and atmosphere must have the same velocity.

A flow path may also be defined as a *one-way* path, allowing flow in one direction only, to simulate the behavior of an idealized check valve. This is done by adding a leading digit of 1 for forward-flow-only, or 2 for reverse-flow-only, to the variable KFLGFL that defines the type of flow path.

A bubble rise model may be specified that includes thermodynamic interactions and, if the RN package is active, RN scrubbing. The calculation of heat and mass transfer is performed for *any* acceptable non-zero value of IBUBF or IBUBT. The *specific* non-zero value is significant only if the RN package is active.

(1) KFLGFL - Type of flow path flag
(type = integer, default = 0, units = dimensionless)
= 0 normal vertical flow path
= 1 atmosphere-first vertical flow path
= 2 pool-first vertical flow path
= 3 normal horizontal flow path
= 4 atmosphere-first horizontal flow path
= 5 pool-first horizontal flow path
= 6 pool velocity = atmosphere velocity, vertical flow
= 7 pool velocity = atmosphere velocity, horizontal flow
= 10 – 17 same as 0 – 7, but only forward flow is permitted
= 20 – 27 same as 0 – 7, but only reverse flow is permitted

(2) KACTFL - Active/inactive flow path flag
(type = integer, default = 0, units = dimensionless)
= 0 active
= 1 inactive ** do not use. Input is accepted, but code does not function correctly for flow paths specified as inactive **

(3) IBUBF - *From* junction bubble rise model switch
(type = integer, default = 0, units = dimensionless)
= 0 no bubble rise physics
= 1 SPARC model with RN aerosol and iodine vapor scrubbing
= -1 SPARC model with no RN scrubbing
= -2 SPARC model with scrubbing of RN aerosols only
= -3 SPARC model with scrubbing of RN iodine vapor only

(4) IBUBT - *To* junction bubble rise model switch
(type = integer, default = 0, units = dimensionless)

= 0 no bubble rise physics
= 1 SPARC model with RN aerosol and iodine vapor scrubbing
= -1 SPARC model with no RN scrubbing
= -2 SPARC model with scrubbing of RN aerosols only
= -3 SPARC model with scrubbing of RN iodine vapor only

FLnnn03 – User specified loss coefficients
$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
Optional

The user can specify forward and reverse loss coefficients and choked flow discharge coefficients. If this record is input, then at least two values must be input. The first two are interpreted as the loss coefficients. The third and fourth values are the forward and reverse choked flow discharge coefficients.

The loss coefficients determine the form loss pressure drop across a flow path; the forward coefficient is used when the velocity is positive and the reverse coefficient is used when the velocity is negative. For additional information refer to Section 1.2.1 of this Users' Guide and Section 5.4 in the CVH/FL Reference Manual

In the test for choking, critical flow is determined from a correlation and then multiplied by a discharge coefficient. The coefficient may be different for forward flow (positive velocity) and reverse flow (negative velocity). A minimum velocity, below which the test is bypassed, can be defined by sensitivity coefficient C4402(1).

(1) FRICFO - Forward loss coefficient
(type = real, default = 1., units = dimensionless)

(2) FRICRO - Reverse loss coefficient
(type = real, default = 1., units = dimensionless)

(3) CDCHKF - Choked flow forward discharge coefficient
(type = real, default = 1., units = dimensionless)

(4) CDCHKR - Choked flow reverse discharge coefficient
(type = real, default = 1., units = dimensionless)

FLnnn04 – Initial atmosphere and pool velocities
$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
Optional

The initial pool and atmosphere velocities may be defined by the user. If this record is present, both velocities must be input; if it is absent, both initial velocities will be taken as 0.0.

(1) VLFLAO - Atmosphere velocity
(type = real, default = none, units = m/s)

(2) VLFLPO - Pool velocity
(type = real, default = none, units = m/s)

FLnnn05 – Length for pool/atmosphere momentum exchange
1 ≤ nnn ≤ 999, nnn is the user-assigned flow path number
Optional

This record defines the length over which momentum exchange occurs when pool and atmosphere flows share the flow path. The value used affects entrainment and flooding by controlling the balance between the resulting force between the two flows (which tends to couple them and reduce slip) and buoyancy (which tends to separate pool from atmosphere). A larger value tends to promote coupling between pool and atmosphere, while a smaller one tends to enhance their separation.

The default for horizontal flow paths is the inertial length defined on record FLnnn01. The default for vertical flow paths is the distance between the lowest point in the flow path (including the junction opening) and the highest point, as defined by the junction elevations on record FLnnn00 and the opening heights from record FLnnn01 (or default). See Section 1.3.2 of the Users' Guide and Section 5.5 of the CVH/FL Reference Manual for more information.

(1) XL2PF - Length for pool/atmosphere momentum exchange
(type = real, default as discussed above, units = m)

FLnnn06 – Flow path connection to EDF
1 ≤ nnn ≤ 999, nnn is the flow path number
Optional

This record directs that the cumulative flows of masses and enthalpies through the flow path be recorded to an external data file. The resulting file can then be used to define mass and energy sources to the CHV package in a subsequent calculation.

If a file is written, each record will contain NUMMAT cumulative masses, the cumulative flow of enthalpy associated with pool material, and the cumulative flow of enthalpy associated with atmosphere materials. Enthalpies are defined with respect to the normal MELCOR reference points.

(1) IP2EDF - User-assigned number of associated EDF FILE
(type = integer, default = none, units = dimensionless)

IP2EDF must be the number of a valid "PUSH" file containing exactly NUMMAT+2 channels. See the EDF Users' Guide for further input requirements, including file names and record frequencies.

FLnnn0F – Junction limits, *from* volume
1 ≤ nnn ≤ 999, nnn is the user-assigned flow path number
Optional

This record defines the junction opening for the *from* volume by directly specifying the range of junction elevations for that volume. If this record is present, the value of FLHGTF from record FLnnn01, whether input or default, will not be used.

(1) ZBJFM - Elevation of bottom of junction opening for the *from* volume. Must lie between bottom of *from* volume and nominal junction elevation (inclusive).
(type = real, default = none, units = m)

(2) ZTJFM - Elevation of top of junction opening for the *from* volume. Must lie between nominal junction elevation and top of *from* volume (inclusive).
(type = real, default = none, units = m)

FLnnn0T – Junction limits, *to* volume
1 ≤ nnn ≤ 999, nnn is the user-assigned flow path number
Optional

This record defines the junction opening for the *to* volume by directly specifying the range of junction elevations for that volume. If this record is present, the value of FLHGTT from record FLnnn01, whether input or default, will not be used.

(1) ZBJTO - Elevation of bottom of junction opening for the *to* volume. Must lie between bottom of *to* volume and nominal junction elevation (inclusive).
(type = real, default = none, units = m)

(2) ZTJTO - Elevation of top of junction opening for the *to* volume. Must lie between nominal junction elevation and top of *to* volume (inclusive).
(type = real, default = none, units = m)

FLnnnBk – Data for blockage of flow by another package
$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
$0 \leq k \leq Z$, k is a continuation character
Optional

Blockage of flow in response to change of geometry in another package (reduction of flow area, redefinition of friction) will be calculated if data are entered on this record. If a dataset *is* entered, no other control of the flow area is possible, and inclusion of a valve (FLnnnVk) record is not permitted. Only one blockage dataset may be entered for a flow path.

(1) PKG - Package defining the blockage
(type = character, default = none, units = dimensionless)

Specification of the defining package is included to allow later generalization, but at this time PKG = COR is the only available option.

Defining Package = COR

The COR flow blockage model can automatically adjust the area and flow resistance of specified flow paths to include the effects of blockage by core debris as modeled by the COR package. It can also model the opening of a flow area between the channel and bypass of a BWR when the separating channel box fails. The user must specify which core cells are to be associated with the flow path; the additional data required are defined below. Fields 2 – 4 are required, field 5 is optional.

(1) PKG - COR
(type = character, default = none, units = dimensionless)

(2) OPTION - Flow geometry to be modeled in this path.
= AXIAL Axial flow geometry. For a BWR, the channel and bypass regions are treated as combined, as in MELCOR 1.8.5
= AXIAL-C Axial flow geometry, considering only the channel region for a BWR.
= AXIAL-B Axial flow geometry, considering only the bypass region for a BWR.
= RADIAL Radial flow geometry. Not recommended for a BWR, because the channel and bypass regions are treated as combined (as in MELCOR 1.8.5).
= RADIAL-B Radial flow geometry, considering only the bypass region for a BWR.

= CHANNEL-BOX Connection between channel and bypass of a BWR that opens when the channel box fails.
(type = character, default = none, units = dimensionless)

(3) ICORC1
(4) ICORC2 - ICORC1 and ICORC2 define the limiting core ring and axial levels to be associated with the flow path by defining two "corner" core cells. Their order is not significant: 103 205, 203 105, 205 103, and 105 203 all specify levels 3 – 5 of rings 1 – 2. Each core cell in the range *must* be associated with either the *from* or the *to* control volume for the flow path as defined on the FLnnn00 record.
(type = character, default = none, units = dimensionless)

(5) FLMPTY - Form loss coefficient for "empty" geometry, to be added to the value from the Ergun correlation.
(type = real, default = 1.0, units = dimensionless)

FLnnnSk – Piping segment parameters
$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
$0 \leq k \leq Z$, k is a continuation parameter
Required

The user must specify several parameters for each segment; at least one segment is required. Some of the parameters are optional. Each record must contain all the data for a segment; the data for a segment cannot be split across records.

(1) SAREA - Segment flow area
(type = real, default = none, units = m^2)

(2) SLEN - Segment length
(type = real, default = none, units = m)

(3) SHYD - Segment hydraulic diameter. The conventional definition is given by 4 times the flow area divided by the wetted perimeter.
(type = real, default = none, units = m)

(4) SRGH - Surface roughness. Optional.
(type = real, default = 5.E-5, units = m)

(5) SLAM - Laminar flow coefficient. Optional. If negative, then control function number –SLAM is used to define the laminar flow coefficient.
(type = real, default = value of sensitivity coefficient C4404(13), whose default value is 16.0, units = dimensionless)

(6) ISFLT - This field is required if and only if an enhanced filter is defined on RN2FLTXXYY records with 21 ≤ YY ≤ 45, in which case ISFLT must be the user number, XX, of the enhanced filter modeled in this segment. See the RN User's Guide for more information. (type = integer, default = 0, units = dimensionless)

FLnnnVk – Valve input

1 ≤ nnn ≤ 999, nnn is the user-assigned flow path number
0 ≤ k ≤ Z, k is a continuation character
Optional

Only one valve may be input for a given flow path. If more than one FLnnnVk record is included, only the one with the lowest value of k will be processed.

Valves may be used to open and close flow paths during the course of a calculation. The flow path area may take on any value between 0 (fully closed) and FLARA (fully open). The fraction open is defined by one or more control functions. It is defined directly by a single control function if no trip is used (although three fields must still be present on the record).

If a trip is specified, a trip control function is used to define "on-forward", "off" and "on-reverse" states. RELAP and TRAC users take note: A MELCOR trip is not what you are used to. The value of the trip control function may be positive ("on-forward"), negative ("on-reverse"), or zero ("off"). Different control functions are used to define the open fraction for "on-forward" and for "on-reverse" states. If the trip is "off", the valve opening remains unchanged from the previous timestep. See Section 1.5 of this document and the CF Users' Guide for more information.

(1) NVTRIP - If positive then NVTRIP is the trip control function number. If negative then a trip is not used and the fraction open is defined by the "on-forward" control function.
(type = integer, default = none, units = dimensionless)

(2) NVFONF - Control function used to defined the fraction open of the flow path for an "on-forward" state of the trip. If no trip is defined, this control function will always define the fraction open.
(type = integer, default = none, units = dimensionless)

(3) NVFONR - Control function used to define the fraction open of the flow path for an "on-reverse" state of the trip. If no trip is defined, this must be a valid control function number (i.e., one defined in MELGEN input), but the value of the control function will not be used.
(type = integer, default = none, units = dimensionless)

FLnnnPk – Pump input data

$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
$0 \leq k \leq Z$, k is a continuation character
Optional

Only one pump may be input for a given flow path. The first field on the first FLnnnPk record for a given flow path is interpreted as the pump type.

(1) PTYPE - Pump type
(type = character, default = none, units = dimensionless)

The additional data required to define a pump depend on the pump type. These data, which may comprise both real and integer values, are entered following the pump type and on continuation records if desired. They are interpreted according to the pump type flag. Because of the variable number and order of data, error checking is not exhaustive; the user is strongly advised to inspect the output of MELGEN in order to verify that the input was correctly interpreted.

PUMP TYPE = FANA

The FANA pump model represents a simple fan, in its normal operating range. It can, however, be used to approximate a constant-velocity coolant pump by appropriate choice of parameters. The input parameters are illustrated in the CVH/FL Reference Manual. Coupling to the momentum equation is explicit in time, and instabilities may arise for large timesteps. The problem may usually be mitigated by increasing the inertial length of the flow path, FLLEN, on record FLnnn01.

(1) PTYPE - FANA
(type = character, default = none, units = dimensionless)

(2) DPMAX - Maximum pressure head
(type = real, default = none, units = Pa)

(3) VPZERO - Volumetric flow rate at zero pressure head. The pressure head is zero for volumetric flow rates greater than or equal to VPZERO.
(type = real, default = none, units = m^3/s)

(4) VPMAX - Volumetric flow rate at maximum pressure head. The pressure head is also set to DPMAX for flows less than VPMAX.
(type = real, default = 0, units = m^3/s)

(5) ITRIP - Pump trip flag. If ITRIP is zero (default), the pump is always on; otherwise, the pump is on and the pressure head is calculated

only if the value of a trip is nonzero. If ITRIP is positive, the value of control function number ITRIP is used for the trip value. If ITRIP is negative, tabular function number –ITRIP is used for the trip value. The tabular function independent argument is time. (type = integer, default = 0, units = dimensionless)

PUMP TYPE = QUICK-CF

The QUICK-CF pump type allows the user to define the pump head through a control function. This function might be as simple as a tabular function of velocity or of time. The complexity of the model is limited only by the ingenuity and patience of the user; an example of a (partial) homologous pump model is shown in the CF User's Guide. Coupling to the momentum equation is explicit in time, and instabilities may arise for large timesteps. The problem may usually be mitigated by increasing the inertial length of the flow path, FLLEN, on record FLnnn01.

(1) PTYPE - QUICK-CF
(type = character, default = none, units = dimensionless)

(2) IPUMCF - Number of control function defining the pressure head; the values from this control function should have units of Pascals.
(type = integer, default = none, units = dimensionless)

FLnnnTk – Time dependent flow path
$1 \leq nnn \leq 999$, nnn is the user-assigned flow path number
$0 \leq k \leq Z$, k is a continuation character
Optional

The velocity through the flow path may be defined using tabular or control functions. The pool and atmosphere velocities are identical. Only one time dependent flow path dataset may be entered for a flow path.

(1) NTFLAG - Time dependent flow path type flag
(type = integer, default = none, units = dimensionless)
= 1 Use tabular function number NFUN to define velocity versus time.
= 2 Use control function number NFUN to define velocity versus time.

(2) NFUN - Tabular or control function number to define the velocity versus time. The interpretation is dependent on the value of NTFLAG.
(type = integer, default = none, units = dimensionless)

FLnnnMk – Momentum flux input data
$1 \leq$ nnn ≤ 999, nnn is the user-assigned flow path number
$0 \leq k \leq Z$, k is a continuation character
Optional

Momentum flux will be calculated for flow path nnn if data are entered on this record. Only one dataset may be entered for a flow path.

(1) NFLFM - Upstream flow path number. If set to 0, an upstream flow velocity of zero will be used to calculate momentum flux.
(type = integer, default = none, units = dimensionless)

(2) NFLTO - Downstream flow path number. If set to 0, a downstream flow velocity of zero will be used to calculate momentum flux.
(type = integer, default = none, units = dimensionless)

(3) XCVAFM - Upstream (*from*) control volume flow area appropriate for flow path nnn (i.e., in the direction of flow)
(type = real, default = none, units = m^2)

(4) XCVATO - Downstream (*to*) control volume flow area appropriate for flow path nnn (i.e., in the direction of flow)
(type = real, default = none, units = m^2)

2.2 MELCOR User Input

Records FLnnn05, FInnn0F, and FLnnn0T may be included in MELCOR input.

Record FLnnn05 defines the length over which momentum exchange occurs between pool and atmosphere flows sharing a flow path. The value used affects entrainment and flooding by controlling the balance between momentum exchange (which tends to couple the two flows and reduce slip) and buoyancy (which tends to separate pool from atmosphere).

Records FLnnn0F and FLnnn0T define the junction openings in the *from* and *to* volumes, respectively, i.e., the range of elevations within those volumes "seen" by the flowpath for purposes of allowing pool and/or atmosphere to flow. In some calculations, use of a restricted opening height may be necessary to prevent the flow of inappropriate phases during relatively quiescent segments of a calculation when gravitational separation should occur. On the other hand, extremely slow running of MELCOR might occur during relatively dynamic segments when entrainment would be expected (see discussion in Sections 1.1.2 and 1.3.1.) Also, the consequences of an initial choice may not become apparent until late in a long calculation. Therefore, MELCOR allows redefinition of the junction opening on restart of a calculation. Although the default definition in MELGEN of

the momentum exchange length for a vertical flow path involves the junction opening heights, inclusion of these records in MELCOR does *not* lead to automatic redefinition of that length.

In addition to these limited modifications to the flow path models and database permitted in MELCOR input, several characteristics of control functions—including bounds on their values—may be modified on restart. This allows limited access to the definitions of pumps and valves. It may be used, for example, to select among a number of scenarios involving different failure paths, *provided that all required paths were provided in the original MELGEN input.*

3. Sensitivity Coefficients

Sensitivity coefficients for thermal hydraulic models are described in the CVH Package Users' Guide.

4. Plot Variables and Control Function Arguments

The flow path package variables that may be used for plot variables and control function arguments are listed and described below. Within slashes (/ /), a 'p' indicates a plot variable and a 'c' indicates a control function argument.

FL-EFLOW.x.n	/cp/	Enthalpy flow rate of pool (x = 'P') or atmosphere (x = 'A') flow through flow path n, with respect to the normal MELCOR reference point (units = W)
FL-FRUNBLK.n	/p/	Fraction of flow path that is unblocked by core debris. This variable is available only for flowpaths where the flow blockage model has been invoked by inclusion of a FLnnnBk record as part of MELGEN input; for flowpaths whose area is controlled by an ordinary valve, the open fraction may be plotted as the value of the related control function, CFVALU.m (units = dimensionless)
FL-I-EFLOW.x.n	/cp/	Integral of enthalpy associated with pool (x = 'P') or atmosphere (x = 'A') flow through flow path n, with respect to the normal MELCOR reference point (units = J)
FL-I-H2O-MFLOW.n	/p/	Integral of mass of water (pool + fog + vapor) flowing through flow path n (units = kg)

FL-I-MFLOW.m.n	/cp/	Integral of mass of material m flowing through flow path n (units = kg)
FL-MFLOW.n	/p/	Total mass flow rate (all hydrodynamic materials) through flow path n (units = kg/s)
FL-MFLOW.m.n	/cp/	Mass flow rate of material m through flow path n (units = kg/s)
FL-V-N-OC.n	/p/	Number of times valve number n has opened or closed. Any area fraction greater than 0.0 is considered "open." (units = dimensionless)
FL-VELLIQ.n	/cp/	Velocity of pool through flow path n (units = m/s)
FL-VELVAP.n	/cp/	Velocity of atmosphere through flow path n (units = m/s)
FL-VOID.n	/cp/	Void fraction in flow path n (units = dimensionless)

5. Example Input

This section gives several examples of input to the FL package. Anything followed by an asterisk is a comment.

In the first example, flow path 12 defines a door between control volumes 10 and 20; positive flow is from volume 10 to volume 20, as a simple opening 1 m wide and 2 m high. The elevation of the floor is 0 m. Both junction altitudes are taken at the center of the door (1 m); both junction opening heights are taken as 2 m to include the full height of the door. The inertial length is estimated as 1 m, representing a length of a few times the thickness of the wall; the segment length is an estimate of the wall thickness, and the hydraulic diameter is 4 times the area (2 m^2) divided by the wetted perimeter (6 m). Form loss is probably more important than wall friction; the loss coefficient is estimated to be 2.0 in both directions.

```
FL01200    'Door'      10    20    1.0  1.0   * Center alt = 1 m
*             A    L   Open H-fm H-to         * Junction openings
FL01201    2.0  1.0   1.0   2.0   2.0         * see full 2 m height
FL01202    3                                  * Normal, horiz
FL01203    2.0  2.0              * Forward and reverse loss coeffs
FL012S1    2.0  0.2   1.33       * Segment L, A, and hyd diam
```

In the second example, flow path 125, represents the vertical connection of the core (control volume 120) to the upper plenum (control volume 150) in a BWR; the direction of positive flow is from core to upper plenum. The elevation of the plane separating them is

10 m. The form loss coefficients are 9.5 for forward flow and 10.5 for reverse flow. From the center of the core to the center of the upper plenum, fluid must travel 2 m (half the height of the core) through a flow area of 4 m^2 and a hydraulic diameter of 0.01 m, and 1.6 m through the more-open upper plenum with an area of 8 m^2 and a hydraulic diameter of 0.8 m. The nominal flow area is taken as 4 m^2. The inertial length was calculated from L/ 4 m^2 = 2 m / 4 m^2 + 1.6 m / 8 m^2, which yields L = 2.8 m; the precise value used is not critical.

```
FL12500    'Core to UP'    120   150  10.0 10.0 * CV120 to CV150
FL12501    8.0   2.8   1.0         * A, L, Open fraction
FL12502    0     0     0     0     * Vert, Active, no SPARC + or -
FL12503    9.5   10.5              * Forward, Reverse form losses
*           A     L    Dhyd
FL125S1    4.0   2.0   0.01        * Segment for half Core
FL125S2    8.0   1.6   0.8         * Segment for half UP
```

Record FL12502 specifies default values, and could be omitted. Because no junction opening heights were included on the FL12501 record, the radius of a circle with area 4 m^2 (1.13 m) will be used in each volume. This is a reasonable fraction of the height of each volume, making use of the default reasonable.

If desired, the height of the junction openings could be reduced by including the desired values on the FL12501 record. This could also be done by specifying the desired limits directly on FL1250F and FL1250T records; for example inclusion of the records

```
FL1250F    9.5   10.0        *'From' opening, 9.5-10.0 m
FL1250T    10.0  11.0        *'To' opening, 10.0-11.0 m
```

would explicitly define the junction openings to see the range of elevations from 9.5 to 10.0 m for forward flow out of volume 120 and 10.0 to 11.0 for reverse flow out of volume 150.

The default momentum exchange length for this flow path might limit countercurrent flow of pool from the upper plenum (volume 150) and atmosphere from the core (volume 120) sufficiently to result in "levitation" of water in the upper plenum under conditions of vigorous boiling in the core. Inclusion of a record such as

```
FL12505    0.2               * Momentum exchange length
```

would substantially increase the limits of countercurrent flow and reduce the levitation of water in the upper plenum.

Addition of the record

```
FL12504    0.0   4.0         * Initial atmos, pool velocity
```

will define an initial pool velocity of 4 m/s from core to upper plenum in the flow path.

Jet pumps in a BWR are frequently modeled as pipe-like flow paths. The partial input

```
FL15100    'Jet Pump'      110  100  9.0  4.0  * From DC to LP
FL15101    0.63 5.0  1.0                *A, L, Open fraction
. . .
FL151S1    0.63 5.0  0.2  5.E-6        *Dhyd for one of 20, smooth
```

represents 20 jet pumps in parallel, each of 0.2 m diameter, with a total area of 0.63 m^2, connecting the downcomer (control volume 110) at 9 m elevation to the lower plenum (control volume 100) at 4 m elevation. Surface roughness is 5 μm rather than the default of 50 μm. The volume of the pumps is usually included in the lower plenum.

Increased flow resistance and blockage of flow paths by core debris may be modeled by use of FLnnnBk records. For example, if flow path 112 connects the lower plenum to the channel region of the core of a BWR, use of the input

```
FL11200    'LP to CHNL'    110  120  4.0  4.0  * CV110 to CV120
. . .
FL112B0    COR  AXIAL-C    104  306  * Channel flow blockage by COR
```

will include the resistance of debris in the channel in rings 1 through 3 of axial levels 4 through 6 of the core in computing flows through flow path 112. The input will be rejected, and MELGEN will not generate an initial restart, unless the channel regions of all core cells involved lie in one of the control volumes (110 or 120) connected by the flow path.

Similar input allows modeling of the opening of a flow path between the channel and bypass regions of a core. If flow path 123 connects the channel and bypass regions, use of the input

```
FL12300    'CH to BP'      120  130  6.0  6.0  * CV120 to CV130
. . .
FL123B0    COR  CHANNEL-BOX    104  306  * Channel box failure
```

will base the open area and flow resistance of flow path 123 on the state of the channel box in rings 1 through 3 of axial levels 4 through 6 of the core. The input will be rejected, and MELGEN will not generate an initial restart, unless the channel and bypass regions are distinguished in all core cells involved. Further, the channel regions of all the cells must lie in one of the control volumes (120 or 130) connected by the flow path, and the bypass regions of all the cells in the other.

Finally, the partial input

```
FL19900    'Pipe'      123  456  20.0 -10.0
FL19901    0.002       30.0 1.0  * A, L, Open fraction
. . .
*          A    L     Dhyd
```

```
FL199S1    .002   0.5 0.05
FL199S3    0.05  29.5 0.25
```

represents a vertical pipe, 30 m long, connecting control volume 123 at 20 m elevation to control volume 456 at –10 m elevation. A short segment has an area of 0.002 m^2, corresponding to a diameter of 50 mm; the remainder has an area of 0.05 m^2, corresponding to a diameter of 0.25 m. Addition of the record

```
FL199V0    -1    20    20    * no trip, open fraction from CF 20
```

includes a simple (untripped) valve in the flow path. The fraction of its area that is open will be obtained from the value of control function 20; a value of 1.0 corresponds to opening to the full 0.002 m^2 nominal area.

If flow path 199 contains a check valve, restricting flow through the flow path to (say) the forward direction, it is preferable to model it as a "one way" flow path rather than by defining a valve. This reduces the number of control functions that must be written, and avoids the small reverse flows that can occur before the CF package can detect the reverse flow and close the valve. (This is a general consequence of the numerically explicit nature of all MELCOR control function models.) The required input record is

```
FL19902    10                 * Vertical, one-way forward
```

In this case, no FL199V0 record is required (or permitted).

Alternatively, addition of the record

```
FL199P0    QUICK-CF   200    * Control function pump
```

includes a pump (momentum source) in the flow path. The pump boost in pressure will be obtained from the value of control function 200. Section 6.7 of the CF Package Users' Guide provides partial input for an appropriate control function to represent a homologous pump model similar to that in TRAC and RELAP.

6. FL Package Output

Each printed edit generated by the FL package in MELGEN and MELCOR contains a snapshot description of the state of all flow paths, with the output organized in tabular form. The integrated (cumulative) flows are included. Many column headings are abbreviated, but most are relatively clear—particularly when it is understood that "LIQ" refers to pool and "VAP" to atmosphere, that "ALPHA" is the fraction of the open area of a flow path occupied by *atmosphere*, and that "P HEAD" refers to *pumps*. For each valve, the number of times its state has changed from fully closed to at least partially open or back is recorded as "NUMBER ON OR OFF." (A complete cycle, closed to open to closed is counted as 2.)

The "FLOW PATH TIME INDEPENDENT EDIT" is generated by the FL package in MELGEN and as part of the first edit for each MELCOR run. This edit list properties of all flow paths, with the input flags, pump data, and valve data interpreted in English. The segment data associated with each flow path are listed, as are the flow paths connected to each control volume.

Users are strongly advised to check the initial edit generated by MELGEN—as well as the contents of the diagnostic file (MEGDIA)—before proceeding with a calculation. This is particularly important if FLnnnBk input records were included in the input to model flow blockage effects in the COR package. When this is done, some of the values input to FL will be redefined for consistency with the geometry of COR. Any such values changed will be flagged by an asterisk ("*") in the edit, with the notation

* MARKS DATA MODIFIED BY BLOCKAGE OR CHANNEL BOX MODEL

7. Diagnostics and Error Messages

Diagnostic messages will be written by MELGEN to report errors or inconsistencies in input. Typical errors include errors in record format and failure to supply all required input records. Inconsistencies between input to different packages are also identified; each of the volumes connected by a flow path must be defined, and must include the specified elevation of the flow path junction; any tabular functions or control functions referred to by pump, valve, or time-dependent flow path input must be properly defined.

Errors may propagate, resulting in messages that are apparently unrelated to the actual input records. In these cases, it is often necessary to rerun MELGEN with the identified errors corrected; the other error messages should then be eliminated or clarified.

No restart file will be written until all errors identified during input processing have been corrected. This does *not*, of course, assure that the accepted input properly describes the physical system that the user intended to model. The analyst should always examine the initial edit produced by MELGEN before proceeding to run MELCOR. We have found that an incorrect definition of control logic for a pump and valve model will frequently not be discovered until the logic is exercised—typically after the investment of significant computer resources. In many cases, the entire calculation must be rerun. A short preliminary run to test the logic, perhaps with simplified input or artificially modified initial conditions is often a good investment.

All time advancement calculations are performed by the CVH package. Errors related to time advancement in MELCOR are described in Section 7.1 of the CVH Package Users' Guide.

Heat Structure (HS) Package
Users' Guide

The MELCOR Heat Structure (HS) package calculates heat conduction within an intact, solid structure and energy transfer across its boundary surfaces into control volumes. The modeling capabilities of heat structures are general and can include pressure vessel internals and walls, containment structures and walls, fuel rods with nuclear or electrical heating, steam generator tubes, piping walls, etc.

This User's Guide provides basic information needed to run the HS package with the rest of MELCOR, including a short discussion of the nodalization scheme and calculational framework of the package and a detailed explanation of the user input and package output for MELGEN and MELCOR. Required and optional input, sensitivity coefficients, control function arguments, plot variables, and error messages are all covered.

More detailed information on the models and numerical solutions employed by the HS package can be found in the HS Package Reference Manual.

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1. Introduction

The Heat Structure (HS) package calculates heat conduction within an intact, solid structure and energy transfer across its boundary surfaces into control volumes. This document is the users' guide for the HS package. It provides information that is necessary to execute the HS package with other packages in the MELCOR Code System.

This section describes the modeling of a heat structure in the MELCOR Code System and provides a brief discussion of the calculation procedure which is used to obtain the temperature distribution for each heat structure and to calculate its interactions with structures in other packages.

A heat structure is an intact, solid structure which is represented by one-dimensional heat conduction with specified boundary conditions at each of its two boundary surfaces. The modeling capabilities of heat structures are general and can include pressure vessel internals and walls, containment structures and walls, fuel rods with nuclear or electrical heating, steam generator tubes, piping walls, etc. Special logic also permits the representation of cylindrical ice columns to model PWR ice condensers.

Figure 1.1 illustrates a heat structure in a control volume. The heat structure is inclined at some angle with respect to the vertical and is partially immersed in a pool. Although the geometry shown here is rectangular, a heat structure may have a rectangular, cylindrical, spherical, or hemispherical geometry.

The heat structure in Figure 1.1 is nodalized with *N* temperature nodes. The nodalization is specified by user input and may be nonuniform, i.e. the distance between temperature nodes need not be the same. Node *1* is the temperature node at the left boundary surface for a rectangular geometry or at the inside boundary surface for a cylindrical, spherical, or hemispherical geometry. Node *N* is the temperature node at the right boundary surface for a rectangular geometry or at the outside boundary surface for the other geometries.

The region between two adjacent temperature nodes is called a mesh interval. Each mesh interval may contain a different material. The name of the material in each mesh interval must be specified by user input. The Material Properties (MP) package provides thermal properties for each material through an interface with the HS package. See the MP Package Users' Guide for details on the default materials and the input which is required for new materials.

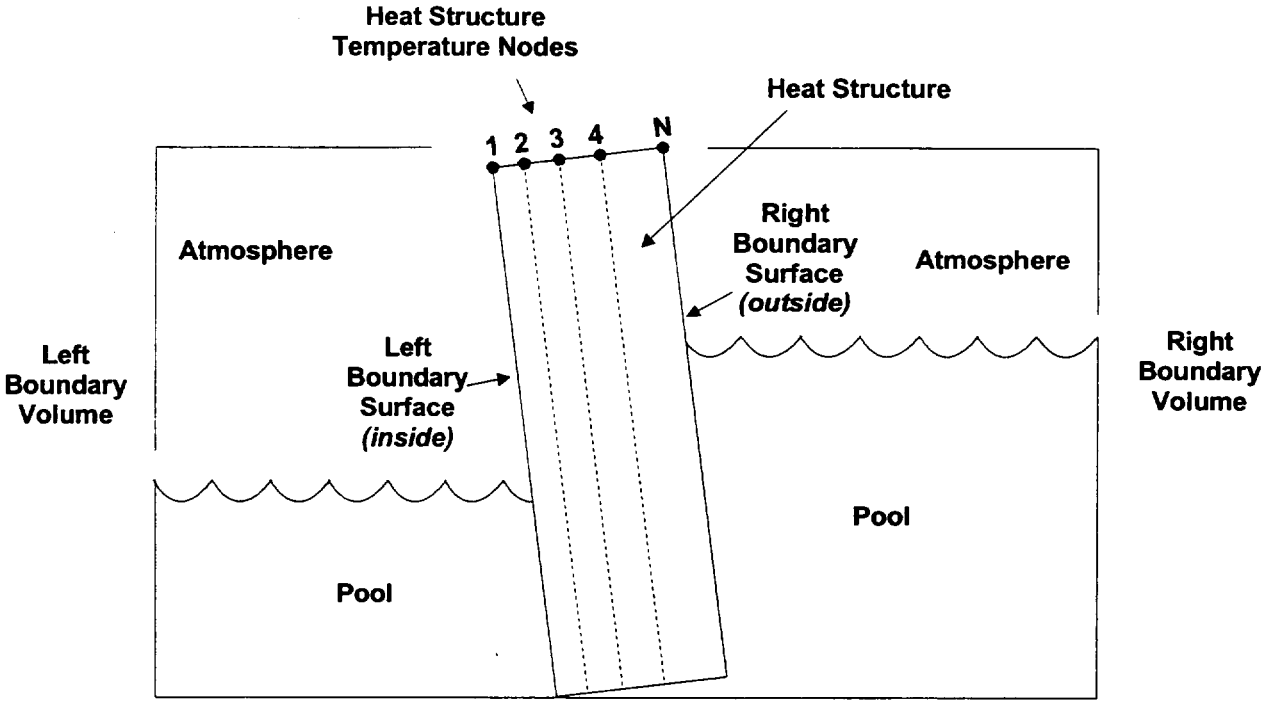


Figure 1.1 Heat Structure in a Control Volume

A pertinent issue for the user of the HS package concerns how finely a heat structure should be nodalized. While no definitive nodalization study is known to exist, the following considerations are useful in resolving this issue*. The mesh interval at a surface should be small enough to accurately respond to changes in the temperature of its boundary volume over a computational cycle. Accurate response is important for correctly calculating energy transfer, condensation-evaporation phenomena, and radionuclide deposition-resuspension. However, the surface mesh interval should not be so small as to encourage temperature oscillations about the boundary volume temperature. Therefore, it is recommended that the size of the surface mesh interval be no smaller than the thermal-diffusion length L_D. That is, ensure that

$$X_{surf} \geq L_D = \sqrt{4\,k\ \ t_{max}/C_p}$$

where

* L.N. Kmetyk, MELCOR Assessment: Gedanken Problems, Volume 1, SAND92-0762, Sandia National Laboratories, Albuquerque, NM (January 1993).

k = thermal conductivity of material in surface mesh interval,

Δt_{max} = maximum computational timestep, and

C_p = volumetric heat capacity (product of density and heat capacity) of material in surface mesh interval.

If this length is greater than the thickness of the heat structure in the direction of energy flow, two temperature nodes are recommended. Otherwise, to minimize the number of temperature nodes, the length of adjacent mesh intervals should increase toward the interior of the heat structure. However, to maintain accuracy while increasing the distance between temperature nodes, it is recommended that the length of adjacent mesh intervals increase by no more than a factor of two within the same material and the length of adjacent mesh intervals be the same at the boundary of dissimilar materials.

Warning !!

If the length of the mesh interval at a surface is less than about half the thermal diffusion length, oscillations in the surface temperatures may occur. However, these oscillations are bounded and usually are damped out in a few computational cycles if the boundary conditions do not change much. To mitigate these oscillations, the current HS package utilizes a fully implicit numerical method rather than the Crank-Nicolson method used in earlier versions.

An internal power source may be specified for a heat structure. Its spatial dependence is specified by user input and may vary for each mesh interval. Its time dependence is given by a user-specified tabular function or control function.

Each heat structure has two boundary surfaces—left and right for rectangular geometries or inside and outside for cylindrical, spherical, or hemispherical geometries. At each boundary surface one of the following boundary conditions is specified:

(1) symmetry (adiabatic),

(2) convective with calculated heat transfer coefficient,

(3) convective with calculated heat transfer coefficient and a specified surface power source function,

(4) convective with specified heat transfer coefficient function,

(5) specified surface temperature function, and

(6) specified surface heat flux function.

If a convective boundary condition is selected for a boundary surface, a control volume must be specified as its boundary volume. No boundary volume is permitted for a symmetry boundary condition or a specified surface temperature boundary condition, and a boundary volume is a user option for the specified heat flux boundary condition. The Control Volume Hydrodynamics (CVH) Package Reference Manual provides information on control volume modeling.

If a boundary volume is specified for a surface, then some additional data are required through user input. For each boundary surface with a boundary volume, these data include:

(1) surface area,

(2) characteristic length (the dimension used in calculating the Reynolds, Grashof, Nusselt, and Sherwood numbers),

(3) axial length (length of structure along boundary surface, used to determine pool fraction),

(4) type of flow over the surface (internal or external; used in calculating the Nusselt number), and

(5) critical pool fractions for pool and atmosphere heat transfer.

The pool fraction of a heat structure boundary surface is the fraction of its surface area in the pool of its boundary volume. The critical value for the pool is the minimum value of the pool fraction for which heat transfer to the pool is calculated. The critical value for the atmosphere is the maximum value of the pool fraction for which heat transfer to the atmosphere and mass transfer at the surface are calculated.

The critical pool fractions provide the user with flexibility for calculating heat transfer at the surface of a heat structure. The user may elect to turn off the calculation of pool or atmosphere heat transfer by appropriate specification of these fractions. Turning off the calculation of pool heat transfer would be useful, for example, in a situation where a heat structure is partially immersed in a pool whose temperature is considerably less than the temperature of the atmosphere. The situation of high pool-atmosphere temperature differences could be calculated by the CVH package with its nonequilibrium thermodynamics option. In this situation, the heat transfer near the pool-atmosphere interface is significant and axial conduction in this region of the heat structure is quite important. The HS package will calculate large energy transfers from the atmosphere to the pool under these conditions, since it calculates one-dimensional internal conduction and boundary conditions using a weighting of pool and atmosphere temperatures and heat transfer coefficients. If during a calculation large temperature differences between the pool and atmosphere are expected or axial conduction is expected to be important, the user should either subdivide a heat structure into structures of acceptable axial dimensions or turn off pool heat transfer by setting the critical pool fraction for pool heat transfer to 1.0.

If a convective boundary condition with calculated heat transfer coefficients is specified, then an extensive set of correlations is available for calculating natural or forced convection to the pool and atmosphere. Pool boiling heat transfer is calculated if the temperature of a heat structure surface is above the boundary volume saturation temperature by using correlations for nucleate boiling, critical heat flux, film boiling, and transition boiling.

Radiation heat transfer from a heat structure surface to the boundary volume pool is calculated during stable film and transition boiling. Radiation heat transfer can also be specified between a heat structure surface and the boundary volume atmosphere. Two options, an equivalent band model and a gray gas model, are currently available. Radiation heat transfer between user-specified pairs of heat structure surfaces may also be modeled.

Mass transfer between a heat structure surface and the boundary volume atmosphere is modeled using correlations or expressions for calculating mass flux. Models include condensation in a pure steam environment, condensation and evaporation in the presence of noncondensibles, and flashing in any environment. Liquid films on heat structure surfaces are also modeled so that condensate transferred from the boundary volume atmosphere and liquid deposited by other packages can be treated. Mass transfer affects the temperature distribution within a heat structure by its energy flux at the surface. When mass transfer occurs at a structure surface, an equation for the surface temperature of the resulting liquid film including the energy flux due to mass transfer is included in the set of conduction (temperature) equations for the structure.

A film-tracking model is available to treat film flow between structures. The user invokes this model by specifying one or more network(s) of connected structures. The model uses a correlation for film thickness as a function of film flow and the conservation of mass to determine the film thickness and total rate of drainage from each structure in the network. The total drainage from each structure is then partitioned among three possible destination types specified by the user for each structure. A user-specified fraction of the total drainage may be directed to one or more other structure surfaces in the network; a user-specified fraction may "rain" from the surface via a user-specified transfer process to the MELCOR Spray package; and the remainder of the total drainage (one minus the sum of all the user-specified fractions listed above) is directed to the CVH pool component of the control volume associated with the structure surface (this is the only destination for drainage from surfaces which are not included in film-tracking networks). The model also allows the user to specify external water sources for any structure through tabular function or control function input. The model is primarily intended to treat the passive containment cooling systems proposed for ALWRs, but it may also be used to track film flow in steam generators, etc.

Finite-difference equations are used to advance the temperature distribution of a heat structure in time during MELCOR execution or to obtain its steady-state temperature distribution during MELGEN execution if specified by user input. These equations are obtained from an integral form of the one-dimensional heat conduction equation and boundary condition equations using a fully implicit numerical method. The finite-difference

approximation is a tridiagonal system of N (N + 1 or N + 2 if there is a liquid film on one or both surfaces of the structure) equations for a heat structure with N (or N + 1 or N + 2) temperature nodes. The solution of this system is obtained using the standard solution algorithm for a tridiagonal system of linear equations. The procedure is iterative because the coefficients are functions of temperature and must be updated between iterations.

A degassing model is provided for the release of gases from materials which are contained in heat structure mesh intervals. Input may be provided, for example, to represent the release of water vapor or carbon dioxide from concrete as its temperature increases. The following information must be input by the user for each gas source in the degassing model:

(1) heat structure surface from which the gas is released,

(2) number of mesh intervals over which the source is distributed, and

(3) name of gas which is released.

Each gas source is characterized by the following information which is provided by user input:

(1) density,

(2) heat of reaction, and

(3) boundaries of temperature range for the release of gas.

The mass of gas that is available for release is the source density times the volume of the mesh intervals over which the source is distributed. The HS package calculates a constant gas release rate over the degassing temperature range and modifies thermal properties over this range to account for the energy which is required for gas production and release. If the initial temperature of the structure exceeds the lower boundary of the degassing temperature range, MELGEN issues a warning message to inform the user that the gas which would have been released below the initial temperature will be ignored and is unavailable for release.

A special application of the degassing model can be used to model ice condensers. In this application the user defines a vertical cylinder with an adiabatic inner boundary and an associated "gas" source that releases liquid water into the pool associated with the outer radial boundary volume. The lower value of the degassing temperature range should be close to but greater than the freezing point of water (273.15 K) to avoid problems with the limits of the tabular functions in the MELCOR material properties libraries. The upper value of the degassing temperature range should be about 373 K to simulate sensible heating of the melted ice by counter-flowing steam. The heat of reaction should include the sensible heating of both the subcooled ice (from its actual temperature) and melted ice in

addition to the latent heat of fusion of water. The gas source density is the density of liquid water. Furthermore, the user is required to specify an initial temperature for the ice, and this temperature should coincide with the lower limit of the degassing range (274 K). The ice condenser modeling logic is activated by including a special keyword in the user input for the outer radial boundary of the cylindrical heat structure (Record HSCCCCC600).

This users' guide contains eight additional sections. Section 2 describes the user input that is required for utilizing this package in MELGEN and MELCOR execution. The sensitivity coefficients and their default values are given in Section 3. Section 4 lists and briefly describes the plot variables and control function arguments which are available in the HS package. Section 5 provides some example input that illustrates the use of this package. Printed output is discussed in Section 6. Section 7 lists the diagnostics and error messages which are provided by this package.

2. Input Requirements

This section provides the input requirements for the MELCOR HS package, including a short description of the input quantities and their units and default values, if any. Further description of the input variables and their use in the models can be found in the HS Package Reference Manual.

2.1 MELGEN User Input

This section contains a detailed description of the MELGEN user input for the HS package. Input record descriptions are found as follows:

Section 2.1.1 Heat Structure input records
Section 2.1.2 Gas Source input records
Section 2.1.3 Film-tracking input records

2.1.1 MELGEN Input for Heat Structures

Input data for heat structures are entered on records with identifiers of the form

HSCCCCCXNN

where

HS	indicates that the record is a Heat Structure record
CCCCC	is the numerical identifier for the heat structure (00000-99999)
X	is the record type
NN	is the record number for record type X

The following input records are required to specify a heat structure. Unless otherwise stated, field variables beginning with I through N are integers and those beginning with A through H or O through Z are real numbers. A complete set of input records must be supplied for each heat structure.

HSCCCCC000 – General Heat Structure Data

00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Required

This record specifies the existence of a heat structure whose numerical identifier is CCCCC.

(1) NP - Number of temperature nodes. This value must be greater than 1 but less than 100.
(type = integer, default = none, units = none)

(2) IGEOM - Indicator for type of geometry.

= 1 rectangular geometry
= 2 cylindrical geometry
= 3 spherical geometry
= 4 hemispherical geometry of the bottom half of a sphere
= 5 hemispherical geometry of the top half of a sphere.
No other values are permitted for this field.
(type = integer, default = none, units = none)

(3) ISS - Steady-state initialization flag. If 0 or positive, or if field 3 is omitted, a steady-state initialization calculation is performed for Heat Structure CCCCC. If a negative value is input, a steady-state initialization calculation is not performed and the initial temperature distribution is input on the HSCCCCC8XX records. The default is that a steady-state initialization will be performed.
(type = integer, default = 0, units = none)

Node 1 is the temperature node at the left boundary for a rectangular geometry or the inside boundary for a cylindrical, spherical, or hemispherical geometry; Node NP is the temperature node at the right boundary for a rectangular geometry or the outside boundary for a cylindrical, spherical, or hemispherical geometry.

HSCCCCC001 – Heat Structure Name

00000 ≤CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional

(1) HSNAME - Name of heat structure. This field may contain no more than 16 characters and imbedded blanks.
(type = character*16, default = none)

If this record is not present, 16 blanks will be stored as the name of Heat Structure CCCCC.

HSCCCCC002 – Heat Structure Elevation and Orientation Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Required

(1) HSALT - Elevation parameter. This value is the elevation of the lowest point on Heat Structure CCCCC. This parameter must satisfy the condition that each boundary surface of this heat structure is contained within its boundary volume.
(type = real, default = none, units = m)

(2) ALPHA - Orientation parameter.

Rectangular geometries: the absolute value of ALPHA is the cosine of the acute angle α between a vertical line and the heat structure surface (see Figure 1.1).

ALPHA = 1:	vertical surface
ALPHA = 0:	horizontal surface with left-hand side on the bottom
0 < ALPHA < 1:	slanted surface with left-hand side on the bottom
ALPHA = -10^{-7}:	horizontal surface with the right-hand side on the bottom
$-1 <$ ALPHA $< -10^{-6}$:	slanted surface with right-hand side on the bottom

Cylindrical geometries: the absolute value of ALPHA is the cosine of the acute angle between a vertical line and the axis of this heat structure. Only the absolute value is used for cylindrical geometries.

Spherical or hemispherical geometries: ALPHA has no meaning and does not need to be entered.

For rectangular and cylindrical geometries, ALPHA must be greater than or equal to - 1.0 and less than or equal to 1.0.
(type = real, default = none, units = none)

If only one field is present on this record, it will be interpreted as HSALT. In this situation, ALPHA will be set equal to 1.0, which corresponds to a vertically oriented heat structure.

NOTE on FLOORS and CEILINGS

In associating horizontal rectangular heat structures with CVH control volumes, the upper surface of the structure should be thought of as a floor for the volume. Therefore, for a heat structure of thickness DELT and ALPHA = 0, HSALT + DELT should be greater than or equal to the lowest elevation in the CVH volume-altitude table for that volume. In this case the right-hand side of the structure is the floor of the CVH volume and the CVH volume number is entered in the IBVR field of Record HSCCCCC600.

If ALPHA = -10^{-7} for the same heat structure, then the description is the same except that the left- and right-hand sides are reversed. The right-hand side is on the bottom and the floor is the left-hand side. The CVH volume number is entered in the IBVL field of Record HSCCCCC400.

The same convention applies to ceilings of control volumes, which should be thought of as the lower surface of a horizontal heat structure.

HSCCCCC003 – Heat Structure Multiplicity
00000 ≤CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional

(1) HSMULT - Multiplicity of heat structure. This value is the number of heat structures in this problem that are identical to Heat Structure CCCCC.
(type = real, default = 1.0, units = none)

HSCCCCC004 – Boundary Fluid Temperature Option
00000 ≤CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional (but generally required for COR radial boundary heat structures; see the COR Package Users' Guide and the descriptions of input records COR00006 and CORZjj02)

This record provides the user the option of which bulk fluid temperature to use on each side in the heat transfer calculations for the specified heat structure.

(1) IOPTL - Option for left (inside) surface of the heat structure.

< 0 Use control function -IOPTL for boundary fluid temperature on the left-hand side.

= 0 Use bulk fluid temperature in left boundary CVH volume (either pool or atmosphere depending on liquid level) for boundary fluid temperature on the left-hand side.

> 0 Use fluid temperature calculated by COR package dT/dz model for core cell IOPTL for boundary fluid temperature on the left-hand side.
(type = integer, default = 0, units = none)

(2) IOPTR - Option for right (outside) surface of the heat structure.

< 0 Use control function -IOPTR for boundary fluid temperature on the right-hand side.

= 0 Use bulk fluid temperature in right boundary CVH volume (either pool or atmosphere depending on liquid level) for boundary fluid temperature on the right-hand side.

No core cell input is allowed for the right-hand surface.
(type = integer, default = 0, units = none)

HSCCCCC100 – Temperature Node Location Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Required

(1) NODLOC - Indicator for location of temperature node location data. If negative, all temperature node location data must be entered for Heat Structure CCCCC on the HSCCCCC1NN records. If a nonnegative integer MMMMM, these data are obtained from the HSMMMMM1NN records for Heat Structure MMMMM, which must exist.
(type = integer, default = none, units = none)

(2) IFRMAT - Format flag for temperature node location data. This value indicates the format for specification of data on the HSCCCCC1NN records.

= 1 Each pair of data on each of these records is interpreted as the location of a temperature node and the number of this node. The intermediate nodes are equally spaced between specified node locations.

= 2 Each pair of data on each of these records is interpreted as a length and the number of consecutive mesh intervals with this length.
No other values are permitted for this field.
(type = integer, default = none, units = none)

(3) XI - Left (inside) boundary location. This value gives the location of the temperature node at the left (inside) boundary surface of this heat structure. XI must be greater than or equal to zero.

Rectangular geometries: XI is relative to any origin.
Cylindrical geometries: XI is relative to the axis of the cylinder.
Spherical geometries: XI is relative to the center of the sphere.
Hemispherical geometries: XI is relative to the center of the sphere which contains the hemisphere.
(type = real, default = none, units = m)

If XI is zero, then either the geometry of this heat structure must be rectangular (IGEOM = 1 on Record HSCCCCC000) or a symmetry boundary condition must be applied to the left boundary surface (IBCL = 0 on Record HSCCCCC400).

HSCCCCC1NN – Temperature Node Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
01 ≤ NN ≤ 99, NN is the sequence number

These record are required if NODLOC on Record HSCCCCC100 is negative. The format of each record is given in the description of Record HSCCCCC100 and the location of Node 1 is known from XI on Record HSCCCCC100. Two fields per record are entered on the HSCCCCC1NN records until the locations of all remaining temperature nodes for Heat Structure CCCCC are specified.

(1) XVALUE - Location of temperature node (IFRMAT = 1)
Length of mesh interval (IFRMAT = 2)
(type = real, default = none, units = m)

(2) NXVALU - Number of temperature node which has location XVALUE (IFRMAT = 1)
Number of consecutive mesh intervals with length XVALUE (IFRMAT = 2)
(type = real, default = none, units = m)

The record numbers need not be sequential. However, for IFRMAT = 1, XVALUE and NXVALU must be strictly monotonically increasing functions of the NN in HSCCCCC1NN. For IFRMAT = 2, the location of the temperature nodes will be ordered by the NN in HSCCCCC1NN.

HSCCCCC200 – Location of Material Composition Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional

(1) MCDLOC - Indicator for location of material composition data. If negative, the material composition data for Heat Structure CCCCC must be entered on the HSCCCCC2NN records. If a nonnegative integer MMMMM, these data are obtained from the HSMMMMM2NN records for Heat Structure MMMMM, which must exist.
(type = integer, default = none, units = none)

If this record is not present, the data for the material composition of Heat Structure CCCCC must be entered on the HSCCCCC2NN records.

HSCCCCC2NN – Material Composition Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
01 ≤ NN ≤ 99, NN is the sequence number

These records are required if either MCDLOC on Record HSCCCCC200 is negative or Record HSCCCCC200 is omitted. The format is two fields per record until materials in the NP-1 mesh intervals of Heat Structure CCCCC are specified, where NP is given on Record HSCCCCC000.

(1) MATNAM - Name of material in mesh interval N, where N is greater than or equal to 1 and less than NP. This field may be a default material name or a new material name. If it is a new material name, then material property input must be provided. See the Material Properties Package Users' Guide for a list of the default materials and the input which is required to specify a new material. MP gases can not be used here. Any gas must be input as "pseudo-gas" with user definition of appropriate values for density, specific heat capacity, and thermal conductivity.

(type = character*24, default = none)

(2) MSHNUM - Mesh interval, N. If the set of all MSHNUM on these records is ordered, the values of MATNUM for a given value of MSHNUM are applied to all mesh intervals between one greater than the next lower value of MSHNUM and the given value of MSHNUM, inclusive.
(type = integer, default = none, units = none)

Record numbers need not be sequential. However, MSHNUM must be a strictly monotonically increasing function of the NN in HSCCCCC2NN.

HSCCCCC300 – Internal Power Source Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Required

(1) ISRC - Internal power source type. If negative or 0, no internal power source exists for Heat Structure CCCCC. If a positive integer TTT (less than 9000), the power must be entered as a function of time in Tabular Function TTT. For ISRC = 9X...X, the power is given by Control Function X...X, where X...X can have from three to eight digits, including leading zeros. The power obtained from the TF or CF is assumed to be given in watts, W.
(type = integer, default = none, units = none)

(2) NSDLOC - Location of internal power source distribution data. If negative and if ISRC on this record is TTT, the internal power source distribution data for Heat Surface CCCCC must be entered on the HSCCCCC3NN records. If a nonnegative integer MMMMM and if ISRC on this record is positive, these data are found on the HSMMMMM3NN records for Heat Structure MMMMM, which must exist.
(type = integer, default = none, units = none)

(3) VSMULT - Internal source multiplier. This number must be entered if ISRC is TTT. It is the fraction of the power from Tabular Function TTT that is applied to this heat structure.
(type = real, default = none, unites = none)

If ISRC is negative or 0, NSDLOC and VSMULT are ignored and do not need to be entered.

HSCCCCC3NN – Internal Power Source Distribution Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
01 ≤ NN ≤ 99, NN is the sequence number

These records are required if ISRC on Record HSCCCCC300 is positive and NSDLOC on Record HSCCCCC300 is negative. The format is two numbers per record until the relative source distribution data are entered for the NP-1 mesh intervals in Heat Structure CCCCC, where NP is given on Record HSCCCCC000.

(1) QFRCIN - Relative source strength. The source values are relative and can be scaled by any factor. These values will be normalized during input processing and multiplied by the internal source multiplier (VSMULT on Record HSCCCCC300) to provide the fraction of power from the appropriate tabular function that is applied to each mesh interval in Heat Structure CCCCC.
(type = real, default = none, units = none)

(2) MSHNUM - Mesh interval number. If the set of all MSHNUM on these records is ordered, the value of QFRCIN for a given value of MSHNUM is applied to all mesh intervals between one greater than the next lower value of MSHNUM and the given value of MSHNUM, inclusive.
(type = integer, default = none, units = none)

Record numbers need not be sequential. However, MSHNUM must be a strictly monotonically increasing function of the NN in HSCCCCC3NN.

HSCCCCC400 – Left (Inside) Boundary Surface Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Required

(1) IBCL - Boundary condition type. The magnitude of IBCL must be one of the following integers to specify the type of boundary condition that is applied at the left (or inside) boundary surface of Heat Structure CCCCC. If the sign of the flag is negative, mass transfer at this surface is not evaluated.

In the following, XXX (referring to a *Tabular Function*) must consist of exactly three digits, including leading zeros if necessary, while X...X (referring to a *Control Function*) may consist of from three to eight digits, possibly including leading zeros.

= 0 A symmetry (insulated) boundary condition is applied.

= 1 A convective boundary condition is applied with the heat transfer coefficients calculated by the HS package.

= 1XXX A convective boundary condition is applied with the heat transfer coefficients calculated by the HS package. A surface power source, whose power is given as a function of time by Tabular Function XXX, is also applied at this surface. The units of quantities obtained from Tabular Function XXX are assumed to be W.

= 2XXX The temperature of this surface is given as a function of time by Tabular Function XXX. The units of quantities obtained from Tabular Function XXX are assumed to be K.

= 3XXX The heat flux from this surface is given as a function of time by Tabular Function XXX. The units of quantities obtained from Tabular Function XXX are assumed to be W/m^2.

= 4XXX A convective boundary condition is applied with the heat transfer coefficients given as a function of time by Tabular Function XXX. The units of quantities obtained from Tabular Function XXX are assumed to be $W/m^2 \cdot K$.

= 5XXX A convective boundary condition is applied with the heat transfer coefficients given as a function of the surface temperature by Tabular Function XXX. The units of quantities obtained from Tabular Function XXX are assumed to be $W/m^2 \cdot K$.

= 6XXX A convective boundary condition is applied with the heat transfer coefficients specified by Control Function X...X. The units of quantities obtained from Control Function XXX are assumed to be $W/m^2 \cdot K$.

= 7XXX A convective boundary condition is applied with the heat transfer coefficients calculated by the HS package. A surface power source, whose power is given by Control Function X...X, is also applied at this surface. The units of quantities obtained from Control Function X...X are assumed to be W.

= 8XXX The temperature of this surface is specified by Control Function X...X. The units of quantities obtained from Control Function X...X are assumed to be K.

= 9XXX The heat flux from this surface is specified by Control Function X...X. The units of quantities obtained from Control Function X...X are assumed to be W/m^2. (type = integer, default = none, units = none)

For details of the input required for tabular functions, see the Tabular Function Package Users' Guide. If control functions are used to specify boundary conditions with IBCL = 6XXX, 7XXX, 8XXX, or 9XXX, their values must be initialized through their respective CFXXX01 records. For details on control function input, see the Control Function Package Users' Guide.

(2) IBVL - Numerical identifier of boundary volume. This value specifies the control volume which is associated with the left (inside) boundary surface of Heat Structure CCCCC. If this value is negative, no control volume is associated with this surface. All fluid quantities required for the heat transfer coefficient calculations are obtained from the appropriate quantities for the boundary volume specified by this value if it is not negative. It is noted that the control volume and heat structure elevations must be specified so that heat structure clearly is located within the control volume. (type = integer, default = none, units = none)

(3) IFLOWL - Indicator for type of flow over left (inside) boundary surface of Heat Structure CCCCC. This value is used to determine the type of convective heat transfer correlation to be used in evaluating the heat transfer coefficient on this surface, see Section 2.6.1 of the HS Reference Manual.

= 'INT' internal flow
= 'EXT' external flow

No other values are permitted for this field.
(type = character*3, default = none)

(4) CPFPL - Critical pool fraction for pool. This is the minimum value of the pool fraction such that heat transfer to the pool is calculated at the left (inside) boundary surface of Heat Structure CCCCC. It must be between 0.0 and 1.0, inclusive. See discussion below. (type = real, default = none, units = none)

(5) CPFAL - Critical pool fraction for atmosphere. This is the maximum value of the pool fraction such that heat and mass transfer to the atmosphere is calculated at the left (inside) boundary surface of Heat Structure CCCCC. It must be between 0.0 and 1.0, inclusive. See discussion below and also see SC4071 for further restrictions on the bounds.
(type = real, default = CPFPL, units = none)

(6) CTDPL - Critical temperature difference for pool heat transfer. If the temperature difference between the structure surface and the pool exceeds this value, then the timestep may be limited in order to ensure both accuracy in the calculated temperature difference and stability in the pool temperature.
(type = real, default = 100., units = K)

(7) CTDAL - Critical temperature difference for atmosphere heat transfer. This value is used in exactly the same way as CTDPL, except it applies to heat transfer from the structure surface to the atmosphere rather than the pool.
(type = real, default = 100., units = K)

(8) XHTFCL - Calculated atmosphere heat transfer scaling factor. Calculated heat transfer coefficients (IBCL = 1, IBCL = 1XXX or IBCL = 7XXX) to the atmosphere are multiplied by this arbitrary scaling factor, which must be nonnegative.
(type = real, default = 1.0, units = none)

(9) XMTFCL - Mass transfer scaling factor. Mass transfer coefficients (IBCL > 0 and IBVL > 0) for the condensation/evaporation of liquid films are multiplied by this arbitrary scaling factor, which must be nonnegative.
(type = real, default = 1.0, units = none)

Control volume assignment (and therefore mass transfer) for adiabatic or specified temperature boundary conditions (IBCL = 0, 2XXX, or 8XXX) is prohibited. For these conditions, IBCL must be less than or equal to zero and fields 2 through 9 are ignored and do not need to be entered. IBVL must be entered for any other boundary condition type.

Mass transfer to a surface with a specified heat flux boundary condition (IBCL = 3XXX or 9XXX) is also prohibited, although the assignment of a control volume in this case is optional. For this condition, IBCL must be negative and IBVL must be entered.

If no control volume is associated with this surface (IBVL < 0), then the boundary condition type must be adiabatic, specified temperature, or specified heat flux (IBCL = 0, 2XXX, 3XXX, 8XXX, or 9XXX). Furthermore, fields 3 through 9 are ignored and do not need to be entered.

For boundary surfaces with specified or calculated heat transfer coefficients (IBCL = 1, 1XXX, 4XXX, 5XXX, 6XXX, or 7XXX), fields 3 and 4 (IFLOWL and CPFPL) are required, although IFLOWL is not used when heat transfer coefficients are specified through 4XXX, 5XXX, or 6XXX.

If the heat flux at both surfaces is specified (IBCL = 0, 3XXX, or 9XXX and IBCR = 0, 3XXX, or 9XXX), then steady-state initialization must not be requested (ISS on Record HSCCCCC000) because a solution is either impossible or arbitrary.

Careful consideration should be given to the selection of values for CPFPL and CPFAL.

If the values of CPFPL and CPFAL are set equal to the same value, heat transfer will occur to either the pool or atmosphere (but not both at the same time) depending upon the value of the pool fraction for the current time.

If CPFPL exceeds CPFAL, there will be no heat transfer to either pool or atmosphere while the value of the pool fraction is between CPFPL and CPFAL.

If CPFAL exceeds CPFPL, there will be heat transfer to both pool and atmosphere while the pool fraction is between CPFPL and CPFAL.

A non-fatal warning message is printed to the output and diagnostic files if the values of CPFPL and CPFAL are not equal.

Refer to the HS Reference Manual for further discussion of the implications of input values for CPFPL and CPFAL. Similar consideration should be given to the inputs for CPFPR and CPFAR which apply to the right boundary surface on Record HSCCCCC600.

HSCCCCC401 – Left (Inside) Boundary Surface Radiation Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional

Inclusion of this record enables radiation heat transfer for the left surface.

(1) EMISWL - Wall emissivity of the left surface. A value of 0. turns radiation heat transfer off at this surface. The wall emissivity is constant

for the transient except when a water film is present. In this case, the emissivity of the wall is calculated using a mechanistic model for radiation on film-covered surfaces.
(type = real, default = none, units = none)

(2) RMODL - Radiation model employed. Two options are currently available. The "-" in the following parameters can be replaced by a space if the parameter is enclosed in single quotes. Upper and lower case characters are equivalent.

= equiv-band equivalent band model
= gray-gas-a gray gas model
(type = character*10, default = none)

(3) PATHL - Radiation path length for the left surface.
(type = real, default = none, units = m)

All three parameters must be entered if this record is present. If the record is not included in the input, no radiation heat transfer is calculated for this surface. See the HS Reference Manual for details on the radiation models available.

HSCCCCC500 – Additional Left (Inside) Boundary Surface Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.

This record is required for the left (inside) boundary surface of each specified heat structure unless either (a) a symmetry or specified temperature boundary condition is applied at this surface (IBCL on Record HSCCCCC400 is 0, 2XXX, or 8XXX) or (b) no boundary volume is specified for this surface (IBVL on Record HSCCCCC400 is negative). In either case (a) or (b) these variables are not needed for the calculation.

(1) ASURFL - Area of boundary surface. This value is the area of the left (inside) boundary surface of Heat Structure CCCCC. ASURFL must be strictly positive. This field is ignored for cylindrical or (hemi)spherical geometries.

Rectangular geometries: the area of this surface and the right (outside) boundary surface (ASURFR on Record HSCCCCC700) must be equal.

Cylindrical geometries: the area of this surface will be calculated from the location of the left (inside) temperature node (XI on Record HSCCCCC100) and the axial length of this structure (BNDZL on this record).

Spherical or hemispherical geometries: the area of this surface will be calculated from the location of the left (inside) temperature node (XI on Record HSCCCCC100).
(type = real, default = none, units = m^2)

(2) CLNL - Characteristic length of boundary surface. This value is the dimension that is used to calculate quantities such as the Reynolds, Grashof, Nusselt, and Sherwood numbers. CLNL must be strictly positive.
(type = real, default = none, units = m)

(3) BNDZL - Axial length of boundary surface. This value is the dimension of the left (inside) boundary surface of Heat Structure CCCCC in a direction perpendicular to the direction of energy flow within this heat structure. BNDZL must be strictly positive. This field is ignored for spherical or hemispherical geometries.

Rectangular or cylindrical geometries: The axial length of this surface and the right (outside) boundary surface (BNDZR on Record HSCCCCC700) must be equal.

Spherical or hemispherical geometries: The axial length is calculated from the location of the left (inside) temperature node (XI on Record HSCCCCC100).
(type = real, default = none, units = m)

HSCCCCC600 – Right (Outside) Boundary Surface Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Required

The fields on this record (IBCR, IBVR, IFLOWR, CPFPR, CPFAR, CTDPR, CTDAR, XHTFCR and XMTFCR) correspond to the fields on Record HSCCCCC400 but apply to the right (outside) boundary surface of Heat Structure CCCCC rather than the left (inside) boundary surface. One additional option IFLOWR = 'ICE' is allowed.

The **ice condenser model** is activated by specifying IFLOWR = ICE. In this case the heat structure should be a cylindrical structure with an adiabatic inner boundary. The associated gas source that releases liquid water is connected to the CVH control volume specified by IBVR. See record HSDGCCCCC1. IBCR = 1, CPFAR = 0.5, and CPFPR = 0.5 should be used. An example is shown in Section 5.2.

The initial temperature specified on Record HSCCCCC8XX should be 274K. It is recommended that the value of HTRSRC on record HSDGCCCCC1 be adjusted

accordingly to include the sensible heat required to raise the temperature of the subcooled ice through the melting point to 274K, plus the sensible energy required to raise the released water to the steam saturation temperature.

CAUTION !!

The ice condenser model will malfunction if any part of the ice condenser becomes submerged in the melt water pool in the outer boundary CVH volume. The user must provide sufficient volume below the bottom of the ice condenser structure to accommodate all of the melted ice. Also an initial ice temperature below 273.15K will cause problems in the material properties routines.

HSCCCCC601 – Right (Outside) Boundary Surface Radiation Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional

The fields on this record (EMISWR, RMODR, and PATHR) correspond to the fields on Record HSCCCCC401 but apply to the right (outside) boundary surface of Heat Structure CCCCC rather than the left (inside) boundary surface.

HSCCCCC700 – Additional Right (Outside) Boundary Surface Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.

This record is required for the right (outside) boundary surface of each specified heat structure unless either (a) a symmetry boundary condition is applied at this surface (IBCR on Record HSCCCCC600 is 0) or (b) no boundary volume is specified for this surface (IBVR on Record HSCCCCC600 is negative). In either case (a) or (b) these variables are not needed for the calculation.

The fields on this record (ASURFR, CLNR, and BNDZR) correspond to the fields on Record HSCCCCC500 but apply to the right (outside) boundary surface of Heat Structure CCCCC rather than the left (inside) boundary surface. However, in geometries for which the area of this surface is calculated, the location of the right (outside) temperature node is used rather than the location of the left (inside) temperature node).

HSCCCCC800 – Initial Temperature Distribution Location
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
Optional

This record and the following one (HSCCCCC800 and HSCCCCC8NN) should not be present if ISS ≥ 0 on Record HSCCCCC000 because a steady-state calculation will be performed to determine the initial temperature distribution. (A warning

message will appear in the MELGEN diagnostics file if these records appear when ISS ≥ 0.)

(1) NTDLOC - Indicator for location of initial temperature distribution. If negative, the initial temperature distribution for Heat Structure CCCCC must be entered on the HSCCCCC8NN records. If a nonnegative integer MMMMM, these data are found on the HSMMMMM8NN records for Heat Structure MMMMM, which must exist.
(type = integer, default = none, units = none)

HSCCCCC8NN – Initial Temperature Distribution Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the heat structure number.
01 ≤ NN ≤ 99, NN is the sequence number.

These records are required if NTDLOC on Record HSCCCCC800 is negative. The format is two fields per record until temperatures for the NP temperature nodes in Heat Structure CCCCC are specified, where NP is given on Record HSCCCCC000.

(1) TEMPIN - Initial temperature. This temperature must be strictly positive.
(type = real, default = none, units = K)

(2) NODNUM - Temperature node number. If the set of all NODNUM on these records is ordered, the value of TEMPIN for a given value of NODNUM is applied to all temperature nodes between one greater than the next lower value of NODNUM and the given value of NODNUM, inclusive.
(type = integer, default = none, units = none)

Record numbers need not be sequential. However, NODNUM must be a strictly monotonically increasing function of the NN in HSCCCCC8NN.

2.1.2 MELGEN Input for Gas Sources

Input data for gas sources for the HS package degassing model are entered on records with identifiers of the form

HSDGCCCCCN

where

HSDG	indicates that the record is a gas source record
CCCCC	is the numerical indicator for the gas source (00000 – 99999)
N	is the record number

The following input records are required to specify a gas source. Unless otherwise stated, if the field record begins with I through N, it is an integer. Unless otherwise stated, if the field variable begins with A through H or O through Z, it is a real number. A complete set of input records must be supplied for each gas source.

HSDGCCCCC0 – General Gas Source Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the gas source number
Required

(1) ISRCHS - Gas release surface. This value indicates from which heat structure boundary surface gas is released from Source CCCCC. The absolute value of ISRCHS is the number of the heat structure which contains this source. If ISRCHS is negative, gas is released from the left (inside) boundary surface of the heat structure; if positive, gas is released from the right (outside) boundary surface. ISRCHS cannot equal 0 and the absolute value of ISRCHS must be the number of an existing heat structure.
(type = integer, default = none, units = none)

(2) ISDIST - Source distribution. This value is the number of mesh intervals over which Source CCCCC is distributed. ISDIST must be greater than or equal to 1 and less than or equal to the number of mesh intervals in the heat structure which contains this source.
(type = integer, default = none, units = none)

(3) GASNAM - Name of released gas. This is the name of the gas which is released from Source CCCCC. It must be the name of a material that is present in the problem. Valid names are:

POOL	-	Pool liquid water
FOG	-	Atmosphere liquid water
H2O-VAP	-	Atmosphere water vapor
H2	-	Hydrogen
O2	-	Oxygen
CO2	-	Carbon dioxide
CO	-	Carbon monoxide
N2	-	Nitrogen
NO	-	Nitrogen monoxide
N2O	-	Nitrous oxide
NH3	-	Ammonia
C2H2	-	Acetylene
CH4	-	Methane

C2H4	-	Ethylene
GASk	-	User-defined gas (k=A, B, ..., J)
SS	-	Steel

The first three are present in all problems. The others must be specified for the problem through Noncondensible Gas (NCG) input. See the NCG Package Users' Guide for details on input for those gases that must be specified.

The SS material type is intended for use in MELCOR calculations where the COR package is employed to model melting of core boundary steel structures. Molten steel is entered into the outer radial ring of the core region at the corresponding elevation. Subsequent relocation of the steel is modeled by the COR package. If COR is not used, the SS source will be ignored. (type = character*8, default = none)

There are several restrictions concerning the "SS" degassing option. These are listed below:

(1) The structure identified by ISRCHS must have an orientation that is either horizontal (ALPHA = 0.0) or vertical (ALPHA = 1.0) as identified on the corresponding input Record HSCCCCC002. If the structure is not horizontal or vertical, MELGEN processing will terminate.

(2) The structures for which SS degassing is desired must lie either along the core or above the core. If along the core, then a structure must align with one of the COR package axial segments as identified by input record CORRZjj01. Structures are not permitted to span across COR axial segments. If the degassing structure lies above the core, then its lowermost elevation must exceed the uppermost core elevation as modeled by the COR package.

(3) Special restrictions apply to changing "SS" degassing input for MELCOR restarts. See Section 2.2.2.

HSDGCCCCC1 – Gas Source Characterization Data
00000 ≤ CCCCC ≤ 99999, CCCCC is the gas source number
Required

(1) RHOSRC - Density of gas source. This value is the density of Gas Source CCCCC. This density times the volume of the mesh intervals over which it is distributed is the mass of gas that can be released by this source. RHOSRC must be greater than or equal to zero. (type = real, default = none, units = kg/m^3)

(2) HTRSRC - Heat of reaction of gas source. This value is the heat of reaction of Gas Source CCCCC. The volumetric heat capacity is increased by the product of HTRSRC and the density of this source (RHOSRC on this record) divided by the temperature range over which gas is released (TEMPU minus TEMPL on this record) to yield the effective volumetric heat capacity of the material in a mesh interval of a degassing heat structure. HTRSRC must be greater than or equal to zero. (type = real, default = none, units = J/kg)

(3) TEMPL - Lower temperature for degassing. This value is the lower boundary of the temperature range for the release of gas from Gas Source CCCCC. TEMPL must be greater than zero. (type = real, default = none, units = K)

(4) TEMPU - Upper temperature for degassing. This value is the upper boundary of the temperature range for the release of gas from Gas Source CCCCC. TEMPU must be greater than TEMPL on this record. (type = real, default = none, units = K)

The next three variables apply only if an **ice condenser structure** has been defined by inputs on Record HSCCCCC600. See the example in Section 5.2.

(5) HTCICE - Ice condenser Nusselt number multiplier. This value is a multiplier for calculated heat and mass transfer coefficients. (type = real, default = none, units = none)

(6) RNDICE - Ice condenser RN deposition surface area enhancement factor. The surface area used in the RN deposition model is equal to the calculated ice surface area (defined below) plus the value of the original ice surface area multiplied by this enhancement factor. A nonzero value for RNDICE is used to account for heat transfer and radionuclide deposition to the wire baskets normally found in ice condensers that remain in place after the ice has melted. (type = real, default = none, units = none)

(7) EXPICE - Ice condenser surface area exponent. The calculated heat and mass transfer surface area of the ice condenser is given by

$$A_O * \left[RNDICE + (1 - RNDICE) * (V/V_O)^{EXPICE}\right],$$

where A_O is the original surface area of the ice (ASURFR on Record HSCCCCC700), V_O is the original volume of the ice, and V is the current volume of the unmelted ice.
(type = real, default = none, units = none)

The values of HTCICE, RNDICE, and EXPICE should be adjusted to obtain the desired ice condenser performance. The value of EXPICE dictates how surface areas changes with melting. A value of 1.0 implies that the area decreases linearly with the volume and is appropriate for transients that lead to rapid axial melting of the ice columns. A value of 0.5 implies a predominantly radial melt typical of slower transients.

2.1.3 MELGEN Input for the Film-Tracking Model

Input data for the film-tracking model are entered on records with identifiers of the form

HSFTijjkk

where

HSFT	indicates that the record is for the film-tracking model with
i	numerical identifier for heat structure networks
jj	sequence number for each heat structure in the network
kk	sequence number for connected drainage heat structures

The following input records are required to describe a network of heat structures connected for the purposes of film tracking. The film-tracking model automatically calculates the total amount of water that drains off of each heat structure surface in the network, and the user provides destination fractions to determine where that drainage goes. The destination fractions allow the user to divide the total drainage among any or all of three types of drainage destinations:

(1) the surface of one or more heat structures in the same network,

(2) the MELCOR Containment Spray (SPR) package (via a user-defined transfer process, see the TP Package Users' Guide) for treatment as "rain" from the surface (this is appropriate for inverted surfaces off which condensation is more likely to drip than drain, e.g. ceilings) and

(3) the pool component of the CVH control volume associated with the given surface.

There may be more than one network in a problem (e.g., one network in the reactor vessel, one network in the steam generators, one network for containment structures, etc.), but no heat structure should be included in more than one network. The heat structures should be listed from the top down on the HSFTijj00 records in the network description; that is, if heat structure A drains to heat structure B, then heat structure A should be listed first (i.e., have a smaller value of jj in its HSFTijj00 record than the value of jj in the HSFTijj00 record that describes heat structure B). Further more, recirculating drainage is not permitted; that is, heat structure B should not drain to heat structure A, if heat structure A is included in the chain of heat structures that drain to heat structure B. All heat structures that receive film drainage from another heat structure or an external source should be included in the network (even though the bottom-most heat structures do not themselves drain to lower structures). Heat structure surfaces which receive film drainage from other heat structures or external sources must support mass transfer; that is, the values of IBCL and IBVL on Record HSCCCCC400 and/or IBCR and IBVR on Record HSCCCCC600 must be positive if drainage is to be tracked on the left and/or right surface(s) of heat structure CCCCC. Finally, the sum of drainage fractions (FRAINs plus all FDRNs for s = L or s = R) for each surface of a heat structure in the network must not exceed one. If the sum of drainage fractions for a surface is less than one, then the excess drainage will go to the pool of the CVH volume associated with that surface.

HSFTi0000 – Network Size Data
$0 \leq i \leq 9$, i is the network identification number
Required

(1) NUMSTR - Number of heat structures in the network
(type = integer, default = none, units = none)

HSFTijj00 – Network Heat Structure Identification and Source Data
i has the same value as i in record HSFTi0000
$01 \leq jj \leq NUMSTR \leq 99$, jj is a sequencing identifier for these records
Required

These records identify and describe the heat structures contained in the network. The first six fields (IDSTRC, NUMDRN, FRAINL, NTPL, FRAINR and NTPR) described below are required. The last four fields should be entered if an external source of water is to be provided for the left and/or right surface(s) of the heat structure.

(1) IDSTRC - Heat structure number (CCCCC value from HSCCCCCxxx records)
(type = integer, default = none, units = none)

(2) NUMDRN - Number of heat structures this structure drains to
(type = integer, default = none, units = none)

(3) FRAINL - Fraction of the total drainage from the left surface of the heat structure that is transferred to the Spray package as "rain."
(type = real, default = none, units = none)

(4) NTPL - The "in" transfer process number for "rain" transfers to the SPR package from the left surface of the structure (enter 0 if FRAINL = 0.; otherwise, enter a positive integer and enter the appropriate TP and SPR input to effect the transfer—see example in Section 5.3.)
(type = integer, default = none, units = none)

(5) FRAINR - Same as FRAINL except for right surface.
(type = real, default = none, units = none)

(6) NTPR - Same as NTPL except for left surface.
(type = integer, default = none, units = none)

(7) IMSRCL - Mass source rate (kg/s) identifier number for left surface; a positive value indicates the source is obtained from tabular function number IMSRCL, a negative value indicates the source is obtained from control function number -IMSRCL and a value of 0 indicates that there is no source.
(type = integer, default = none, units = none)

(8) IESRCL - Specific enthalpy (J/kg) source identifier number for source associated with IMSRCL; a positive value indicates a tabular function, a negative value indicates a control function and 0 indicates there is no source.
(type = integer, default = none, units = none)

(9) IMSRCR - Same as IMSRCL except for right surface of heat structure CCCCC.
(type = integer, default = none, units = none)

(10) IESRCR - Same as IESRCL except it is associated with IMSRCR.
(type = integer, default = none, units = none)

HSFTijjkk – Data for Drainage Heat Structures
i has the same value as i in HSFTi0000
jj has the same value as jj in HSFTijj00
$01 \leq kk \leq NUMDRN \leq 99$, kk is a sequence number for these records
Required if NUMDRN on record HSFTijj00 is positive
Must have NUMDRN of these records

These records identify and describe the heat structures that receive film drainage from heat structure IDSTRC on corresponding HSFTijj00 record.

(1) IDSDRN - The heat structure number (CCCCC value from HSCCCCCxxx records) of the structure receiving the film drainage.
(type = integer, default = none, units = none)

(2) FDRNL - The fraction of the total film drainage from the left surface of heat structure IDSTRC that goes to the left surface of heat structure IDSDRN.
(type = real, default = none, units = none)

(3) FDRNR - Same as FDRNL except applies to right surface of heat structures.
(type = real, default = none, units = none)

2.1.4 MELCOR Input for Structure-to-Structure Radiation

Input data for the structure-to-structure radiation model are input on records of the form HSRDCCCCC0, where CCCCC is a user-defined five digit integer for a given pair of surfaces. Each surface pair must be unique in that the surfaces associated with one pair must not be associated with another. The number of allowable surface pairs is not restricted and is limited only by the amount of computer storage available to the database.

The following record defines the input data required.

HSRDCCCCC0 – Structure-to-Structure Radiation
Optional

(1) IHSRD1 - Heat structure number for the first surface of the pair. A left side surface is identified by the use of a negative structure number while a right side surface is identified by a positive structure number.
(type = integer, default = none, units = none)

(2) IHSRD2 - Heat structure number for the second surface of the pair. The left and right side conventions are the same as above for surface 1.
(type = integer, default = none, units = none)

(3) VIEW - View factor between surface 1 and surface 2.
(type = integer, default = none, units = none)

(4) ICFRD1 - Optional real-valued control function index whose value is the emissivity of surface 1.
(type = integer, default = 0 (see below), uints = none)

(5) ICFRD2 - Optional real-valued control function index whose value is the emissivity of surface 2.
(type = integer, default = 0 (see below), units = none)

The input of 0 or blank for the control function indices specifies the default use of COR Package Reference Manual relation (Equation. 2.10) for determining the emissivity as a function of temperature.

The user should note that use of this model is restricted to the surfaces of structures for which the boundary condition flags (IBCL – input Record HSCCCCC400 and IBCR – Record HSCCCCC600) do not specify either temperature or heat flux. Thus, the options 0, 2XXX, 3XXX, 8XXX, or 9XXX are not permitted for IBCL or IBCR. All other options are permitted.

If the use of control functions is employed, the emissivity is bounded between 0.0 and 1.0, inclusive, prior to its use in determining the radiative exchange. The radiative exchange is zeroed if either of the surface emissivities is zero, if the input view factor is zero, or if either of the surfaces of the pair is covered by a water pool in its adjacent CVH volume.

2.2 MELCOR User Input

This section discusses MELCOR user input for the HS package. All HS package input records are optional for MELCOR execution. Input records are supplied for MELCOR execution only to make permitted changes to the existing data base for the HS package. MELCOR input and these changes are discussed as follows:

Section 2.2.1	Heat Structure input records
Section 2.2.2	Gas Source input records
Section 2.2.3	Film-Tracking input records
Section 2.2.4	MELCOR Input for Structure-to-Structure Radiation

2.2.1 MELCOR Input for Heat Structures

All HS package input records (except for structure-to-structure radiation) are optional for MELCOR execution. Input records for heat structures are supplied for MELCOR execution

only to make changes to time-independent data or temperature distributions on a restart. Any change to the data for a given heat structure is permitted except one which changes the geometry or involves changes in the number of temperature nodes for this heat structure. At present a heat structure may not be added or deleted on a restart. All changes will be propagated through subsequent restarts unless rescinded by their input records.

The following items pertaining to input processing by the HS package during a restart are important and must be conformed to by all MELCOR input for heat structures:

(1) Although a complete set of records does not need to be supplied for each heat structure with data changes during MELCOR execution, each included record must be complete as described in Section 2.1.1. Thus, all fields on a record preceding and following the field which contains the datum to be changed must be present.

One exception to this is modifying the boundary conditions for a heat structure on a restart. If it is desired to change any of the fields on **either** the HSCCCCC400 (401) or HSCCCCC600 (601) boundary surface data records on a restart, then **both** the HSCCCCC400 (401) and HSCCCCC600 (601) records for that heat structure must be included in the MELCOR input.

(2) All fields on each record must conform to the criteria or restrictions as described in Section 2.1.1.

(3) All data location indicators which are described in Section 2.1.1 will be interpreted by the HS package input processor during MELCOR execution as applying to data for Heat Structure MMMMM rather than to data on HSMMMMMXNN records. Therefore, one should provide records containing the new data for Heat Structure CCCCC if the corresponding data will be changed for Heat Structure MMMMM, since the executive input processor sorts records and the desired changes will not be made if CCCCC is less than MMMMM. To be safe, it is recommended that output from MELCOR restarts be examined after a very short test run to ensure that all user changes were correctly processed.

2.2.2 MELCOR Input for Gas Sources

All HS package gas source input records are optional for MELCOR execution. Input records for gas sources are supplied for MELCOR execution only to make changes to time-independent data on a restart. Any change to the data for a given gas source is permitted. At present a gas source may not be added or deleted on a restart. Gas Source CCCCC may be made effectively inactive on a restart by setting its source density (RHOSRC on Record HSDGCCCCC1) to zero. All changes will be propagated through subsequent restarts unless rescinded by their input records.

The following items pertaining to input processing by the HS package during a restart are important and must be conformed to by all MELCOR input for gas sources:

(1) Although a complete set of records does not need to be supplied for each gas source with data changes during MELCOR execution, each included record must be complete as described in Section 2.1.2. Thus, all fields on a record preceding and following the field which contains the datum to be changed must be present.

(2) All fields on each record must conform to the criteria or restrictions as described in Section 2.1.2.

(3) The ISRCHS, ISDIST, and GASNAM input data as identified by input record HSDGCCCCC0 are not permitted to change for "SS" degassing sources.

2.2.3 MELCOR Film-Tracking Model Input

All HS package film-tracking model input records are optional for MELCOR execution. Input records for the film-tracking model are supplied for MELCOR execution only to make changes to time-independent data on a restart. The only data that may be changed are values of FRAINL, NTPL, FRAINR, NTPR, IMSRCL, IESRCL, IMSRCR, IESRCR, FDRNL and FDRNR. Networks and the heat structures included in them may not be added or deleted. Restart changes are primarily provided to alter drainage patterns. The value of NUMSTR specified on record HSFTi0000 for a restart should be equal to the number of heat structures in network i which are to be modified. Similarly, the value of NUMDRN on record HSFTijj00 should be equal to the number of drainage heat structures which are to have their values of FDRNL and/or FDRNR modified.

2.2.4 MELCOR Input Controlling Structure-to-Structure Radiation

Although no MELCOR input is allowed for the structure-to-structure radiation model, the model may be effectively turned on and off for individual radiation pairs by using the control function method of specifying surface emissivities (ICFRD1 and ICFRD2) on MELGEN input records HSRDCCCCC0. For periods during a MELCOR calculation when the calculation of radiation is not desired (between given surfaces previously active in the radiation model), the user can structure the control function such that a zero emissivity (and thus zero radiation heat transfer) is produced. Because control function input is allowed upon MELCOR restarts, this method allows user control of the radiation model during all parts of the MELCOR calculation.

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the the MELCOR EXEC Users' Guide.

3.1 HS Sensitivity Coefficients

The sensitivity coefficients for the Heat Structure package have identifier numbers between 4000 and 4299. These are reserved as follows:

4000 – 4049:	Analytic Functions
4050 – 4059:	Iteration Parameters
4060 – 4079	Parameter Ranges for Atmosphere Heat Transfer
4080 – 4099:	Parameter Ranges for Pool Heat Transfer
4100 – 4149:	Atmosphere Heat Transfer Correlations
4150 – 4199:	Pool Heat Transfer Correlations
4200 – 4249:	Mass Transfer Parameters and Correlations
4250 – 4299:	Liquid Film Parameters and Correlations

This section describes the sensitivity coefficients that are presently used in the HS package and gives their default values, units, and EQUIVALENCE names. See the MELCOR/MELGEN Executive Package Users' Guide for details on the use of Sensitivity Coefficient records.

Warning!!

In the present version of the MELCOR Code System, no error testing of the new value of a sensitivity coefficient in the HS package is performed. Therefore, the user is warned that the indiscriminate change of a coefficient may result in nonphysical results or an aborted calculation.

4000 – Surface Tension

The surface tension of water, σ, is given as a function of temperature by:

$$\sigma(T) = C4000(1)x[C4000(2) + C4000(3)xT_R]xT_R^{C4000(4)} + C4000(5)$$

where

$\sigma(T)$ = surface tension, N/m

T = temperature, K

T_R = C4000(6) – T/C4000(7)

C4000(1) - constant coefficient
(default = 0.2358, units = N/m, equiv = none)

C4000(2) - additive constant
(default = 1.0, units = none, equiv = none)

C4000(3) - constant coefficient
(default = -0.625, units = $1/K^{-1}$, equiv = none)

C4000(4) - constant coefficient
(default = 1.256, units = none, equiv = none)

C4000(5) - additive constant
(default = 0.0, units = N/m, equiv = none)

C4000(6) - additive constant
(default = 1.0, units = none, equiv = none)

C4000(7) - critical temperature for water
(default = 647.3, units = K, equiv = none)

4051 – Steady-State Iteration Parameters

These coefficients are iteration parameters which are used for steady-state heat conduction calculations.

C4051(1) - maximum number of permitted steady-state iterations
(default = 400, units = none, equiv = XITMXS)

C4051(2) - desired relative error tolerance for steady-state calculations; iterations will be performed until the relative error in the temperature profile is less than this value or until XITMXS iterations have been performed (see C4051(5) below).
(default = 1.0×10^{-5}, units = none, equiv = ERRSS)

C4051(3) - initial steady-state timestep
(default = 1.0×10^{5}, units = s, equiv = DTSS)

C4051(4) - maximum relative error tolerance for film mass
(default = 1.0×10^{-2}, units = none, equiv = ERFSS)

C4051(5) - maximum relative error tolerance for steady-state calculations; failure will be declared if the relative error in the temperature profile exceeds this value after XITMXS iterations (default = 1.0×10^{-2}, units = none, equiv = ERDIES)

4052 – Steady-State Iteration Weight Parameters

These coefficients are iteration weight parameters which are used for steady-state heat conduction calculations to mitigate nonconvergence by oscillation. Refer to Section 3.1 of the HS Reference Manual for details on the use of steady-state iteration parameters.

4052(1) - steady-state boiling heat transfer coefficient weight (default = 0.0, units = none, equiv = WTBSST)

4052(2) - error tolerance for steady-state boiling heat transfer coefficient (default = 0.05, units = none, equiv = ERBSST)

4055 – Transient Iteration Parameters

These coefficients are iteration parameters which are used for transient conduction calculations.

C4055(1) - maximum number of permitted transient iterations (default = 30, units = none, equiv = XITMAX)

C4055(2) - desired relative error tolerance for transient conduction calculations; NOTE: the conduction calculation is declared converged when the maximum relative error in the temperature profile within the structure is less than this value, normally. However, if degassing or mass transfer (condensation/ evaporation) is occurring, then the iteration continues until the maximum relative error in the temperature profile (including the film surfaces) is less than the value specified by C4055(6) described below. If the relative error is still larger than C4055(6) but smaller than C4055(2) after XITMAX iterations, then the solution is accepted as converged (see C4055(8) below). (default = 5.0×10^{-4}, units = none, equiv = ERRTRN)

C4055(3) - minimum number of iterations to limit timestep (default = 31, units = none, equiv = XITCUT)

C4055(4) - minimum relative error tolerance for material property determination
(default = 0.01, units = none, equiv = RETMIN)

C4055(5) - matrix solver precision limit
(default = 1.0×10^{-10}, units = none, equiv = EPSILL)

C4055(6) - override value for ERRTRN during degassing/mass transfer—see the NOTE for C4055(2) above
(default = 5.0×10^{-6}, units = none, equiv = ERRSML)

C4055(7) - maximum relative error tolerance for film mass
(default = 1.0×10^{-2} units = none, equiv = ERFTRN)

C4055(8) - maximum relative error tolerance for transient calculations; failure will be declared and a request made to repeat the cycle with a smaller timestep if the relative error in the temperature profile exceeds this value after XITMAX iterations
(default = 5.0×10^{-3}, units = none, equiv = ERDIET)

4056 – Transient Iteration Weight Parameters

These coefficients are iteration weight parameters which are used for transient heat conduction calculations to mitigate nonconvergence by oscillation. Refer to Section 3.1 of the HS Reference Manual for details on the use of transient iteration parameters.

C4056(1) - transient boiling heat transfer coefficient weight
(default = 0.9, units = none, equiv = WTBTRN)

C4056(2) - error tolerance for transient boiling heat transfer coefficient
(default = 0.05, units = none, equiv = ERBTRN)

4060 – Atmosphere Natural and Forced Convection Ranges

These coefficients define the limits of natural and forced convection heat transfer to the atmosphere. In general, a mixed convection regime is also considered, and the convection heat transfer to the atmosphere is determined by the following criteria:

Natural Convection if $Re^2 <$ C4060(1)xGr
Forced Convection if $Re^2 >$ C4060(2)xGr
Mixed Convection if C4060(1)x$Gr \leq Re^2 \leq$ C4060(2)xGr

where

Re = Reynolds number for atmosphere

Gr = Grashof number for atmosphere

However, if C4060(1) < 0 or C4060(2) ≤ C4060(1), convection heat transfer to the atmosphere is assumed to be given by the greater of the values defined by the natural and forced convection correlations.

C4060(1) - constant coefficient
(default = 1.0, units = none, equiv = none)

C4060(2) - constant coefficient
(default = 10.0, units = none, equiv = none)

4061-4063 – Atmosphere Laminar and Turbulent Natural Convection Ranges

These coefficients define the limits of laminar and turbulent natural convection heat transfer to the atmosphere. In general, a transition regime is also considered, and the natural convection heat transfer to the atmosphere is determined by the following criteria:

Laminar if Ra < C406m(1)
Turbulent if Ra > C406m(2)
Transition if C406m(1) ≤ Ra ≤ C406m(2)

where

Ra = Rayleigh number for atmosphere

m = 1 for rectangular geometries

= 2 for cylindrical geometries

= 3 for spherical or hemispherical geometries

However, if C406m(1) < 0 or C406m(2) ≤ C406m(1), natural convection heat transfer to the atmosphere is assumed to be given by the greater of the values defined by the laminar and turbulent natural convection correlations.

<u>Rectangular</u>
C4061(1) - Rayleigh number upper limit for atmosphere laminar natural convection
(default = 10^9, units = none, equiv = none)

C4061(2) - Rayleigh number lower limit for atmosphere turbulent natural convection
(default = 10^{10}, units = none, equiv = none)

Cylindrical

C4062(1) - Rayleigh number upper limit for atmosphere laminar natural convection
(default = 10^{9}, units = none, equiv = none)

C4062(2) - Rayleigh number lower limit for atmosphere turbulent natural convection
(default = 10^{10}, units = none, equiv = none)

(Hemi)spherical

C4063(1) - Rayleigh number upper limit for atmosphere laminar natural convection
(default = 10^{9}, units = none, equiv = none)

C4063(2) - Rayleigh number lower limit for atmosphere turbulent natural convection
(default = 10^{10}, units = none, equiv = none)

4064-4066 – Atmosphere Laminar and Turbulent Forced Convection Ranges

These coefficients define the limits of laminar and turbulent forced convection heat transfer to the atmosphere. In general, a transition regime is also considered, and the forced convection heat transfer to the atmosphere is determined by the following criteria:

Laminar if Re < C406m(1)
Turbulent if Re > C406m(2)
Transition if C406m(1) ≤ Re ≤ C406m(2)

where

m = 4 for rectangular geometries

= 5 for cylindrical geometries

= 6 for spherical or hemispherical geometries

However, if C406m(1) < 0 or C406m(2) ≤ C406m(1), forced convection heat transfer to the atmosphere is assumed to be given by the greater of the values defined by the laminar and turbulent forced convection correlations.

Rectangular

C4064(1) - Reynolds number upper limit for atmosphere laminar forced convection
(default = $3x10^5$, units = none, equiv = none)

C4064(2) - Reynolds number lower limit for atmosphere turbulent forced convection
(default = $6x10^5$, units = none, equiv = none)

Cylindrical

C4065(1) - Reynolds number upper limit for atmosphere laminar forced convection
(default = 2000, units = none, equiv = none)

C4065(2) - Reynolds number lower limit for atmosphere turbulent forced convection
(default = 10^4, units = none, equiv = none)

(Hemi)spherical

C4066(1) - Reynolds number upper limit for atmosphere laminar forced convection
(default = 2000, units = none, equiv = none)

C4066(2) - Reynolds number lower limit for atmosphere turbulent forced convection
(default = 10^4, units = none, equiv = none)

4071 – Bounds on Critical Pool Fractions

As described in Section 2.4 of the Heat Structures Package Reference Manual, heat transfer from a heat structure surface to the pool and/or atmosphere of an adjacent control volume is controlled by user input critical pool fractions on the HSCCCCC400 and HSCCCCC600 input records. These sensitivity coefficients impose bounds on the user-input values, to prevent transfer of heat to insignificant fluid masses.

C4071(1) - Lower bound imposed on input values of CPFPL and CFFPR
(default = 0.02, units = none, equiv = none)

C4071(2) - Upper bound imposed on input values of CPFAL and CFPAR

(default = 0.98, units = none, equiv = none)

4080 – Pool Natural and Forced Convection Ranges

These coefficients define the limits of natural and forced convection heat transfer to the pool. In general, a mixed convection regime is also considered, and the convection heat transfer to the pool is determined by the following criteria:

Natural Convection if $Re^2 < C4080(1) \times Gr$
Forced Convection if $Re^2 > C4080(2) \times Gr$
Mixed Convection if $C4080(1) \times Gr \leq Re^2 \leq C4080(2) \times Gr$

where

Re = Reynolds number for pool

Gr = Grashof number for pool

However, if C4080(1) < 0 or C4080(2) ≤ C4080(1), convection heat transfer to the pool is assumed to be given by the greater of the values defined by the natural and forced convection correlations.

C4080(1) - constant coefficient
(default = 1.0, units = none, equiv = none)

C4080(2) - constant coefficient
(default = 10.0, units = none, equiv = none)

4081 – 4083 – Pool Laminar and Turbulent Natural Convection Ranges

These coefficients define the limits of laminar and turbulent natural convection heat transfer to the pool. In general, a transition regime is also considered, and the natural convection heat transfer to the pool is determined by the following criteria:

Laminar if *Ra* < C408m(1)
Turbulent if *Ra* > C408m(2)
Transition if C408m(1) ≤ *Ra* ≤ C408m(2)

where

Ra = Rayleigh number for pool

m = 1 for rectangular geometries

= 2 for cylindrical geometries

= 3 for spherical or hemispherical geometries

However, if C408m(1) < 0 or C408m(2) ≤ C408m(1), natural convection heat transfer to the pool is assumed to be given by the greater of the values defined by the laminar and turbulent natural convection correlations.

Rectangular

C4081(1) - Rayleigh number upper limit for pool laminar natural convection (default = 10^9, units = none, equiv = none)

C4081(2) - Rayleigh number lower limit for pool turbulent natural convection (default = 10^{10}, units = none, equiv = none)

Cylindrical

C4082(1) - Rayleigh number upper limit for pool laminar natural convection (default = 10^9, units = none, equiv = none)

C4082(2) - Rayleigh number lower limit for pool turbulent natural convection (default = 10^{10}, units = none, equiv = none)

(Hemi)spherical

C4083(1) - Rayleigh number upper limit for pool laminar natural convection (default = 10^9, units = none, equiv = none)

C4083(2) - Rayleigh number lower limit for pool turbulent natural convection (default = 10^{10}, units = none, equiv = none)

4084-4086 – Pool Laminar and Turbulent Forced Convection Ranges

These coefficients define the limits of laminar and turbulent forced convection heat transfer to the pool. In general, a transition regime is also considered, and the forced convection heat transfer to the pool is determined by the following criteria:

Laminar if Re < C408m(1)
Turbulent if Re > C408m(2)
Transition if C408m(1) ≤ Re ≤ C408m(2)

where

m = 4 for rectangular geometries

= 5 for cylindrical geometries

= 6 for spherical or hemispherical geometries

However, if C408m(1) < 0 or C408m(2) ≤ C408m(1), forced convection heat transfer to the pool is assumed to be given by the greater of the values defined by the laminar and turbulent forced convection correlations.

Rectangular

C4084(1) - Reynolds number upper limit for pool laminar forced convection (default = 3×10^5, units = none, equiv = none)

C4084(2) - Reynolds number lower limit for pool turbulent forced convection (default = 6×10^5, units = none, equiv = none)

Cylindrical

C4085(1) - Reynolds number upper limit for pool laminar forced convection (default = 2000, units = none, equiv = none)

C4085(2) - Reynolds number lower limit for pool turbulent forced convection (default = 10^4, units = none, equiv = none)

(Hemi)spherical

C4086(1) - Reynolds number upper limit for pool laminar forced convection (default = 2000, units = none, equiv = none)

C4086(2) - Reynolds number lower limit for pool turbulent forced convection (default = 10^4,units = none, equiv = none)

4101-4112 – Atmosphere Natural Convection

The atmosphere natural convection heat transfer correlations have the following form:

$$Nu = C41mm(1) \times Ra^{C41mm(2)} + C41mm(3)$$

where

Nu = Nusselt number

Ra = Rayleigh number

mm = 01 (04) for laminar (turbulent) correlations for rectangular geometries in internal flow

= 02 (05) for laminar (turbulent) correlations for cylindrical geometries in internal flow

= 03 (06) for laminar (turbulent) correlations for spherical or hemispherical geometries in internal flow

= 07 (10) for laminar (turbulent) correlations for rectangular geometries in external flow

= 08 (11) for laminar (turbulent) correlations for cylindrical geometries in external flow

= 09 (12) for laminar (turbulent) correlations for spherical or hemispherical geometries in external flow

The default values of the coefficients for the atmosphere natural convection heat transfer correlations are summarized in Table 3.1. All are dimensionless and have no assigned EQUIVALENCE names.

Table 3.1 Default Values for Sensitivity Coefficients 4101 – 4124

Atmosphere Related					
Array	Type of Flow	1	2	3	4
C4101	L,I,R,NC	0.046	1/3	0	-
C4102	L,I,C,NC	0.046	1/3	0	-
C4103	L,I,S,NC	0.228	0.226	0	-
C4104	T,I,R,NC	0.046	1/3	0	-
C4105	T,I,C,NC	0.046	1/3	0	-
C4106	T,I,S,NC	0.228	0.226	0	-
C4107	L,E,R,NC	0.59	0.25	0	-
C4108	L,E,C,NC	0.59	0.25	0	-
C4109	L,E,S,NC	0.43	0.25	2.0	-
C4110	T,E,R,NC	0.10	1/3	0	-
C4111	T,E,C,NC	0.10	1/3	0	-
C4112	T,E,S,NC	0.43	0.25	2.0	-
C4113	L,I,R,FC	8.235	0	0	0
C4114	L,I,C,FC	48/11	0	0	0
C4115	L,I,S,FC	48/11	0	0	0
C4116	T,I,R,FC	0.023	0.8	1/3	0
C4117	T,I,C,FC	0.023	0.8	1/3	0
C4118	T,I,S,FC	0.023	0.8	1/3	0

Atmosphere Related					
Array	Type of Flow	1	2	3	4
C4119	L,E,R,FC	0.664	0.5	1/3	0
C4120	L,E,C,FC	0.664	0.5	1/3	0
C4121	L,E,S,FC	0.60	0.5	1/3	2.0
C4122	T,E,R,FC	0.037	0.8	1/3	0
C4123	T,E,C,FC	0.037	0.8	1/3	0
C4124	T,E,S,FC	0.60	0.5	1/3	2.0

L=Laminar, T=Turbulent, I=Internal, E=External, R=Rectangular, C=Cylindrical, S=(Hemi)spherical, NC=Natural Convection, FC=Forced Convection

4113-4124 – Atmosphere Forced Convection

The atmosphere forced convection heat transfer correlations have the following form:

$$Nu = C41mm(1) x \mathrm{Re}^{C41mm(2)} x \mathrm{Pr}^{C41mm(3)} + C41mm(4)$$

where

Nu = Nusselt number

Re = Reynolds number

Pr = Prandtl number

mm = 13 (16) for laminar (turbulent) correlations for rectangular geometries in internal flow

= 14 (17) for laminar (turbulent) correlations for cylindrical geometries in internal flow

= 15 (18) for laminar (turbulent) correlations for spherical or hemispherical geometries in internal flow

= 19 (22) for laminar (turbulent) correlations for rectangular geometries in external flow

= 20 (23) for laminar (turbulent) correlations for cylindrical geometries in external flow

= 21 (24) for laminar (turbulent) correlations for spherical or hemispherical geometries in external flow

The default values of the coefficients for the atmosphere forced convection heat transfer correlations are summarized in Table 3.1. All are dimensionless and have no assigned EQUIVALENCE names.

4151-4162 – Pool Natural Convection

The pool natural convection heat transfer correlations have the following form:

$$Nu = C41mm(1)xRa^{C41mm(2)} + C41mm(3)$$

where

Nu = Nusselt number

Ra = Rayleigh number

mm = 51 (54) for laminar (turbulent) correlations for rectangular geometries in internal flow

= 52 (55) for laminar (turbulent) correlations for cylindrical geometries in internal flow

= 53 (56) for laminar (turbulent) correlations for spherical or hemispherical geometries in internal flow

= 57 (60) for laminar (turbulent) correlations for rectangular geometries in external flow

= 58 (61) for laminar (turbulent) correlations for cylindrical geometries in external flow

= 59 (62) for laminar (turbulent) correlations for spherical or hemispherical geometries in external flow

The default values of the coefficients for the pool natural convection heat transfer correlations are summarized in Table 3.2. All are dimensionless and have no assigned EQUIVALENCE names.

Table 3.2 Default Values for Sensitivity Coefficients 4151 – 4174

Pool Related					
Array	Type of Flow	1	2	3	4

Pool Related					
Array	Type of Flow	1	2	3	4
C4151	L,I,R,NC	0.046	1/3	0	-
C4152	L,I,C,NC	0.046	1/3	0	-
C4153	L,I,S,NC	0.228	0.226	0	-
C4154	T,I,R,NC	0.046	1/3	0	-
C4155	T,I,C,NC	0.046	1/3	0	-
C4156	T,I,S,NC	0.228	0.226	0	-
C4157	L,E,R,NC	0.59	0.25	0	-
C4158	L,E,C,NC	0.59	0.25	0	-
C4159	L,E,S,NC	0.43	0.25	2.0	-
C4160	T,E,R,NC	0.10	1/3	0	-
C4161	T,E,C,NC	0.10	1/3	0	-
C4162	T,E,S,NC	0.43	0.25	2.0	-
C4163	L,I,R,FC	8.235	0	0	0
C4164	L,I,C,FC	48/11	0	0	0
C4165	L,I,S,FC	48/11	0	0	0
C4166	T,I,R,FC	0.023	0.8	1/3	0
C4167	T,I,C,FC	0.023	0.8	1/3	0
C4168	T,I,S,FC	0.023	0.8	1/3	0
C4169	L,E,R,FC	0.664	0.5	1/3	0
C4170	L,E,C,FC	0.664	0.5	1/3	0
C4171	L,E,S,FC	0.60	0.5	1/3	2.0
C4172	T,E,R,FC	0.037	0.8	1/3	0
C4173	T,E,C,FC	0.037	0.8	1/3	0
C4174	T,E,S,FC	0.60	0.5	1/3	2.0

L=Laminar, T=Turbulent, I=Internal, E=External, R=Rectangular, C=Cylindrical, S=(Hemi)spherical, NC=Natural Convection, FC=Forced Convection

4163-4174 – Pool Forced Convection

The pool forced convection heat transfer correlations have the following form:

$$Nu = C41mm(1) x \mathrm{Re}^{C41mm(2)} x \mathrm{Pr}^{C41mm(3)} + C41mm(4)$$

where

Nu = Nusselt number

Re = Reynolds number

Pr = Prandtl number

mm = 63 (66) for laminar (turbulent) correlations for rectangular geometries in internal flow

= 64 (67) for laminar (turbulent) correlations for cylindrical geometries in internal flow

= 65 (68) for laminar (turbulent) correlations for spherical or hemispherical geometries in internal flow

= 69 (72) for laminar (turbulent) correlations for rectangular geometries in external flow

= 70 (73) for laminar (turbulent) correlations for cylindrical geometries in external flow

= 71 (74) for laminar (turbulent) correlations for spherical or hemispherical geometries in external flow

The default values of the coefficients for the pool forced convection heat transfer correlations are summarized in Table 3.2. All are dimensionless and have no assigned EQUIVALENCE names.

4180 – Nucleate Boiling Heat Flux

The nucleate boiling heat flux is obtained through the Rohsenow relation,

$$\left[\frac{C_{pl}(T_{surf}-T_{sat})}{h_{fg}}\right] = C4180(1)x\,\mathrm{Pr}^{C4180(3)}\,x\left[\frac{q''_{NB}}{\mu h_{fg}}\left\{\frac{\sigma}{g(\rho_l-\rho_v)}\right\}^{1/2}\right]^{C4180(4)}$$

where

q''_{NB} = nucleate boiling heat flux, W/m^2

c_{pl} = heat capacity of liquid at T_{sat}, J/kg • K

T_{surf} = temperature of surface, K

T_{sat} = saturation temperature in boundary volume, K

h_{fg} = latent heat in boundary volume of this surface, J/kg

Pr = Prandtl number of liquid in boundary volume

μ = dynamic viscosity of liquid at T_{avg}, kg/m • s

T_{avg} = $(T_{surf} + T_{sat})/2$, K

σ = surface tension at T_{avg}, N/m

g = acceleration of gravity, m/s^2

ρ_l = density of liquid at T_{sat}, kg/m^3

ρ_v = density of vapor at T_{sat}, kg/m^3

C4180(1) - constant determined empirically for different surfaces and fluids (default = 0.013, units = none, equiv = none)

C4180(2) - unused

C4180(3) - Prandtl number exponent (default = 1.0, units = none, equiv = none)

C4180(4) - exponent (default = 0.33, units = none, equiv = none)

4181 – Critical Heat Flux

The critical heat flux is given by Zuber as

$$q_c'' = C4181(1) x \rho_v h_{fg} \left[\sigma(\rho_l - \rho_v) g / \rho_v^2\right]^{C4181(2)} x \left[\rho_l / (\rho_l + \rho_v)\right]^{C4181(3)}$$

where

q_c'' = critical heat flux, W/m^2

ρ_v = density of vapor at T_{sat}, kg/m^3

ρ_l = density of liquid at T_{sat}, kg/m^3

h_{fg} = latent heat in boundary volume, J/kg

g = acceleration of gravity, m/s^2

σ = surface tension at T_{avg}, N/m

T_{avg} = $(T_{surf} + T_{sat}) / 2$, K

T_{sat} = saturation temperature in boundary volume, K

T_{surf} = temperature of this surface, K

C4181(1) - constant coefficient
(default = 0.18, units = none, equiv = none)

C4181(2) - exponent
(default = 0.25, units = none, equiv = none)

C4181(3) - exponent
(default = 0.5, units = none, equiv = none)

4182 – Minimum Film Boiling Heat Flux

The minimum film boiling heat flux is given by Zuber as

$$q''_{mfilm} = C4182(1)\rho_v h_{fg}\left[\sigma(\rho_l - \rho_v)g / \rho_l^2\right]^{C4182(2)} x\left[\rho_l(\rho_l + \rho_v)\right]^{C4182(3)}$$

where

q''_{mfilm} = minimum film boiling heat flux, W/m^2

C4182(1) - constant coefficient
(default = 0.09, units = none, equiv = none)

C4182(2) - exponent
(default = 0.25, units = none, equiv = none)

C4182(3) - exponent
(default = 0.5, units = none, equiv = none)

4183 – Film Boiling Heat Flux

The film boiling heat flux is given by Bromley as

$$q''_{film} = C4183(1)x\left[\rho_v(\rho_l - \rho_v)g\,k_v^3\left(h_{fg} + \frac{1}{2}c_{pv}\Delta T\right)/\mu_v L_c\right]^{C4183(2)} x\Delta T^{C4183(3)}$$

where

q''_{film} = film boiling heat flux, W/m^2

L_c = characteristic length of this surface, m

ΔT = $T_{surf} - T_{sat}$, K

T_{surf} = temperature of this surface, K

T_{sat} = saturation temperature in boundary volume, K

g = acceleration due to gravity, m/s^2

h_{fg} = latent heat in boundary volume, J/kg

ρ_l = density of liquid at T_{sat}, kg/m^3

ρ_v = density of vapor at T_{sat}, kg/m^3

c_{pv} = heat capacity of vapor at T_{sat}, J/kg • K

T_{avg} = (T_{surf} + T_{sat}) / 2, K

μ_v = dynamic viscosity of vapor at T_{avg}, kg/m • s

k_v = thermal conductivity of vapor at T_{avg}, W/m • K

C4183(1) - constant coefficient
(default = 0.943, units = none, equiv = none)

C4183(2) - exponent
(default = 0.25, units = none, equiv = none)

C4183(3) - exponent
(default = 0.75, units = none, equiv = none)

4184 – Radiation to Pool Heat Flux (Plane Model)

The radiation to pool heat flux is given by

$$q''_{rad} = C4184(1) x \sigma \left(T^4_{surf} - T^4_{pool} \right)$$

where

q''_{rad} = radiation to pool heat flux, W/m^2

T_{surf} = temperature of surface, K

T_{pool} = temperature of pool in boundary volume, K

σ = Stefan-Boltzmann constant, 5.669×10^{-8} $W/m^2 \cdot K^4$

C4184(1) - constant coefficient
(default = 1.0, units = none, equiv = none)

4200 – Mass Transfer Flux Model Transition Parameter

The condensation/evaporation mass flux is not limited by the presence of noncondensible gases if the ratio of the steam partial pressure to the total pressure in the bulk atmosphere exceeds this parameter.

C4200(1) - ratio of steam partial pressure to total pressure in bulk atmosphere
(default = 0.9995, units = none, equiv = VPFRAC)

4201 – Sherwood Number for Diffusion Mass Transfer

A Sherwood Number Correlation is used to calculate a diffusion mass transfer coefficient. The correlation has the following form:

$$Sh = C4201(1) x Nu^{C4201(2)} x Sc^{C4201(3)} x \mathrm{Pr}^{C4201(4)}$$

where

Nu = Nusselt number

Sc = Schmidt number

Pr = Prandtl number

C4201(1) - constant coefficient
(default = 1.0, units = none, equiv = none)

C4201(2) - Nusselt number exponent
(default = 1.0, units = none, equiv = none)

C4201(3) - Schmidt number exponent
(default = 1/3, unit = none, equiv = none)

C4201(4) - Prandtl number exponent
(default = 1/3, units = none, equiv = none)

4202 – Film Flashing Heat Transfer Coefficient

This parameter is used to limit the rate of film evaporation calculated by the mechanistic formula used when noncondensibles are present. The mechanistic formula is

$$\dot{m}_c = h_D \rho_v \ln(\Delta P_{srf} / \Delta P_{atm})$$

where

$\dot{m}_c$ = mass flux at this surface, kg/m^2 • s

h_D = mass transfer coefficient, m/s

ρ_v = density of vapor at $T_{sat}(P_{tot})$, kg/m^3

ΔP_{srf} = P_{tot} - P_{srf} = noncondensible partial pressure at the surface temperature, Pa

ΔP_{atm} = P_{tot} - P_{stm} = noncondensible partial pressure in the bulk atmosphere, Pa

P_{tot} = total control volume pressure, Pa

P_{srf} = saturation pressure of steam at the surface temperature, Pa

P_{stm} = steam partial pressure in the control volume, Pa

Because this equation is singular when the P_{srf} reaches P_{tot} it is necessary to bound the rate of evaporation as the surface temperature reaches T_{sat} (P_{tot}). This is done by using a flashing heat transfer coefficient to limit the rate of evaporation as follows:

$$\dot{m}_e = h_e \min(0, T_{dew} - T_{srf})/h_{fg}$$

$$\dot{m} = \max(\dot{m}_c, \dot{m}_e)$$

where

h_e = maximum flashing heat transfer coefficient, $W/m^2 \cdot K$

h_{fg} = latent heat of vaporization for steam, J/kg

T_{dew} = control volume dew point temperature, K

T_{srf} = surface temperature, K

and h_e has been implemented as sensitivity coefficient 4202, with a default value of $5. \times 10^5$ $W/m^2 - K$ as follows.

C4202(1) - maximum evaporative heat transfer coefficient (default = $5.x10^5$, units = $W/m^2 \cdot K$, equiv = HTFLSH)

4203 – CVH Steam Depletion Control Parameters

These parameters determine what corrective measure is applied if the calculated condensation rates cause excessive steam depletion in a CVH control volume. Steam depletion is considered excessive if the mass of steam condensed during any timestep exceeds C4203(2) x $M_{stm,0}$, where $M_{stm,0}$ is the initial mass of steam in the control volume at the beginning of the timestep. When excessive condensation occurs, one of two corrective actions is taken. By default, the recommended procedure is to repeat the cycle with a smaller timestep to avoid the problem. The alternative, which is invoked any time the current timestep is less than the value of C4203(1), is to scale the calculated condensation fluxes in the offending control volume by a calculated factor less than one, which will eliminate the excessive condensation. The scaling method is not recommended, except as a last resort, because it can artificially limit the true rate of condensation. As an alternative to scaling the condensation rate or limiting the timestep, it may be preferable to renodalize the problem to reduce the ratio of the HS structure surface area to the CVH volume in the region of the excessive condensation.

C4203(1) - fallback/scaling time-step size transition parameter (default = -1.0, units = s, equiv = none)

C4203(2) - maximum steam mass fraction which may condense per timestep (default = 0.9, units = none, equiv = none)

4205 – Stainless Steel Melting (degassing) Parameters

These parameters control the melting of stainless steel heat structures via the degassing model.

C4205(1) - mass of unmelted steel below which the heat structure is deactivated and the remaining mass relocated to the COR package
(default = 10., units = kg, equiv = none)

4210-4232 – Film Heat Transfer Coefficient Correlations

Laminar or turbulent heat transfer through the condensate film is determined by the following criteria:

Laminar if Re_f < C42m0(1)
Turbulent if Re_f > C42m0(2)
Transition if C42m0(1) ≤ Re_f ≤C42m0(2)

where

Re_f = Reynolds number for the film flow

The laminar heat transfer coefficient through the film, $h_{f,l}$, is given by

$$h_{f,l} = (k_f / L) \; x \; Nu_{f,l}$$

where the laminar film Nusselt number, $Nu_{f,l}$, is given by

$$Nu_{f,l} = C42m1(1) x \{ g \; \rho_f (\rho_f - \rho_v) h_{fg} L^3 \sin\theta / [\mu_f k_f (T_{sat} - T_{srf})] \}^{C42m1(2)}$$

The turbulent heat transfer coefficient through the film, $h_{f,t}$, is given by

$$h_{f,t} = \left\{ k_f / \left[(\mu_f / \rho_f)^2 / g \right]^{C42m2(1)} \right\} x \; Nu_{f,t}$$

where the turbulent film Nusselt number, $Nu_{f,t}$ is given by

$$Nu_{f,t} = \left(\mathrm{Re}_f^{\,C42m2(2)} + C42m2(3)\mathrm{Re}_f^{C42m2(4)}\,\mathrm{Pr}_f^{C42m2(5)}\right)^{C42m2(6)}$$

The transition heat transfer coefficient through the film, $h_{f,tr}$, is given by linear interpolation of Re_f as

$$h_{f,tr} = h'_{f,l} + \left[h'_{f,t} - h'_{f,l}\right]x\left[\mathrm{Re}_f - C42m0(1)\right]/\left[C42m0(2) - C42m0(1)\right]$$

In each of these equations,

k_f = thermal conductivity of film

L = characteristic length of surface

ρ_f = density of film

ρ_v = density of vapor

g = acceleration of gravity

h_{fg} = latent heat of vaporization corrected for sensible heat

$$\left(h_{fg} + 0.68\,c_{p,f}\left(T_f - T_{srf}\right)\right)$$

$c_{p,f}$ = specific heat capacity of film

T_f = temperature of film/atmosphere interface

T_{srf} = temperature of film/structure interface

μ_f = viscosity of film

θ = angle between horizontal and structure surface or axis (cyl.)

$h'_{f,l}$ = $h_{f,l}$ evaluated with Re_f = C42m0(1)

$h'_{f,t}$ = $h_{f,t}$ evaluated with Re_f = C42m0(2)

and

m = 1 for upward-facing rectangular geometries

= 2 for horizontal cylindrical geometries

= 3 for spherical or hemispherical geometries

For downward-facing rectangular geometries, the laminar/turbulent transition criteria are given by:

Laminar if Ra_f < C4213(2)
Turbulent, otherwise

where

Ra_f = Rayleigh number for the film flow

The heat transfer coefficient through the film is given by

$$h_f = \{k_f / [\sigma_f / g(\rho_f - \rho_v)\cos\theta]\}^{1/2} x Nu_f$$

where the film Nusselt number is given by

$$Nu_f = C4214(1) x \{\max[C4213(1), Ra_f]\}^{C4214(2)}$$

for laminar film flow, and

$$Nu_f = C4215(1) x \{\min[C4213(3), Ra_f]\}^{C4215(2)}$$

for turbulent film flow.

Rectangular (upward facing)

C4210(1) - Reynolds number upper limit for laminar film flow (default = 30.0, units = none, equiv = none)

C4210(2) - Reynolds number lower limit for turbulent film flow (default = 100.0, units = none, equiv = none)

C4210(3) - (do not use)

C4210(4) - Sine of minimum angle from horizontal (default = 0.1686289, units = none, equiv = none)

C4211(1) - Laminar correlation leading coefficient

(default = 0.943, units = none, equiv = none)

C4211(2) - Laminar correlation exponent
(default = 0.25, units = none, equiv = none)

C4212(1) - Turbulent correlation exponent
(default = 0.3333333, units = none, equiv = none)

C4212(2) - Turbulent correlation exponent
(default = - 0.44, units = none, equiv = none)

C4212(3) - Turbulent correlation coefficient
(default = 5.82×10^{-6}, units = none, equiv = none)

C4212(4) - Turbulent correlation exponent
(default = 0.8, units = none, equiv = none)

C4212(5) - Turbulent correlation exponent
(default = 0.3333333, units = none, equiv = none)

C4212(6) - Turbulent correlation exponent
(default = 0.5, units = none, equiv = none)

Rectangular (downward facing)

C4213(1) - Lower constraint on Ra_f
(default = 10^6, units = none, equiv = none)

C4213(2) - Transition value of Ra_f
(default = 10^8, units = none, equiv = none)

C4213(3) - Upper constraint on Ra_f
(default = 10^{10}, units = none, equiv = none)

C4214(1) - Laminar correlation leading coefficient
(default = 0.6, units = none, equiv = none)

C4214(2) - Laminar correlation exponent
(default = 0.2, units = none, equiv =none)

C4215(1) - Turbulent correlation leading coefficient
(default = 0.72, units = none, equiv = none)

C4215(2) - Turbulent correlation exponent
(default = 0.19, units = none, equiv = none)

NOTE: To avoid potential numerical difficulties the laminar and turbulent correlations must be continuous at the transition Ra_f number given by C4213(2).

Horizontal Cylindrical

C4220(1) - Reynolds number upper limit for laminar film flow (default = 30.0,units = none, equiv = none)

C4220(2) - Reynolds number lower limit for turbulent film flow (default = 100.0, units = none, equiv = none)

C4220(3) - (do not use)

C4220(4) - Cosine of maximum angle from horizontal (default = 0.9715642, units = none, equiv = none)

NOTE: If the value of C4220(4) is set equal to 0., then the cylindrical correlations will be applied to all cylinders. As long as the radius of the cylinder is very large compared to the film thickness, use of the correlations, irrespective of the angle of inclination, is probably justified. Since many important structures are vertical cylinders (e.g., containment vessels, reactor vessels, core shrouds and baffles), the matter should be given careful consideration.

C4221(1) - Laminar correlation leading coefficient (default = 0.729, units = none, equiv = none)

C4221(2) - Laminar correlation exponent (default = 0.25, units = none, equiv = none)

C4222(1) - Turbulent correlation exponent (default = 0.3333333, units = none, equiv = none)

C4222(2) - Turbulent correlation exponent (default = - 0.44, units = none, equiv = none)

C4222(3) - Turbulent correlation coefficient (default = 5.82×10^{-6}, units = none, equiv = none)

C4222(4) - Turbulent correlation exponent (default = 0.8, units = none, equiv = none)

C4222(5) - Turbulent correlation exponent
(default = 0.3333333, units = none, equiv = none)

C4222(6) - Turbulent correlation exponent
(default = 0.5, units = none, equiv = none)

(Hemi)spherical

C4230(1) - Reynolds number upper limit for laminar film flow
(default = 30.0, units = none, equiv = none)

C4230(2) - Reynolds number lower limit for turbulent film flow
(default = 100.0, units = none, equiv = none)

C4231(1) - Laminar correlation leading coefficient
(default = 0.815, units = none, equiv = none)

C4231(2) - Laminar correlation exponent
(default = 0.25, units = none, equiv = none)

C4232(1) - Turbulent correlation exponent
(default = 0.3333333, units = none, equiv = none)

C4232(2) - Turbulent correlation exponent
(default = - 0.44, units = none, equiv = none)

C4232(3) - Turbulent correlation coefficient
(default = 5.82×10^{-6}, units = none, equiv = none)

C4232(4) - Turbulent correlation exponent
(default = 0.8, units = none, equiv = none)

C4232(5) - Turbulent correlation exponent
(default = 0.3333333, units = none, equiv = none)

C4232(6) - Turbulent correlation exponent
(default = 0.5, units = none, equiv = none)

4251 – Minimum and Maximum Liquid Film Thickness

These coefficient represent the minimum and maximum thickness of a liquid film on a surface. The maximum film thickness will be ignored if film tracking is active.

C4251(1) - constant minimum film thickness
(default = 10^{-9}, units = m, equiv = FILMIN)

C4251(2) - constant maximum film thickness
(default = 0.0005, units = m, equiv = FILMAX)

4253 – Film-Tracking Model Correlation Parameters

The film thickness, δ_f, is given as a function of the Reynolds number of the film flow by the following correlation

$$\delta_f = C4253(1)\cdot\delta^*\cdot \mathrm{Re}_f^{C4253(2)}, \text{ if } \mathrm{Re}_f < C4253(5)$$

$$= C4253(3)\cdot\delta^*\cdot \mathrm{Re}_f^{C4253(4)}, \text{ if } \mathrm{Re}_f < C4253(6)$$

= value determined by linear interpolation between boundary limits

and, during film tracking, the heat transfer coefficient through the film is given by

$$h_f = k_f/\delta_f, \text{ if } \mathrm{Re}_f < C4253(5)$$

$$= (k_f/\delta^*)\left[\mathrm{Re}_f^{C4253(7)} + C4253(8)\mathrm{Re}_f^{C4253(9)}\mathrm{Pr}_f^{C4253(10)}\right]^{C4253(11)}, \text{if } \mathrm{Re}_f > C4253(6)$$

= value determined by linear interpolation between boundary limits

where

$$\delta^* = \left[(\mu_f \rho_f)^2/(g\cdot\sin\theta)\right]^{1/3}$$

And k_f, μ_f, ρ_f, and Pr_f are the thermal conductivity, viscosity, density and Prandtl number of the film, respectively, and θ is the angle of the surface with respect to horizontal.

C4253(1) - low Reynolds number film thickness correlation constant
(default = 0.909, units = none, equiv = none)

C4253(2) - low Reynolds number film thickness correlation exponent
(default = 0.3333333, units = none, equiv = none)

C4253(3) - high Reynolds number film thickness correlation constant
(default = 0.115, units = none, equiv = none)

C4253(4) - high Reynolds number film thickness correlation exponent

(default = 0.6, units = none, equiv = none)

C4253(5) - low Reynolds number limit
(default = 1000., units = none, equiv = none)

C4253(6) - high Reynolds number limit
(default = 3000., units = none, equiv = none)

C4253(7) - high Reynolds number film heat transfer coefficient exponent
(default = -0.44, units = none, equiv = none)

C4253(8) - high Reynolds number film heat transfer coefficient constant
(default = $5.82 \cdot 10^{-6}$, units = none, equiv = none)

C4253(9) - high Reynolds number film heat transfer coefficient exponent
(default = 0.8, units = none, equiv = none)

C4253(10) - high Reynolds number film heat transfer coefficient exponent
(default = 0.3333333, units = none, equiv = none)

C4253(11) - high Reynolds number film heat transfer coefficient exponent
(defaut = 0.5, units = none, equiv = none)

4. Plot Variables and Control Function Arguments

Section 4 lists and describes the plot variables and control function arguments which are currently available for the Heat Structure package. Within slashes (/ /) a 'p' denotes a plot variable and a 'c' denotes a control function argument.

HS-CPUC	/p/	Total CPU time used for HS package calculations (s)
HS-CPUE	/p/	Total CPU time used for HS package edits (s)
HS-CPUR	/p/	Total CPU time used for HS package restarts (s)
HS-DEGAS-ENERGY.GGGG	/cp/	Total energy of released gas from Gas Source GGGGG (J)
HS-DEGAS-MASS.GGGGG	/cp/	Total mass of released gas from Gas Source GGGGG (kg)

HS-DEGAS-RATE.GGGGG	/cp/	Degassing rate of Gas Source GGGGG (kg/s)
HS-DEGAS-STEELM-GGGGG	/p/	Steel mass melted during the system cycle for steel degassing source GGGGG (kg)
HS-DEGAS-CSTEELM-GGGGG	/p/	Cumulative mass of steel melted for steel degassing source GGGGG (kg)
HS-DELE-ATMS-L.CCCCC	/cp/	Integrated energy transfer to boundary volume atmosphere of left (inside) boundary surface of Heat Structure CCCCC due to mass transfer (J)
HS-DELE-ATMS-R.CCCCC	/cp/	Integrated energy transfer to boundary volume atmosphere of right (outside) boundary surface of Heat Structure CCCCC due to mass transfer (J)
HS-DELE-POOL-L.CCCCC	/cp/	Integrated energy transfer to boundary volume pool of left (inside) boundary surface of Heat Structure CCCCC due to mass transfer (J)
HS-DELE-POOL-R.CCCCC	/cp/	Integrated energy transfer to boundary volume pool of right (outside) boundary surface of Heat Structure CCCCC due to mass transfer (J)
HS-FILM-TEMP-L.CCCCC	/cp/	Temperature of film/atmosphere interface at left boundary surface of Heat Structure CCCCC (K)
HS-FILM-TEMP-R.CCCCC	/cp/	Temperature of film/atmosphere interface at right boundary surface of Heat Structure CCCCC (K)
HS-DELM-DROP-L.CCCCC	/cp/	Integrated droplet (fog) mass transfer to boundary volume atmosphere of left (inside) boundary surface of Heat Structure CCCCC (kg)
HS-DELM-DROP-R.CCCCC	/cp/	Integrated droplet (fog) mass transfer to boundary volume atmosphere of right (outside) boundary surface of Heat Structure CCCCC (kg)

HS-DELM-POOL-L.CCCCC	/cp/	Integrated water mass transfer to boundary volume pool of left (inside) boundary surface of Heat Structure CCCCC (kg)
HS-DELM-POOL-R.CCCCC	/cp/	Integrated water mass transfer to boundary volume pool of right (outside) boundary surface of Heat Structure CCCCC (kg)
HS-DELM-STEAM-L.CCCCC	/cp/	Integrated vapor (steam) mass transfer to boundary volume atmosphere of left (inside) boundary surface of Heat Structure CCCCC (kg)
HS-DELM-STEAM-R.CCCCC	/cp/	Integrated vapor (steam) mass transfer to boundary volume atmosphere of right (outside) boundary surface of Heat Structure CCCCC (kg)
HS-ENERGY-FLUX-L.CCCCC	/p/	Energy flux associated with HS-MASS-FLUX-L.CCCCC (W/m^2)
HS-ENERGY-FLUX-R.CCCCC	/p/	Energy flux associated with HS-MASS-FLUX-R.CCCCC (W/m^2)
HS-ENERGY-INPUT.CCCCC	/cp/	Energy input to Heat Structure CCCCC by internal and surface power sources and by other packages (J)
HS-ENERGY-STORED.CCCCC	/p/	Stored energy of Heat Structure CCCCC (J)
HS-FILM-ENTH-L.CCCCC	/p/	Specific enthalpy of liquid film on left (inside) boundary surface of Heat Structure CCCCC (J/kg)
HS-FILM-ENTH-R.CCCCC	/p/	Specific enthalpy of liquid film on right (outside) boundary surface of Heat Structure CCCCC (J/kg)
HS-FILM-MASS-L.CCCCC	/p/	Mass of liquid film on left (inside) boundary surface of Heat Structure CCCCC (kg)

HS-FILM-MASS-R.CCCCC	/p/	Mass of liquid film on right (outside) boundary surface of Heat Structure CCCCC (kg)
HS-FILM-THICK-L.CCCCC	/p/	Thickness of liquid film on left (inside) boundary surface of Heat Structure CCCCC (m)
HS-FILM-THICK-R.CCCCC	/p/	Thickness of liquid film on right (outside) boundary surface of Heat Structure CCCCC (m)
HS-HTC-ATMS-L.CCCCC	/cp/	Atmosphere heat transfer coefficient at left (inside) boundary surface of Heat Structure CCCCC ($W/m^2 \cdot K$)
HS-HTC-ATMS-R.CCCCC	/cp/	Atmosphere heat transfer coefficient at right (outside) boundary surface of Heat Structure CCCCC ($W/m^2 \cdot K$)
HS-HTC-POOL-L.CCCCC	/cp/	Pool heat transfer coefficient at left (inside) boundary surface of Heat Structure CCCCC ($W/m^2 \cdot K$)
HS-HTC-POOL-R.CCCCC	/cp/	Pool heat transfer coefficient at right (outside) boundary surface of Heat Structure CCCCC ($W/m^2 \cdot K$)
HS-ITER-FREQ	/p/	Average iteration frequency over all heat structures
HS-MASS-FLUX-L.CCCCC	/cp/	Mass flux to left (inside) boundary surface of Heat Structure CCCCC ($kg/m^2 \cdot s$)
HS-MASS-FLUX-R.CCCCC	/cp/	Mass flux to right (outside) boundary surface of Heat Structure CCCCC ($kg/m^2 \cdot s$)
HS-MTC-L.CCCCC	/p/	Diffusion mass transfer coefficient at left (inside) boundary surface of Heat Structure CCCCC (m/s)
HS-MTC-R.CCCCC	/p/	Diffusion mass transfer coefficient at right (outside) boundary surface of Heat Structure CCCCC (m/s)

HS-POOL-FRAC-L.CCCCC	/cp/	Fraction left (inside) boundary surface of Heat Structure CCCCC in pool of its boundary volume
HS-POOL-FRAC-R.CCCCC	/cp/	Fraction of right (outside) boundary surface of Heat Structure CCCCC in pool of its boundary volume
HS-QFLUX-ATMS-L.CCCCC	/cp/	Heat flux to atmosphere at left (inside) boundary surface of Heat Structure CCCCC (W/m^2)
HS-QFLUX-ATMS-R.CCCCC	/cp/	Heat flux to atmosphere at right (outside) boundary surface of Heat Structure CCCCC (W/m^2)
HS-QFLUX-POOL-L.CCCCC	/cp/	Heat flux to pool at left (inside) boundary surface of Heat Structure CCCCC (W/m^2)
HS-QFLUX-POOL-R.CCCCC	/cp/	Heat flux to pool at right (outside) boundary surface of Heat Structure CCCCC (W/m^2)
HS-QTOTAL-ATMS-L.CCCCC	/p/	Time and surface integral of heat flux to atmosphere at left (inside) boundary surface of Heat Structure CCCCC (J)
HS-QTOTAL-ATMS-R.CCCCC	/p/	Time and surface integral of heat flux to atmosphere at right (outside) boundary surface of Heat Structure CCCCC (J)
HS-QTOTAL-POOL-L.CCCCC	/p/	Time and surface integral of heat flux to pool at left (inside) boundary surface of Heat Structure CCCCC (J)
HS-QTOTAL-POOL-R.CCCCC	/p/	Time and surface integral of heat flux to pool at right (outside) boundary surface of Heat Structure CCCCC (J)
HS-TEMP.CCCCCMN	/cp/	Temperature at node MN of Heat Structure CCCCCC (K)

5. Example Input

This section provides example input for a problem which uses the Heat Structure package for MELGEN and MELCOR execution. This problem is included to provide a nontrivial example of the input for the HS package and is not intended to be a reactor safety application of the MELCOR Code System.

Consider a boiling water reactor (BWR) with a Mark II containment. The reactor produces 3226 MW thermal power from 47,368 nuclear fuel rods. The example problem whose input is discussed here is a boil-off with the core initially 85% covered. The following packages are used in this calculation:

(1) Heat Structure Package

(2) Control Volume Hydrodynamics Package

(3) Flow Path Package

(4) Material Properties Package

(5) Control Function Package

(6) Tabular Function Package

This example problem does not use the Core package. The core is represented by a single fuel rod heat structure with multiplicity 47,368. The following sections contain illustrations of input for this problem.

5.1 Example MELGEN Input

A subset of the MELGEN input that will create a restart file to execute the boil-off problem is given here. This input contains records not only for heat structures but also for some concomitant gas source, noncondensible gas, material properties, and tabular function input.

5.1.1 Heat Structure Input

The following illustrates complete input records for 3 of 21 heat structures in the example problem. These provide examples of various nodalizations, material composition, geometries, power sources, and boundary conditions for heat structures. Refer to Section 2.1.1 for details on MELGEN heat structure inputs.

The following records are comments (records beginning with the symbol*) and a complete set of input for an intact fuel rod in the LaSalle nuclear reactor. This heat structure is a

vertical structure with a cylindrical geometry. It has a multiplicity equal to the number of fuel rods in the core. There are 12 temperature nodes. Each fuel rod is composed of uranium dioxide fuel, a helium gap, and a Zircaloy cladding. The decay-heat power after scram is represented by an internal power source whose power is given as a function of time by a tabular function. A symmetry boundary condition is applied at the center and a convective boundary condition for external flow with calculated heat transfer coefficient is applied at the surface.

```
*INTACT FUEL RODS (5.4943-9.3043 M) - HEAT TRANSFER TO CORE
HS10100000  12          2
HS10100001  'FUEL ROD'
HS10100002  5.4943      1.0
HS10100003  4.7368E4
HS10100100  -1          1       0.0
HS10100102  8.678160E-4         2
HS10100103  1.735632E-3         3
HS10100104  2.603448E-3         4
HS10100105  3.471264E-3         5
HS10100106  4.339080E-3         6
HS10100107  5.206896E-3         7
HS10100108  5.321196E-3         8
HS10100109  5.524421E-3         9
HS10100110  5.727646E-3         10
HS10100111  5.930871E-3         11
HS10100112  6.134096E-3         12
HS10100201  uranium-dioxide     6
HS10100202  helium              7
HS10100203  zircaloy            11
HS10100300  500     -1 2.0889E-5
HS10100301  1.0     6
HS10100302  0.0     11
HS10100400  0
HS10100600  1       101     EXT     0.5     0.5
HS10100601  .5      EQUIV-BAND      .1
HS10100700  1.429449E-1 1.226819E-2     3.70884
```

The following records are comments and a complete set of input for the upper head of the pressure vessel for the reactor. The upper head has a hemispherical geometry and is made of carbon steel. A convective boundary condition for internal flow with calculated heat transfer coefficients is applied at the interior surface of the reactor and a convective boundary condition with heat transfer coefficient that is obtained from a tabular function is applied at the exterior surface. The exterior surface boundary condition represents the insulation on the pressure vessel.

```
* UPPER HEAD - UPPER PLENIUM TO DRYWELL HEAT TRANSFER
*
HS10402000  5       5       -1
```

```
HS10402001  'UPPER HEAD'
HS10402002  18.53
HS10402100  -1       1      3.226
HS10402101  3.334    5
HS10402200  -1
HS10402201  CARBON-STEEL  4
HS10402300  -1
HS10402400  1        104    INT      0.5      0.5
HS10402401  .75      EQUIV-BAND     3.
HS10402500  50.59    3.226 3.226
HS10402600  5120     205    EXT      0.5      0.5
HS10402601  .3       EQUIV-BAND     15.
HS10402700  54.55    3.334 3.334
HS10402800  -1
HS10402801  560.0    5
```

The following records are comments and a complete set of input for the wetwell floor of the containment for the nuclear power plant. It is represented as a rectangular, horizontal heat structure which is made of concrete. At both surfaces a convective boundary condition with calculated heat transfer coefficient is applied.

```
* WETWELL FLOOR
* WETWELL TO SECONDARY CONTAINMENT HEAT TRANSFER
HS20002000  5          1              -1
HS20002001  'WETWELL FLOOR'
HS20002002  -28.7274 0.0
HS20002100  -1         2              0.0
HS20002101  0.7620     4
HS20002200  -1
HS20002201  CONCRETE 4
HS20002300  -1
HS20002400  1      300    EXT         0.5      0.5
HS20002401  .8     EQUIV-BAND         15.
HS20002500  548.0     26.416       26.416
HS20002600  1      200   'EXT'        0.5      0.5
HS20002601  .8     EQUIV-BAND         18.
HS20002700  548.0 26.416            26.416
HS20002800  -1
HS20002801  325.0 5
```

5.1.2 Gas Source Input

The following records are a complete set for a gas source which models the degassing of limestone concrete by the release of free water. Refer to Section 2.1.2 for details on MELGEN gas source input.

The source releases water vapor into the boundary volume of the left boundary surface of Heat Structure 20001 between the temperatures 360 K and 380 K. It is distributed over the entire heat structure and can release as much as 2.211×10^5 kg of water vapor.

```
HSDG200110  -20001      4           H2O-VAP
HSDG200111  110.0       1.808E6     360.0       380.0
```

Limestone concrete can also release water vapor from bound water and carbon dioxide from calcium carbonate as its temperature increases. The following records are input for the HS package degassing model for gas sources for the degassing of the concrete in Heat Structure 20001.

```
HSDG200120  -20001      4    CO2
HSDG200121  72.0        6.912E6     500.0       520.0
HSDG200130  -20001      4    H2O-VAP
HSDG200131  110.0       2.909E7     360.0       380.0
```

5.1.3 Noncondensible Gas (NCG) Input

The following records specify the noncondensible gases for the example problem. The carbon dioxide specification must be present since it is released by a gas source for the degassing model. The water vapor which is released by some gas sources is a material that is present in all problems. Refer to the NCG Package Users' Guide for details on NCG MELGEN input.

```
NCG004  H2      4   *   HYDROGEN
NCG005  N2      5   *   NITROGEN
NCG006  CO2     6   *   CARBON DIOXIDE
```

5.1.4 Material Property (MP) Input

The following records illustrate the material properties input which is required for the new material 'CONCRETE'. For this problem, input for the new materials carbon steel and helium must also be present. Tabular functions 106, 107, and 108 must also be provided for the thermal conductivity, heat capacity, and density of concrete. Refer to the MP Package Users' Guide for details on MP MELGEN input.

```
MPMAT10600  CONCRETE
MPMAT10601  THC 106
MPMAT10602  CPS 107
MPAT10603   RHO 108
```

5.1.5 Tabular Function (TF) Input

The following records are input for Tabular Function 120, which is the heat transfer coefficient as a function of temperature for the insulated exterior of the reactor pressure

vessel. This function specifies a constant heat transfer coefficient of 10 W/m^2 • K. Refer to the TF Package Users' Guide for details on TF MELGEN input.

```
TF12000  'HTC OUT VESS'      2          1.0        0.0
TF12010  273.15   10.0       5000.0     10.0
```

The following records are input for Tabular Function 500, which is the decay-heat power as a function of time for the LaSalle reactor core. This function specifies an initial power of 3326 MW with a decay that is typical of a BWR core after scram.

```
TF50000     'DECAY-HEAT POWER'     22    3.326E9     0.0
TF50011  0.0   1.000000   0.1   0.900689
TF50012  0.2   0.274300    0.3   0.153171
TF50013  0.4   0.110821    0.5   0.091625
TF50014  0.6   0.083212    0.8   0.073556
TF50015  1.0   0.064777    1.5   0.063089
TF50016  2.0   0.059854    3.0   0.057265
TF50017  4.0   0.055204    6.0   0.052085
TF50018  8.0   0.049776    10.0   0.047947
TF50019  15.0   0.044575    20.0   0.042176
TF50020  30.0   0.038783    40.0   0.036348
TF50021  60.0   0.031546    1.0E5   0.001460
```

5.2 Example MELGEN Input for Ice Condenser Model

An example of heat structure, gas source and tabular value input that was used to model a PWR ice condenser is provided below. See the description related to input Record HSCCCCC600 for details.

```
HS00500000  2  2  -1  *  two nodes
HS00500001  'Ice Condenser'       * name of structure
HS00500002  10.0  1.0     * elevation is vertical
HS00500003  1000.     * multiplicity
HS00500100  -1 1  0.0  * node data
HS00500101  0.15  2    * location node 2
HS00500200  -1      * index for material
HS00500201  basket 1    * mat. name and mesh interval
HS00500300  0     * no internal heat source
HS00500400  0     * adiabatic left surface
HS00500600  1     1  ice  0.5  0.5  * convective H.T.C.
HS00500700  1.0  0.3  14.60  * CLNR is diameter
HS00500800  -1     * input option parameter
HS00500801  274. 2    * initial temperature
*
HSDG000010  500   1      pool * ice water to pool
HSDG000011  1000. 754419.  274.  373.  1.2  0.33  1.
*
```

```
* basket properties
*
MPMAT01200 basket
MPMAT01201 rho 300
MPMAT01202 cps 400
MPMAT01203 thc 500
*
TF30000   'basket rho'  1  1.0
TF30010   274.  1.
TF40000   'basket cps'  1  1.0
TF40010   274.  485.7
TF50000   'basket thc'  1  1.0
TF50010   274.  5.
*
```

5.3 Example MELGEN and MELCOR Input for Film-Tracking Model

An example of heat structure, film-tracking, tabular function, spray and transfer process input that was used to model a passive containment cooling system for a hypothetical containment dome is provided below. See the film-tracking input described in Sections 2.1.3 and 2.2.3 for details.

The MELGEN input for the film-tracking model is as follows:

```
cv00100  'containment'  2  2  7
cv001a1  pvol  1.0e5  tatm 348.  rhum  1.0  mlfr.4  1.0
cv001b1  0.0    0.0  6.0   169.646  9.0    226.195
cv001c1  ae   100  2
*
cv00200  'environment'  2  2  6
cv002a1  pvol  1.0e5  tatm 298.  rhum  0.5  mlfr.4  1.0
cv002b1  0.0    0.0  48.0   1.e10
*
tf10000  'enthalpy source' 4  1.0   * simulates containment heating
tf10010  0.0  0.0 10.  0.0 10.1  1.0e7  1.e4 1.0e7
*
hs00100000      2 2                    *  2 nodes
hs00100001      'bot. cyl.'            *  cyl. bottom section
hs00100002      0.0  1.0               *  elevation, vertical
hs00100003      1.                     *  multiplicity
hs00100100      -1  1  3.              *  temp and node, loc.
hs00100101      3.05  2                *  location node 2
hs00100200      -1                     *  index for material
hs00100201      'stainless-steel'  1   *  material, mesh loc.
hs00100300      0                      *  no internal power
hs00100400      1  1  int  0.5  0.5    *  convective h.t.c.
hs00100500      1.  3.e-0 3.0          *  clnl is radius
```

```
hs00100600      1  2  ext 0.5   0.5   *  convective h.t.c.
hs00100700      1.  3.e-0 3.0          *  clnl is radius
*
hs00200000      2  2                   *  2 nodes
hs00200001      'mid. cyl.'            *  cyl. middle section
hs00200002      3.0  1.0               *  elevation, vertical
hs00200003      1.                     *  multiplicity
hs00200100      -1  1  3.              *  temp and node, loc.
hs00200101      3.05  2                *  location node 2
hs00200200      -1                     *  index for material
hs00200201      'stainless-steel'  1   *  material, mesh loc.
hs00200300      0                      *  no internal power
hs00200400      1  1  int  0.5  0.5    *  convective h.t.c.
hs00200500      1.  3.e-0 3.0          *  clnl is radius
hs00200600      1  2  ext 0.5   0.5    *  convective h.t.c.
hs00200700      1   3.e-0 3.0          *  clnl is radius
*
hs00300000      2  5                   *  2 nodes
hs00300001      'top hemi.'            *  hemispherical dome
hs00300002     6.0  1.0                *  elevation, vert. (unused)
hs00300003      1.                     *  multiplicity
hs00300100      -1  1  3.              *  temp and node, loc.
hs00300101      3.05  2                *  location node 2
hs00300200      -1                     *  index for material
hs00300201      'stainless-steel'  1   *  material, mesh loc.
hs00300300      0                      *  no internal power
hs00300400      1  1  int  0.5  0.5    *  convective h.t.c.
hs00300500      1.  3.e-0 3.0          *  clnl is radius
hs00300600      1  2  ext 0.5   0.5    *  convective h.t.c.
hs00300700      1.  3.e-0 3.0          *  clnl is radius
*
hsft00000       3
hsft00100       300  1   0.5  100  0.0  0  0  0  10  20
hsft00101       200  0.5 1.0
hsft00200       200  1   0.0  0    0.0  0
hsft00201       100  1.0 1.0
hsft00300       100  0   0.0  0    0.0  0
*
tf01000  'water source' 3 1.0          *  passive containment cooling
tf01010  0.0  3.e0  1.5e3  3.e0  4.e3  7.0
*
tf02000  'water enthalpy'  2  1.0      *  water at about 300 K
tf02010  0.0  1.e5  1.e4   1.e5
*
sprsr0100 'rain'  1  8.                *  rain from HS 300
sprsr0101 300     0. -1  -1  100       *  "out" Trans. Pr. 100
sprsr0102 3.e-3   1.                   *  drop size (3 mm)
```

```
*
tpin10000 1   1                              *  water mass, temp.
tpot10000 1   100   def.1                    *  from "in" TP 100
*
```

The MELCOR input (to change the drainage partitioning on the left surface of structure 300) is as follows:

```
*
hsft00000         1
hsft00100         300   1    0.2 100 0.0 0 *  dec. left rain
hsft00101         200   0.8  1.0            *  inc. left
*
```

6. Example Output

Both time-independent and time-dependent data from the data base for the Heat Structure package are printed during MELGEN and MELCOR execution. Sections 6.1 and 6.2 discuss the printed output from these data, respectively. Additional information is printed during MELGEN and MELCOR execution. The output containing this information is discussed in Sections 6.3 and 6.4.

6.1 Time-independent Data Output

During MELGEN execution after all input data are processed and all initialization calculations are completed and during MELCOR execution prior to commencing the first cycle of a restart, time-independent data are printed. For the HS package, this output follows the header:

EDIT FOR HEAT STRUCTURE PACKAGE
(TIME-INDEPENDENT DATA)

For Heat Structure CCCCC with user input name HSNAME, the following information is printed in the section "HEAT STRUCTURE CCCCC HSNAME":

(1) number of temperature nodes

(2) location of temperature nodes

(3) geometry type

(4) altitude of base

(5) orientation parameter

(6) multiplicity

(7) name of material in each mesh interval

(8) mass in each mesh interval

(9) total mass of structure

(10) volume in each mesh interval

(11) total volume of structure

(12) internal power source information (tabular function number for power table if source exists or statement that no internal power source exists)

(13) power fractions for each mesh interval if an internal power source exists or statement that all power fractions are zero if no internal power source exists

(14) boundary volume numerical identifier for each boundary surface

(15) type of boundary condition which is applied at each boundary surface

(16) type of flow (internal/external) over each boundary surface

(17) surface power source information for each boundary surface (tabular function number for power table if source exists or statement that no surface power source exists)

(18) statement indicating whether or not mass transfer calculations are performed for each boundary surface

(19) area of each boundary surface

(20) characteristic length of each boundary surface

(21) axial length of each boundary surface

(22) critical pool fractions for pool and atmosphere heat transfer

At each boundary surface whose critical pool fraction for pool heat transfer exceeds its fraction for atmosphere heat transfer, heat transfer to neither the pool nor atmosphere will be calculated for pool fractions between these values. If at least one surface has such a specification, information is printed for each such surface in the section which follows the statement,

> WARNING – HEAT TRANSFER MAY NOT BE CALCULATED AT THE FOLLOWING SURFACES:

This information includes the following:

(1) identification number of heat structure,

(2) side of the heat structure – left (inside) or right (outside) – for which no heat transfer might be calculated, and

(3) range of pool fraction for which no heat transfer will be calculated.

If no gas sources for the HS package degassing model are present the statement

NO GAS SOURCES FOR THE DEGASSING MODEL ARE PRESENT IN THIS PROBLEM

Is printed. If Gas Source CCCCC exists for a problem, the following information is printed in the section "GAS SOURCE CCCCC":

(1) mesh intervals over which source is distributed

(2) name of gas which is released and number of control volume into which it is released

(3) density

(4) heat of reaction

(5) boundaries of temperature range over which gas is released

(6) total mass of gas that can be released

The following is an example of the kind of time-independent output obtained when the film-tracking model is active (there is no time-dependent output from the model):

6.2 Time-Dependent Data Output

During MELGEN execution after all input data are processed and all initialization calculations are completed and during MELCOR execution at user specified time intervals, time-dependent data are printed. For the HS package, this output follows the header:

EDIT FOR HEAT STRUCTURE PACKAGE
(TIME-DEPENDENT DATA)
TIME = 0.000E+00 CYCLE = 000000000

The version number and creation date of the HS package and its associated manuals are printed at the top of the page containing this header. The units for each output quantity are given following this header.

The output for the heat structures is printed in the following four sections:

(1) HEAT STRUCTURE TEMPERATURE DISTRIBUTIONS

(2) HEAT TRANSFER DATA

(3) MASS TRANSFER DATA

(4) ENERGY TRANSFER DATA

The temperature at each node in each heat structure is printed in the section "HEAT STRUCTURE TEMPERATURE DISTRIBUTIONS". The temperatures for Heat Structure CCCCC with name HSNAME are printed on lines following a left justified "HEAT STRUCTURE CCCCC HSNAME".

The following data for the boundary surfaces of each heat structure are printed in the section "HEAT TRANSFER DATA":

(1) boundary volume

(2) surface temperature

(3) pool fraction (fraction of surface in pool of its boundary volume)

(4) atmosphere convective heat transfer coefficient

(5) atmosphere radiation heat transfer coefficient

(6) pool heat transfer coefficient

(7) atmosphere heat transfer flow regime

(8) pool heat transfer flow regime

The following data for each boundary surface of each heat structure are printed in the section "MASS TRANSFER DATA":

(1) boundary volume

(2) pool fraction

(3) mass flux

(4) liquid film thickness

(5) liquid film mass

(6) changes in mass of steam, fog droplets, and pool in boundary volume due to mass transfer at the surface

The following data for each heat structure are printed in the section "ENERGY TRANSFER DATA":

(1) stored energy

(2) energy input by internal and surface power sources and by transfers from other packages

The following data are printed in this section for each boundary surface:

(3) specific enthalpy of its liquid film

(4) time and surface integral of its atmosphere and pool heat fluxes

(5) energy transferred to atmosphere and pool of its boundary volume due to mass transfer

The information printed in this section at different times is sufficient to establish the global conservation of energy for the HS package.

If gas sources are present in the problem, the following data are printed for each gas source in the section "DEGASSING SOURCE DATA":

(1) number of heat structure which contains source

(2) control volume into which gas is released

(3) degassing rate

(4) total mass of gas released

(5) total energy consumed by gas release

An example of the time-independent edit obtained when the film-tracking model is active follows:

```
********** FILM-TRACKING MODEL SETUP **********

THE FIRST SET OF STRUCTURES COUPLED FOR PURPOSES
OF FILM TRACKING CONSISTS OF 3 STRUCTURES:
```

```
1 - STRUCTURE  300
RECEIVES WATER ON THE RIGHT (OUTSIDE) SURFACE VIA:
MASS SOURCE TABULAR FUNCTION  10
AND ENTHALPY SOURCE TABULAR FUNCTION  20
DRAINAGE FROM THE LEFT SIDE IS PARTITIONED AS FOLLOWS:
RAIN TO TRANSFER PROC.  100  = 5.0000E-01
TO HEAT STRUCTURE  200       = 5.0000E-01
DRAINAGE FROM THE RIGHT SIDE IS PARTITIONED AS FOLLOWS:
TO HEAT STRUCTURE  200       = 1.0000E+00

2 - STRUCTURE  200
DRAINAGE FROM THE LEFT SIDE IS PARTITIONED AS FOLLOWS:
TO HEAT STRUCTURE  100       = 1.0000E+00
DRAINAGE FROM THE RIGHT SIDE IS PARTITIONED AS FOLLOWS:
TO HEAT STRUCTURE  100       = 1.0000E+00

3 - STRUCTURE  100
DRAINAGE FROM THE LEFT SIDE IS PARTITIONED AS FOLLOWS:
TO POOL OF CONTROL VOL     1 = 1.0000E+00
DRAINAGE FROM THE RIGHT SIDE IS PARTITIONED AS FOLLOWS:
TO POOL OF CONTROL VOL     2 = 1.0000E+00
```

6.3 Additional MELGEN Output

Prior to the time-independent data edit, the following information is given for the HS package during MELGEN execution:

(1) number of input errors detected during processing of input records which are internal to the HS package (pass-one processing),

(2) total number of heat structures and gas sources

(3) data-base memory requirements for the HS package

(4) CPU time which was required for pass-one input processing

(5) scratch memory requirements for the HS package

(6) number of input errors detected which result from inconsistencies with other packages (pass-two processing)

(7) number of iterations which were required for steady-state temperature convergence for each heat structure whose input requested steady-state initialization

6.4 Additional MELCOR Output

Additional MELCOR output which is provided by the HS package is discussed in this section.

Each edit includes the section "HEAT STRUCTURE PACKAGE STATISTICS" which documents the performance of the HS package. For the entire problem and for the portion of the problem between the past and present edits, the following information is printed:

(1) CPU time for calculation, edit, and restart

(2) average iteration frequency per heat structure

7. Diagnostics and Error Messages

The Heat Structure package prints a message if any of the following occur:

(1) an error is detected during MELGEN input processing

(2) temperature convergence during steady-state initialization in MELGEN execution is not achieved

(3) an error is detected during MELCOR input processing

(4) during MELCOR execution the HS package requests repeating a computational cycle with a reduced timestep

The messages are discussed in Section 7.1 through 7.3.

7.1 MELGEN input Errors

Error messages are printed by the HS package when errors are detected during input processing in MELGEN execution. Such errors occur if input specifications are violated or if input data are inconsistent. In general any input which violates a "must" imperative in the user input descriptions of Sections 2.1.1 and 2.1.2 will be detected as an error. All such error messages are self-explanatory and indicate the input record which must be corrected. Error messages are also printed if materials, control volumes, or tabular functions which are specified in heat structure input are not present in a problem. Concomitant with the detection of an error during MELGEN input processing is a directive to not create a restart file.

Failure to converge in a steady-state initialization temperature iteration usually indicates a problem associated with the user inputs related to the heat structure nodalization or CVH boundary volume. In this case the user should re-examine the input for errors or unrealistic

conditions. As a last resort, the user can abandon steady-state initialization for that heat structure and prescribe a temperature profile with the HSCCCCC800 and HSCCCCC801 input records.

7.2 MELCOR Input Errors

Error messages are printed by the HS package when errors are detected during input processing in MELCOR execution. All such error messages are self-explanatory and indicate the input record which must be corrected. Error messages are also printed if materials, control volumes or tabular functions which are specified in heat structure input are not present in a problem. Concomitant with any input error message during MELCOR execution is a directive to not proceed with a transient calculation.

7.3 Requests to Repeat a Computational Cycle

The HS package prints a diagnostics message during MELCOR execution whenever it requests repeating a computational cycle with a reduced timestep because of numerical difficulties. MELCOR only terminates execution after a time-step reduction if the new time-step is less than the minimum specified by the user. In such a situation, a restart file is written and an edit of all current data is performed.

Material Properties (MP) Package Users' Guide

The MELCOR Material Properties (MP) package models the physical properties needed by many of the various physics packages. This is done by using analytical laws, correlations, or linear tables. New materials and their properties may be defined through user input, and properties for default materials may be redefined by user input.

This Users' Guide gives a list of the default materials and the properties defined in the package, describes the user input, and lists some sample input and output.

The default property values and functions used in the MP package along with their references are provided in the MP Package Reference Manual.

Contents

List of Tables

1. Default Material Properties

The MELCOR Material Properties (MP) package models many common properties needed by the various phenomenological packages through the use of analytical laws, correlations, and tabulated values. These properties include thermodynamic state and transport properties needed for structural materials, as well as transport properties for water and noncondensible gases. (Thermodynamic state properties for these fluids are provided separately by the H2O and NCG packages; see the NCG/H2O Reference Manual.)

In a few cases, stand-alone codes that have been wholly integrated into MELCOR still use properties defined within those codes; a notable example is CORCON, which has been integrated into the Cavity (CAV) package. Also, properties unique to a package, such as those for trace species used in the RadioNuclide (RN) package, are generally modeled within that package. The Core (COR), Fuel Dispersal Interactions (FDI), and Heat Structures (HS) packages use principally the structural materials properties, while the Control Volume Hydrodynamics (CVH), Engineered Safety Features (ESF), Containment Sprays (SPR), and RN packages use principally the fluid transport properties.

The following 35 materials, listed with their mnemonic identifiers, are defined in the Material Properties package:

Table 1.1 MP Materials and Mnemonic Identifiers

1.	Water (WATER)	19.	Carbon Dioxide (CO2)
2.	Steam (STEAM)	20.	Carbon Monoxide (CO)
3.	Air (AIR)	21.	Nitrogen (N2)
4.	Hydrogen (H2)	22.	Nitric Oxide (NO)
5.	Helium (HE)	23.	Nitrous Oxide (N2O)
6.	Argon (AR)	24.	Ammonia (NH3)
7.	Deuterium (D2)	25.	Acetylene (C2H2)
8.	Zircaloy (ZR)	26.	Methane (CH4)
9.	Zirconium Oxide (ZRO2)	27.	Ethylene (C2H4)
10.	Uranium Dioxide (UO2)	28.	Uranium Hexafluoride (UF6)
11.	Stainless Steel (SS)	29.	Aluminum (ALUM)
12.	Stainless Steel Oxide (SSOX)	30.	Aluminum Oxide (AL2O3)
13.	Boron Carbide (B4C)	31.	Cadmium (CADM)
14.	Silver-Indium-Cadmium (AGINC)	32.	Stainless Steel 304 (SS304)
15.	Uranium Metal (UMETL)	33.	Lithium Aluminum (LIAL)
16.	Graphite (GRAPH)	34.	Uranium Aluminum (UAL)
17.	Concrete (CON)	35.	Carbon Steel (CS)
18.	Oxygen (O2)		

Material 11, Stainless Steel (SS), is a type 347 stainless steel and is typically used in the Core package, whereas material 32 (SS304) is a type 304 stainless steel.

The following properties are defined in the package:

Table 1.2 Defined Material Properties (Mnemonic)

1	Enthalpy as a function of temperature (ENH)	Tabular	J/kg
2.	Temperature as a function of enthalpy (TMP)	Tabular	K
3.	Specific Heat Capacity as a function of temperature (CPS)	Tabular	J/kg-K
4.	Thermal Conductivity as a function of temperature (THC)		
	a. From tables	Tabular	W/m-K
	b. From Eucken correlation and Wassijewa equation	Calculated	W/m-K
5.	Dynamic Viscosity as a function of temperature		
	a. From tables (VIS)	Tabular	kg/m-s
	b. From Chapman-Enskog equations and Lennard-Jones potential parameters (SIG, EPS)	Calculated	kg/m-s
6.	Binary Diffusion Coefficient		
	a. Function of temperature and pressure	Calculated	m^2/s
	b. From Chapman-Enskog equations and Lennard-Jones potential parameters	Calculated	
7.	Density		
	a. Constant (DEN)	Constant	kg/m^3
	b. Function of temperature (RHO)	Tabular	kg/m^3
	c. Function of temperature and pressure (N/A)	Calculated	kg/m^3
8.	Melting Temperature (MLT)	Constant	K
9.	Latent Heat of Fusion (LHF)	Constant	J/kg

Default values are provided for some, but not all, combinations of materials and physical properties.

Table 1.3 summarizes the properties for which default values are available. A 'T' indicates that the default function can be changed through user-defined tabular functions (see the Tabular Function Package Users' Guide) and an MPMATnnnmm input record. A 'C' indicates that the default function can be changed through user-defined constant values input on an MPMATnnnmm record. An 'X' indicates that the default function cannot be changed through user input. A blank space indicates that no default is provided, but may be supplied by the user, although in some cases that property for that material may not be used by MELCOR.

Also shown are the mnemonic identifiers used to add new values or alter the default values through user input for those properties which can be changed.

Two materials, AIR and UF6, are not currently defined in the NCG package and, as such, should not be used.

In those cases where both tabular data and correlational data exists for a given material, the tabular data are the default. For example, H2 viscosity data exists in tabular form and as Chapman-Enskog input parameters. The code will use the tabular form unless the user specifies the use of Chapman-Enskog parameters.

Table 1.3 Default material properties, property mnemonics, and user input capabilities

Property*:	1	2	3	4a	4b	5a	5b	6a	6b	7a	7b	7c	8	9
Mnemonic:	ENH	TMP	CPS	THC	SIG	VIS	SIG	n/a	SIG	DEN	RHO	n/a	MLT	LHF
WATER				T		T								
STEAM				T	C	T	C		C			X		
AIR				T	C	T	C		C			X		
H2					C	T	C		C					
HE					C		C		C					
AR					C		C		C					
D2					C	T	C		C					
ZR	T	T	T	T						C	T		C	C
ZRO2	T	T	T	T						C	T		C	C
UO2	T	T	T	T						C	T		C	C
SS	T	T	T	T						C	T		C	C
SSOX	T	T	T	T						C	T		C	C
B4C	T	T	T	T						C	T		C	C
AGINC	T	T	T	T						C	T		C	C
UMETL	T	T	T	T						C	T		C	C
GRAPH	T	T	T	T						C	T		C	
CON			T	T							T			
O2					C		C		C					
CO2					C		C		C					
CO					C		C		C					
N2					C		C		C					
NO					C		C		C					
N2O					C		C		C					
NH3					C		C		C					
C2H2					C		C		C					
CH4					C		C		C					
C2H4					C		C		C					
UF6					C		C		C					
STEAM + AIR								X						
STEAM + H2								X						
ALUM	T	T	T	T						C	T		C	C
AL2O3	T	T	T	T						C	T		C	C
CADM	T	T	T	T						C	T		C	C
SS304	T	T	T	T						C	T		C	C
LIAL	T	T	T	T						C	T		C	C
UAL	T	T	T	T						C	T		C	C
CS	T	T	T	T						C	T		C	C

T - The default function can be changed using tabular functions and an MPMATnnnmm input record.
C - The default function can be changed using constant values input on an MPMATnnnmm record.
X - The default function cannot be changed through user input.
* - See page 5 for a full description of these properties.

2. User Input

2.1 MELGEN Input

The user may define new materials for the material properties package. This is done by naming the material and defining the properties for that material through a tabular function or a constant value input. If the input material name matches the name of one of the 34 default materials, the input properties are used instead of the default properties for that material. One set of the following records is required for each new material or for each redefinition of a pre-defined material.

MPMATnnn00 - Material Name
$0 \leq nnn \leq 999$, nnn is the user-defined material id number
Required

This record defines the name of the material. The name may be a default material name or a newly defined name. Any name containing spaces must be enclosed in single quotes. Alternatively, a dash (-) can be used in place of a space. Upper and lower case letters are considered equivalent.

(1)MATNAM - Default or user-defined material name.
(type = character * 24)

Table 2.1 Default Material Names

1.	WATER	19.	CARBON DIOXIDE
2.	STEAM	20.	CARBON MONOXIDE
3.	AIR	21.	NITROGEN
4.	HYDROGEN	22.	NITRIC OXIDE
5.	HELIUM	23.	NITROUS OXIDE
6.	ARGON	24.	AMMONIA
7.	DEUTERIUM	25.	ACETYLENE
8.	ZIRCALOY	26.	METHANE
9.	ZIRCONIUM OXIDE	27.	ETHYLENE
10.	URANIUM DIOXIDE	28.	URANIUM HEXAFLUORIDE
11.	STAINLESS STEEL	29.	ALUMINUM
12.	STAINLESS STEEL OXIDE	30.	ALUMINUM OXIDE
13.	BORON CARBIDE	31.	CADMIUM
14.	SILVER-INDIUM-CADMIUM	32.	STAINLESS STEEL 304
15.	URANIUM METAL	33.	LITHIUM ALUMINUM
16.	GRAPHITE	34.	URANIUM ALUMINUM
17.	CONCRETE	35.	CARBON STEEL

18.	OXYGEN		

MPMATnnnmm - Property, Tabular Function Pairs
$0 \leq nnn \leq 999$, nnn is the user-defined material id number
$01 \leq mm \leq 49$, mm is used for ordering the input
Required

These records define the properties by data pairs. The first field in a pair is a property mnemonic, and the second field is the number of the tabular function to be used for that property. There may be an arbitrary number of pairs on a record, but a pair may not be split across a record. If a property for a material is given more than once, the last definition is used.

(1) PROP - Property mnemonic.
(type = character * 3)

Must be one of the following property mnemonics:

ENH - enthalpy vs temperature
TMP - temperature vs enthalpy
CPS - specific heat vs temperature
THC - thermal conductivity vs temperature
VIS - viscosity vs temperature
RHO - density vs temperature

(2) ITBPRP - Number of the tabular function for property, PROP. See the Tabular Function (TF) Package Users' Guide.
(type = integer, default = none, units = dimensionless)

or

Character string 'C-E' to specify the use of Chapman-Enskog relationships for THC or VIS properties (see PROP above). If Chapman-Enskog relationships are specified, the Lennard-Jones potential parameters SIG and EPS may be defined by the user or changed from the defaults provided, as described in the next section.
(type = character *3)

MPMATnnnmm - Property, Constant Value Pairs
$0 \leq nnn \leq 999$, nnn is the user-defined material id number
$50 \leq mm \leq 98$, mm is used for ordering the input
Required

These records define the constant properties by data pairs. The first field in a pair is a property mnemonic, and the second field is the constant value to be used for that property. There may be an arbitrary number of pairs on a record, but a pair may not be split across a record. If a property for a material is given more than once, the last definition is used.

(1) PROP - Mnemonic for a constant property.
(type = character * 3)

Must be one of the following property mnemonics:

DEN - constant density
MLT - melting temperature
LHF - latent heat of fusion
SIG - Lennard-Jones potential parameter, σ
EPS - Lennard-Jones potential parameter, ε/k

(2) CPROPV - Constant property value to be used for property, PROP.
(type = real, defaults = see MP Reference Manual, units = kg/m**3 for 'DEN', K for 'MLT', J/kg for 'LHF', Å (10^{-10}m)for 'SIG', K for 'EPS')

MPMATnnn99 - Steel Composition
$0 \leq nnn \leq 999$, nnn is the user-defined material id number for stainless steel (SS)
Optional

This record allows the user to override the default stainless steel composition (74% iron, 18% chromium, 8% nickel, 0% carbon) used by the Core package. The values will be normalized if required to ensure that the sum of the material fractions equals 1.0.

(1) XFE - Relative mass fraction of iron (must be greater than 0.0).
(type = real, default = 0.74, units = dimensionless)

(2) XCR - Relative mass fraction of chromium.
(type = real, default = 0.18, units = dimensionless)

(3) XNI - Relative mass fraction of nickel.
(type = real, default = 0.08, units = dimensionless)

(3) XCAR - Relative mass fraction of carbon.
(type = real, default = 0.0, units = dimensionless)

2.2 MELCOR Input

There is at present no MELCOR input to the material properties package.

3. Sensitivity Coefficients

There are no sensitivity coefficients currently used in the material properties package.

4. Plot Variables and Control Function Arguments

There are no plot variables or control function arguments currently available in the material properties package.

5. Example MELGEN Input

```
*****************************************************
*          MELGEN INPUT FOR USER'S GUIDE            *
*****************************************************
*
TITLE      'USERS GUIDE'
*
*********
* FILES *
*********
*
OUTPUTF    MPUSERS.GOUT
DIAGF      MPUSERS.GDIA
RESTARTF   MPUSERS.RST
*
CRTOUT
*
************************************************************
* CHANGE NH3 THERMAL CONDUCTIVITY AND VISCOSITY THROUGH    *
* LENNARD-JONES POTENTIAL PARAMETERS, SIG AND EPS          *
************************************************************
*
MPMAT00200    'AMMONIA'
MPMAT00250    SIG      3.000              * CONSTANT SIG (ANGSTROMS)
MPMAT00251    EPS      600.0                     * CONSTANT EPS (K)
*
*
**********************************
* CHANGE B4C MELTING TEMPERATURE *
**********************************
```

```
*
MPMAT00300    'BORON CARBIDE'
MPMAT00350    MLT       2750.0                          * CONSTANT MLT (K)
*
*
*****************************************************************
* ADD LENNARD-JONES POTENTIAL PARAMETERS FOR A NEW GAS, HELIUM *
*****************************************************************
*
MPMAT00400    'GASA'    * MUST USE NAME COMPATIBLE WITH NCG PACKAGE
MPMAT00450    SIG       2.551    * CONSTANT SIG (ANGSTROMS)
MPMAT00451    EPS       10.22    * CONSTANT EPS (K)
*
*                              * NOTE:  GASA (HELIUM) PARAMETERS MUST
*                                *        BE DEFINED USING NCG CARDS
```

6. Example MELGEN Output (Partial Listing)

```
TOTAL NUMBER OF PROPERTIES =       7
TOTAL NUMBER OF MATERIALS  =      35
TOTAL NUMBER OF PROPERTIES FOR ALL MATERIALS =    245


USING                 FOR
DEFAULT TABLE     29 WATER thermal conductivity vs temperature
DEFAULT TABLE     32 WATER viscosity vs temperature
DEFAULT TABLE     30 STEAM thermal conductivity vs temperature
DEFAULT TABLE     33 STEAM viscosity vs temperature
DEFAULT TABLE     31 AIR thermal conductivity vs temperature
DEFAULT TABLE     34 AIR viscosity vs temperature
CHAPMAN-ENSKOG 2000 HYDROGEN thermal conductivity vs temperature
DEFAULT TABLE     42 HYDROGEN viscosity vs temperature
CHAPMAN-ENSKOG 2000 HELIUM thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 HELIUM viscosity vs temperature
CHAPMAN-ENSKOG 2000 ARGON thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 ARGON viscosity vs temperature
CHAPMAN-ENSKOG 2000 DEUTERIUM thermal conductivity vs temperature
DEFAULT TABLE     83 DEUTERIUM viscosity vs temperature
DEFAULT TABLE      1 ZIRCALOY enthalpy vs temperature
DEFAULT TABLE      8 ZIRCALOY temperature vs enthalpy
DEFAULT TABLE     15 ZIRCALOY specific heat vs temperature
DEFAULT TABLE     22 ZIRCALOY thermal conductivity vs temperature
DEFAULT TABLE     35 ZIRCALOY density vs temperature
DEFAULT TABLE      2 ZIRCONIUM-OXIDE enthalpy vs temperature
DEFAULT TABLE      9 ZIRCONIUM-OXIDE temperature vs enthalpy
DEFAULT TABLE     16 ZIRCONIUM-OXIDE specific heat vs temperature
DEFAULT TABLE     23 ZIRCONIUM-OXIDE thermal conductivity vs
```

```
                    temperature
DEFAULT TABLE    36 ZIRCONIUM-OXIDE density vs temperature
DEFAULT TABLE     3 URANIUM-DIOXIDE enthalpy vs temperature
DEFAULT TABLE    10 URANIUM-DIOXIDE temperature vs enthalpy
DEFAULT TABLE    17 URANIUM-DIOXIDE specific heat vs temperature
DEFAULT TABLE    24 URANIUM-DIOXIDE thermal conductivity vs
                    temperature
DEFAULT TABLE    37 URANIUM-DIOXIDE density vs temperature
DEFAULT TABLE     4 STAINLESS-STEEL enthalpy vs temperature
DEFAULT TABLE    11 STAINLESS-STEEL temperature vs enthalpy
DEFAULT TABLE    18 STAINLESS-STEEL specific heat vs temperature
DEFAULT TABLE    25 STAINLESS-STEEL thermal conductivity vs
                    temperature
DEFAULT TABLE    38 STAINLESS-STEEL density vs temperature
DEFAULT TABLE     5 STAINLESS-STEEL-OXIDE enthalpy vs temperature
DEFAULT TABLE    12 STAINLESS-STEEL-OXIDE temperature vs enthalpy
DEFAULT TABLE    19 STAINLESS-STEEL-OXIDE specific heat vs
                    temperature
DEFAULT TABLE    26 STAINLESS-STEEL-OXIDE thermal conductivity vs
                    temperature
DEFAULT TABLE    39 STAINLESS-STEEL-OXIDE density vs temperature
DEFAULT TABLE     6 BORON-CARBIDE enthalpy vs temperature
DEFAULT TABLE    13 BORON-CARBIDE temperature vs enthalpy
DEFAULT TABLE    20 BORON-CARBIDE specific heat vs temperature
DEFAULT TABLE    27 BORON-CARBIDE thermal conductivity vs
                    temperature
DEFAULT TABLE    40 BORON-CARBIDE density vs temperature
DEFAULT TABLE     7 SILVER-INDIUM-CADMIUM enthalpy vs temperature
DEFAULT TABLE    14 SILVER-INDIUM-CADMIUM temperature vs enthalpy
DEFAULT TABLE    21 SILVER-INDIUM-CADMIUM specific heat vs
                    temperature
DEFAULT TABLE    28 SILVER-INDIUM-CADMIUM thermal conductivity vs
                    temperature
DEFAULT TABLE    41 SILVER-INDIUM-CADMIUM density vs temperature
DEFAULT TABLE    51 URANIUM-METAL enthalpy vs temperature
DEFAULT TABLE    52 URANIUM-METAL temperature vs enthalpy
DEFAULT TABLE    50 URANIUM-METAL specific heat vs temperature
DEFAULT TABLE    49 URANIUM-METAL thermal conductivity vs
                    temperature
DEFAULT TABLE    48 URANIUM-METAL density vs temperature
DEFAULT TABLE    56 GRAPHITE enthalpy vs temperature
DEFAULT TABLE    57 GRAPHITE temperature vs enthalpy
DEFAULT TABLE    55 GRAPHITE specific heat vs temperature
DEFAULT TABLE    54 GRAPHITE thermal conductivity vs temperature
DEFAULT TABLE    53 GRAPHITE density vs temperature
DEFAULT TABLE    45 CONCRETE specific heat vs temperature
DEFAULT TABLE    46 CONCRETE thermal conductivity vs temperature
```

```
DEFAULT TABLE     47 CONCRETE density vs temperature
CHAPMAN-ENSKOG 2000 OXYGEN thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 OXYGEN viscosity vs temperature
CHAPMAN-ENSKOG 2000 CARBON-DIOXIDE thermal conductivity vs
                    temperature
CHAPMAN-ENSKOG 2000 CARBON-DIOXIDE viscosity vs temperature
CHAPMAN-ENSKOG 2000 CARBON-MONOXIDE thermal conductivity vs
                    temperature
CHAPMAN-ENSKOG 2000 CARBON-MONOXIDE viscosity vs temperature
CHAPMAN-ENSKOG 2000 NITROGEN thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 NITROGEN viscosity vs temperature
CHAPMAN-ENSKOG 2000 NITRIC-OXIDE thermal conductivity vs
                    temperature
CHAPMAN-ENSKOG 2000 NITRIC-OXIDE viscosity vs temperature
CHAPMAN-ENSKOG 2000 NITROUS-OXIDE thermal conductivity vs
                    temperature
CHAPMAN-ENSKOG 2000 NITROUS-OXIDE viscosity vs temperature
CHAPMAN-ENSKOG 2000 AMMONIA thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 AMMONIA viscosity vs temperature
CHAPMAN-ENSKOG 2000 ACETYLENE thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 ACETYLENE viscosity vs temperature
CHAPMAN-ENSKOG 2000 METHANE thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 METHANE viscosity vs temperature
CHAPMAN-ENSKOG 2000 ETHYLENE thermal conductivity vs temperature
CHAPMAN-ENSKOG 2000 ETHYLENE viscosity vs temperature
CHAPMAN-ENSKOG 2000 URANIUM-HEXAFLUORIDE viscosity vs temperature
DEFAULT TABLE     58 ALUMINUM enthalpy vs temperature
DEFAULT TABLE     59 ALUMINUM temperature vs enthalpy
DEFAULT TABLE     60 ALUMINUM specific heat vs temperature
DEFAULT TABLE     61 ALUMINUM thermal conductivity vs temperature
DEFAULT TABLE     62 ALUMINUM density vs temperature
DEFAULT TABLE     84 ALUMINUM-OXIDE enthalpy vs temperature
DEFAULT TABLE     85 ALUMINUM-OXIDE temperature vs enthalpy
DEFAULT TABLE     86 ALUMINUM-OXIDE specific heat vs temperature
DEFAULT TABLE     87 ALUMINUM-OXIDE thermal conductivity vs
                     temperature
DEFAULT TABLE     88 ALUMINUM-OXIDE density vs temperature
DEFAULT TABLE     63 CADMIUM enthalpy vs temperature
DEFAULT TABLE     64 CADMIUM temperature vs enthalpy
DEFAULT TABLE     65 CADMIUM specific heat vs temperature
DEFAULT TABLE     66 CADMIUM thermal conductivity vs temperature
DEFAULT TABLE     67 CADMIUM density vs temperature
DEFAULT TABLE     68 STAINLESS-STEEL-304 enthalpy vs temperature
DEFAULT TABLE     69 STAINLESS-STEEL-304 temperature vs enthalpy
DEFAULT TABLE     70 STAINLESS-STEEL-304 specific heat vs
                     temperature
DEFAULT TABLE     71 STAINLESS-STEEL-304 thermal conductivity vs
```

```
                    temperature
DEFAULT TABLE    72 STAINLESS-STEEL-304 density vs temperature
DEFAULT TABLE    73 LITHIUM-ALUMINUM enthalpy vs temperature
DEFAULT TABLE    74 LITHIUM-ALUMINUM temperature vs enthalpy
DEFAULT TABLE    75 LITHIUM-ALUMINUM specific heat vs temperature
DEFAULT TABLE    76 LITHIUM-ALUMINUM thermal conductivity vs
                    temperature
DEFAULT TABLE    77 LITHIUM-ALUMINUM density vs temperature
DEFAULT TABLE    78 URANIUM-ALUMINUM enthalpy vs temperature
DEFAULT TABLE    79 URANIUM-ALUMINUM temperature vs enthalpy
DEFAULT TABLE    80 URANIUM-ALUMINUM specific heat vs temperature
DEFAULT TABLE    81 URANIUM-ALUMINUM thermal conductivity vs
                    temperature
DEFAULT TABLE    82 URANIUM-ALUMINUM density vs temperature
DEFAULT TABLE    89 CARBON-STEEL enthalpy vs temperature
DEFAULT TABLE    90 CARBON-STEEL temperature vs enthalpy
DEFAULT TABLE    91 CARBON-STEEL specific heat vs temperature
DEFAULT TABLE    92 CARBON-STEEL thermal conductivity vs
                    temperature
DEFAULT TABLE    93 CARBON-STEEL density vs
```

The following constant properties table is available. If negative, then that property for that material is undefined.

DENSITY (KG/M**3)	MELT TEMP.(K)	LAT.HT.FUS. (J/KG)	LJ SIGMA (ANG)	LJ EPSILON (K)	MATERIAL
-1.0000E+03	-1.0000E+03	-1.0000E+03	-1.0000E+03	-1.0000E+03	WATER
-1.0000E+03	-1.0000E+03	-1.0000E+03	2.6410E+00	8.0910E+02	STEAM
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.7110E+00	7.8600E+01	AIR
-1.0000E+03	-1.0000E+03	-1.0000E+03	2.8270E+00	5.9700E+01	HYDROGEN
-1.0000E+03	-1.0000E+03	-1.0000E+03	2.5510E+00	1.0220E+01	HELIUM
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.5420E+00	9.3300E+01	ARGON
-1.0000E+03	-1.0000E+03	-1.0000E+03	2.9480E+00	3.9300E+01	DEUTERIUM
6.5000E+03	2.0980E+03	2.2500E+05	-1.0000E+03	-1.0000E+03	ZIRCALOY
5.6000E+03	2.9900E+03	7.0700E+05	-1.0000E+03	-1.0000E+03	ZIRCONIUM-OXIDE
1.0960E+04	3.1130E+03	2.7400E+05	-1.0000E+03	-1.0000E+03	URANIUM-DIOXIDE
7.9300E+03	1.7000E+03	2.6800E+05	-1.0000E+03	-1.0000E+03	STAINLESS-STEEL
5.1800E+03	1.8700E+03	5.9800E+05	-1.0000E+03	-1.0000E+03	STAINLESS-STEEL-OXIDE
2.5200E+03	2.7500E+03	5.0000E+05	-1.0000E+03	-1.0000E+03	BORON-CARBIDE
9.6894D+03	1.0750E+03	9.8000E+04	-1.0000E+03	-1.0000E+03	SILVER-INDIUM-CADMIUM
1.8210E+04	1.4060E+03	5.0250E+04	-1.0000E+03	-1.0000E+03	URANIUM-METAL
1.7300E+03	3.8660E+03	-1.0000E+03	-1.0000E+03	-1.0000E+03	GRAPHITE
-1.0000E+03	-1.0000E+03	-1.0000E+03	-1.0000E+03	-1.0000E+03	CONCRETE
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.4670E+00	1.0670E+02	OXYGEN
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.9410E+00	1.9520E+02	CARBON-DIOXIDE
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.6900E+00	9.1700E+01	CARBON-MONOXIDE
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.7980E+00	7.1400E+01	NITROGEN
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.4920E+00	1.1670E+02	NITRIC-OXIDE
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.8280E+00	2.3240E+02	NITROUS-OXIDE
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.0000E+00	6.0000E+02	AMMONIA

DENSITY (KG/M**3)	MELT TEMP.(K)	LAT.HT.FUS. (J/KG)	LJ SIGMA (ANG)	LJ EPSILON (K)	MATERIAL
-1.0000E+03	-1.0000E+03	-1.0000E+03	4.0330E+00	2.3180E+02	ACETYLENE
-1.0000E+03	-1.0000E+03	-1.0000E+03	3.7580E+00	1.4860E+02	METHANE
-1.0000E+03	-1.0000E+03	-1.0000E+03	4.1630E+00	2.2470E+02	ETHYLENE
-1.0000E+03	-1.0000E+03	-1.0000E+03	5.9670E+00	2.3680E+02	URANIUM-HEXAFLUORIDE
2.3650E+03	9.3300E+02	3.9780E+05	-1.0000E+03	-1.0000E+03	ALUMINUM
4,0000E+03	2.3270E+03	1.0700E+06	-1.0000E+03	-1.0000E+03	ALUMINUM-OXIDE
7.5900E+03	5.9400E+02	5.5000E+04	-1.0000E+03	-1.0000E+03	CADMIUM
7.7006D+03	1.7000E+03	2.6920E+05	-1.0000E+03	-1.0000E+03	STAINLESS-STEEL-304
2.3280E+03	9.1700E+02	3.9845D+05	-1.0000E+03	-1.0000E+03	LITHIUM-ALUMINUM
3.1819D+03	1.3380E+03	2.9000E+05	-1.0000E+03	-1.0000E+03	URANIUM-ALUMINUM
-1.0000E+00	-1.0000E+00	-1.0000E+00	2.5510E+00	1.0220E+01	GASA
7.7529E+03	1.8109E+03	2.7196E+05	-1.0000E+03	-1.0000E+03	CARBON-STEEL

7. Diagnostic and Error Messages

An error message is printed when the range of a property table is exceeded if extrapolation is not allowed. The material name, property name, independent variable value and acceptable range are printed. For example,

```
ERROR IN SUBROUTINE MPDFVL, CALLED FROM COR
ARGUMENT OUT OF RANGE FOR ZIRCALOY SPECIFIC HEAT VS TEMPERATURE
ARGUMENT =   2.70374D+02, RANGE =  2.73150D+02,  5.00000D+03
```

Noncondensible Gas (NCG) Package Users' Guide

Noncondensible gases (NCGs) in the Control Volume Hydrodynamics (CVH) package are modeled as ideal gases. The constant volume heat capacity is approximated as an analytic function of temperature. This document describes user input requirements for specifying a noncondensible gas to be present in calculation and defining or changing its equation of state.

More detailed information on the constitutive relations and the default values for the existing library of predefined noncondensible gases can be found in the NCG Reference Manual.

Contents

1. Introduction

Noncondensible gases in the Control Volume Hydrodynamics (CVH) package are modeled as ideal gases and are characterized by their molecular weight, energy of formation, and specific heat capacity at constant volume, c_v, calculated from the general analytic form

$$c_v(T) = c_{v0} + c_{v1}T + c_{v2}T^2 + c_{v3}T^3 + \frac{c_{vsqrt}}{\sqrt{T}} + \frac{c_{vm1}}{T} + \frac{c_{vm2}}{T^2} \qquad (1.1)$$

for the temperature range $T_{low} \le T \le T_{up}$, and held fixed at the boundary value for temperatures below T_{low} or above T_{up}. Each of the coefficients in Equation (1.1), as well as T_{low} and T_{up}, can be specified via user input.

All MELCOR calculations are assumed to involve water in the pool, liquid water in the atmosphere and water vapor in the atmosphere. Because of this, water in the pool (which may be two-phase) is automatically defined as material number one, referred to as "POOL", liquid water in the atmosphere is automatically defined as material number two, referred to as "FOG", and water vapor in the atmosphere is automatically defined as material number three, referred to as "H2O-VAP". Noncondensible gases must be defined by the user as higher numbered materials if desired for a calculation. A library of data for gases of interest is available for use. The available gases and their associated coefficients for Equation (1.1) are defined in the NCG Reference Manual, and include hydrogen (H2), oxygen (O2), carbon dioxide (CO2), carbon monoxide (CO), nitrogen (N2), methane (CH4), helium (HE), argon (AR), and deuterium (D2).

Only the thermal equation of state of noncondensible gases is defined by the NCG package. The thermal equation of state for water is defined by the H2O package and is based on the analytic expression for the Helmholtz function, $\psi(\rho,T)$, that was used to generate the Keenan and Keyes Steam Tables. Transport properties such as viscosity, thermal conductivity, and binary diffusivity are treated in the Material Properties (MP) package. In order to evaluate the viscosity and thermal conductivity of control volume atmospheres, those properties must be defined for all noncondensible gases present in the calculation. Input to the MP package is therefore required in any calculation involving user-defined gases (GASA through GASJ). In addition, the user has the option of modifying the properties used for gases in the NCG default library.

2. MELGEN User Input

The user must specify which noncondensible gases are in the calculation and any desired changes in the default coefficients and other constants defining the equation of state (called "material properties" below). Liquid and vapor water are always materials one, two

and three and do not need to be defined for a calculation. To include a material in the calculation, a record of the following form must be in the MELGEN input:

NCGnnn – Identifier Field
000 ≤ nnn ≤ zzz used for ordering
Required

The minimum amount of information is the MELCOR name and material number. Library data are used unless the user inputs the material property data. Material property data is input pairwise. The first data pair identifies the material property and the second is the material property value. An arbitrary number of data pairs may be input on a single record but a data pair may not be split across two records. More than one record may have the same MELCOR name and material number if more than one are required to define the material properties. Although they need not be defined in order, no gaps in the material numbers are allowed. Water and steam are always materials one through three. All data for user-defined gases GASA-GASJ must be input.

(1) MNAME - MELCOR material name, e.g., O2 for oxygen.
(type = character, default = none, units = dimensionless)

(2) MNUMBER - MELCOR material number. This material will be referred to by this number through the calculation.
(type = integer, default = none, units = dimensionless)

(3) MP NAME - Material property name. Refer to the following table of allowed material properties.
(type = character, default = none, units = dimensionless)

(4) MP VALUE - Material property value. Refer to the following table for units.
(type = real, default = none, units = depends on property)

.
.
.
additional MP NAME/VALUE pairs

Material Property Name	Units	Physical Interpretation
CV0	J/(kg K)	c_{v0} coefficient in $c_v(T)$
CV1	J/(kg K^2)	c_{v1} coefficient in $c_v(T)$
CV2	J/(kg K^3)	c_{v2} coefficient in $c_v(T)$
CV3	J/(kg K^4)	c_{v3} coefficient in $c_v(T)$

Material Property Name	Units	Physical Interpretation
CVSQRT	$J/(kg\sqrt{K})$	c_{vsqrt} coefficient in $c_v(T)$
CVM1	J/kg	c_{vm1} coefficient in $c_v(T)$
CVM2	(J K)/kg	c_{vm2} coefficient in $c_v(T)$
TLOW	K	T_{low} lowest temperature for fit to $c_v(T)$
TUP	K	T_{up} highest temperature for fit to $c_v(T)$
WM	kg/mol	molecular weight
EF	J/kg	e_f energy of formation
SZ	J/(kg K)	s_0 entropy at natural temperature (not used currently)

After all the records have been processed, all material numbers between 1 and the largest number used as a hydrodynamic material number in CVH input must be defined. (Of course, materials 1, 2, and 3 are automatically defined.) There can be no gaps in the material numbers. For example, if only materials one, two, three and six are defined, then an error will occur because materials four and five are not defined.

3. MELCOR User Input

Currently, the noncondensible gases database and models cannot be changed via MELCOR input.

4. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the MELCOR EXEC Users' Guide.

4.1 NCG Sensitivity Coefficients

Only one sensitivity coefficient is used. It is the temperature T_n that appears in the integral of specific heat $c_v(T)$ to determine the specific internal energy and enthalpy (see the NCG Reference Manual).

2090 – Natural Temperature

(1) - The lower temperature limit used in the integral of $c_v(T)$ to calculate specific internal energy and enthalpy.

(default = 298.15, units = K, equiv = none)

5. Plot Variables and Control Function Arguments

There are no plot variables or control function arguments for the NCG package.

6. Example Input

Materials one, two, and three are always water in the pool (may be two-phase), liquid water in the atmosphere (fog), and water vapor in the atmosphere, respectively. The example input set below defines four as hydrogen and material five as oxygen with a modified value for c_{v0} of 3000. Note that the sequencing order does not matter as long as there are no gaps in material numbers after completion of NCG processing.

```
NCG000     O2    5     CV0   3000.
NCG010     H2    4
```

7. Example Output

No example output is included in this document.

8. Diagnostic and Error Messages

Diagnostic and error messages can originate from bad user input. The messages will be self-explanatory.

Passive Autocatalytic Recombiner (PAR) Package Users' Guide

The MELCOR ESF Package models the phenomena for the various engineered safety features (ESFs) in a nuclear power plant. The Passive Autocatalytic Recombiner (PAR) package constitutes a subpackage within the ESF package, and calculates the removal of hydrogen from the atmosphere due to the operation of passive hydrogen reaction devises. This Users' guide provides basic information needed to run the PAR model with the rest of MELCOR, including a detailed explanation of the user input and package output for MELGEN, MELCOR, and HISPLT. Required and optional input, control function arguments, plot variables, and error messages are all covered.

More detailed information on the phenomenological modeling and numerical solution schemes implemented in the PAR package can be found in the PAR Package Reference Manual.

Contents

1. Introduction

The MELCOR ESF package models the thermal-hydraulic behavior of various engineered safety features (ESFs) in nuclear power plants. One such device is the passive autocatalytic hydrogen recombiner.

The MELCOR PAR model is based on the Fischer model (see the PAR Package Reference Manual), which is a parametric model developed for the most common PAR design. The user input provides correlation coefficients for the general mathematical form of the model. These coefficients are used by the code to calculate the total gas flow rate through a PAR unit. From the PAR gas flow rate together with user provided PAR efficiencies, transient relaxation times, delay times, and the internally calculated hydrogen mole fractions, a per-PAR-unit hydrogen reaction rate is calculated. This rate is then multiplied by the current timestep and the user provided number of active PAR units to determine the change in hydrogen, oxygen, and steam masses. These differential masses are then passed to CVH as source/sink terms.

2. Input Requirements

This section gives the input requirements for the MELCOR PAR package, including a short description of the input quantities and their units and default values, if any. Further description of the input variables and their meaning in the models can be found in the PAR Package Reference Manual.

Input record identifiers for the PAR model all begin with the character string "ESFPAR". Multiple hydrogen recombiner types can be specified, and input is grouped into sets for each hydrogen recombiner modeled, identified by the three digits "nnn".

2.1 MELGEN Input

ESFPARnnn00 – Hydrogen Recombiner Name
$1 \leq nnn \leq 999$, where nnn is the PAR number
Required

This record specifies a user-supplied name for the hydrogen recombiner for purposes of easy identification. This record is required. The following character field (limited to 16 characters) must be present:

(1) FPRNAM - PAR name.
(type = character*16, default = none)

ESFPARnnn01 – Hydrogen Recombiner Interface and Control Integers
$1 \leq$ nnn ≤ 999, where nnn is the PAR number
Required

This record specifies the control volume to which the PAR unit is interfaced, a control function/flag to switch between the basic model and a user provided model, and a control function/flag to switch between the constant efficiency and a user provided variable efficiency. This record is required, but only the first field must be present.

(1) IPAR - Hydrogen Recombiner control volume number.
(type = integer, default = none, units = none)

(2) IPROPT - Flag for selection of the Hydrogen Recombiner flow model. If this number is specified as zero, the basic Fischer model will be used. Otherwise this field should correspond to the identifier number of a control function that provides the PAR unit total gas volumetric flow rate.
(type = integer, default = 0, units = none)

(3) IETAPR - Flag for selection of the Hydrogen Recombiner efficiency model. If this number is specified as zero, a constant efficiency (EPAR, provided on the 02 record) will be used for the PAR efficiency. Otherwise this field should correspond to the identifier number of a control function that provides the PAR efficiency.
(type = integer, default = 0, units = none)

ESFPARnnn02 – Hydrogen Recombiner Parameters
$1 \leq$ nnn ≤ 999, where nnn is the PAR number
Optional

This record specifies the Fischer model flow rate correlation coefficients, the transient effect parameters and the PAR multiplicity. This record is optional, but if any of the fields require changes from default values, the entire set of six parameters must be supplied.

(1) APAR - Hydrogen Recombiner correlation coefficient.
(type = real, default = 0.67, units = m^3/s)

(2) BPAR - Hydrogen Recombiner exponential parameter.
(type = real, default = 0.307, units = none)

(3) EPAR - Hydrogen Recombiner efficiency.
(type = real, default = 0.85, units = none)

(4) TAUPAR - Hydrogen Recombiner transient relaxation time.
(type = real, default = 1800.0, units = s)

(5) TPARD - Hydrogen Recombiner operation delay time.
(type = real, default = 0.0, units = s)

(6) FPARD - Number of hydrogen recombiners of this type. Note that this does not have to be a whole number of units. The degraded operation of one or more units can be simulated by using a fraction of a PAR unit.
(type = real, default = 1.0, units = none)

ESFPARnnn03 – Hydrogen Recombiner Combustion Limit Data
$1 \leq nnn \leq 999$, where nnn is the PAR number
Required

This record specifies the on/off reactant concentration limits of the PAR unit. The first two fields specify the minimum hydrogen mole fraction for which the unit will start operating (startup point) and the minimum hydrogen mole fraction to which the unit will reduce the hydrogen concentration (shutoff point). The 3rd and 4th fields specify the same values for the oxygen concentration limits. This record is optional, but if any of the fields require changes from default values the entire set of four parameters must be supplied.

NOTE: Care must be exercised to ensure that the shutoff concentrations are always less than the startup concentrations. Also, due to lack of data, the default values used here are not technically defensible.

(1) HPAR0 - Minimum H_2 mole fraction for PAR startup.
(type = real, default = 0.02, units = none)

(2) HPARR - Minimum H_2 mole fraction for PAR shutdown.
(type = real, default = 0.005, units = none)

(1) OPAR0 - Minimum O_2 mole fraction for PAR startup.
(type = real, default = 0.03, units = none)

(2) OPARR - Minimum O_2 mole fraction for PAR shutdown.
(type = real, default = 0.005, units = none)

2.2 MELCOR Input

No input for the H_2 recombiner model is processed during MELCOR execution.

3. Sensitivity Coefficients

Because the required model parameters are all accessible through the input record, sensitivity coefficients for the Hydrogen Recombiner model are not required.

4. Plot Variables and Control Function Arguments

The plot variables and control function arguments currently included in the PAR model are listed below, along with a brief description. Within slashes (/ /) a 'p' indicates a plot variable and a 'c' indicates a control function argument.

ESF-PAR-DMH2.n	/pc/	Per PAR unit H_2 removal rate for PAR n. (units = kg/s)
ESF-PAR-INH2.n	/pc/	Total H_2 removed for all FPARD units of PAR n. (units = kg)
ESF-PAR-DVOL.n	/pc/	Per PAR unit total gas flow rate for PAR n. (units = m^3/s)
ESF-PAR-IVOL.n	/pc/	Total volume of gas processed in all FPARD units of PAR n. (units = m^3)
ESF-PAR-TOUT.n	/pc/	Outlet gas temperature for PAR n. (units = m^3/s)
ESF-PAR-FMOL.n	/pc/	Outlet gas H_2 mole fraction for PAR n. (units = m^3)

5. Example Input

The following are sample MELGEN input records for the PAR model. No MELCOR input records are necessary to run the PAR model.

```
*      PASSIVE AUTOCATALYTIC RECOMBINER INPUT
*
ESFPAR10100    'NISPAR1'
*
*               IPAR     IPROPT   IETAPR
ESFPAR10101     100       101      102
*
*                APAR      BPAR     EPAR    TAUPAR   TPARD   FPARD
ESFPAR10102      0.75     0.300     0.75    1800.0    0.0     20.0
*
*               HPAR0      HPARR     OPAR0     OPARR
ESFPAR10103     0.01       0.001      0.02     0.001
*
```

```
**
*
*        CONTROL FUNCTION FOR H2 RECOMBINER FLOW RATE
*
*        PAR GAS FLOW RATE USING FISHER MODEL (NO TRANSIENT)
*     FOR CONTROL VOLUME 100 @ HYDROGEN AS MATERIAL 6.
*
CF10100   'PAR-FLOW'   POWER-R  1  0.67  0.0
CF10103   0.307
CF10110   1.0  0.0  CVH-X.6.100
*
*
*        CONTROL FUNCTION FOR H2 RECOMBINER EFFICIENCY
*
*        PAR EFFICIENCY USING A CONSTANT
*
CF10200   'PAR-EFF'   EQUALS  1  1.0  0.0
CF10210   0.0  0.75  TIME
*
```

6. PAR Model Output

In general, the PAR model output is self-explanatory. The hydrogen removal rate, gas flow rate, total reacted hydrogen, total volume of processed gas, PAR outlet gas temperature and H_2 mole fraction are output for each PAR unit.

7. Diagnostic and Error Messages

Diagnostics and error messages generated during MELGEN are concerned with input processing and are generally self-explanatory. Currently, no messages are generated during MELCOR execution.

RadioNuclide (RN) Package
Users' Guide

This document includes a brief description of the models employed in the RadioNuclide (RN) package, detailed descriptions of the input format, discussion of the output, sensitivity coefficients, and plot variables, and example input for a typical plant calculation. Details on the various models employed in the RadioNuclide package can be found in the RN Package Reference Manual.

Contents

List of Tables

1. Introduction

The RadioNuclide (RN) package models the behavior of fission product aerosols and vapors and other trace species, including release from fuel and debris, aerosol dynamics with vapor condensation and revaporization, deposition on structure surfaces, transport through flow paths, and removal by engineered safety features. The package also allows for simplified chemistry controlled by the user.

Boundary conditions for the various models are obtained from other MELCOR packages: fluid conditions are obtained from the Control Volume Hydrodynamics (CVH) package, fuel and debris temperatures are obtained from the Core (COR) and Cavity (CAV) packages, and structure surface temperatures are obtained from the Heat Structures (HS) package. The COR and CAV packages also provide information regarding bulk debris relocation, allowing the RN package to perform relocation of unreleased fission products. Likewise, advection of radionuclides between control volumes is done using CVH flows, and wash-off of radionuclides deposited on heat structures is determined from drainage of water films calculated by the HS package. The RN package determines decay heat power for current radionuclide inventories from the Decay Heat (DCH) package when requested by both of these packages.

This document includes a brief description of the models employed in the RN package, detailed descriptions of the input format, discussion of the output, specification of the sensitivity coefficients, and plot variables, and example input for a typical plant calculation. Details on the various models employed in the RadioNuclide package can be found in the RN Package Reference Manual.

2. Description Of Models

The RadioNuclide (RN) package in MELCOR calculates the release and transport behavior of fission product vapors and aerosols. The models and concepts included in the RN package are discussed in detail in the RN Package Reference Manual. Only a brief overview is included in this section as a guide to understanding user input requirements.

2.1 General Framework

The RN package operates on the basis of material classes, which are groups of elements that have similar chemical properties. The number of classes is specified on the RN1001 input record, with a default of 16 classes. The grouping of the different elements into these classes is shown in Table 1. Classes are generally referred to by their class name or representative element. Combination of masses in these classes upon release to form compounds in other classes, such as Cs + I to CsI, is permitted subject to stoichiometric constraints (e.g., excess Cs is retained in the Cs class). For the RN package, the classes

must be in numerical order without any gaps. A maximum of 30 classes can presently be employed.

Some models in the RN package use groupings of elements different from the groupings defined in Table 1. Transfers of masses between various models must therefore use *mapping* strategies, which are described in the RN Package Reference Manual. These mappings may be changed with the input records described in Section 3.1.1.

Warning: If a class is redefined from the default values, or if a new class is added, all of the properties, including mappings, should be evaluated and possibly redefined through the RN sensitivity coefficients. Default values for these properties are defined based on the default elements in each class. Whether default values are appropriate when classes are modified must be determined by the user. Note that the DCH package might also have to be redefined in a consistent manner.

Table 1. RN Class Compositions

Class	Name	Representative	Member Elements
1	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	Alkaline Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	Halogens	I	F, Cl, Br, I, At
5	Chalcogens	Te	O, S, Se, Te, Po
6	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	Early Transition Elements	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10	Uranium	U	U
11	More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
12	Less Volatile Main Group	Sn	Ga, Ge, In, Sn, Ag
13	Boron	B	B, Si, P
14	Water	H_2O	H_2O
15	Concrete	- - -	- - -
16	Cesium iodide	CsI- - -	CsI- - -

2.2 Initial Radionuclide Inventories

Initial inventories and distributions of radionuclides must be specified for the core, for the cavity, and for control volume pools and atmospheres. (Inventories for some locations may

be zero initially.) Radionuclide masses can be distributed among core cells according to radial and axial decay heat power profiles in the core. In addition, a fraction of the radionuclides in a core cell can be designated as residing in the fuel-cladding gap.

Total radioactive class masses are normally determined by the DCH package from the operating power of the reactor and the mass of each element in the class per unit of operating power (see the DCH Package Reference Manual and Users' Guide). RN package input generally defines only the initial distribution of these masses in the core and cavity through reference values and multipliers specified on the RNFPNijjXX input records. However, options are provided to use these records to specify the class masses directly. These options are useful for analysis of experiments.

2.3 Release of Radionuclides

Release of radionuclides can occur from the core fuel (with nonradioactive releases from other core structures), from the fuel-cladding gap, and from material in the cavity. At present, no material can be released from the reactions treated in the FDI (fuel dispersal) package. The radionuclides residing in the COR package fuel are assumed to be in elemental form and therefore to have only radioactive mass (no associated molecular mass). Upon release from fuel, the total class masses are converted to compound form with a corresponding increase in mass from the added nonradioactive material (e.g., the hydroxide mass in CsOH). For core materials other than the fuel, such as the fuel rod cladding, the entire mass is nonradioactive.

Three options are currently available for the release of radionuclides from the core components; the CORSOR, CORSOR-M or CORSOR-Booth model may be specified on input record RNFP000. The CORSOR-BOOTH model contains low and high burn-up options. In addition, the CORSOR and CORSOR-M release rates can be modified to be a function of the component surface-to-volume ratio as compared to a base value, derived from the experimental data on which CORSOR is based. The reduction in release rate of the tellurium class by the presence of unoxidized zirconium is also modeled using the parameters in sensitivity coefficient array 7105.

By default the release models are used only to calculate the release of radioactive radionuclides from core fuel material (i.e. UO_2), which exists in the intact fuel component, in refrozen fuel material on other components and in particulate debris. However, the same release correlations can be used to calculate the release of nonradioactive structural material from core components at their individual temperatures (e.g. Zr from the cladding as a function of the cladding temperature), if the user provides optional input to override the default (refer to sensitivity coefficient array 7100).

The release model also can provide for the combination of different donor classes into a new class based on the elemental molecular weights. An example could be the combination upon release of Cs and I atoms to form CsI molecules, which is modeled by

moving stoichiometric amounts of Cs and I mass from the Cs and I classes into a new CsI class. The number of moles of each class that combine is defined by RNCLSNNXX input data. This combination occurs instantaneously upon release and is only limited by the availability of the released mass during that time step. If there is an excess of any donor class during the time step, that excess material stays in the original class.

It is assumed that the gaps in each radial ring can communicate axially between core cells, so when the cladding temperature in any core cell reaches or exceeds the cladding failure temperature specified for that cell, or when the cladding intact geometry has been lost, the entire gap inventory in that ring is released. A default temperature is provided, but may be overridden for any core cell using the RNGAPijj00 input record. This cladding failure temperature is only used in the RN package for gap releases and is not related to any COR package parameters.

For release of radionuclides from the cavity due to core-concrete interactions, the VANESA model has been implemented in MELCOR and is coupled to CORCON during every time step. If a water pool is present, pool scrubbing calculations are performed to apportion the released mass between the pool and the atmosphere.

2.4 Aerosol Dynamics

The calculation of aerosol agglomeration and deposition processes is based on the MAEROS computer code, but without direct inclusion of condensation or evaporation within the MAEROS solution framework. Vapor condensation on and evaporation from aerosol particles are handled separately to reduce the stiffness of the differential equation set and to ensure consistency with the calculation of these processes by other models and packages.

MAEROS is a multisectional, multicomponent aerosol dynamics code that evaluates the size distribution of each type of aerosol mass, or *component*, as a function of time. This size distribution is described by the mass in each size bin, or *section*, as depicted in Figure 2.4.1 of the RN Package Reference Manual. Each section may have a different chemical composition as described by the masses of various components for that section. In other words, a section is an aerosol size grouping and a component is a particular type of aerosol material.

Since MELCOR operates on a radionuclide class structure, a mapping between RN classes and MAEROS aerosol components must be specified by the user. The most accurate representation would be obtained with a one-to-one correspondence between classes and components. However, the computational cost of using 15 components in MAEROS can be high, and the increased accuracy is not thought to be justified, in general. Combination of the 15 material classes two MAEROS components is the current default. For a small increment in resources, the component representing only water droplets (class 14 aerosols) was added to improve the calculation of effects related to the condensation

and evaporation of water. Note that calculations with additional components can be performed for comparison, if desired.

Aerosols can directly deposit onto heat structure and water pool surfaces through a number of processes, including gravitational settling, diffusion to surfaces, thermophoresis (a Brownian process causing migration of particles toward lower temperatures), and diffusiophoresis (deposition induced by condensation of water vapor onto structural surfaces). All heat structure surfaces are automatically designated as deposition surfaces for aerosols using information from the HS package. The surface orientation can be changed or deposition on a surface can be disabled through user input on the RNDS record series.

Aerosols can also *settle* from one control volume to another through *flowthrough areas* (i.e., the gravitational settling and Brownian diffusion kernels in MAEROS described below are applied to flowthrough areas in addition to HS and pool surfaces). Such areas will ordinarily correspond to open flow paths between the control volumes, through which aerosols and radionuclide vapors are also advected. The appropriate flow area, path elevation, etc. are specified in the RNSETXXX input records. Aerosols are not transported through these areas if the flow path is blocked by a water pool.

Finally, aerosols can agglomerate and become larger than the user-specified maximum diameter. These aerosols are assumed to immediately deposit onto water pools or horizontal heat structure surfaces or to settle from one control volume to another through *flowthrough areas* defined as part of RN input. The term *fallout* in MELCOR is used exclusively for this immediate deposition or settling of aerosols larger than the maximum user-specified diameter. All control volumes must have at least one upward-facing deposition surface (floor) or flowthrough area defined to receive fallout aerosols generated by this mechanism. If there is more than one, fallout is distributed in proportion to the total area of each surface. During MELGEN a check is made for the existence of at least one such area; if none is present, an error message is generated and no restart file is written.

A number of time-dependent aerosol sources (specified on record RN1001) can also be specified for a control volume by the user (see the RNASXXX input record series). The aerosols can be put in either the control volume pool or atmosphere, with the time rate of the source specified by a tabular function.

2.5 Condensation/Evaporation and Hygroscopic Behavior

Fission products and water can condense onto or evaporate from aerosols, heat structure surfaces, and water pools. Aerosol water is identified with "fog" in the CVH package. The change in fog mass is determined by thermodynamics calculated within the CVH package and is then distributed over aerosol sections in the RN package by applying the Mason equation. Additionally, for water soluble aerosols, a solubility, or hygroscopic, effect is considered whereby the particles can grow by absorbing water vapor from moist,

unsaturated atmospheres. Water condensation and evaporation for heat structure and water pool surfaces are treated solely in the HS and CVH packages, respectively.

The condensation and evaporation of fission product vapors to and from heat structures, pool surfaces, and aerosols are evaluated in RN with the same equations as in the TRAP-MELT2 code. The fission product vapor masses in the control volume atmosphere and condensed on the aerosol and heat structure surfaces are determined by rate equations based on the surface areas, mass transfer coefficients, atmosphere concentration, and the saturation concentrations corresponding to the temperatures of the surfaces.

2.6 Decay Heat Distribution

The decay heat released by radionuclides in the control volume atmosphere and from those deposited on the various heat structure surfaces can be apportioned according to user specifications on the RNDH records. The apportionment is among the volume atmosphere, the surfaces of heat structures in that volume, and the pool surface (if a pool is present). Fractions may also be specified as going to the atmosphere and surfaces of other volumes to simulate decay radiation transmitted through flow paths. All decay heat released by radionuclides in a control volume pool is assumed to be absorbed by that pool.

An approximate correction is made for the reduced deposition of decay heat in small or low density atmospheres when the thickness becomes comparable to or less than the range of typical beta radiation from fission product decay.

2.7 ESF Models

Models are currently available for the removal of radionuclides by pool scrubbing, filter trapping, and spray scrubbing. These models are controlled by the parameters input on the RN2PLSXX, RN2FLTXXKK, and RN2SPRXX records. The normal RN deposition and condensation models, including a surface area enhancement factor, are applied to heat structures used to model ice condensers (see the HS Package Users' Guide).

The pool scrubbing models, adapted from the SPARC90 code, include the effects of steam condensation at the pool entrance and aerosol deposition by Brownian diffusion, gravitational setting, and inertial impaction, subject also to evaporative forces, for the rising bubble. Decontamination is calculated only for those flow paths activated on the FLnnn02 input record (see the FL Package Users' Guide). As further specified by the user on input record RN2PLSXX, the model treats regular flow paths that vent through pools, as well as gases generated by core-concrete interactions flowing through overlying pools. Iodine vapor is also scrubbed. See Section 2.7.1 of the RN Package Reference Manual.

The MELCOR RN package contains a simple filter model. When aerosols and vapors are transported through flow paths with the bulk fluid flow of pool and/or atmosphere calculated

by the CVH package, some fraction of the transported RN materials may be removed by the action of filters in the flow path. A single filter can remove either aerosols or fission product vapors, but not both. However, a flow path can contain more than one filter. The efficiency of each filter is defined by decontamination factors, specified by user input. By default, a single decontamination factor is applied to all RN classes *except* water, for which the default DF is 1.0. Additional user input may be used to modify the DF on a class-by-class basis, *including the water class.* The parameters for the filter characteristics are specified on the RN2FLTXXYY input record series.

The effect of filter mass loading on the flow resistance of the associated flow path may be modeled through user input. A maximum loading may be specified for each filter; when this loading is reached, no further RN materials will be removed (i.e., the DF is set to unity).

Several additional features are available to represent a variety of filter degradation and failure characteristics. These include radiolytic and thermal desorption of iodine (vapor) from charcoal filters, release of iodine from a charcoal filter due to charcoal combustion, and aerosol filter failure resulting from excessive mass loading. These models, developed for application of MELCOR to non-LWR plants, are not currently described in the RN Package Reference Manual.

The MELCOR Containment Sprays (SPR) package, which calculates the thermal-hydraulic behavior associated with spray systems, is coupled to the RadioNuclide package for the calculation of aerosol washout and atmosphere decontamination by the sprays. The spray model includes vapor adsorption and aerosol removal by diffusiophoresis, inertial interception and impaction, and Brownian diffusion. Aerosols and fission products removed by the sprays are deposited in the pool associated with the control volume or a user-specified sump pool.

2.8 Fission Product Chemistry

Chemistry effects can be simulated in MELCOR through the class reaction and class transfer processes using the RNRCTIIYY and RNTRNIIYY records. Reversible and irreversible reactions can be used to model adsorption, chemisorption, and chemical reactions. Only fission product vapors can react with surfaces and only vapors and ions produced from them can undergo chemical transformations in the pool.

2.9 Iodine Pool Chemistry Model

An iodine pool model has been implemented in MELCOR for use in predicting iodine in the containment atmosphere during the late phase of accident sequences. The model uses known iodine chemistry to predict what factors affect the iodine concentration in the atmosphere, while allowing for additional chemical reactions. In the containment atmosphere, where gas phase behavior is important, there are submodels relating the

radiolysis of the air and cable insulation to the generation of nitric acid and hydrochloric acid, respectively. On the structural surfaces, provision is made to account for the type of surface, thus allowing the extension to treat the effects of different paints and other surface coatings on iodine behavior. In the water pool, where liquid phase behavior is important, the model determines the pH based upon the user controlled boric acid and phosphate buffering, the effects of cesium hydroxide, cesium iodide and control rod silver released by the accident scenario chosen, and the effects of the acids introduced from the containment atmosphere due to radiolysis. The aqueous pool chemistry model then determines the speciation of iodine, particularly the important elemental, molecular, and organic forms, over the range of pH from 4 to 12. Thus, chemical systems that control pool pH can be examined as well as pools and films on surfaces that have no pH controls. With this combination of features, the iodine pool model provides the ability to conduct sensitivity studies and to incorporate new effects found in the course of ongoing research.

3. User Input

3.1 MELGEN Input

The input description for the RN package for MELGEN follows. As noted occasionally below, several input parameters define models or options not used with the LWR version of MELCOR, and which are not described in the LWR COR or RN reference manuals.

3.1.1 General Control, Options, and Mappings

These input records define various dimensions, options, and mappings that control the framework and structure of the models in the RN Package.

RN1000 Record – Activates RN Package
Optional

This record activates the RN package in MELCOR.

(1) IACTV - Activation switch for RN package.
= 0, RN package Active
= 1, RN package Not Active
(type = integer, default=1 (not active), units = none)

RN1001 Record – Dimension Record
Optional

This record defines the dimensions for the database. It specifies the size of the aerosol problem as well as the number of tabular input sources. The number of material classes cannot be greater than 30.

(1) NUMSEC - Number of sections in the aerosol calculation.
(type = integer, default=10, units = none)

(2) NUMCMP - Number of aerosol components.
(type = integer, default=2, units = none)

(3) NUMCLS - Number of material classes, must be the same as the number of classes specified in the DCH input.
(type = integer, default=15, units = none)

(4) NCLSW - Material class of water.
(type = integer, default=14, units = none)

(5) NCLSBX - Material class of B_2O_3.
(type = integer, default=13, units = none)

(6) NUMSRA - Number of tabular aerosol sources.
(type = integer, default=0, units = none)

(7) NUMSRV - Number of tabular vapor sources.
(type = integer, default=0, units = none)

(8) NCLCSI - Material class of CsI.
(type = integer, default=16, units = none)

(9) NUMCA - Number of chemisorption classes.
(type = integer, default=6, units = none)

RN1002 Record – Activates Hygroscopic Model
Optional

This record activates the hygroscopic model in MELCOR.

(1) IHYGRO - Activation switch for hygroscopic model.
= 0, hygroscopic model off
= 1, hygroscopic model on
(type = integer, default=0 (not active), units = none)

RN1003 Record – Additional array dimensions
Optional

(1) NCLS2 - Number of secondary RN classes.
(type = integer, default=0, units = none)

This parameter is the number of RN classes that do not get the full RN treatment. The secondary classes are transported, but do not vaporize or form aerosols. Any secondary classes must have ID numbers after the regular RN classes. This is not currently used but is reserved for future development.

(2) NCA2 - Number of extended deposition classes.
(type = integer, default=0, units = none)

This parameter is the number of additional surface deposition classes besides the chemisorption classes. Currently, the only model that uses these is the iodine pool model, for deposited iodine and methyl iodide on steel and painted surfaces, and for hydrochloric and nitric acid. If the iodine pool model is on, NCA2 must be at least 6 to account for the deposited iodine, methyl iodide, and nitric and hydrochloric acids. The classes used are:

1. deposited methyl iodine
2. chemically bound methyl iodine
3. deposited iodine
4. chemically bound iodine
5. nitric acid
6. hydrochloric acid

RN2001 Record – Options Record
Optional

(1) ICONV - Convection option switch.
= 0, Flow path convection of radionuclides will be calculated
= 1, Flow path convection will not be calculated
(type = integer, default=0, units = none)

RNCRCLXX Records – Core Material to RN Class Map
$00 \leq XX \leq 99$, XX is a sequencing parameter
Optional

The mapping of the nonradioactive core mass to the RN material class structure is determined by this input. This mapping is discussed in more detail in the model description section.

(1) ICRMT - Core material:
1 = fuel material in COR package,
2 = unoxidized Zirconium in COR package,
3 = oxidized Zirconium in COR package,
4 = control rod unoxidized steel in COR package,
5 = control rod oxidized steel in COR package,
6 = control rod poison in COR package,
(type = integer, default = see below, units = none)

(2) ICLSS - RN material class (see Table 1).
(type = integer, default = see below, units = none)

(3) FRAC - Fraction of the core material, ICRMT, that is in class ICLSS
(type = real, default = see below, units = none)

Default values are:

ICRMT	ICLSS	Fraction
1	10 (U)	1.0
2	8 (Ce)	1.0
3	8 (Ce)	1.0
4	7 (Mo)	1.0
5	7 (mo)	1.0
6	13 (B)	1.0 (for BWRs)
6	11 (Cd)	0.05 (for PWRs)
6	12 (Sn)	0.95 (for PWRs)

RNCLVNXX Records – RN Class to VANESA Group Map
$00 \leq XX \leq 99$, XX is a sequencing parameter
Optional

When debris enters the cavity, the associated radionuclides are converted to the VANESA group structure and maintained in that form until released from the melt. The mapping of the RN class masses to the masses in the VANESA structure is determined by this input. This input was provided for maximum flexibility to allow a user to redefine RN classes. Input should be consistent with the RN class structure; nondefault values should be used with great care, if at all. The complete list of VANESA group numbers is described in the RN Package Reference Manual.

(1) ICLSS - RN Material Class Number.
(type = integer, default = see below, units = none)

(2) ICLSSV - VANESA Group Number.
(type = integer, default = see below, units = none)

Default values are:

ICLSS	ICLSSV
1 (Xe)	27 (Xe; released instantaneously)
2 (Cs)	19 (Cs)
3 (Ba)	20 (Ba)
4 (I)	26 (I; immediately forms CsI)
5 (Te)	9 (Te)
6 (Ru)	6 (Ru)
7 (Mo)	5 (Mo)
8 (Ce)	23 (Ce)
9 (La)	22 (La)
10 (U)	17 (U)
11 (Cd)	8 (Sb)
12 (Sn)	7 (Sn)
13 (B)	(RN class not present in fuel)
14 (H_2O)	(RN class not present in fuel)
15 (Concrete)	(RN class not present in fuel)

Masses for RN classes 13, 14, and 15 are not present in the fuel, so no mapping is required for these classes.

RNVNCLXX Records – VANESA Group to RN Class Map
$00 \leq XX \leq 99$, XX is a sequencing parameter
Optional

On release, VANESA group masses are converted to RN class form. The mapping of the VANESA group masses to the RN class masses is input on this record series. This input was provided for maximum flexibility to allow a user to redefine RN classes. Input should be consistent with the RN class structure; non-default values should be used with great care, if at all. The complete list of VANESA group numbers is described in the RN Package Reference Manual.

(1) ICLSSV - VANESA Group Number
(type = integer, default = see below, units = none)

(2) ICLSS - RN Material Class Number
(type = integer, default = see below, units = none)

Default values are:

ICLSSV	ICLSS	ICLSSV	ICLSS
1 (gases)	none	14 (Na)	15 (concrete)
2 (Fe)	7 (Mo)	15 (K)	15 (concrete)
3 (Cr)	7 (Mo)	16 (Si)	15 (concrete)
4 (Ni)	6 (Ru)	17 (U)	10 (U)
5 (Mo)	7 (Mo)	18 (Zr)	8 (Ce)
6 (Ru)	6 (Ru)	19 (Cs)	2 (Cs)
7 (Sn)	12 (Sn)	20 (Ba)	3 (Ba)
8 (Sb)	11 (Cd)	21 (Sr)	3 (Ba)
9 (Te)	5 (Te)	22 (La)	9 (La)
10 (Ag)	12 (Sn)	23 (Ce)	8 (Ce)
11 (Mn)	7 (Mo)	24 (Nb)	7 (Mo)
12 (Ca)	15 (concrete)	25 (CsI)	2 (Cs) and 4 (I)
13 (Al)	15 (concrete)	26 (I)	None
		27 (Xe)	None

CsI (group 25) receives special treatment, as described in the RN Package Reference Manual. Bulk gases from CORCON (group 1) are released by the CAV package to the CVH package. I (group 26) is automatically combined with Cs by VANESA, and Xe (group 27) is released instantaneously by VANESA; no mapping is needed for these groups.

3.1.2 Initial Radionuclide Inventories

The initial inventories of radionuclides in the core, cavity, and control volumes are given by these records. These data determine the amount of decay heat in the core and cavity and, when released, the decay heat in the aerosols produced from the core and cavity. If these data are not input, there will be no decay heat in the problem from material released from the core or cavity. Decay heat will be generated for the initial radionuclide masses and from sources depending on the radioactive fractions specified. If the RN package is not active, the total decay heat value calculated by the Decay Heat Power (DCH) package will be split between the core and the cavity according to the amount of fuel in each location.

RNFPNijjXX Records – Initial Core Fuel and Cavity Radionuclide Inventories

Cavity record

i = 0, cavity input

$00 \le jj \le 99$, jj is the user-specified cavity number

$01 \le XX \le 99$, XX is a sequencing parameter

Core record
$1 \leq i \leq 9$, i is the core radial node number
$01 \leq jj \leq 99$, jj is the core axial node number
$01 \leq XX \leq 99$, XX is a sequencing parameter

Each record specifies the fission product mass in a given location or the multiplier on the total mass for each class. The total mass is the mass used in the Decay Heat package for each class except for class 10 (uranium), which is taken from the COR package data base (i.e., user-specified fuel distribution).

(1) NINP - Flag to determine type of input
(type = integer, default = none, units = none)
< 0, ABS(NINP) = ijj is the reference node for the radionuclide inventory in the present node, where i is the core radial ring number and jj is the core axial segment number for the reference node
= 0, use the total mass of each class as given in Decay Heat or Core package input
> 0, NINP is the class for the radionuclide mass read in on the next entry

(2) RINP1 - Variable which depends on value of NINP
(type = real, default = none, units = none or kg)
If NINP ≤ 0, Multiplier on this reference inventory for the present node, for example, an axial node multiplier
If NINP > 0, Initial radionuclide mass (in kg) of class NINP

(3) RINP2 - Multiplier on this reference inventory for the present node, for example, a radial node multiplier
(type = real, default = none, units = none)
If NINP ≤ 0, Mass = Mass (defined by NINP value) x RINP1 x RINP2
If NINP > 0, Mass = Mass (RINP1 value) x RINP2

The information on these records is additive.

RNGAPijjXX Records – Initial Fuel-Cladding Gap Inventory Fractions
$1 \leq i \leq 9$, i is the core radial node number
$01 \leq jj \leq 99$, jj is the core axial node number
$01 \leq XX \leq 99$, XX is a sequencing parameter
Optional

The amount of core radionuclide material in the gap region is specified on these records. Note that the <u>total</u> amount of radionuclides in the fuel and the gap is given

on the RNFPNijjXX record series. The present record series is used to distribute the total amount between the fuel and the gap. Upon cladding failure, the gap inventory of the entire radial ring is released to the appropriate control volume. In addition, any release of radionuclides from the fuel is held up in the gap until cladding failure. Therefore, a puff-type release is usually seen when the cladding fails.

(1) NINP - Flag to determine type of input
(type = integer, default = none, units = none)
< 0, ABS(NINP) is the reference node for the gap inventory fractions in the present node
> 0, NINP is the class for the gap fraction input on the next entry

(2) RINP1 - Variable that depends on the value of NINP
(type = real, default = none, units = none)
If NINP < 0, Multiplier on radioactive and total inventories in the reference node for the present node
If NINP > 0, Fraction of total node inventory of class NINP that is in the gap.

(3) RINP2 - Ratio of total mass to radioactive mass, if NINP > 0. If NINP < 0, this field must still be present, but it is ignored.
(type = real, default = none, units = none)

RNAGXXX Records – Initial Aerosol Masses in Atmosphere
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

These records allow the user to input an initial mass of aerosol in the gas phase (atmosphere) of any CVH control volume.

(1) IVOL - User-specified number of the control volume containing initial aerosol masses.
(type = integer, default = none, units = none)

(2) ICLSS - Class of input aerosol masses.
(type = integer, default = none, units = none)

(3) RFRAC - Radioactive fraction of the aerosol masses.
(type = real, default = none, units = none)

(4) XMASS(1) - Initial aerosol mass of class ICLSS in section 1 in atmosphere of control volume IVOL.
(type = real, default = none, units = kg)

...
...
(N+3) XMASS(N)
- Initial aerosol mass of class ICLSS in section N in atmosphere of control volume IVOL.
(type = real, default = none, units = kg)

A total of NUMSEC values is required. This list may be continued on additional RNAGXXX records.

Input from multiple RNAGXXX records for the same control volume and class is additive.

RNALXXX Records – Initial Aerosol Masses in Pool
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

These records allow the user to input an initial mass of aerosol in the liquid phase (pool) of any volume.

(1) IVOL - User volume for input masses.
(type = integer, default = none, units = none)

(2) ICLSS - Class of input aerosol masses.
(type = integer, default = none, units = none)

(3) RFRAC - Radioactive fraction of masses.
(type = real, default = none, units = none)

(4) XMASS - Initial aerosol mass of class ICLSS in pool of volume IVOL.
(type = real, default = none, units = kg)

Input from multiple RNALXXX records for the same control volume and class is additive.

RNVGXXX Records – Initial Fission Product Vapor Masses in Atmosphere
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

Initial fission product vapor masses in the atmosphere can be input on these records.

(1) IVOL - User volume for input masses.
(type = integer, default = none, units = none)

(2) RFRAC - Radioactive fraction of masses.
(type = real, default = none, units = none)

(3) XMASS(1) - Initial vapor mass of class 1 in atmosphere of control volume IVOL.
(type = real, default = none, units = kg)

...
...
(N+2) XMASS(N)
- Initial vapor mass of class N in atmosphere of control volume IVOL.
(type = real, default = none, units = kg)

A total of NUMCLS values is required in the class order specified in Table 1. This list may be continued on additional RNVGXXX records.

Input from multiple RNVGXXX records for the same control volume is additive.

RNVLXXX Records – Initial Fission Product Vapor Masses in Pool
$000 \leq XXX \leq 999$, XXX is a sequencing parameter
Optional

Initial fission product vapors in the pool can be input through these records.

(1) IVOL - User volume for input masses.
(type = integer, default = none, units = none)

(2) RFRAC - Radioactive fraction of masses.
(type = real, default = none, units = none)

(3) XMASS(1) - Initial vapor mass of class 1 in pool of control volume IVOL.
(type = real, default = none, units = kg)

...
...
(N+2) XMASS(N)
- Initial vapor mass of class N in pool of control volume IVOL.
(type = real, default = none, units = kg)

A total of NUMCLS values is required in the class order specified in Table 1. This list may be continued on additional RNVLXXX records.

Input from multiple RNVLXXX records for the same control volume is additive.

3.1.3 Release Model Parameters

RNFP000 Record – Core Release Model
Optional

(1) ICRLSE - Release model indicator for the core
(type = integer, default = -2, units = none)

For oxide fuels, ICRLSE is interpreted as follows:

= -1, original CORSOR model with surface-to-volume ratio option
= 1, original CORSOR model without surface-to-volume ratio option
= -2, CORSOR-M model with surface-to-volume ratio option
= 2, CORSOR-M model without surface-to-volume ration option
= -3, CORSOR-Booth model for high burn-up fuel
= 3, CORSOR-Booth model for low burn-up fuel

WARNING: The default coefficients used in all of the CORSOR models are for the 15 default material classes. For material class definitions other than the default specification, the user may need to alter the CORSOR models through sensitivity coefficients (7101 through 7107). The corresponding Vapor Pressure (7110), Vapor Diffusivity (7111) and Class Molecular Weights (7120) sensitivity coefficient arrays may also need to be altered for consistent release modeling. DCH package input must also be modified in a consistent manner.

For metallic fuels, oxidation-based releases are always calculated. The following interpretations for ICRLSE are used to determine how non-oxidation based releases are calculated. These models are not used in the LWR version of MELCOR.

= 0, no non-oxidation based releases calculated
= 1, non-oxidation releases based on the Birney model applied to the original radionuclide inventory (linear release over time).
= -1, non-oxidation releases based on the Birney model applied to the time-dependent inventory (exponential release over time).
= 2, non-oxidation releases using an Arrhenius model applied to the original inventory (linear release over time).

= -2, non-oxidation releases using an Arrhenius model applied to the time-dependent inventory (exponential release over time).

RNGAPijj00 Record – Gap Release Temperature
$1 \leq i \leq 9$, i is the core radial node number
$01 \leq jj \leq 99$, jj is the core axial node number
$00 \leq XX \leq 99$, XX is a sequencing parameter
Optional

(1) CLFAIL - Cladding failure temperature for gap release for core cell ijj.
(type = real, default=1173., units = K)

If CLFAIL = -1, the cladding does not fail until the core cell goes from intact geometry to debris geometry.

RNCLSNNXX Records – Parameters for Class Combination at Release
$00 \leq NN \leq 99$, NN is an arbitrary ID for the class combination
$00 \leq XX \leq 99$, XX is a sequencing parameter
Optional

These records specify the combination of masses in one or more donor classes into a new acceptor class, e.g., masses from the Cs and I classes into the CsI class. This combination is only applied to masses at initial release from core materials.

RNCLSNN00 (i.e., XX = 00)

(1) NCLCN - Acceptor class number
(type = integer, default = none, units = none)

RNCLSNNXX ($01 \leq XX \leq 99$)

(1) NCLSD - Donor class number
(type = integer, default = none, units = none)

(2) XMRAT - Ratio of the number of moles transferred from the donor class to the number of moles received by the acceptor class (e.g., 1.0 for Cs or I to CsI).
(type = real, default = none, units = none)

3.1.4 Aerosol Modeling Parameters

RN1100 Record – Aerosol Sectional Parameters
Optional

This record determines the size boundaries and nominal density for the aerosol calculations. If this record is input, and if the aerosol coefficients are read in on the RNCFXXX record series, the values are checked to see if valid aerosol coefficients have been read in. If not, the code will abort in MELGEN. If the coefficients are calculated, the values on this record will be used to perform the coefficient evaluation.

(1) DMIN - Lower bound aerosol diameter.
(type = real, default = 0.1E-6, units = m)

(2) DMAX - Upper bound aerosol diameter.
(type = real, default = 50.E-6, units = m)

(3) RHONOM - Nominal density of aerosols.
(type = real, default = 1000., units = kg/m^3)

RNACOEF Record – Aerosol Coefficients
Optional

In general, the aerosol coefficients are calculated by the code. In order to facilitate the use of these coefficients in subsequent calculations, the values can be read in. If the coefficients are calculated as determined by the RNACOEF record, the RNCFXXX record series values are written out to file ACOEFF by MELCOR. The coefficients can be read in with a redirected input file (R*I*F) mode.

(1) ICOEFF - Index for the aerosol coefficients calculation,
(type = integer, default = -1, units = none)

= 1, Calculate the coefficients
= -1, Read in the coefficients on the RNCFXXX record series (default)

On modern computers, where CPU usage is not a problem, the +1 option should be routinely used since it eliminates file handling errors.

RNPT000 Record – Conditions for Aerosol Coefficients
Optional

This information determines the conditions at which aerosol coefficients are evaluated. The coefficients are evaluated in MELGEN at each of the four combinations of low and high pressures and temperatures specified on this record (i.e., low-T/low-P, low-T/high-P, high-T/low-P, and high-T/high-P). Bilinear interpolation is then used to calculate values of the aerosol coefficients for intermediate values of pressures and temperatures calculated by the code. If the conditions are outside of the range of these coefficients, the end values are used (i.e., no extrapolation is performed).

(1) PGAS1 - Lowest gas pressure for coefficients.
(type = real, default = 1.0E5, units = Pa)

(2) PGAS2 - Highest gas pressure for coefficients.
(type = real, default = 2.0E7, units = Pa)

(3) TGAS1 - Lowest gas temperature for coefficients.
(type = real, default = 273., units = K)

(4) TGAS2 - Highest gas temperature for coefficients.
(type = real, default = 2000., units = K)

RNCFXXX Record Series – Aerosol Coefficient Input
$000 \leq XXX \leq 999$, where XXX is a sequencing parameter
Optional

This information is calculated first by the code. It may be reinput through this record series for subsequent calculations. See the discussion for the RNACOEF record for more information.

RNCFDS Record

(1) NCOFG - Number of sections used to generate the aerosol coefficients on Record Series RNCFXXX.
(type = integer, default = none, units = none)

(2) DMING - Lower bound diameter used in generation of aerosol coefficients.
(type = real, default = none, units = m)

(3) DMAXG - Upper bound diameter used in generation of aerosol coefficients.
(type = real, default = none, units = m)

(4) RHOG - Nominal density used in generation of aerosol coefficients. (type = real, default = none, units = kg/m^3)

RNCFPT Record

(1) PGAS1G - PGAS1 used in generation of coefficients. (type = real, default = none, units = Pa)

(2) PGAS2G - PGAS2 used in generation of coefficients. (type = real, default = none, units = Pa)

(3) TGAS1G - TGAS1 used in generation of coefficients. (type = real, default = none, units = K)

(4) TGAS2G - TGAS2 used in generation of coefficients. (type = real, default = none, units = K)

RNCFXXX Records

(1) ACF - Aerosol coefficient. (type = real, default = none, units depend on the particular coefficient generated in MELGEN; see the RN Package Reference Manual)

RNMS000 Record – Miscellaneous Aerosol Dynamics Constants
Optional

The miscellaneous coefficients used for the aerosol dynamic processes are input on this record.

(1) CHI - Aerosol dynamic shape factor. (type = real, default = 1.0, units = none)

(2) GAMMA - Aerosol agglomeration shape factor. (type = real, default = 1.0, units = none)

(3) FSLIP - Particle slip coefficient. (type = real, default = 1.257, units = none)

(4) STICK - Particle sticking coefficient. (type = real, default = 1.0, units = none)

(5) TURBDS - Turbulence dissipation rate. (type = real, default = 0.001, units = m^2/s^3)

(6) TKGOP - Ratio of the thermal conductivity of the gas over that for the particle.
(type = real, default = 0.05, units = none)

(7) FTHERM - Thermal accommodation coefficient.
(type = real, default = 2.25, units = none)

(8) DELDIF - Diffusion boundary layer thickness.
(type = real, default = 1.0E-5, units = m)

If desired, these data can be split between two records with ID's of RNMS000 and RNMS001 with four parameters on each record.

RNCCXXX Records – Class/Component Map
000 ≤ XXX ≤ 999, XXX is arbitrary, and only the lowest-numbered record will be read.
Optional

This record determines the mapping between the material classes, NUMCLS, and the aerosol components, NUMCMP. If NUMCMP = 1 (*which is not the default, nor is it recommended*), all classes are assigned to component 1. If NUMCMP > 1, the code by default places water class (class NCLSW) alone in component 2. If NUMCMP > 2, the code by default assigns the volatiles, Cs, I and CsI (NCLI2, NCLCS, and NCLCSI) to component 3. If NUMCMP > 3, there are no default assignments to the additional components. A warning will be issued during initialization if any component has no material classes assigned to it.

(1) IX(1) - Aerosol component number of material class 1
. . .
. . .
. . .
(N) IX(N) - Aerosol component number of material class N

If any IX values are input, then NUMCLS values are required.
[type = integer, default = as described, units = none]

RNDSXXX Records – Radionuclide Deposition Surfaces
000 ≤ XXX ≤ 999, where XXX is a sequencing parameter
Optional

Heat structure surfaces are also deposition surfaces for radionuclides, and are defined by HS package input. The RN Package Reference Manual details the default orientations of heat structures as used for deposition purposes in RN. These

records are used to override the heat structure information; the orientation can be altered or heat structure surfaces designated as inactive for deposition.

(1) IDS - User heat structure number defined in the HS input.
(type = integer, default = none, units = none)

(2) ISDE - Desired surface of heat structure.
(type = character, default = none, units = none)

= LHS, Left side of heat structure
= RHS, Right side of heat structure

(3) ITYP - Orientation of heat structure surface for deposition of radionuclides,
(type = character, default = as defined in HS input, units = none)

= CEILING, Ceiling
= WALL, Vertical Wall
= FLOOR, Floor
= INACTIVE, Not a Deposition Surface

RNSETXXX Records – Flowthrough Areas for Intervolume Transport
$000 \leq XXX \leq 999$, XXX is a sequencing parameter
Optional

These records specify the area available for the settling of aerosols from volume to volume without bulk flow. For example, if the floor of a control volume is an arbitrary boundary, specification of a flowthrough area will allow aerosols to settle through this arbitrary boundary. This settling is in addition to, and independent of, transport by intervolume flow.

(1) IVOLF - User control volume number for the *from* volume,
(type = integer, default = none, units = none)

(2) IVOLT - User control volume number for the *to* volume.
(type = integer, default = none, units = none)

(3) ELEV - Elevation of the flowthrough area.
(type = real, default = none, units = m).
If the water level is above this elevation, no transport occurs.

(4) AREA - Area for the transport.
(type = real, default = none, units = m^2)

WARNING: If IVOLF and IVOLT are defined as the same control volume, i.e., the volume settles into itself, physically unrealistic results may be calculated. Currently, when the pool disappears from any such volume the aerosols that were suspended in the liquid are resuspended in the largest section of the gas phase aerosol and allowed to settle where they will. Similarly, vapors that were held in the liquid phase are put into the gas phase. Users are encouraged to always provide a heat structure at the bottom of a control volume onto which vapors and aerosols can deposit. This should result in the most realistic treatment of fission products.

RNASXXX Records – Aerosol Source Records
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
NUMSRA sets required

A source of aerosol mass can be input with these records, defined by a tabular or control function. If the source is directed to the liquid phase (pool) and none is present, the source will be accumulated and added to the pool if it reappears.

(1) IVOL - User volume for aerosol source.
(type = integer, default = none, units = none)

(2) IPHS - Phase to receive aerosol source mass.
(type = integer, default = none, units = none)

= 1, Liquid phase (pool)
= 2, Vapor phase (atmosphere)

(3) ICLSS - Class of aerosol source.
(type = integer, default = none, units = none)

(4) RFRS - Radioactive fraction of mass source.
(type = real, default = none, units = none)

(5) XM - Mass addition rate, multiplies the value of tabular or control function specified by ITAB below.
(type = real, default = none, units = kg/s)

(6) ITAB - Definition of the time dependence of the mass addition rate XM.
(type = integer, default = none, units = none)

> 0, use tabular function ITAB
< 0, use control function |ITAB|

(7) IDIST - Sectional distribution parameter, only necessary for atmosphere sources (IPHS = 2).
(type = integer, default = none, units = none)

= 1, Uniform source with respect to log diameter (i.e., log uniform), no additional values

= 2, Log-normal distribution with respect to log diameter, 2 additional values described below needed on new record (add 1 to XXX).

(7A) GEOMM - Source mean diameter (also denoted AMMD), if greater than zero the value is the mass median diameter, if less than zero, the absolute value is the geometric mean diameter
(type = real, default = none, units = m)

(7B) GSD - Source geometric standard deviation
(type = real, default = none, units = none)
= 3, Section by section distribution specified, NUMSEC additional values for FRC below needed on new record (add 1 to XXX)

(7A) FRC - Fraction of source in each section, values are normalized after they are read.
(type = real, default = 1.0, units = none)

RNARXXX Records – Aerosol Resuspension Parameters
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

The size distribution of resuspended aerosols is determined by this input. Because no resuspension models are currently included in MELCOR, this input will not be used.

(1) IDISTP - Distribution parameter.
(type = integer, default = 3, units = none)

= 1, Uniform distribution with respect to log diameter, or log uniform, no additional values

= 2, Lognormal distribution with respect to log diameter, 2 additional values needed on new record

E(1A)GEOMM Source mean diameter (also denoted AMMD), if greater than zero, the value is the mass median diameter, if less than zero, the absolute value is the geometric mean diameter
(type = real, default = none, units = m)

D (1B) GSD Geometric standard deviation.
(type = real, default = none, units = none)

= 3, Section by section distribution specified, NUMSEC additional values needed on new record

C (1A) FRC Mass fraction of resuspended aerosols in each section, values are normalized after they are read
(type = real, default=1.0, units = none)

3.1.5 Condensation/Evaporation Models

RNACOND Record – Aerosol Condensation Index
Optional

This record determines whether water will condense on all aerosol particles or just on aerosol particles containing water (see Section 2.5.1 of the RN Package Reference Manual). If ICOND = 0 (the default), condensation of water on all aerosol particles will be evaluated. If ICOND = 1, water will condense only on aerosol particles containing water (i.e., CVH "fog"). For either process, the amount of water that condenses on existing particles can be rate-limited. If this is the case, any excess water that must condense to maintain thermodynamic equilibrium (saturation) conditions is added to the aerosol distribution in the smallest size section. For evaporation, no rate limitation is applied; as much water will evaporate as is necessary to maintain saturation. The total amount of water that condenses or evaporates during a time step is determined by the CVH package.

(1) ICOND - Index for condensation calculations in aerosol dynamics.
(type = integer, default = 0, units = none)

= 0, Condensation onto all existing aerosols is evaluated (default)

= 1, Condensation only onto existing water aerosols (CVH "fog")

RNVSXXX Records – Vapor Source Records
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
NNSRV sets required

Sources of fission product vapors are input on this record series.

(1) IVOL - User volume for vapor source.
(type = integer, default = none, units = none)

(2) IPHS - Phase for vapor source.
(type = integer, default = none, units = none)

= 1, Liquid phase
= 2, Gas phase

(3) ICLSS - Class of vapor source.
(type = integer, default = none, units = none)

(4) RFRC - Radioactive fraction of mass source.
(type = real, default = none, units = none)

(5) XM - Mass addition rate, time dependence is included through the tabular or control function specified by ITAB below.
(type = real, default = none, units = kg/s)

(6) ITAB - Definition of the time dependence of the mass addition rate XM.
(type = integer, default = none, units = none)

> 0, use tabular function ITAB
< 0, use control function |ITAB|

3.1.6 Decay Heat Distribution

Decay heat generated by radionuclides residing in the control volume atmosphere or on heat structure surfaces in a control volume is distributed among the volume atmosphere, the surfaces of heat structures in that volume, the pool surface (if a pool is present), and the atmospheres and surfaces of other control volumes, as defined by the following input. Splits are the same for all classes.

RNDHLENXXX Records – Length for Absorption of Decay Betas
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

Deposition of decay heat in a volume atmosphere results primarily from absorption of beta radiation. The fractions specified by SPVOL1 (Record RNDHVXXX) or SPSUR2 (Record RNDHSXXX) are interpreted as the values appropriate for complete absorption. They must be reduced for small volumes or low densities, where the thickness of the atmosphere is insufficient to permit complete absorption of beta rays. The fractions absorbed are based on the range of a typical beta ray (given in sensitivity coefficient array 7002), and the characteristic path for absorption in the control volume, specified on this record. Any reduced deposition is compensated for by proportionate increase in energy distributed to other components specified by the parameters SPVOL2-SPVOL4 or SPSUR3-SPSUR5 entered on the RNDHVXXX or RNDHSXXX input records or their default values. (The calculation is bypassed if the sum of these other split coefficients is zero.)

(1) IVOL - User-specified control volume number.
(type = integer, default = none, units = none)

(2) CVPATH - Characteristic path for absorption of beta radiation in control volume.
(type = real, default = MIN(VOLUME$^{1/3}$, CVARA$^{1/2}$), units = m)

VOLUME is defined by the volume/altitude table (CVnnnBk records) and CVARA is the volume flow area (CVnnn03 record, or its default).

RNDHVXXX Records – Decay Heat Split for Control Volumes
000 ≤ XXX ≤ 999
Optional

The split of the decay heat from radionuclides in the volume atmosphere is specified on these records. The decay heat may go to any heat structures or other volumes depending on the data. All the decay heat from radionuclides in the water stays in the water phase.

(1) IVOL - User control volume number.
(type = integer, default = none, units = none)

(2) SPVOL1 - Fraction of the atmosphere decay heat that goes to the control volume atmosphere.
(type = real, default = 0.50, units = none)

(3) SPVOL2 - Fraction of the atmosphere decay heat that goes to the surfaces in that volume.
(type = real, default = 0.50, units = none).

Note that surfaces include the heat structures that are exposed to the atmosphere as well as the surface of the pool, and that surface area weighting is used.

(4) SPVOL3 - Fraction of the atmosphere decay heat that goes to other volumes,
(type = real, default = 0.0, units = none).

The details of this split are given by the RNDHVSXXX Records.

(5) SPVOL4 - Fraction of the atmosphere decay heat that goes to other heat structure surfaces.
(type = real, default = 0.0, units = none).

The details of this split are given by the RNDHVSXXX Records.

RNDHVSXXX Records – Control Volume Decay Heat Split to Other Components
$000 \leq XXX \leq 999$, XXX is a sequencing parameter
Optional

These records are only needed if the RNDHVXXX Records specify that decay heat goes to other control volumes or heat structures not in the control volume where the heat is released, i.e., if SPVOL3 and/or SPVOL4 are non-zero. In this case, this record series specifies which other control volumes or heat structures receive decay heat.

(1) IVOL - User-specified control volume number for the source of decay heat.
(type = integer, default = none, units = none)

(2a) ID1 - ID of the receiving component.
This is either a user-specified control volume number or a user-specified heat structure number. If the latter, an extra field is required (ID2 below) to specify the left or right surface (thus requiring four fields total for this input record).
(type = integer, default = none, units = none).

(2b) ID2 - If input, ID2 is the pointer to the correct surface of the heat structure.
(type = integer, default = none, units = none).

= -1, Left side of heat structure.
= 1, Right side of heat structure

(3) FRAC - Fraction of the split decay heat that goes to control volume ID1 or heat structure surface ID1/ID2.
(type = real, default = 0.00, units = none).

These values should sum to 1.0 for each volume and/or heat structure subset.

RNDHSXXX Records – Decay Heat Split for Heat Structures
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

These records determine the split of the decay heat from radionuclides on heat structure surfaces. The decay heat may be split between the heat structure itself, the atmosphere in the associated control volume, other surfaces in that volume, and neighboring volumes and heat structures.

(1) IDHS1 - User-specified heat structure number.
(type = integer, default = none, units = none)

(2) IDHS2 - Pointer to surface of heat structure on which decay occurs.
(type = integer, default = none, units = none)

= -1, Left side of heat structure
= 1, Right side of heat structure

(3) SPSUR1 - Fraction of the surface decay heat that goes to that surface.
(type = real, default = 0.50, units = none)

(4) SPSUR2 - Fraction of the surface decay heat that goes to the atmosphere of the control volume in which the surface resides.
(type = real, default = 0.25, units = none)

(5) SPSUR3 - Fraction of the surface decay heat that goes to other surfaces in that volume, including the pool if present, using surface area weighting.
(type = real, default = 0.25, units = none)

(6) SPSUR4 - Fraction of the surface decay heat that goes to the atmosphere of other control volumes.
(type = real, default = 0.00, units = none).

Details of the split are given by the RNDHSS Records.

(7) SPSUR5 - Fraction of the surface decay heat that goes to heat structure surfaces in other control volumes.
(type = real, default = 0.00, units = none).

Details of the split are given by the RNDHSS Records.

RNDHSSXXX Records – Surface Decay Heat Split to Other Components
000 ≤ XXX ≤ 999, XXX is a sequencing parameter
Optional

These records are only needed if the RNDHSXXX Records specify that decay heat goes to the atmospheres of other control volumes or to heat structures in other control volumes, i.e., if SPSUR4 and/or SPSUR5 are nonzero. In that case, this record series specifies which other volumes or heat structures receive decay heat.

(1) IDHS - User heat structure number for the source of decay heat.
(type = integer, default = none, units = none)

(2) IDHS2 - Pointer to side of heat structure.
(type = integer, default = none, units = none).

= -1, Left side of heat structure
= 1, Right side of heat structure

(3a) ID1 - ID of the receiving component.
This is either a user-specified control volume number or a user-specified heat structure number. If the latter, an extra field is required (ID2 below) to specify the left or right surface (thus requiring five fields total for this input record).
(type = integer, default = none, units = none).

(3b) ID2 - If input, ID2 is the pointer to the correct surface of the heat structure.
(type = integer, default = none, units = none).

= -1, Left side of heat structure.
= 1, Right side of heat structure

(4) FRAC - Fraction of the split decay heat that goes to control volume ID1 or heat structure surface ID1/ID2.
(type = real, default = 0.00, units = none).

These values should sum to 1.0 for each volume and/or heat structure subset.

3.1.7 ESF Parameters

RN2PLSXX Record – Pool Scrubbing Record
00 < XX < 99, XX is a sequencing parameter

Pool scrubbing of aerosols and/or iodine vapor can be treated for all flow paths and flow directions for which the RN SPARC model is enabled (see IBUBF and IBUBT on the FL Package FLnnn02 record), and for all gas flows from the cavity model which have RN aerosol and/or iodine vapor scrubbing enabled (see input record CAVnn00). This input allows the user to vary the parameters used in each such application of the model.

(1) FPPLS - Pool scrubbing user flow path number. Regular flow paths and cavity water pools can be handled as discussed below.
Regular Flow Paths – If the number is negative, the pool scrubbing parameters apply in the *from* volume. If the number is positive, the parameters are for the *to* volume.
Cavity Water Pools – The flow path number for a cavity water pool is 1000 plus the cavity number.
(type = integer, default = none, units = none)

(2) AVENT - Flow area of the vent (or individual holes in multi-hole vents)
(type = real, default = FLARA (FL Package) for regular Flow Paths and a CORCON calculated value for Cavity Water Pools, units = m^2)

(3) MVENT - Type of vent (1=multi-hole sparger/quencher, 2=downcomer, 3=horizontal vent).
(type = integer, default = 3, units = none)

(4) NVENT - Number of holes in the vent (usually 1 except for vents of type MVENT=1).
(type = integer, default = 1, units = none)

(5) NTYPE - Number of identical vents in use (normally 1).
(type = integer, default = 1, units = none)

RN2FLTXXYY Record Series – Filter Parameters
01 < XX < 99, XX is the user filter number
YY is a record identifier
Optional

RN2FLTXX00 – Filter Specification

This record gives the location of the filter and the performance characteristics for the filter.

(1) IFLTFP - Filter user flow path number. The filter is located in this flow path for aerosol and fission product vapor removal.
(type = integer, default = none, units = none)

(2) CTYPE - Type of filter. Removal of either aerosols or fission product vapors is given by this parameter. The character string AEROSOL means that aerosols will be removed while the string FPVAPOR removes fission product vapors.
(type = character, default = none, units = none)

(3) DFG - Global decontamination factor for the filter.

DFG ≡ (mass entering filter) / (mass not removed by filter) must be ≥ 1.0

This decontamination factor is used for all classes but water, except as modified below by the RN2FLTXXKK records. The value for the water class is 1.0, regardless of the value of DFG, unless another value is specified for the water class on a RN2FLTXXKK record.
(type = real, default = 1.0, units = none)

(4) XMASG - Limit on total mass removed by the filter. If the value is negative, there is no total mass limit.
(type = real, default = – 1.0, units = kg)

(5) ICVTYP - Control volume type associated with the filter for editing and accounting purposes. Normally, this entry should be the same as the ICVTYP entry on the CVnnn00 record associated with the control volume from which the filter removes fission products (see CVH Package Users' Guide).
(type = integer, default = 99, units = none)

RN2FLTXXKK – Filter Class Parameters
$01 \leq KK \leq 20$
Optional

This record modifies the global parameters specified on the previous record for specific classes.

(1) ICLSS - Class number to be modified.
(type = integer, default = none, units = none)

(2) DFC - Class decontamination factor (Note: DFC must be ≥ 1.0).
(type = real, default = DFG, units = none)

(3) XMASC - Limit on class mass removed by the filter (see description for XMASG on previous record.
(type = real, default = -1.0, units = kg)

Optional records RN2FLTxx21 through RNFLTxx45 below activate models that represent the specific characteristics of specialized filters. These models (developed for application of MELCOR to non-LWR plants) are not currently described in the RN Package Reference Manual. If data are provided on these records, a value must also be provided (in FL Package input, on record FLnnnSk) that identifies the flow path segment within which filter XX resides. The value of the sixth data field on Record FLnnnSk must then match the value for XX on the following records.

RN2FLTXXKK – Initialization of Filter RN Mass
$21 \leq KK \leq 40$
Optional

These records allow initialization of masses for up to 20 RN classes.

(1) ICLSS - RN class for which an initial mass is to be placed on filter XX
(type = integer, default = none, units = none)

(2) XMFLTI - Initial (total) mass of ICLSS material
(type = real, default = 0.0, units = kg)

(3) XMFRAC - Fraction of XMFLTI that is radioactive
(type = real, default = 1.0, units = none)

RN2FLTXX41 – Performance Characteristics of Aerosol Filters
Optional

(1) XMNSZA - Minimum aerosol size (mean diameter) for which decontamination factors defined by Records RN2FLTXX00 and RN2FLTXX01 apply. Aerosols with smaller diameters will not be affected by the filter.
(type = real, default = 0.0, units = m)

(2) FAILDP - Pressure drop (segment pressure loss) at which filter XX fails. On "failure", the filter decontamination factor is reset to 1.0, a fraction FAILRL of the RN mass deposited on the filter is released, and the value for SLAM input on Record FLnnnSk is reset to 0.
(type = real, default =-1.0, units = Pa)

(3) FAILRL - Fraction of RN mass (applied to all classes, and to both radioactive and nonradioactive fractions) that will be released from filter XX on failure. The released mass will be evenly distributed among the sections of the aerosol distribution above diameter XMNSZA
(type = real, default = 1.0, units = none)

(4) DHRELS - Fraction of the total decay heat generated by RN material (of all classes) on filter XX that contributes to heating the gases passing through the filter. The remaining fraction (1-DHRELS) is assumed to be lost to the environment.
(type = real, default = 1.0, units = none)

RN2FLTXX42 – Performance Characteristics of Charcoal (Vapor) Filters
Optional

From 1 to 4 values may be entered; unspecified parameters retain their default values.

(1) AGE - Service life of charcoal filter
(type = real, default = 0.0, units = months)

(2) XMBEDI - Initial mass of charcoal in filter
(type = real, default = 827.35, units = kg)

(3) DHRELS - Fraction of the total decay heat generated by RN material (of all classes) on charcoal filter XX which goes to heating the charcoal and the gases passing through the filter. The remaining fraction (1-DHRELS) is assumed to be lost to the environment. For most applications, this value should be the same as the value of DHRELS used for the aerosol filter.
(type = real, default = 1.0, units = none)

(4) SPECHT - Specific heat of charcoal
(type = real, default = 711.78, units = J/kg K)

RN2FLTXX43 – Thermal Desorption Data for Charcoal Filters
Optional

If absent, thermal desorption is not modeled. One or both values may be entered.

(1) ITHCOF - Thermal desorption coefficient index
(type = integer, default = 0, units = none)

= 0, No thermal desorption
= 1, Use correlation for thermal desorption rate from the FISH6 code
= 2, Use correlation for thermal desorption rate from the ROOM code
< 0, Use Tabular Function |ITHCOF| to specify desorption rate (fraction released / s) as a function of temperature (K)

(2) THAGE - Age coefficient index
(type = real, default = 0.0, units = none

= 0., Use expression consistent with correlation specified by ITHCOF
> 0., Use constant age coefficient THAGE

RN2FLTXX44 – Radiolytic Desorption Data for Charcoal Filters
Optional

If absent, radiolytic desorption is not modeled. One to three values may be entered.

(1) IRDCOF - Radiolytic desorption coefficient index
(type = integer, default = none, units = none)

= 0, Use correlation for radiolytic desorption rate from the ROOM code
< 0, Use Tabular Function |IRDCOF| to specify desorption rate (fraction released / s) as a function of exposure

(2) RADAGE - Age coefficient index
(type = real, default = 0, units = none)

= 0., Use the expression for the age coefficient in the ROOM code
> 0., Use constant age coefficient RADAGE

(3) EXTIMI - Initial radiation exposure time
(type = real, default = 0.0, units = s)

RN2FLTXX45 – Charcoal Combustion Data for Charcoal Filters
Optional

If absent, charcoal combustion is not modeled.

(1) BURNRT - Burn rate expression index
(type = real, default = 0.0, units = none or kg/m^2 s)

= 0., Charcoal burning is not modeled
=-1., Use expression for burn rate described in the RN Reference Manual (from coal conversion technology)
> 0., Constant burn rate of BURNRT (kg/m^2 s)

(2) TMPIGN - Charcoal ignition temperature
(type = real, default = 573.0, units = K)

(3) APPRHO - Apparent charcoal particle density
(type = real, default = 520.6, units = kg/m^3)

(4) AVPDIA - Average charcoal particle diameter
(type = real, default = 0.0016, units = m)

(5) XMFREM - Mass of charcoal remaining after burn is complete. Burn then consumes XMBEDI – XMFREM.
(type = real, default = 0.0, units = kg)

(6) PROCON - Proportionality coefficient between fraction of initial charcoal mass consumed by burning and fraction of iodine mass on filter (at time of ignition) that is released (i.e., ratio of charcoal combustion rate to iodine release rate) PROCON > 1.0
(type = real, default = 1.0, units = none)

RN2SPRXX Record Series – Spray Parameters
XX is a record identifier
Optional

The following records describe the washout of radionuclides by the Containment Sprays (SPR) package. The user should refer to the SPR Users' Guide for important information on the interactions between the SPR and RN packages.

RN2SPR00 – Iodine Class
Optional

This record gives the class of iodine for vapor spray removal. All material in that class is assumed to be chemically similar to iodine, and is subjected to the removal calculation.

(1) IICLS - Class of iodine for spray removal calculation.
(type = integer, default = 4, units = none)

RN2SPRXX – Spray Partition Coefficient
XX ≥ 01, XX is a sequencing parameter
Optional

This record specifies the partition coefficient used for the sprays as defined in the SPR package.

(1) ISPNUM - User-defined spray source number.
(type = integer, default = none, units = none)

(2) HPART - Iodine partition coefficient for this spray source. The partition coefficient is defined as the ratio of the concentration of iodine in the liquid droplets to the concentration of iodine in the gas under equilibrium conditions. It is normally much greater than one. Recommended values for this parameter are as follows:
(type = real, default = 1.0, units = none)

Recommended Iodine Partition Coefficient Values

Spray Type	Conservative	Best Estimate
Sodium Hydroxide	2,000	5,000
Sodium Thiosulfate	---	100,000
Hydrazine	---	5,000
Boric Acid	500	2,500

As many pairs as needed for multiple spray sources are input on these records. The pairs may not be split between records.

3.1.8 Radionuclide Chemistry

RNRCTIIYY Records – Class Reaction Information
00 ≤ II ≤ 99, II is the reaction number
00 ≤ YY ≤ 99, YY is an input type number
Optional

These records specify the chemical reactions that will be considered in MELCOR for vapors in the gas phase. The stoichiometric reaction is specified, and forward or reverse reactions may occur depending on the values of the reaction mass transfer data. For evaluation of the reacted mass, the total rate based on mass transfer plus the specified reaction rate is used. In addition, a deposition velocity may be input which is the total rate including mass transfer. The energy associated with the reaction may also be specified. These rates may be input as control functions or tabular functions depending on the complexity desired.

The first *from* class is the fission product vapor in the atmosphere that undergoes the reaction. All other *from* classes as well as the *to* classes are assumed to be on the surface. The reactions are limited by the availability of the appropriate classes. For example, if the reaction is a forward reaction, and, for example, the second *from* class is not on the surface, the reaction will not take place. Remember, all states must be vapor states as only vapors undergo reactions – aerosol states do not react but only act as surfaces where the reactions can occur.

RNRCTII00 – *From* Class Specification

(1) ICLASF - The *from* reacting classes
(type = integer, default = none, units = none)

(2) FRACF - The mole fraction for this class based on a stoichiometric reaction
(type = real, default = 0.0, units = none)

As many pairs as necessary may be specified.

RNRCTII01 – *To* Class Specification

(1) ICLAST - The *to* reacting classes
(type = integer, default = none, units = none)

(2) FRACT - The mole fraction for this class based on a stoichiometric reaction
(type = real, default = 0.0, units = none)

As many pairs as necessary may be specified.

RNRCTII02 – Translation Array

(1) FRACFT - The mass fraction of the *from* classes forming each of the *to* classes is specified by these records. This information is needed to properly allocate the radioactive masses. The order is the fraction of each *from* class to all of the *to* classes starting with the first *from* class. For example, given the reaction A + B → C + D, the order of the input would be fraction A to C, A to D, B to C, and B to D.
(type = real, default = 0.0, units = none)

For example, consider the reaction

$H_2O + CO \rightarrow CO_2 + H_2$

The mass fraction input would be 0.89 (wt of O divided by wt of H_2O), 0.11 , 1. , 0. The number of required mass fractions is the number of *from* classes times the number of *to* classes.

RNRCTII03 – Control Volumes

(1) IVOL - The control volumes in which these reactions may occur. More than one CV can be given on this record.
(type = integer, default = none, units = none)

RNRCTII04 – States

(1) ISTAT - The states within the control volumes where the reactions can occur
(type = character, default = none, units = none)

= HS.x.y, vapors on HS x on side y, x is the user HS number and y is either -1 or 1 depending on specification of the left or right side, respectively
= AG, aerosols in the vapor phase
= LP, liquid pool

(2) IRSTTW - Flag to determine if the reaction will occur if there is water present on or in the reaction medium ISTAT (heat structure, atmosphere, or pool).
(type = integer, default = 0, units = none)

= 0, reaction will stop if water is present
= 1, reaction will continue if water is present.

As many pairs as necessary may be specified.

RNRCTII10 – Forward Reaction Mass Transfer Data

(1) CFMF - Location of the forward reaction mass transfer data (type = integer, default = 0, units = none)

- < 0, the data are given as a function of time by tabular function number ABS(CFMF)
- = 0, no forward reaction.
- > 0, the data are given by control function number CFMF

Only one entry is allowed on this record. Note that function number 0 cannot be used. If the value of the function is positive, the value is a rate constant which does not include mass transfer effects and the units of the function must be fraction per second. If the value of the function is negative or zero, the absolute value is a deposition velocity in m/s which includes mass transfer effects and is a net transfer rate. See the RN Package Reference Manual for further details.

RNRCTII11 – Backward Reaction Mass Transfer Data

(1) CFMB - Location of the backward reaction mass transfer data (type = integer, default = 0, units = none)

- < 0, the data are given as a function of time by tabular function number ABS(CFMB)
- = 0, no backward reaction.
- > 0, the data are given by control function number CFMB

Only one entry is allowed on this record. Note that function number 0 cannot be used. The value of the function is the reverse reaction constant in units of kg/s. If the forward reaction data is a deposition velocity, this value is not used. See the RN Package Reference Manual for further details.

RNRCTII20 – Forward Reaction Energy Transfer Data

(1) CFEF - Location of the forward reaction energy transfer data (type = integer, default = 0, units = none)

- < 0, the data are given as a function of time by tabular function number ABS(CFEF)
- = 0, no energy transfer for the forward reaction.
- > 0, the data are given by control function number CFEF

Only one entry is allowed on this record. The units of the function are J per kg of mass transferred of the first *from* class. The energy is added to the atmosphere in the case of aerosols, to the pool for reactions in the pool, and to the heat structure for the heat structure case.

RNRCTII21 – Backward Reaction Energy Transfer Data

(1) CFTO - Location of the backward reaction energy transfer data
(type = integer, default = 0, units = none)

< 0, the data are given as a function of time by tabular function number ABS(CFTO)
= 0, no energy transfer for the backward reaction.
> 0, the data are given by control function number CFTO

Only one entry is allowed on this record. See the above record for discussion of the units of the function.

RNTRNIIYY Records – Class Transfer Information
$00 \leq II \leq 99$, II is the transfer number
$00 \leq YY \leq 99$, YY is an input type number
Optional

These records specify the class transfers that will be considered in MELCOR to simulate rapid chemical reactions. The stoichiometric reaction is specified, and only forward transfers may occur. The energy associated with the transfer may also be specified. These rates may be input as control functions or tabular functions depending on the complexity desired. These records can also be used to change states of masses, i.e., to change from deposited aerosols, which do not undergo chemical reactions, to deposited vapors, which can react.

RNTRNII00 – *From* Class Specification

(1) ICLASF - The *from* transfer classes
(type = integer, default = none, units = none)

(2) FRACF - The mole fraction for this class based on a stoichiometric reaction
(type = real, default = 0.0, units = none)

As many pairs as desired may be specified.

RNTRNII01 – *To* Class Specification

(1) ICLAST - The *to* transfer classes
(type = integer, default = none, units = none)

(2) FRACF - The mole fraction for this class based on a stoichiometric reaction
(type = real, default = 0.0, units = none)

As many pairs as desired may be specified.

RNTRNII02 – Translation Array

(1) FRACFT - The mass fraction of the *from* classes forming each of the *to* classes is specified by these records. This information is needed to properly allocate the radioactive masses. The order is the fraction of each *from* class to all of the *to* classes starting with the first *from* class. For example, given the reaction A+B $\rightarrow$ C+D, the order of the input would be fraction A to C, A to D, B to C, and B to D. The number of required mass fraction is the number of *from* classes times the number of *to* classes.
(type = real, default = 0.0, units = none)

RNTRNII03 – Control Volumes

(1) IVOL - The control volumes in which these transfers may occur are specified. More than one CV can be given on this record.
(type = integer, default = none, units = none)

RNTRNII04 – States

(1) ISTATF - The *from* states within the control volumes where the transfers can occur
(type = character, default = none, units = none)

= ALL,	all states, the *from* states and to states are the same
= HSA.x.y,	aerosols on HS x on side y, x is the user number and y is either -1 or 1 depending on specification of the left or right side, respectively
= HSV.x.y,	vapors on HS x on side y
= AG,	aerosols in the vapor phase
= AL,	aerosols in the liquid phase
= VG,	vapors in the vapor phase

= VL, vapors in the liquid phase

(2) ISTATT - The *to* states within the control volumes where the transfers can occur
(type = character, default = none, units = none).

= ALL, all states, the *from* states and to states are the same
= HSA.x.y, aerosols on HS x on side y, x is the user number and y is either -1 or 1 depending on specification of the left or right side, respectively
= HSV.x.y, vapors on HS x on side y
= AG, aerosols in the vapor phase
= AL, aerosols in the liquid phase
= VG, vapors in the vapor phase
= VL, vapors in the liquid phase

(3) ITSTTW - Flag to determine if the transfer will occur if there is water present for the above states
(type = integer, default = 0, units = none)

= 0, transfer will continue if water is present
= 1, transfer will stop if water is present for the *from* state
= 2, transfer will stop in water is present for the *to* state
= 3, transfer will stop if water is present for the either state
= 4, transfer will stop if water is present for the both states

As many sets as desired may be specified.

RNTRNII10 – Mass Transfer Data

(1) CFM - Location of the mass transfer data
(type = integer, default = 0, units = none)

< 0, the data are given as a function of time by tabular function number ABS(CFM)
= 0, no transfer, (no mass or energy transfer)
> 0, the data are given by control function number CFM

Note that function number 0 cannot be used. The units of the function are kg/sec of the first *from* class. If the function value is negative, all the mass is transferred. No reverse transfer is permitted.

RNTRNII11 – Energy Transfer Data

(1) CFE - Location of the energy transfer data
(type = integer, default = 0, units = none)

< 0, the data are given as a function of time by tabular function number ABS(CFE)
= 0, no energy transfer
> 0, the data are given by control function number CFE

Only one entry is allowed on this record. The units of the function are J per kg of mass transferred of the first *from* class. The energy is added to the atmosphere in the case of aerosols, to the pool for reactions in the pool, and to the heat structure for the heat structure case.

3.1.9 Chemisorption

RNCA100 Record – Chemisorption Activation Flag

(1) ICAON - Chemisorption activation flag, 1 = ON, 0 = OFF.
(type = integer, default = 1, units = none)

RNCAONxx Records – Chemisorption Class Activation Flags
$00 \leq xx \leq 99$, xx is a sequencing parameter

This is the CA (Chemisorption Activation) class card, used to set CA classes on or off and to set up new classes.

(1) ICACL - CA class number.

(2) ICACON - CA class flag, 0=on, 1=off.

(3) ICAST - Surface material type for CA class.
1 = Stainless steel
2 = Inconel (currently not in material database)
3 = Zircaloy

NOTE: Chemisorption currently can only be done on materials in the MELCOR database, and does not function for user-defined materials. Currently, Inconel is not in the database. Also, note that the CsOH class must be ON if the CsI class is ON, as iodine released in the CsI chemisorption reaction is released via the CsOH vapor deposition class. The first four classes are default ON, and the next two (tellurium)

are OFF because current data suggests that tellurium does not chemisorb in the presence of an oxide film on the surface.

RNCACMxx Records – Chemisorption Class to Radionuclide Vapor Mapping
$00 \leq xx \leq 99$, xx is a sequencing parameter

(1) ICA - CA class number

(2) ICL - Radionuclide vapor class number

3.1.10 Iodine Pool Model

RNIOD100 Record – Iodine model activation flags
Optional

(1) IODON - Iodine pool model activation flag, 1 = ON, 0 = OFF.
(type = integer, default = 0, units = none)

(2) IRCOPT - Set of chemical equations to use
(type = integer, default=0, units = none)

This parameter selects the set of chemical equations to use in the aqueous pool chemistry. The only set that has been tested is the default INSPECT-Powers set, and the others should be regarded as placeholders for the present.

= 0 INSPECT-Powers set
= 1 INSPECT
= 2 Boyd, Carter and Dixon
= 3 minimum iodine set

(3) IODFLG - Iodine pool chemistry activation flag
(type = integer, default = 0, units = none)

This parameter is used to select between having the pool chemistry activate in a control volume only when iodine is present (the default behavior) and having the pool chemistry activate whether or not iodine is present, as long as the other activation criteria are satisfied. This allows calculation of water hydrolysis species without requiring iodine in the pool.

= 0 pool chemistry activates only with iodine present (default)
= 1 chemistry activates if other conditions are satisfied.

(4) IPCOEF1 - Partition coefficient flag for I^0 . 1 = ON, 0 = OFF (default)
(type = integer, default = 0, units = none)

This coefficient is used to switch the partition coefficient for I^0 on and off. The default is off (no atomic iodine released from the pool to the atmosphere).

(5) IPCOEF2 - Partition coefficient flag for HOI. 1 = ON, 0 = OFF
(type = integer, default = 0, units = none)

This coefficient is used to switch the partition coefficient for HOI on and off. The default is off (no HOI released from the pool to the atmosphere).

Note that use of the iodine pool model requires definition of at least 4 additional RN classes in the DCH module, which must be named as follows:

CH3I – methyl iodine
HCL – hydrochloric acid
HNO3 – nitric acid
IM – pool iodine bound in chemical species other than iodine or CsI.

If pool buffering is desired, 2 buffer classes may also be defined: HBO2, boric acid, and HPO4, sodium triphosphate. A third buffer class is recognized but not used currently: LIBO, lithium borate. Including the effect of silver in binding pool iodine will require defining the silver iodide class, AGI. The additional classes must be named as given for the pool model to recognize them. Also, methane, carbon dioxide, hydrogen, and carbon monoxide must be defined in the NCG input.

RNIOD200 Record – Iodine pool model start time
Optional

(1) TIOBEG - Iodine pool model start time.
(type = real, default = -1.0E30, units = sec)

The iodine pool chemistry model does not start until the problem time reaches TIOBEG. Calculation of atmospheric radiolysis to produce nitric and hydrochloric acid is not affected by the pool model start time and begins at the problem start time. This card may be used to delay startup of the pool chemistry model until later times in a plant accident scenario, where iodine is of most interest. The pool chemistry solver can take a significant amount of CPU time, so this is another reason to delay pool startup.

RNPHxxx – Ph Calculation Type
$1 \leq xxx \leq 999$, xxx is the control volume number containing the pool this record applies to.

Optional.

This record selectes the time-dependent input source for the pool Ph in a control volume, or alternatively the Ph is calculated internally if no RNPH record is specified.

(1) PHSRC - Ph input source, which can be a table, control function, or external data file. The allowed values for PHSRC are
TF.nnn – source from table function nnn.
CF.nnn – source from control function nnn.
EDF.nnn.mmm – source from channel mmm of EDF nnn.

RNDOSxxxy – Dose input record
$1 \leq xxx \leq 999$ where xxx is the control volume number,
$0 \leq y \leq 9$ where y is a sequencing number
Optional.

This record is used to specify the dose rate to the atmosphere, pool, wall, and electric cable in a control volume. These rates will be used in the relevant parts of the iodine pool model to calculate radiolysis reactions. The atmosphere dose rate is used in homogeneous iodine reactions and nitric acid formation, the pool dose rate applies to aqueous chemistry, the wall dose rate is used in surface reactions of iodine and methyl iodine, and the cable dose rate is used for generation of hydrochloric acid (by release of chlorine from plastics).

(1) DOSID - identifies site for dose rate
(type = character, default = none, units = none)

= ATMO – atmospheric dose rate
= POOL – pool dose rate
= WALL – wall dose rate
= CABL – cable dose rate

(2) DOSSRC - source for time-dependent dose rate (Grays/s).
(type = character, default = none, units = none)

= OFF – dose rate is 0.
= DC – source is decay heat.
= TF.nnn – source from table function nnn.
= CF.nnn – source from control function nnn.
= EDF.nnn.mmm – source from channel mmm of EDF nnn.

(3) SCALE - (type = real, default = 1.0, units = none)
Optional

SCALE is an optional scale factor that multiplies the radiation dose source.

RNCBxxx – Cable mass input
$1 \leq xxx \leq 999$, xxx is the control volume number.
Optional.

This record specifies the cable mass in a control volume to be used in calculating the release of chlorine from plastics as a result of the radiation dose rate.

(1) CABM - Cable mass in control volume
(type = real, default = 0.0, units = kg).

RNSCyyy – Surface coating on walls
yyy is a sequence number
Optional

If this record is omitted, the heat structure surface will be assumed to be the same as the material specified for the surface heat structure node. Up to13 of items (1) -(3) can input on the same record.

(1) IDS - Heat structure ID
(type = integer, default = none, units = none)

(2) SIDE - Surface side
(type = character, default = none, units = none)

= LHS, left hand side
= RHS, right hand side

(3) COAT - Surface coating
(type = character, default = none, units = none)

= NONE, no coating, surface same as surface material.
= PAINT, painted surface.
= STEEL, steel surface.
= CONCRETE, concrete surface.

RNIOPyyy – Iodine pool species to be output on plot file.
yyy is a sequencing number.
Optional.

This record specifies the aqueous pool species available for plotting on the plot file.

(1) SPCNAM - The species name from the following list. Up to six species names may be on a record. The maximum total number of species that can be output is currently 10.

Table 2. Aqueous Species Names

E-	OH0	H0	H2O2	HO2-	HO20
O-	O2-	O3-	I2-	I3-	I0
HOI-	I2AQ	I2OH-	HOI0	OI-	IO0
I2O2	HIO20	IO2-	IO20	HIO3-	IO32-
HOI30	IO3-	IO30	HI-	FE2+	CH3
CH3I	CH3I+	CH4I0	CH2O	CH3O	CH3OH
FE3+	H+	H2AQ	OH-	O2AQ	I-

3.2 MELCOR Input

The MELCOR input available for the RN package is as follows:

RNEDTFLG Record – RN Edit Flags
Optional

Input is available in MELCOR to tailor the edits to the problem at hand.

(1) IFLGDM - Edit flag for deposited RN masses, 0 bypasses the edits, 1 prints the edits
(type = integer, default = 0, units = none)

(2) IFLGGM - Edit flag for gas RN masses, 0 bypasses the edits, 1 prints the edits
(type = integer, default = 0, units = none)

(3) IFLGLM - Edit flag for liquid RN masses, 0 bypasses the edits, 1 prints the edits
(type = integer, default = 0, units = none)

(4) IFLGCA - Edit flag for chemisorption masses, 0 bypasses the edits, 1 prints the edits
(type = integer, default = 0, units = none)

(5) IFLGI2 - Edit flag for iodine pool model, 0 bypasses the edits, 1 prints the edits
(type = integer, default = 0, units = none)

RNIOD200 Record – Iodine pool model start time
Optional

(1) TIOBEG - Iodine pool model start time.
(type = real, default = -1.0E30, units = sec)

The iodine pool chemistry model does not start until the problem time reaches TIOBEG. Calculation of atmospheric radiolysis to produce nitric and hydrochloric acid is not affected by the pool model start time and begins at the problem start time. This card may be used to delay startup of the pool chemistry model until later times in a plant accident scenario, where iodine is of most interest. The pool chemistry solver can take a significant amount of CPU time, so this is another reason to delay pool startup.

4. Sensitivity Coefficients

7000 – Differential Equation Convergence

These values are used to control the solution of the aerosol dynamics equations. At each time step, the equations are solved by one of two available methods, depending on the rate of change of the sectional mass distribution. If the rate is not excessive, then the distribution is updated using the start-of-step derivatives in an explicit Euler step. For larger rates, the equations are integrated by the RKF45 routine developed at Sandia National Laboratories.

		default	units	equiv
1	RKF45 absolute error tolerance	1.0E-18	none	none
2	RKF45 relative error tolerance, and relative tolerance for conservation of component masses in RN	1.0E-3	none	none
3	Maximum fractional decrease in any sectional density permitted during an explicit step	0.1	none	none
4	Maximum fractional increase in any sectional density permitted during an explicit step	0.1	none	none
5	Sectional density below which the fractional change restrictions are ignored	1.0E-12	kg/m^3	none

7001 – Aerosol Coefficient Criteria

These values are used to control the evaluation of the aerosol dynamics coefficients. These values are used to determine if the numerical integration performed is satisfactory.

(1) - Aerosol coefficient absolute error,
(default = 1.0E-18, units = none, equiv = none)

(2) - Aerosol coefficient relative error,
(default = 1.0E-3, units = none, equiv = none)

7002 – Fission Product Decay Beta Range

This value defines the range of characteristic beta radiation from fission product decay, and is used to modify the fraction of decay heat which is deposited in a control volume atmosphere. SPVOL1 (records RNDHVXXX) and SPSUR2 (records RNDHSXXX) are multiplied by a factor

min [1.0, Atmosphere_density x CVPATH / C7002(1)],

where CVPATH is the characteristic path in the volume (see description of RNDHLEN records). Any reduced deposition is compensated by proportionate increase in energy distributed to other components specified by SPVOL2-SPVOL4 or SPSUR3-SPSUR5. (The calculation is bypassed if the sum of these other split coefficients is zero.)

(1) - Characteristic range of beta radiation fission product decay,
(default = 1.2, units = kg/m^2, equiv = RANGE)

7100 – COR Material Release Multipliers

These values are used to scale the nominal release rates obtained from the CORSOR release models described below. All values must be between 0.0 and 1.0, inclusive. By default the scale factor is unity for the fuel material and zero for all other core materials because the CORSOR models are strictly applicable to the fuel material.

		default	units	equiv
1	Fuel material multiplier	1.0	none	none
2	Structural Zr multiplier	0.0	none	none
3	Oxidized Zr multiplier	0.0	none	none
4	Structural steel multiplier	0.0	none	none
5	Oxidized steel multiplier	0.0	none	none

		default	units	equiv
6	Control rod poison multiplier	0.0	none	none
7	Structural inconel multiplier	0.0	none	none

7101 – CORSOR Coefficients

These values are used to determine the release of aerosols and vapors from the fuel in the core during heating. Default values of these coefficients are the generally accepted CORSOR values. The release rate is

Release Rate (fraction / min) = A exp (BT)

The coefficients are in C7101(i,j,k) where
i – Location index, dimensioned 3
j – Type of parameter,
= 1, Temperature value, °C
= 2, CORSOR coefficient A value, fraction/min
= 3, CORSOR coefficient B value, $°C^{-1}$
k – RN material class, dimensioned 20

The interpretation of the values is as follows:

For a temperature between C7101(i,1,k) and C7101(i + 1,1,k), the CORSOR A and B coefficients C7101(i,2,k) and C7101(i,3,k) are used for the releases. For temperature values less than C7101(1,1,k), no releases are evaluated. For temperatures greater than C7101(3,1,k), the values C7101(3,2,k) and C7101(3,3,k) are used. The default values of the coefficients are:

	C7101(1,1,k)	C7101(2,1,k)	C7101(3,1,k)
All Classes except Class 5	900.E0	1400.E0	2200.E0
	C7101(1,1,5)	C7101(2,1,5)	C7101(3,1,5)
Class 5	900.E0	1600.E0	2000.E0

The A and B values are:

		C7101(1,j,k)	C7101(2,j,k)	C7101(3,j,k)
Class 1	A	7.02E-9	2.02E-7	1.74E-5
	B	0.00886	0.00667	0.00460
Class 2	A	7.53E-12	2.02E-7	1.74E-5
	B	0.0142	0.00667	0.00460
Class 3	A	7.50E-14	8.26E-9	1.38E-5
	B	0.0144	0.00631	0.00290
Class 4	A	7.02E-9	2.02E-7	1.74E-5

		C7101(1,j,k)	C7101(2,j,k)	C7101(3,j,k)
	B	0.00886	0.00667	0.00460
Class 5	A	1.62E-11	9.04E-8	6.02E-6
	B	0.0106	0.00552	0.00312
Class 6	A	1.36E-11	1.36E-11	1.40E-6
	B	0.00768	0.00768	0.00248
Class 7	A	5.01E-12	5.93E-8	3.70E-5
	B	0.0115	0.00523	0.00200
Class 8	A	6.64E-12	6.64E-12	1.48E-7
	B	0.00631	0.00631	0.00177
Class 9	A	5.00E-13	5.00E-13	5.00E-13
	B	0.00768	0.00768	0.00768
Class 10	A	5.00E-13	5.00E-13	5.00E-13
	B	0.00768	0.00768	0.00768
Class 11	A	1.90E-12	5.88E-9	2.56E-6
	B	0.0128	0.00708	0.00426
Class 12	A	1.90E-12	5.88E-9	2.56E-6
	B	0.0128	0.00708	0.00426
Class 13 to 20	A	0.	0.	0.
	B	0.	0.	0.

7102 – CORSOR-M Coefficients

The values of the CORSOR-M coefficients from CORSOR-M are in this record series. This model uses an Arrhenius form of the release equation, or

Release Rate (fraction / min) = k_o exp (-Q / RT)

The values in the expression designated k_o, Q, and T are in units of min^{-1}, kcal/mol, and K, respectively. The value of R is 1.987E-3 in the appropriate units. The default values in MELCOR for each class are

Class	k_o (C7102(1,i))(1./min)	Q (C7102(2,i))(kcal/mole)
1	2.00E5	63.8
2	2.00E5	63.8
3	2.95E5	100.2
4	2.00E5	63.8
5	2.00E5	63.8
6	1.62E6	152.8
7*	23.15*	44.1*
8	2.67E8	188.2
9**	1.46E7 **	143.1**

Class	k_o (C7102(1,i))(1./min)	Q (C7102(2,i))(kcal/mole)
10	1.46E7	143.1
11**	5.95E3**	70.8**
12	5.95E3	70.8
13-30	0.	0.

Note. The CORSOR-M model does not consider release from Class 7 (Moly), Class 9 (La) or Class 11 (Cd) to be significant. Previous versions of MELCOR used zero values for these classes when using CORSOR-M. In MELCOR 1.8.5 non-zero release coefficients are supplied as described.

* Coefficients for CORSOR-M class 7 (Moly) are based on a curve fit to the CORSOR release model for Class 7.

** Coefficients for CORSOR-M Class 7 are set identical to the CORSOR-M Class 8 values, following the same assumption as used in the CORSOR model for Class 7. Likewise for Class 11 and 12.

7103 – CORSOR-Booth Class Scaling Factors: Nominal Values

The release rate for species other than cesium is given by multiplying the cesium release rate by an appropriate scaling factor for each RN class:

Release Rate(k) = Release Rate(Cs) x C7103(k)

Class	C7103(k)	Class	C7103(k)
1	1.0	8	3.34E-5
2	1.0	9	1.0E-4
3	3.33E-3	10	1.0E-4
4	1.0	11	5.0E-2
5	1.0	12	5.0E-2
6	1.0E-4	13-30	0.0
7	1.0E-3		

7104 – Release Surface-to-Volume Ratio

This value is the base value for the CORSOR and CORSOR-M releases when the surface-to-volume ratio option is specified. The rates are modified as follows

Release Rate = Release Rate (CORSOR or CORSOR-M)

$$\times (S/V)_{structure} / (S/V)_{base}$$

where the $(S/V)_{base}$ is derived from the CORSOR test data.

(1) - Surface-to-volume base ratio,
(default = 4.225E2, units = m^{-1}, equiv = none)

7105 – Modification of Release Rates

These values are used to modify the CORSOR or CORSOR-M coefficients as determined by conditions other than used in the release expressions. For example, the release of tellurium is affected by the amount of cladding oxidation as discussed in Section 2.3.1 of the RN Package Reference Manual. At present, this mechanism is the only one addressed in this sensitivity coefficient series. In this case, the CORSOR or CORSOR-M release rate is used when the amount of cladding oxidation is greater than the cut-off value or when there is no cladding present. When the amount of cladding oxidation is less then the cut-off value, the release rate is multiplied by the multiplier given below. The default values are:

(1) - Tellurium Class,
(default = 5, units = none, equiv = none)

(2) - Cladding oxidation fraction cut-off point,
(default = 0.70, units = none, equiv = none)

(3) - Release rate multiplier (Used when amount of oxidation is less than the cut-off value),
(default = 1/40 = 0.025, units = none, equiv = none)

7106 – CORSOR-Booth Transient Release Parameters for Cesium

The classical or effective diffusion coefficient for cesium in the fuel matrix is given by

$D = D0 \times EXP(-Q / RT)$

where R is the universal gas constant, T is the temperature, Q is the activation energy and D0 is the pre-exponential factor given by this sensitivity coefficient below.

The CORSOR-Booth method gives the cesium release fraction as a function of $D \times TIME / A^2$ where A is the equivalent sphere radius for the fuel grain.

(1) - low burn-up value of D0
(default = 5.E-8, units = m^2/s, equiv = none)

(2) - high burn-up value of D0
(default = 2.5E-7, units = m^2/s, equiv = none)

(3) - burn-up value at which value of D0 changes
(default = 3.E4, units = MWD/MTU, equiv = none)

(4) - activation energy Q
(default = 3.8E5, units = J/kg-mole, equiv = none)

(5) - equivalent sphere radius of fuel grain
(default = 1.0E-5, units = m, equiv = none)

7107 – CORSOR-Booth Class Scaling Factors: Oxidation Modified

The scaling factors given by C7103(k) above must be modified under certain conditions of cladding oxidation.

When the oxide mass fraction exceeds C7107(1,k) and the temperature (TEMP) exceeds C7107(2,k), the class k scaling factor is given by:

SFACT(k) = C7107(3,k) x EXP(C7107(4,k) x MIN(TEMP , C7107(5,k)))

when the oxide mass fraction is below C7107(6,k) the class k scaling factor is given by:

SFACT(k) = C7107(7,k)

Class	C7107(i,k)						
	i = 1	i = 2	i = 3	i = 4	i = 5	I = 6	i = 7
1-2	1.1	0.0	0.0	0.0	0.0	-1.0	0.0
3	1.1	0.0	0.0	0.0	0.0	0.05	0.05
4	1.1	0.0	0.0	0.0	0.0	-1.0	0.0
5	1.1	0.0	0.0	0.0	0.0	0.70	0.025
6	.75	2300.	1.06792E-20	0.0159923	2700.	-1.0	0.0
7-8	1.1	0.0	0.0	0.0	0.0	-1.0	0.0
9	1.1	0.0	0.0	0.0	0.0	0.05	0.10
10	1.1	0.0	0.0	0.0	0.0	-1.0	0.0
11-12	0.75	2000.	3.194E-9	0.008283	2300.	-1.0	0.0
13-30	1.1	0.0	0.0	0.0	0.0	-1.0	0.0

7110 – Vapor Pressure

The vapor pressure curves for the fission product vapors are included in these sensitivity coefficients. These values determine the amount of fission product vapor released from the core and the amount condensed onto the heat structures and aerosol particles. These coefficients give the vapor pressure through the following relationship:

$$\log_{10}[\text{Pressure (mm Hg)}] = -A / T + B + C \log_{10}(T)$$

The values of A, B, and C are stored in the C7110(i,j,k) array where

- i - Location index, dimensioned 3
- j - Type of parameter,
  - = 1, Temperature value, K
  - = 2, Coefficient A
  - = 3, Coefficient B
  - = 4, Coefficient C
- k - RN material class, dimensioned 20

The interpretation of these values is as follows:

For a temperature value C7110(1,1,k) equal to -1.E0, the class is always an aerosol, or, in other words, the vapor pressure is 0. It is **not** recommended that users define classes which are radioactive (i.e., generate decay heat) to be always an aerosol because they may overheat surfaces on which they are deposited. Even the most refractory of materials will vaporize and discontinue heating a surface when the temperature becomes high enough (above 4000 K). If the first coefficient A value, C7110(1,2,k) is equal to -1.E0, the class is always a vapor. For other values, if the temperature is between the i and i+1 temperature values, the coefficients at i are used. For temperatures lower than the first temperature value, the vapor pressure is 0. For temperatures higher than the last temperature value, the last range coefficient values are extrapolated and used. The values presently in the code are given below. They are based on preliminary data in (see RN Reference Manual), but values flagged by * have been adjusted slightly to give a continuous variation of vapor pressure as a function of temperature. Class 16 values are for CsI, the normal application of this user-defined class. Classes 3 and 6 – 13 now have vapor pressure curves; classes 14 – 15 and 17 – 30 have the same values, which are representative of a nonvolatile (refractory) oxide (the values are actually those for UO_2 above 3000 K). Hence, these classes will not vaporize until the temperature exceeds 3000 K.

		C7110(1,j,k)	C7110(2,j,k)	C7110(3,j,k)
Class 1	T	0.	10000.	
	A	-1.E0 (always a vapor)		
Class 2	T	600.	1553.	
	A	9400.	6870.778	
	B	21.59	7.994503	
	C	-3.75	0.0	
Class 3	T	1000.	10000.	
	A	7836.		
	B	6.44		

		C7110(1,j,k)	C7110(2,j,k)	C7110(3,j,k)
	C	0.0		
Class 4	T	298.	387.	457.
	A	3578.	3205.	2176.912045
	B	17.72	23.66536	7.637352
	C	-2.51	-5.18	0.0
Class 5	T	298.	10000.	
	A	13940.		
	B	23.51		
	C	-3.52		
Class 6	T	1500.	10000.	
	A	33200.		
	B	10.6088		
	C	0.0		
Class 7	T	1500.	10000.	
	A	32800.		
	B	9.68		
	C	0.0		
Class 8	T	1500.	10000.	
	A	21570.		
	B	8.74		
	C	0.0		
Class 9	T	1500.	10000.	
	A	21800.		
	B	8.683		
	C	0.0		
Class 10	T	1500.	10000.	
	A	32110.		
	B	11.873		
	C	0.0		
Class 11	T	1000.	10000.	
	A	13730.		
	B	8.43		
	C	0.0		
Class 12	T	1000.	10000.	
	A	15400.		
	B	8.15		
	C	0.0		
Class 13	T	1000.	10000.	
	A	19520.		
	B	11.125		
	C	0.0		

		C7110(1,j,k)	C7110(2,j,k)	C7110(3,j,k)
Class 14 to 15	T	3000.	10000.	
	A	18000.		
	B	8.875		
	C	0.0		
Class 16	T	600.	894.	1553.
	A	10420.	9678.	7303.903158
	B	19.70	20.34569	7.58405103
	C	-3.02	-3.52	0.0
Class 17 to 30	T	3000.	10000.	
	A	18000.		
	B	8.875		
	C	0.0		

7111 – Vapor Diffusivity Constants

These values are used to determine the fission product vapor diffusivity. The diffusivity values are used in the determination of the transport of condensed vapors to the walls and aerosols in each volume. The values in 7111 are for the RN material class masses. For each class, two different values are specified. They are:

C7111(1,i) = Sigma, Angstroms
C7111(2,i) = E/K, Deg K

The sigma and E/K values are Lennard-Jones parameters where sigma is a characteristic diameter of the molecule and E/K is the characteristic energy of interaction between the molecules divided by the Boltzmann constant. The default values of these parameters are

Class	Sigma (C7111(1,i) (Angstroms)	E/K (C7111(2,i) (K)
1	4.055	229.
2 – 3	3.617	97.
4	4.982	550.
5 - 30	3.617	97.

Most of the classes are defaulted to water vapor values due to the lack of information.

[Sensitivity coefficients 7112 and 7115, previously used in calculation of diffusivities of RN vapors through atmosphere gases, have been eliminated. The calculation now uses modeling and data in the Materials Properties (MP) package.]

7120 – Class Molecular Weights

Two class molecular weights are specified by these coefficients. The first value represents the molecular weight as the species exists in the fuel (typically an elemental value), which will be used in the class combination model to determine the total number of moles released which are available for combination with other classes. The second value represents a compound molecular weight (if data are available) after the species reacts with nonradioactive mass (oxygen or water) when it is released. For example, the Cs class might have an elemental mass equal to Cs and a compound mass equal to CsOH. The compound molecular weight is used in the diffusivity calculations and in the reaction mass transfer calculations. These values are stored as follows:

C7120(1,i) = Molecular Weight – Elemental
C7120(2,i) = Molecular Weight – Compound

The units are kg/kg-mole. The default values in the code are:

Class	MW-E [C7120(1,i)]		MW-C [C7120(2,i)]	
1	Xe	131.3	Xe	131.3
2	Cs	132.905	CsOH	149.913
3	Ba	137.34	Ba	137.34
4	I_2	253.8008	I_2	253.8008
5	Te	127.6	TeO	143.6
6	Ru	101.07	Ru	101.07
7	Mo	95.94	Mo	95.94
8	Ce	140.12	Ce	140.12
9	La	138.91	La	138.91
10	U	238.03	UO_2	270.03
11	Cd	112.4	Cd	112.4
12	Sn	118.69	Sn	118.69
13	B_2O_3	69.622	B_2O_3	69.622
14	H_2O	18.016	H_2O	18.016
15, 17-30	conc.	28.97	conc.	28.97
16	CsI	259.8054	CsI	259.8054

Sensitivity coefficient arrays 7130, 7131, 7132, and 7134 described below pertain to metallic fuels and are not applicable to the LWR version of MELCOR. The models are not described in the RN Package Reference Manual.

7130 – Oxidation-Based Release Coefficients for Metallic Fuels

When a metallic fuel oxidizes, a substantial change occurs in the structure of the fuel matrix. This change allows many fission products to escape almost instantaneously as the fuel is oxidized. The oxidation- based release model assumes that the release rate of each fission product is proportional to the rate of fuel oxidation. Thus, the release equation takes the form

$$I = k F$$

where I is the integrated release fraction, F is the fraction of the fuel that is oxidized, and k is a proportionality constant specified in this coefficient. This model is applied to each core cell and fuel element independently in order to properly account for varying fission product concentrations throughout the core. The default values in MELCOR for each class are:

Class	k [C7130(i)]	Class	k [C7130(i)]
1	1.00	8	0.01
2	0.30	9	0.01
3	0.01	10	0.01
4	1.00	11	0.01
5	1.00	12	0.01
6	0.05	13-30	0.00
7	0.01		

This model is not used with the LWR COR package.

7131 – Birney Non-Oxidation Release Coefficients for Metallic Fuel

When metallic fuels melt in a non-oxidizing environment, the release of fission products is gradual over time and dependent upon the vapor pressure of the fission product class. The release correlation takes the form

$$dM/dt = -R\,M_o \text{ where } R = k\,(P/P_o)^v,$$

where M_o is the initial mass, R is the Birney release rate (fraction/minute), k is a proportionality constant (fraction/minute), v is a normalization constant (none) for the ratio of partial pressures, and P and P_o are the vapor pressure of the fission product at the current temperature and the reference temperature (1473 K), respectively, as calculated using the form in sensitivity coefficient 7110. The values of k, v and a maximum allowed release rate R_m are specified here in coefficient 7113. This model is applied to each core cell and fuel element independently to

properly account for varying fission product concentration throughout the core. The default values in MELCOR are:

Class	k[(C7131(1,j)] (1./min)	v [C7131(2,j)] (none)	R_m[C7131(3,j)] (1./min)
1	0.050	0.70	1.0E5
2	0.00048	0.70	1.0E5
3	0.00010	0.70	1.0E5
4	0.00320	0.70	1.0E5
5	0.00170	0.70	1.0E5
6	0.00010	0.70	1.0E5
7	0.00010	0.70	1.0E5
8	0.00010	0.70	1.0E5
9	000010	0.70	1.0E5
10	2.50E-6	0.70	1.0E5
11	0.00010	0.70	1.0E5
12	0.00010	0.70	1.0E5
13-30	0.00	0.70	1.0E5

This model is not used with the LWR COR package.

7132 – Arrhenius Non-Oxidation Release Coefficients for Metallic Fuel

When metallic fuels melt in a non-oxidizing environment, the release of fission products is gradual over time and dependent upon the vapor pressure of the fission product class. The release correlation takes the form

$$dM/dt = -R\,M_o \text{ where } R = k_o \exp(-Q/R_{gas}\,T),$$

where R is the Arrhenius release rate (fraction/minute), k_o is a proportionality constant (fraction / minute), R_{gas} is the universal gas constant in units of kcal/(mole K), Q is a correlation constant in units of kcal/mole, and T is the fuel temperature (K). The values of k_o, Q and a maximum allowed release rate R_m are specified in this coefficient. This model is applied to each core cell and fuel element independently in order to properly account for varying fission product concentration throughout the core. The default values in MELCOR for each class are

Class	k_o [C7132(1,j)] (1./min)	Q [C7132(2,j)] (kcal/mole)	R_m [C7132(3,j)] (1./min)
1	0.00	0.00	1.0E5
2	0.00	0.00	1.0E5
3	0.00	0.00	1.0E5

Class	k_o [C7132(1,j)] (1./min)	Q [C7132(2,j)] (kcal/mole)	R_m [C7132(3,j)] (1./min)
4	0.00	0.00	1.0E5
5	0.00	0.00	1.0E5
6	0.00	0.00	1.0E5
7	0.00	0.00	1.0E5
8	0.00	0.00	1.0E5
9	0.00	0.00	1.0E5
10	0.00	0.00	1.0E5
11	0.00	0.00	1.0E5
12	0.00	0.00	1.0E5
13-30	0.00	0.00	1.0E5

This model is not used with the LWR COR package.

7135 – Noble Gas Release on Failure of Metallic Fuel

Metallic fuel elements normally fail through cladding rupture. When the cladding ruptures, much of the noble gas inventory is released in a puff. The failure itself is calculated in the COR Package, but the noble gas release is calculated in the RN package using this coefficient.

(1) - Noble gas class
(default = 1.0, units = none, equiv = none)

(2) - Fraction of the noble gas inventory in the fuel element and cell that is released on fuel failure. The remainder is left in the fuel to be released using the time-dependent release models.
(default = 0.80, units = none, equiv = none)

(3) - Fraction of the released gas that is placed in the center channel when the inner fuel fails. The remainder is placed in the inner annulus.
(default = 0.50, units = none, equiv = none)

(4) - Fraction of the released gas that is placed in the inner annulus when the outer fuel fails. The remainder is placed in the outer annulus.
(default = 0.50, units = none, equiv = none)

This model is not used with the LWR COR package.

7136 – Solubility of RN Classes in Water Films

If part or all of a water film drains from a surface of a heat structure to the pool in the associated control volume, any fission products deposited on that surface are

normally relocated with the water in proportion to the fraction of the film that is drained. These coefficients allow the film fission product relocation behavior to be modified by changing the fraction of fission product deposits which are assumed to be dissolved in—and therefore relocate with—the film.

C7136(i) is the fraction of class i deposited on a surface that is treated as dissolved in any water film on that surface. Thus,

fraction_of_class_i_relocated = C7136(i) x fraction_of_film_relocated.

Class	C7136(i)
1-30	1.0

Sensitivity coefficient arrays 7140, 7141, 7142, 7143, and 7144 described below pertain to metallic fuels and are not applicable to the LWR version of MELCOR. The models are not described in the RN Package Reference Manual.

7140 – Release from Molten U-Al Pools

These values are used to alter the release rates of fission products from pools of molten U-Al. The model is described in more detail in the pool release model reference.

This model is not used with the LWR COR package.

(1) - Contact angle of an escaping bubble with the pool surface.
(default = 170.0, units = degrees, equiv = none)

(2) - The contact angle of a nucleating bubble with the nucleation site at bubble departure. The departure diameter is determined from
Departure_diameter = 0.0208 x C7140(2) x $\sqrt{(\sigma / g)}$
(default = 10.0, units = degrees, equiv = none)

(3) - Coefficient of bubble coalescence and breakup.
n_{bub}/t = C7140(3) x r^3_{bub} x n^2_{bub} + nucleation – rise
(default = 1.0, units = none, equiv = none)

(4) - Minimum permitted bubble diameter.
(default = 1.0E-4, units = m, equivalence = none)

(5) - Mean size of nucleation cavity openings.
(default = 1.0E-4, units = m, equiv = none)

(6) - Standard deviation of normal distribution of nucleation cavity openings.
(default = 3.6E-5, units = m, equiv = none)

(7) - Maximum concentration of nucleation sites present in the pool for a temperature between the solidus and liquidus temperatures of the fuel.
(default = 6.5E6, units = number/kg, equiv = none)

(8) - Concentration of permanent nucleation sites existing at all temperatures.
(default = 100.0, units = number/kg, equiv = none)

(9) - Coefficient in correlation for Sherwood (Nusselt) number used to calculate mass transfer at the pool surface.
$Sh = C7140(9)\ Ra^{C(7140(10))}$, Ra = Rayleigh number
(default = 0.2, units = none, equiv = none)

(10) - Exponent in above correlation.
(default = 0.26, units = none, equiv = none)

(11) - Fraction (between 0.0 and 1.0) of pool surface open for collection of bubbles.
(default = 1.0, units = none, equiv = none)

(12) - Diffusivity of all RN classes in molten metal pool.
(default = 1.0E-11, units = m^2/s, equiv = none)

(13) - Switch defining limits on nucleation of fission products.
= 1.0 No limits; fission product material immediately available to nucleation site
= 2.0 Diffusion limited; nucleation limited by the rate at which fission products diffuse to nucleation sites
= 3.0 Convection and diffusion limited; nucleation is limited by the rate at which fission products convect and diffuse to nucleation sites
(default = 1.0, units = none, equiv = none)

7141 – Solubility of Classes in Al-U Alloy

Solubility of each fission product class in a molten metal pool, used as the concentration below which it is assumed that there is no driving force present for the release of that class. That is, for lower concentrations there will be no release of the class by the pool release model.

This model is not used with the LWR COR package.

(n) - Solubility of class n (1 to 30).
(default = 0.0, units = moles/liter, equiv = none)

7142 – Debris Particle of Average Surface Area

This dimension defines the surface-to-volume ratio for debris. This model is not used with the LWR COR package.

(1) - Dimension of particle with average surface area.
(default = 3.2E-4, units = m, equiv = none)

7143 – Molten Fraction Criterion for Release from U-Al Pools

Below this mole fraction, the CORSOR or CORSOR-M model of fission product release will be applied. At higher molten fractions, the fission product release calculation will switch to the molten pool model.

This model is not used with the LWR COR package.

(1) - Molten fraction at which release calculation switches to the molten pool model.
(default = 0.62, units = none, equiv = none)

7144 – Temperature Criterion for Release from Intact Fuel

No release will be calculated from intact fuel below this temperature.

This model is not used with the LWR COR package.

(1) - Threshold temperature for FP release from intact fuel.
(default = 933.0, units = K, equiv = none)

7150 – SPARC-90 Model Parameters

These parameters are used to control the SPARC-90 Pool Scrubbing model.

(1) - Number of spatial steps taken in tracking the ascent of the bubbles as they rise through the pool.
(default = 10., units = none, equiv = XNRISE)

(2) - Number of angular steps taken between 0 and 180 degrees in calculating heat and mass transfer from the interior to the surface of the rising bubbles.
(default = 5., units = none, equiv = XNCIRC)

(3) - Error tolerance in the calculation of the saturation ratio in the rising bubbles.
(default = 1.E-4, units = none, equiv = ERRSMX)

(4) - Maximum number of iterations permitted during the calculation of the saturation ratio.
(default = 25., units = none, equiv = XITSMX)

(5) - Error tolerance in the calculation of the energy transfer in the rising bubbles.
(default = 1.E-4, units = none, equiv = ERREMX)

(6) - Maximum number of iterations permitted during the calculation of the energy transfer in the rising bubbles.
(default = 25., units = none, equiv = XITEMX)

(7) - Error tolerance in the calculation of the temperature in the rising bubbles.
(default = 1.E-3, units = none, equiv = ERRTMX)

(8) - Maximum number of iterations permitted during the calculation of the temperature in the rising bubbles.
(default = 25., units = none, equiv = XITTMX)

(9) - Maximum decontamination factor. Calculated decontamination factors that exceed this value will result in the complete removal (i.e., absorption into the pool) of the associated vapor or aerosol.
(default = 1.E12, units = none, equiv = DFMAX)

(10) - Vent exit condensation decontamination factor scaling factor. This factor is applied to the decontamination factor that is calculated as a result of steam condensation in the vent exit region that occurs when the bubbles are thermally equilibrated with the pool temperature. GE's Moody suggested a value of 3. at one time according to the authors of SPARC-90.
(default = 1.0, units = none, equiv = ECMULT)

7151 – SPARC-90 Globule Size Correlation

This correlation relates the initial size of the globule formed to the Weber number of the gas exiting the vent with velocity V_o. The cube of the initial diameter of the gas globule is given by

$$D_g^3 = 1.5\, v_n\, D_o^2 \left(\sigma/\rho_l\, g\right)^{1/2}$$

where D_o is the equivalent diameter of the vent, σ and ρ_l are the surface tension and density of the pool and the normalized volume v_n is given by

$$v_n = a\, We^b \quad (We = \rho_l D_o V_o^2 / \sigma)$$

and the constants a and b are given by constants C7151(1,i) and C7151(2,i), respectively for vent type i = MVENT.

i (vent type)	C7151(1,i)	C7151(2,i)
1 (sparger)	3.45	0.46
2 (downcomer)	0.0891	0.616
3 (horizontal)	0.857	0.73

7152 – SPARC-90 Bubble Size/Shape Model

The volume mean diameter of bubbles formed at the vent exit is given by

$$d_{vm} = C7152(1) \cdot 10^{C7152(2) + (C7152(3) + C7152(4)\ x_{nc})^{C7152(5)}}$$

where x_{nc} is the noncondensible gas fraction in the gas exiting the vent. The bubbles are modeled as oblate spheroids with a major to minor axis ratio given by

$$\frac{a}{b} = C7152(6) + C7152(7)\, d_{vm} + C7152(8)\ d_{vm}^2$$

(1) - Initial bubble diameter correlation coefficient.
(default = 7.E-3, units = m, equiv = DIAMI)

(2) - Initial bubble diameter correlation exponent constant.
(default = -0.2265, units = none, equiv = none)

(3) - Initial bubble diameter correlation exponent constant.
(default = 0.0203, units = none, equiv = none)

(4) - Initial bubble diameter correlation exponent constant.
(default = 0.0313, units = none, equiv = none)

(5) - Initial bubble diameter correlation exponent constant.
(default = 0.5, units = none, equiv = none)

(6) - Oblate spheroid major/minor axis ratio correlation constant.
(default = 0.817, units = none, equiv = none)

(7) - Oblate spheroid major/minor axis ratio correlation constant.
(default = 1.13466, units = cm^{-1}, equiv = none)

(8) - Oblate spheroid major/minor axis ration correlation constant.
(default = -0.3795. units = cm^{-2}, equiv = none)

7153 – SPARC-90 Bubble Rise Velocity Model

The bubble rise velocity relative to the liquid is given by the following correlation

$$V_r = C7153(1)\,(\sigma / \rho_l)^{1/4}\ \text{(cm/s) for}\ d_{vm} \le 0.5\ \text{cm}$$

$$V_r = C7153(3)\,V_r(d_{vm} = 0.5\ \text{cm})\,d_{vm}^{C7153(4)}\ \text{(cm/s) otherwise}$$

where σ and ρ_l are the surface tension and density of the liquid, respectively.

(1) - Coefficient for rise velocity correlation of small bubbles.
(default = 7.876, units = cm/s, equiv = none)

(2) - Transition diameter from small to large bubble rise velocity correlations.
(default = 0.5, units = cm, equiv = none)

(3) - Coefficient for rise velocity correlation of large bubbles.
(default = 1.40713, units = none, equiv = none)

(4) - Exponent for diameter in rise velocity correlation of large bubbles.
(default = 0.49275, units = none, equiv = none)

7154 – SPARC-90 Swarm Velocity Model

The bubble swarm velocity correlation is given by

$$\overline{V}_s = \text{MIN}\left\{ 0.5\left[V_s(x=0) + V_s(x=h_p)\right] C7154(5)\right\}$$

where

$$V_s(x) = \{[(Q_s + C7154(1)\ ]/C7154(2)\}^{C7154(3)}[1 - C7154(4)x](cm/s)$$

x is the vertical distance from the surface of the pool and h_p is the depth of the pool at the vent exit.

(1) - Constant in the swarm velocity correlation.
(default = 5.33, units = liter/s, equiv = none)

(2) - Constant in the swarm velocity correlation.
(default = 3.011E-3, units = liter-s/cm^2, equiv = none)

(3) - Exponent in the swarm velocity correlation.
(default = 0.5, units = none, equiv = none)

(4) - Coefficient of x in equation for $V_s(x)$.
(default = -3.975E-4, units = cm^{-1}, equiv = none)

(5) - Maximum permitted value of the swarm velocity.
(default = 170., units = cm/s, equiv = VSWRMX)

7155 – SPARC-90 Particle Impaction Model

If gas leaves the vent exit at a high velocity, the initial globules rapidly lose that velocity. The forward globular interface, as it slows and stops, can capture particles if they have sufficient inertia. Inertia and drag of particle size i is represented by the Stokes number

$$Stk_i = \frac{\rho_i V_e d_i^2}{9\,\mu\, D_0}$$

where

d_i = particle diameter
ρ_i = particle density
V_e = vent exit gas velocity (before equilibration with pool)
μ = gas viscosity
D_o = vent exit orifice diameter

The decontamination factor for this impaction process is given by

$$DF_{II,i} = (1-\alpha_i)^{-1}$$

where

$$\alpha_i = C7155(1) \cdot C7155(2)^{C7155(3)^{\sqrt{Stk_i}}} \text{ if } \sqrt{Stk_i} \le C7155(4)$$

$$\alpha_i = C7155(5) \cdot C7155(6)^{C7155(7)^{\sqrt{Stk_i}}} \text{ otherwise}$$

and α_i is limited to a maximum value of C7155(8).

(1) - Constant in α_i correlation for small Stokes number.
(default = 1.79182, units = none, equiv = none)

(2) - Constant in α_i correlation for small Stokes number.
(default = 3.3437E-11, units = none, equiv = none)

(3) - Constant in α_i correlation for small Stokes number.
(default = 5.9244E-3, units = none, equiv = none)

(4) - Transition value of SQRT(Stk_i) for changing from small to large Stokes number correlation for α_i.
(default = 0.65868, units = none, equiv = none)

(5) - Constant in α_i correlation for large Stokes number.
(default = 1.13893, units = none, equiv = none)

(6) - Constant in α_i correlation for large Stokes number.
(default = 1.4173E-6, units = none, equiv = none)

(7) - Constant in α_i correlation for large Stokes number.
(default = 4.25973E-3, units = none, equiv = none)

(8) - Maximum permitted value of α_i.
(default = 0.99, units = none, equiv = none)

7156 – SPARC-90 Solute Ionization Correlations

The van't Hoff ionization factors are used in modeling hygroscopic effects that promote steam condensation on hygroscopic aerosol particles even in subsaturated atmospheres. The temperature-dependent correlations have the form

$I_{sol}[T^\circ C] = I_{sol}[C7156(9)][1 + C7156(8)\{T-C7156(9)\}]$ (sol = CsOH or CsI)

$I_{CsOH}[C7156(9)] = C7156(6) + C7156(7)[n_{CsOH}/n_T]$

$I_{CsI}[C7156(9)] = C7156(1) + C7156(2)[n_{CsI}/n_T]$ for $n_{CsI}/n_T \leq C7156(3)$

$I_{CsI}[C7156(9)] = C7156(4) + C7156(5)[n_{CsI}/n_T]$ otherwise

$I_{sol'}[T^\circ C] = C7156(10)$ for all other solutes in the droplet

where $n_T = n_{CsOH} + n_{CsI} + n_{sol} + n_w$ is the total number of moles and $n_{sol'}$ is the number of moles of soluble material excluding CsOH and CsI in the growing droplet/aerosol.

(1) - Additive constant in low concentration CsI correlation.
(default = 1.79417, units = none, equiv = none)

(2) - Multiplicative constant in low concentration CsI correlation.
(default = -3.34363, units = none, equiv = none)

(3) - Transition CsI molar ratio between CsI correlations.
(default = 0.021, units = none, equiv = none)

(4) - Additive constant in high concentration CsI correlation.
(default = 1.63439, units = none, equiv = none)

(5) - Multiplicative constant in high concentration CsI correlation.
(default = 4.30022, units = none, equiv = none)

(6) - Additive constant in CsOH correlation.
(default = 1.75467, units = none, equiv = none)

(7) - Multiplicative constant in CsOH correlation.
(default = 20.7974, units = none, equiv = none)

(8) - Multiplicative constant in temperature correction correlation.
(default = -0.002321, units = none, equiv = none)

(9) - Reference temperature for CsI and CsOH van't Hoff ionization correlations.
(default = 25., units = C, equiv = none)

(10) - Temperature independent van't Hoff ionization constant for other solutes.
(default = 2., units = none, equiv = XIVH)

7157 – SPARC-90 Settling Velocity Correlation

A set of empirical correlations are used to determine the Reynolds number, Re, from which $V_{g,i}$, the settling velocity of particles of size *i* in the rising bubbles, follows as

$$V_{g,i} = (\mu\, Re\,)/(\rho_g d_i\,)$$

where μ and ρ_g are the viscosity and density of the gas, respectively, and d_i is the diameter of the particle. The empirical correlations are

$$f\,(\mathrm{Re}) = \left(4\,\rho_i\,\rho_g\,g\,d_i^3\right)/\left(3\,\mu^2\,\right)$$

$$\mathrm{Re} = [f(\mathrm{Re})/C7157(2)]^{C7157(3)} \text{ if } C7157(1) < f(\mathrm{Re}) < C7157(4)$$

$$= [f(\mathrm{Re})/\,C7157(5)]^{C7157(6)} \text{ if } C7157(4) \le f(\mathrm{Re}) < C7157(7)$$

$$= [f(\mathrm{Re})/\,C7157(8)]^{C7157(9)} \text{ if } C7157(7) \le f(\mathrm{Re}) < C7157(10)$$

$$= [f(\mathrm{Re})/\,C7157(11)]^{C7157(12)} \text{ if } C7157(10) \le f(\mathrm{Re}) < C7157(13)$$

$$= [f(\mathrm{Re})/\,C7157(14)]^{C7157(15)} \text{ if } C7157(13) \le f(\mathrm{Re})$$

For particles with a diameter less than about 70 microns, the gravitational settling velocity follows Stokes law and is given by

$$V_{g,i} = \left(\rho_i\,g\,S_i\,d_i^2\right)/(18\mu) \text{ if } f(\mathrm{Re}) \le C7157(1)$$

where S_i is the Cunningham slip correction factor for particles of size *i*.

(1) - First bound on *f*(Re) in settling velocity correlation.
(default = 9.6, units = none, equiv = none)

(2) - First denominator in settling velocity correlation.
(default = 27.00, units = none, equiv = none)

(3) - First exponent in settling velocity correlation.
(default = 1./1.130, units = none, equiv = none)

(4) - Second bound on *f*(Re) in settling velocity correlation.
(default = 93.6, units = none, equiv = none)

(5) - Second denominator in settling velocity correlation.
(default = 24.32, units = none, equiv = none)

(6) - Second exponent in settling velocity correlation.
(default = 1./1.227, units = none, equiv = none)

(7) - Third bound on *f*(Re) in settling velocity correlation.
(default = 410., units = none, equiv = none)

(8) - Third denominator in settling velocity correlation.
(default = 15.71, units = none, equiv = none)

(9) - Third exponent in settling velocity correlation.
(default = 1./1.417, units = none, equiv = none)

(10) - Fourth bound on *f*(Re) in settling velocity correlation.
(default = 1.07E4, units = none, equiv = none)

(11) - Fourth denominator in settling velocity correlation.
(default = 6.477, units = none, equiv = none)

(12) - Fourth exponent in settling velocity correlation.
(default = 1./1.609, units = none, equiv = none)

(13) - Fifth bound on *f*(Re) in settling velocity correlation.
(default = 2.45E5, units = none, equiv = none)

(14) - Fifth denominator in settling velocity correlation.
(default = 1.194, units = none, equiv = none)

(15) - Fifth exponent in settling velocity correlation.
(default = 1./1.867, units = none, equiv = none)

7158 – SPARC-90 HOI Correlation

The partition coefficient for organic iodine (CH_3I) is given by the following correlation

$$H_{OI} = T/10^{C7158(1)/T+C7158(2)}$$

with the temperature, T, given in degrees K.

(1) - First constant in exponent of correlation for H_{OI}.
(default = -1388.89, units = K, equiv = none)

(2) - Second constant in exponent of correlation for H_{OI}.
(default = 6.461, units = none, equiv = none)

7159 – SPARC-90 I2 Chemistry Model Parameters

The first eleven parameters are used to calculate the temperature-dependent equilibrium constants for the five chemical reactions considered in the I_2 scrubbing model. The reactions considered are

$$I_{2(g)} \leftrightarrow I_{2(aq)}$$

$$I_{2(aq)} + I^- \leftrightarrow I_3^-$$

$$I_{2(aq)} + H_2O \leftrightarrow H^+ + I^- + HIO$$

$$I_{2(aq)} + H_2O \leftrightarrow H_2OI^+ + I^-$$

$$H_2O \leftrightarrow H^+ + OH^-$$

The equilibrium constant for the i^{th} reaction (i = 1,..,4) is given by

$$EQK(i) = C7159(2 \cdot i - 1)\exp[C7159(2*i)/T]$$

while the equilibrium constant for the dissociation of water is given by

$$EQK(5) = C7159(9)\exp\left[C7159(10)\ /T + C7159(11)/T^2\right]$$

The twelfth parameter is a value of gaseous iodine concentration (moles/cm^3) that is used to indicate when saturation of the pool prevents continued iodine scrubbing. If the iodine vapor concentration in the bubbles exceeds this value but scrubbing is prevented by a large iodine concentration in the pool, then a message is issued to notify the user of the condition. The thirteenth parameter is the relative error tolerance used in iteratively solving the system of iodine chemistry equilibrium equations for the iodine partition coefficient.

(1) - Coefficient of the equilibrium constant for the first iodine chemistry reaction.
(default = 1.3882E-3, units = none, equiv = none)

(2) - Constant used in the exponent of the equilibrium constant for the first iodine chemistry reaction.
(default = 3279.3, units = K, equiv = none)

(3) - Coefficient of the equilibrium constant for the second iodine chemistry reaction.
(default = 7.7606, units = moles^{-1}, equiv = none)

(4) - Constant used in the exponent of the equilibrium constant for the second iodine chemistry reaction.
(default = 1370., units = K, equiv = none)

(5) - Coefficient of the equilibrium constant for the third iodine chemistry reaction.
(default = 1.0423E-2, units = moles^2, equiv = none)

(6) - Constant used in the exponent of the equilibrium constant for the third iodine chemistry reaction.
(default = -7148., units = K, equiv = none)

(7) - Coefficient of the equilibrium constant for the fourth iodine chemistry reaction.
(default = 4.2271E-9, units = moles, equiv = none)

(8) - Constant used in the exponent of the equilibrium constant for the fourth iodine chemistry reaction.
(default = -1748.5, units = K, equiv = none)

(9) - Coefficient used in the equilibrium constant for the dissociation of water. (default = 1.56531E-13, units = moles^2, equiv = none)

(10) - First constant used in the exponent of the dissociation constant for water. (default = 5462.81, units = K, equiv = none)

(11) - Second constant used in the exponent of the dissociation constant for water. (default = -1.87376E6, units = K^2, equiv = none)

(12) - Minimum iodine vapor concentration required to issue a message indicating the cessation of scrubbing due to pool saturation. (default = 1.E-6, units = moles/cm^3, equiv = CGITST)

(13) - Relative error tolerance used in solving the iodine equilibrium equations. (default = 1.E-3, units = none, equiv = ERRTOL)

7160 – Chemisorption

The coefficients give the chemisorption rate for species j on surface type i through the following equation:

$$k_{ij} = a_{ij} e^{\frac{-E_{ij}}{RT_i}}$$

The values of a and E are stored in the array C7160(i,j) where

i - Type of parameter,
= 1, chemisorption coefficient a, m/s
= 2, activation energy E, J/kg

j - CA class, dimensioned 10 (maximum number of CA classes).

7170 – Hygroscopic Aerosol Parameters

The user-adjustable parameters for the hygroscopic aerosol model contained in coefficient array C7170 are described in the following. The coefficients allow the user to input the water solubility of RN class materials as a linear function of temperature, to adjust the ionization factor for the RN material (basically the number of ions formed upon dissolving in water), and to input/adjust the material density of the RN class compound.

The solubility in water of an RN class "N" can be specified at two temperatures, between which the solubility is assumed to vary linearly. Outside of this temperature range the solubility is held constant at the value associated with the temperature

range boundary value. Usually the temperature range is specified in reference books as "cold" water, taken to be 273K and "hot" water, taken to be 373K. The user can adjust these temperature limits. The material solubility is expressed in units of kg of solute per kg of water (*note, not kg solution*). Upon being dissolved in water the RN class compound is assumed to form 2 ions, as would be the case for $CsI \rightarrow Cs^{+} + I^{-}$. The user can modify this to some other value to represent a more complex dissolution process. In order to assure smoothness in the model behavior as higher temperature is approached (eg. approaching the water critical point), the RN class solubility is gradually reduced to zero over a temperature range, normally between 600K and 647K). The solubility or ionization factor is also reduced to zero over this same temperature range.

For each RN class material the following C7170 coefficients can be adjusted. The coefficient array is doubly dimensioned where the first index is the specific coefficient value, and the second index is the RN class number.

(1,N) - Reference temperature for low temperature saturation solubility.
(default = 273.0, units = K , equiv = none)

(2,N) - Reference temperature for high temperature saturation solubility.
(default = 373.0, units = K , equiv = none).

(3,N) - Saturation solubility at low temperature reference.
(default =See Table 3, units = [kg/kg H_2O], equiv = none)

(4,N) - Saturation solubility [kg/kg H_2O] at high temperature reference.
(default = See Table 3, units = [kg/kg H_2O], equiv = none)

(5,N) - Temperature to begin linearly reducing solubility factor.
(default = 600.0, units = K , equiv = none).

(6,N) - Temperature above which solubility factor is zero.
(default = 647.0, units = K , equiv = none).

(7,N) - Value of ionization factor below C7170(5).
(default = 2.0, units = dimensionless , equiv = none).

(8,N) - Value of ionization factor above C7170(6). The default value is 0.
(default = 0.0, units = dimensionless , equiv = none).

(9,N) - Class compound material density.
(default = See Table 3, units = [kg/m^3], equiv = none)

The following table provides those default values for C7170 that are unique to a specific RN class. The user may also want to modify the RN class compound molecular weight when modeling specific aerosol materials that are not default RN class compounds, such as NaOH or MgO. These are accessible through sensitivity coefficient array C7120(2,N).

Table 3. Default Hygroscopic Properties of RN Class Compounds.

RN Class "N"	Compound Density [kg/m^3]	Compound Solubility At 273K [kg/kg H_2O]	Compound Solubility At 373K [kg/kg H_2O]	Ionization Factor
Sensitivity Coefficient ⇒	**C7170(9,N)**	**C7170(3,N)**	**C7170(4,N)**	**C7170(7,N)**
1. Noble Gases: Xe	1	0	0	--
2. Alkali Metals: CsOH	3675	3.95	3.95	2
3. Alkaline Earths: BaO	5720	0	0	2
4. Halogens: I_2	1	0	0	2
5. Chalcogens: Te	5680	0	0	2
6. Platinoids: Ru	6970	0	0	2
7. Transition: Mo	7470	0	0	2
8. Tetravalent: Ce	7000	0	0	2
9. Trivalents: La	6510	0	0	2
10. Uranium: UO2	10960	0	0	2
11. Cd	8150	0	0	2
12. Sn	6446	0	0	2
13. Boron	2520	0	0	2
14. Water: H2O	1000	--	--	0
15. Concrete	2250	0	0	2
16. CsI	4510	.44	2.25	2

7180 - Iodine Pool Model Mass Transfer Parameters

These mass transfer parameters are used to calculate the pool-to-atmosphere and atmosphere-to-surface transfer rates, and the nitric/hydrochloric acid atmosphere-to-surface deposition rates. Default values for Pool-atmosphere and iodine-steel wall give good agreement with the ISP-41 test problem. The values for iodine-painted wall are unknown and the defaults are the same as for the steel wall.

(1) - Pool-atmosphere mass transfer rate.
(default = 0.003, units = m/s, equiv = none).

(2) - HCl acid deposition rate.
(default = 0.003, units = m/s, equiv = none).

(3) - H_2NO_3 acid deposition rate.
(default = 0.003, units = m/s, equiv = none).

(4) - Iodine-steel wall adsorption rate.
(default = 0.0009, units = m/s, equiv = none).

(5) - Iodine-steel wall desorption rate.
(default = 9E-7, units = 1/s, equiv = none).

(6) - Iodine-painted wall adsorption rate.
(default = 0.0009, units = m/s, equiv = none).

(7) - Iodine-painted wall desorption rate.
(default = 9E-7, units = 1/s, equiv = none).

7181 - Iodine Pool Chemistry Iteration Parameters

These are used to control the solution of the iodine pool chemistry equations. The defaults give good convergence on the ISP-41 test problem. The difference between parameter (3) and parameters (4) and (5) is that parameter (3) is applied to each chemical species after solution by the chemistry solver; parameters (4) and (5) are passed to the solver to determine a local convergence for each species.

(1) - ODE chemistry solver effective time step.
(default = 1.0, units = s, equiv = none).

(2) - ODE chemistry solver maximum number of timesteps.
(default = 4000, units = none, equiv = none).

(3) - Chemistry solver species relative error tolerance.
(default = 0.0001, units = none, equiv = none).

(4) - Chemistry solver absolute convergence error.
(default = 1E-13, units = kmole/m^3, equiv = none).

(5) - Chemistry solver relative convergence error.
(default = 0.0001, units = none, equiv = none).

7182 - Iodine Pool Chemistry Activation Limits

These are used to define when the pool chemistry solution is activated. These are used because the chemistry solution has a limited range of validity. The parameters are consistent with late-time conditions in a plant accident scenario.

(1) - Minimum iodine concentration in pool.
(default = 1E-10, units = kmole/m^3, equiv = none).

(2) - Maximum atmosphere pressure.
(default = 1E6, units = Pa, equiv = none).

(3) - Minimum atmosphere volume.
(default = 0.1, units = m^3, equiv = none).

(4) - Maximum atmosphere temperature.
(default = 500, units = K, equiv = none).

(5) - Maximum pool temperature.
(default = 425, units = K, equiv = none).

(6) - Minimum pool volume.
(default = 0.0, units = m^3, equiv = none).

5. Plot Keys And Control Function Variables

The plot keys and control function arguments for the RN package are given below. Within slashes (/ /) a 'p' indicates a plot variable and a 'c' indicates a control function argument.

Note that many of these quantities are available ONLY as control function arguments. These can be plotted by inclusion of PLOTxxx input records in MELGEN and MELCOR input. See the Executive (EXEC) Package Users' Guide for details. While inconvenient, this was found necessary to avoid generation of excessively large plot files.

RN1-CPUC	/p/	Total time for the run routines of the RN1 package. (units = s)
RN1-CPUE	/p/	Total time for the edit routines of the RN1 package. (units = s)
RN1-CPUR	/p/	Total time for the restart routines of the RN1 package. (units = s)
RN1-CPUT	/p/	Sum of the run, edit and restart times of the RN1 package. (units = s)
RN1-ATMG.cv	/p/	Total mass of aerosol (radioactive plus nonradioactive) in the gas phase, for each control volume cv. (units = kg)
RN1-ARMG.cv	/p/	Total mass of radioactive aerosol in the gas phase, for each control volume cv. (units = kg)

RN1-VTMG.cv	/p/	Total mass of fission product vapor (radioactive plus nonradioactive) in the gas phase, for each control volume cv. (units = kg)
RN1-VRMG.cv	/p/	Total mass of radioactive fission product vapor in the gas phase, for each control volume cv. (units = kg)
RN1-ATML.cv	/p/	Total mass of aerosol (radioactive plus nonradioactive) in the liquid phase, for each control volume cv. (units = kg)
RN1-ARML.cv	/p/	Total mass of radioactive aerosol in the liquid phase, for each control volume cv. (units = kg)
RN1-VTML.cv	/p/	Total mass of fission product vapor (radioactive plus nonradioactive) in the liquid phase, for each control volume cv. (units = kg)
RN1-VRML.cv	/p/	Total mass of radioactive fission product vapor in the liquid phase, for each control volume cv. (units = kg)
RN1-XMRLSE-x-y.cv	/cp/	Total mass of class x released from COR components in control volume cv. The parameter y specifies total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-XMRLSET	/cp/	Total non-radioactive plus radioactive mass released from COR components. (units = kg)
RN1-XMRLSER	/cp/	Total radioactive mass released from COR components. (units = kg)
RN1-AMG-w-x-y.cv	/c/	Aerosol mass of section w, class x, in the atmosphere of control volume cv not including aerosols deposited on heat structures. The parameter y specifies total mass (y=1) or radioactive mass only (y=2). (units = kg.)
RN1-VMG-x-y.cv	/c/	Vapor mass of class x, in the atmosphere of control volume cv not including vapor deposited on heat structures. The parameter y specifies total mass (y=1) or radioactive mass only (y=2). (units = kg)

RN1-AML-x-y.cv	/c/	Aerosol mass of class x, in the pool of control volume cv not including aerosols deposited on heat structures. The parameter y specifies total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-VML-x-y.cv	/c/	Vapor mass of class x, in the pool of control volume cv not including vapor deposited on heat structures. The parameter y specifies either total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-ADEP-s-x-y.hs	/c/	Aerosol mass of class x, deposited on side s (s=1 is the LHS, s=2 is the RHS) of heat structure hs. The parameter y specifies total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-VDEP-s-x-y.hs	/c/	Vapor mass of class x, deposited on side s (s=1 is the LHS, s=2 is the RHS) of heat structure hs. The parameter y specifies total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-ATMT	/p/	Total radioactive plus non-radioactive aerosol mass in the atmosphere and pool regions, not including deposited aerosols on heat structures. (units = kg)
RN1-ATMR	/p/	Total radioactive aerosol mass in the atmosphere and pool regions, not including deposited aerosols on heat structures. (units = kg)
RN1-VTMT	/p/	Total radioactive plus non-radioactive fission product vapor mass in the atmosphere and pool regions, not including deposited vapors on heat structures. (units = kg)
RN1-VTMR	/p/	Total radioactive fission product vapor mass in the atmosphere and pool regions, not including deposited vapors on heat structures. (units = kg)
RN1-TMT	/p/	Total radioactive and non-radioactive aerosol and fission product vapor masses in the atmosphere and pool regions. Equal to RN1-ATMT plus RN1-VTMT variables. (units = kg)

RN1-TMR	/p/	Total radioactive aerosol and fission product vapor masses in the atmosphere and pool regions. Equal to RN1-ATMR plus RN1-VTMR variables. (units = kg)
RN1-MDTT-n-y	/p/	Total radioactive and non-radioactive mass deposited on heat structure n (user number) on side y. The values of y are 1 for the LHS and 2 for the RHS. (units = kg)
RN1-MDTR-n-y	/p/	Total radioactive mass deposited on heat structure n (user number) on side y. The values of y are 1 for the LHS and 2 for the RHS. (units = kg)
RN1-TMDTT	/p/	Total radioactive and non-radioactive mass deposited on all heat structures. (units = kg)
RN1-TMDTR	/p/	Total radioactive mass deposited on all heat structures. (units = kg)
RN1-DHTOT	/p/	Total decay heat calculated by RadioNuclide package for all locations of radionuclides. (units = W)
RN1-DHCOR	/p/	Total decay heat from the radionuclides in the core. (units = W)
RN1-DHCAV	/p/	Total decay heat from the radionuclides in the cavity. (units = W)
RN1-DHDEP	/p/	Total decay heat from the radionuclides deposited on the heat structures. (units = W)
RN1-DHATM	/p/	Total decay heat from airborne radionuclides. (units = W)
RN1-DHPOL	/p/	Total decay heat from radionuclides in the pool. (units = W)
RN1-AMGT-x-y.cv	/c/	Aerosol mass of class x in the atmosphere of control volume cv (sum of sections), not including aerosols deposited on heat structures. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2). (units = kg)
RN1-CVCLT-x-y.cv	/c/	Total mass of class x as aerosol and vapor in control volume cv. Includes mass in pool and atmosphere, but not that

		deposited on heat structures. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2). (units = kg)
RN1-TYCLT-x-1.ty	/c/	Total mass of class x in all control volumes of type ty, including mass deposited on heat structures associated with the control volumes. (units = kg)
RN1-TYCLT-x-2.ty	/cp/	Radioactive mass of class x in all control volumes of type ty, including mass deposited on heat structures associated with the control volumes. (units = kg)
RN1-CVTOT-y.cv	/c/	Mass of radionuclides in control volume cv. Includes mass in pool and atmosphere, but not that deposited on heat structures. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2). (units = kg)
RN1-TYTOT-1.ty	/c/	Sum of total masses of radionuclides in all control volumes of type ty. Includes mass in pool and atmosphere, but not that deposited on heat structures. (units = kg)
RN1-TYTOT-2.ty	/cp/	Sum of radioactive masses of radionuclides in all control volumes of type ty. Includes mass in pool and atmosphere, but not that deposited on heat structures. (units = kg)
RN1-MMDW.cv	/p/	Mass median diameter of the wet aerosol distribution in the gas phase for each control volume cv. (units = m)
RN1-GSDW.cv	/p/	Geometric standard deviation of the wet aerosol distribution in the gas phase for each control volume cv. (units = none)
RN1-MMDD.cv	/p/	Mass median diameter of the dry aerosol distribution in the gas phase for each control volume cv. (units = m)
RN1-GSDD.cv	/p/	Geometric standard deviation of the dry aerosol distribution in the gas phase for each control volume cv. (units = none)
RN1-PH.nnn	/p/	pH of pool in control volume nnn. (units = none)

RN1-IOP-cccccc.nnn	/c/	Concentration of aqueous species cccccc in control volume nnn. Although this is available as a plot variable, the "c" means that the pool species must be specified on record RNIOPyyy before it can be output. This is done because there are many pool species (39) and the user does not necessarily want them all on the plot file, increasing the size of the plot output file. The species cccccc can be one of the names in the table in the RNIOP record description. (units = kmole/m^3)
RN1-IOT-x-y-.cv	/c/	Total mass of iodine pool surface deposition class x deposited on surfaces in control volume cv. The parameter y specifies either total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-IOD-s-x-y.hs	/c/	Mass of iodine pool surface deposition class x deposited on side s of heat structure hs. The parameter y specifies either total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-CAT-x-y-.cv	/c/	Total mass of chemisorption surface deposition class x deposited on surfaces in control volume cv. The parameter y specifies either total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-CAD-s-x-y.hs	/c/	Mass of chemisorption surface class x deposited on side s of heat structure hs. The parameter y specifies either total mass (y=1) or radioactive mass only (y=2). (units = kg)
RN1-TMCAT	/p/	Total mass of chemisorbed species deposited on all heat structures. (units = kg)
RN1-TMCAR	/p/	Total radioactive mass of chemisorbed species deposited on all heat structures. (units = kg)
RN1-MCAT-n-y	/p/	Total mass chemisorbed on side y of heat structure n (user number). The LHS is y=1 and the RHS is y=2. (units = kg)
RN1-MCAR-n-y	/p/	Total radioactive mass chemisorbed on side y of heat structure n (user number). The LHS is y=1 and the RHS is y=2. (units = kg)

RN1-MMDC-x.cv	/p/	Mass median diameter of component x in the aerosol distribution in the gas phase for each control volume cv. (units = m)
RN1-GSDC-x.cv	/p/	Geometric standard deviation of component x in the aerosol distribution in the gas phase for each control volume cv. (units = none)
RN2-CPUC	/p/	Total time for the run routines of the RN2 package. (units = s)
RN2-CPUE	/p/	Total time for the edit routines of the RN2 package. (units = s)
RN2-CPUR	/p/	Total time for the restart routines of the RN2 package. (units = s)
RN2-CPUT	/p/	Sum of the run, edit and restart times of the RN2 package. (units = s)
RN2-AMFLT-x.f	/c/	Total aerosol mass of class x on filter f, where f is the filter number. (units = kg.)
RN2-AMFLT.f	/cp/	Total aerosol mass on filter f (sum of RN2-AMFLT-x.f) (units = kg)
RN2-VMFLT-x.f	/c/	Total vapor mass of class x on filter f. (units = kg)
RN2-VMFLT.f	/p/	Total vapor mass on filter f (sum of RN2-VMFLT-x.f). (units = kg)
RN2-FLT-QTOT.f	/p/	Total decay heat from all radionuclides deposited on filter f. (units = W)
RN2-FLT-QLOS.f	/p/	Heat loss from filter f (portion of RN2-FLT-QTOT that is assumed to be lost from the system). (units = W)
RN2-VFLT-TMP.f	/p/	Temperature of charcoal bed in vapor filter f. (units = K)
RN2-VFLT-RAD.f	/p/	Radiolytic desorption rate of fission product vapors from filter f. (units = kg/s)
RN2-VFLT-THR.f	/p/	Thermal desorption rate of fission product vapors from filter f. (units = kg/s)

RN2-VFLT-BUR.f	/p/	Rate of fission product vapor release from filter f due to charcoal combustion. (units = kg/s)
RN2-DFBUB-w.ip	/p/	Instantaneous decontamination factor of aerosols in mass section w from pool scrubbing associated with path ip. (ip=10*NFL+1 for the *from* volume associated with flow path NFL, ip=10*NFL+2 for the *to* volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.)
RN2-DFBUB-a.ip	/p/	(a=NUMSEC+1) Instantaneous decontamination factor of total aerosol mass from pool scrubbing associated with path ip. (ip=10*NFL+1 for the *from* volume associated with flow path NFL, ip=10*NFL+2 for the *to* volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.)
RN2-DFBUB-v.ip	/p/	(v=NUMSEC+1+x) Instantaneous decontamination factor of vapor in class x from pool scrubbing associated with path ip. (ip=10*NFL+1 for the *from* volume associated with flow path NFL, ip=10*NFL+2 for the *to* volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.) Currently, only x=4 is calculated.
RN2-DFBBT-w.ip	/p/	Cumulative decontamination factor of aerosols in mass section w from pool scrubbing associated with path ip. (ip=10*NFL+1 for the *from* volume associated with flow path NFL, ip=10*NFL+2 for the *to* volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.)
RN2-DFBBT-a.ip	/p/	(a=NUMSEC+1) Cumulative decontamination factor of total aerosol mass from pool scrubbing associated with path ip. (ip=10*NFL+1 for the *from* volume associated with flow path NFL, ip=10*NFL+2 for the *to* volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.)
RN2-DFBBT-v.ip	/p/	(v=NUMSEC+1+x) Cumulative decontamination factor of vapor in class x from pool scrubbing associated with path ip. (ip=10*NFL+1 for the *from* volume associated with flow path

NFL, ip=10*NFL+2 for the *to* volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.) Currently, only x=4 is calculated.

6. Example Input

The following input is typical of that for a full plant calculation. The CORSOR-Booth model is used instead of the default CORSOR-M model, and a 16th class for CsI is used. A second aerosol component is used for better treatment of water aerosols, and the modeled size range for aerosols is extended. Initial radionuclide inventories in the core fuel are set for a three-ring, five-level core, with the bottom of active fuel at the sixth core level, and fractions of those inventories for five classes that have already been released to the fuel-cladding gap are initialized. Example input for flowthrough areas and heat structure deposition surfaces is provided, and a filter having decontamination factor of 4.0 and able to remove up to 0.1 kg of aerosols independent of class is placed in a flow path.

```
RN1000      0    * activate RN package
*
* declare 2 aerosol components (one for water)
* and add 16th class for CsI
*           NUMSEC NUMCMP NUMCLS NCLSW CLSBX NUMSRA NUMSRV NCLCSI
RN1001      5      2      16     14    13    0      0      16
*
* combine Cs and I to form CsI
RNCLS0100  16          * acceptor class number
RNCLS0101   2    1.0   * one mole class 2 (Cs) per mole CsI
RNCLS0102   4    0.5   * one-half mole class 4 (I2) per mole CsI
*
* define new CsI "element" - call it CI to put in class 16
*           ELMNAM  ELMMAS
DCHNEM0100  CI      1.E-6    * must establish nonzero initial mass
*
* define decay curve for "CI" - combination of Cs and I curves
*           TIME     DCHEAT     TIME     DCHEAT     TIME     DCHEAT
DCHNEM0101  0.       5.0211E5   6.12     4.0919E5   11.88    3.8675E5
DCHNEM0102  18.      3.5494E5
DCHNEM0103  29.88    3.1747E5   61.2     2.8612E5   118.8    2.4439E5
DCHNEM0104  241.2    2.3141E5   612.     2.1557E5   1188.    1.9989E5
DCHNEM0105  3600.    1.5937E5   5400.    1.3421E5   7200.    1.2565E5
DCHNEM0106  14400.   8.3485E4   21600.   6.8352E4   28800.   5.8241E4
DCHNEM0107  36000.   5.1511E4   43200.   4.3972E4   54000.   3.8938E4
DCHNEM0108  72000.   3.1424E4   86400.   2.6405E4   129600.  1.7206E4
DCHNEM0109  172800.  1.3019E4   259200.  8.8273E3   345600.  6.4804E3
DCHNEM0110  518400.  4.5686E3   691200.  3.5628E3   864000.  3.0797E3
*
* define decay heat for class 16
```

```
DCHCLS0160  CSI    * new class name
DCHCLS0161  CI     * element "CI" defined with DCHNEM records
*
RNCLVN01    16   25    * RN class 16 maps into VANESA group 25
RNVNCL01    25   16    * VANESA group 25 maps back into RN class 16
*
RNFP000     -3    * use CORSOR-Booth model for high burn-up fuel
*
* initialize core radionuclide masses as fractions of total
* 40% rings 1 and 2, 20% ring 3
* 15% level 6, 25% level 7, 30% level 8, 20% level 9, 10% level10
*            NINP    RINP1    RINP2
RNFPN11001  0        0.1      0.4    *  4% of total mass in cell 110
RNFPN10901  0        0.2      0.4    *  8% of total mass in cell 109
RNFPN10801  0        0.3      0.4    * 12% of total mass in cell 108
RNFPN10701  0        0.25     0.4    * 10% of total mass in cell 107
RNFPN10601  0        0.15     0.4    *  6% of total mass in cell 106
*
RNFPN21001  0        0.1      0.4    *  4% of total mass in cell 210
RNFPN20901  0        0.2      0.4    *  8% of total mass in cell 209
RNFPN20801  0        0.3      0.4    * 12% of total mass in cell 208
RNFPN20701  0        0.25     0.4    * 10% of total mass in cell 207
RNFPN20601  0        0.15     0.4    *  6% of total mass in cell 206
*
RNFPN31001  0        0.1      0.2    *  2% of total mass in cell 310
RNFPN30901  0        0.2      0.2    *  4% of total mass in cell 309
RNFPN30801  0        0.3      0.2    *  6% of total mass in cell 308
RNFPN30701  0        0.25     0.2    *  5% of total mass in cell 307
RNFPN30601  0        0.15     0.2    *  3% of total mass in cell 306
*
RNFPN00001  0        0.0      0.0    *  no initial cavity inventory
*
*                                     100% total
*
* initialize gap fractions - constant throughout core
NINP     RINP1    RINP2
RNGAP11001  1        0.03     1.0    * 3% of class 1 (Xe) in gap
RNGAP11002  2        0.05     1.0    * 5% of class 2 (Cs) in gap
RNGAP11003  3        1.E-6    1.0    * .0001% of class 3 (Ba) in gap
RNGAP11004  4        0.017    1.0    * 1.7% of class 4 (I) in gap
RNGAP11005  5        0.0001   1.0    * .01% of class 5 (Te) in gap
*
RNGAP10901  -110     1.0      1.0    * same fractions as in cell 110
RNGAP10801  -110     1.0      1.0    * same fractions as in cell 110
RNGAP10701  -110     1.0      1.0    * same fractions as in cell 110
RNGAP10601  -110     1.0      1.0    * same fractions as in cell 110
*
```

```
RNGAP21001  -110     1.0      1.0    * same fractions as in cell 110
RNGAP20901  -110     1.0      1.0    * same fractions as in cell 110
RNGAP20801  -110     1.0      1.0    * same fractions as in cell 110
RNGAP20701  -110     1.0      1.0    * same fractions as in cell 110
RNGAP20601  -110     1.0      1.0    * same fractions as in cell 110
*
RNGAP31001  -110     1.0      1.0    * same fractions as in cell 110
RNGAP30901  -110     1.0      1.0    * same fractions as in cell 110
RNGAP30801  -110     1.0      1.0    * same fractions as in cell 110
RNGAP30701  -110     1.0      1.0    * same fractions as in cell 110
RNGAP30601  -110     1.0      1.0    * same fractions as in cell 110
*
* change minimum and maximum aerosol sizes
*           DMIN     DMAX     RHONOM
RN1100      5.E-7    5.E-4    1000.
*
RNACOEF      1    * calculate the aerosol coefficients (don't read)
*
* set water (class 14) to aerosol component 2
RNCC001      1  1  1  1  1  1  1  1  1  1  1  1  2  1  1
*
* declare flowthrough areas at bottom of CV 301
*           IVOLF    IVOLT    ELEV     AREA
RNSET001    301      302      12.0     75.0
RNSET002    301      303      12.0     25.0
*
* override heat structure 10501 orientation for RN deposition
*           IDS      ISDE     ITYP
RNDS001     10501    RHS      FLOOR     * default orientation "WALL"
RNDS002     10501    LHS      CEILING   * default orientation "WALL"
*
* place aerosol filter in flow path 321
* with global DF of 4.0 and maximum loading of 0.1 kg
*           IFLTFP   CTYPE    DFG       XMASG
RN2FLT0100  321      AEROSOL  4.0       0.1
```

RN input for initial aerosol and vapor inventories and time-dependent sources is more appropriate for simulating experiments or just a portion of an accident in a plant. To initialize class aerosol masses in a control volume and to set up aerosol and vapor sources, the following input could be used:

```
* declare tabular aerosol and vapor sources
*           NUMSEC   NUMCMP   NUMCLS   NCLSW    NCLSBX   NUMSRA   NUMSRV
RN1001      5        2        16       14       13       1        1
*
* initial CsI aerosol masses in CV 301
*           IVOL     ICLS     RFRAC
```

```
RNAG001     301      16       1.0
*           XMASS for each of NUMSEC sections
RNAG002     0.1      0.1      0.1      0.1      0.1
*
* CsI aerosol source defined by TF 101 with log-normal dist.
*           IVOL     IPHS     ICLS     RFRAC    XM       ITAB     IDIST
RNAS000     301      2        16       1.0      1.0      101      2
* mass median diameter = 10.0 microns, standard deviation = 2.0
*           AMMD     GSD
RNAS001     10.E-6   2.
*
* aerosol TF linearly decreasing from 0.1 kg/s to zero at 100 s
*           TFNAME             NTFPAR   TFSCAL   TFADCN
TF10100     AEROSOL-SOURCE     2        1.0      0.0
*           TIME     RATE
TF10110     0.0      0.1
TF10111     100.0    0.0
*
* iodine vapor source defined by TF 102
*           IVOL     IPHS     ICLS     RFRAC    XM       ITAB
RNVS000     301      2        4        1.0      1.0      102
*
* vapor TF linearly constant at 0.05 kg/s
*           TFNAME             NTFPAR   TFSCAL   TFADCN
TF10200     VAPOR-SOURCE       1        1.0      0.0
*           TIME     RATE
TF10210     0.0      0.05
*
```

7. Error Messages

The error messages from the MELGEN program are concerned with the input and should be self-explanatory. There are three error and informative messages from MELCOR, two concerning the aerosol calculations and one concerning the decay heat split.

The first message from MELCOR informs the user that the RN package had to cut the time step while doing the aerosol time integration. The format is as follows:

```
RN1 PACKAGE TIME STEP CUT
CALLED BY AEROSOL RUNGE-KUTTA INTEGRATOR
IN CONTROL VOLUME xxxxx
```

It indicates that the numerical integration routine in MAEROS was unable to complete its integration through the timestep. If this error occurs frequently, relay this information to the MELCOR group so appropriate action can be taken.

The second error message is similar to the first, but occurs when the error in component mass conservation exceeds the specified tolerance given by C7000(2) for some component. The message is

```
RN1 PACKAGE TIME STEP CUT
EXCESSIVE ERROR IN AEROSOL CALCULATION
IN CONTROL VOLUME xxxxx
AEROSOL COMPONENT = xx   RELATIVE ERROR =  x.xxxxxEee
```

and, if it appears frequently, the MELCOR development group should be notified.

The third error message notes a problem with the decay heat split in that all the decay heat is not used. The message is:

```
PROBLEM WITH DECAY HEAT SPLIT AT TIME =  X.XXXXEXX
DIFF    =  X.XXXXEXX
SUMTOT  =  X.XXXXEXX
TOTDH   =  X.XXXXEXX
```

Here DIFF is the difference between the total power from decay of radionuclides in control volumes or on the surfaces (TOTDH) and the sum of the powers distributed to control volume contents and heat structure surfaces (SUMTOT). The occurrence of this message should be relayed to the MELCOR staff for resolution.

Containment Sprays (SPR) Package Users' Guide

The MELCOR containment spray package models the heat and mass transfer between spray water droplets and the containment building atmosphere.

This Users' Guide describes the input to the SPR package, including a brief description of the models employed, the input format, sample input, discussion of the output, sensitivity coefficients, plot variables, and control variables. Details on the models can be found in the SPR Package Reference Manual.

Contents

1. Introduction

The MELCOR Containment Spray (SPR) package models the heat and mass transfer between spray water droplets and the containment building atmosphere. The modeling in the SPR package is taken virtually intact from the HECTR 1.5 code. The model assumes, among other things, that spray droplets are spherical and isothermal and that they fall through containment at their terminal velocity and that there is no horizontal velocity component. In a special application, the spray model is used to treat condensation from the Heat Structures (HS) package's film-tracking model that "rains" from inverted surfaces into the containment atmosphere.

An arbitrary number of spray sources may be placed in any containment control volume. The source of water (reservoir) for each spray may be identified with the pool of any CVH control volume, or it may be left unidentified. If a CVH pool is designated as the spray source reservoir, then the spray will operate only if the pool has sufficient water. The user provides input in the form of pool heights in the reservoir to determine whether there is sufficient water for spray operation. The user may set a flag to stop the calculation if the water level in any reservoir falls below the specified minimum requirement. Radionuclides dissolved in the reservoir water will not be transported along with the water to the spray source (i.e., it is assumed that there is a perfect filter for all radionuclides between the reservoir and the spray).

For each spray source, except for sources associated with "rain" from the HS film-tracking model, the user must specify an initial droplet temperature and flow rate, each of which may be controlled by a control function. The user may turn the sprays on and off with a separate control function for each spray source. A droplet size distribution may also be input for each spray source. In other words, the spray droplets for each source may be divided into a number of different size bins, with individual drops representing the average droplet size being tracked during their fall through the control volume; the total heat and mass transfer for the spray source is obtained by summing the heat and mass transfers calculated for all sizes.

For spray sources associated with "rain" from the HS film-tracking model, the user must define an "out" transfer process in the MELCOR Transfer Process (TP) package that retrieves the "rain" from an associated "in" transfer process that is accessed by the HS film-tracking model. In this special application of the spray package model, the user should not specify control functions for the droplet temperature or flow rate or a CVH pool as the source reservoir. Refer to Section 5.4 of the Heat Structures Package Users' Guide for an example of Spray package and Transfer Process package input for the special HS film-tracking "rain" application. Note that radionuclides associated with the condensate film in the HS package currently are not transferred with the "rain" to the Spray package; they stay with the remaining film on the structure.

For each droplet type, the following computation is done in each control volume in the spray train. Spray droplet heatup and cooldown in a steam environment are modeled using a correlation for forced convection heat transfer coefficients. Similarly, evaporation and condensation are modeled using a correlation for mass transfer coefficients. The heat and mass transfer correlations have been formulated specifically for high temperature atmospheres, such as might be encountered during a hydrogen burn.

These coefficients are used to compute heat and mass transfer rates, which are integrated by a Runge-Kutta method over the fall height of the spray droplet to obtain the final droplet mass and temperature. By comparing the droplet mass and temperature at the bottom of the compartment to the inlet conditions, the heat transfer and mass transfer to a given droplet are computed. Total heat and mass transfer rates are calculated by multiplying the rates for one droplet by the total number of droplets of that size and summing over all droplet sizes. It is assumed that this total heat and mass transfer rate is constant over a given timestep, and it is also assumed that the containment atmosphere conditions do not change significantly during the fall time of the drop.

The user can describe how droplets falling from one control volume are to be carried over to lower control volumes. The user may designate that specified fractions of those droplets be transferred to one or more additional control volumes for continued heat and mass transfer to the atmosphere. (These droplets are currently treated independently of other spray trains involving those control volumes.) Alternatively, a separate control volume may be designated as the containment spray sump. Droplets reaching the bottom of a control volume and not carried over to other volumes will be placed in the pool of the sump control volume. Otherwise, droplets reaching the bottom of a control volume and not carried over to other volumes nor placed in a separate sump are put into the pool of that control volume.

It should be noted that the SPR package does not model interactions between spray droplets and other structures (nor does any other MELCOR package). Thus, it is not possible to model either core sprays or steam generator auxiliary feed water sprays properly using the SPR package.

WARNING

The SPR Package is coupled to the MELCOR Radionuclide (RN) package for the calculation of aerosol washout and atmosphere decontamination by the sprays. Current limitations of this interface require some restrictions on the input to the SPR package to avoid nonphysical results associated with multiple calculations in the same control volume. When the SPR and RN packages are both active, the user should limit the spray input so that only one spray train passes through each control volume and only a single drop size is used in this spray train.

2. User Input

2.1 MELGEN Input

2.1.1 Spray Source Data

The user must define the control volumes in which the spray sources are located. The user may optionally define the elevations of the spray sources if the sources are not at the top of the control volumes. The user may optionally input the numbers of the control functions determining whether the spray sources are on or off. Also, for each source the user must define the droplet initial temperature, the spray flow rate, and the droplet size distribution.

SPRSRnn00 – Spray Source Name, Control Volume, Control Function
01 ≤ nn ≤ 99, nn is the user-defined spray source number (may be any value—contiguous numbers are not necessary).
Required

This record allows the user to define a spray source name, the number of the control volume containing the spray source, and the elevation of the source in that control volume. The user can define an optional control function determining whether the spray source is on or off, a control volume containing the water reservoir, a flag to stop the calculation if the reservoir becomes dry, the pool elevation below which the reservoir is declared to be "dry" and the pool elevation that must be reached before spray operation can resume following "dryout."

(1) SPNAME - Character string defining a name for spray source.
(type = character*16, default = none)

(2) IVOL - Number of control volume containing the spray source.
(type = integer, default = none)

(3) FALLHS - Elevation of the spray source in control volume IVOL source. If this number is not input, the top elevation of control volume IVOL will be used. The value of FALLHS must be between the bottom and top elevations of control volume IVOL.
(type = real, default = top elevation of control volume IVOL, units = m)

(4) ISPCON - Number of logical control function to be used in determining whether spray source is on or off. If the control function value is .TRUE., the spray source is on, if the value is .FALSE., the spray

source is off. If no number is input, or if the number is not greater than zero, the spray source is assumed to be always on.
(type = integer, default = -1)

(5) IVOLRS - Number of control volume containing reservoir (pool) for spray source. If no number is input, then the spray source is unidentified.
(type = integer, default = no entry)

(6) IFDRY - Reservoir "dryout" option flag: enter 0 to inactivate spray upon reservoir "dryout", enter 1 to stop calculation upon reservoir "dryout."
(type = integer, default = 0)

(7) ELDRY - Reservoir pool elevation at "dryout."
(type = real, default = CVBOT + 0.01*(CVTOP – CVBOT))

(8) ELWET - Reservoir pool elevation to resume spray after "dryout"
(type = real, default = ELDRY + 0.04*(CVTOP – CVBOT))

SPRSRnn01 – Spray Droplet Temperature and Flow Rate
$01 \leq nn \leq 99$, nn is the user-defined spray source.
Required

This record allows the user to define the initial spray droplet temperature and flow rate for the spray source. These values may be defined either as constants or by control functions. The optional fifth field is only used in conjunction with the Heat Structures (HS) package film-tracking "rain" model.

(1) TDROPO - Initial temperature of all droplets from this source. Used if control function ITMPCF is not input. The value of TDROPO must be between 273.15 and 647.245 even if the value will not be used because ITMPCF is input.
(type = real, default = none, units = K)

(2) SPFLO - Total spray volumetric flow rate from this source. Used if control function IFLOCF is not input. The value of SPFLO must be greater than or equal to zero even if the value will not be used because IFLOCF is input.
(type = real, default = none, units = m^3/s)

(3) ITMPCF - Number of real-valued control function whose value is the initial temperature (K) of all droplets from this source. The value of the control function must be between 273.15 and 647.245. This field

is optional. If it is positive, the control function ITMPCF will be used for the droplet temperature and TDROPO is not used.
(type = integer, default = 0)

(4) IFLOCF - Number of a real-valued control function whose value is the total spray flow rate (m^3/s) for this source. The value of the control function must be greater than or equal to zero. This field is optional. If it is positive, the control function IFLOCF will be used for the flow rate and SPFLO is not used.
(type = integer, default = -1)

(5) IHSTP - "Out" transfer process number associated with the "in" transfer process that the Heat Structures package uses to transfer "rain" from the film-tracking model to the Spray package. If IHSTP is input, the specifications of temperature (TDROPO or ITMPCF) and flow (SPFLO or IFLOCF) will not be used.
(type = integer, default = "not used")

SPRSRnnmm – Spray Droplet Size Distribution
$01 \leq nn \leq 99$, nn is the user-defined spray source.
$02 \leq mm \leq 99$, mm is used for ordering the input.
Required

This record allows the user to define the initial spray droplet diameter and relative frequency for a droplet type in the spray source. One record per droplet type, maximum number of droplet types per source is 5.

Note: When the RadioNuclide package is active, radionuclide washout by sprays is automatically calculated. However, the radionuclide washout calculations used with caution when multiple spray droplet sizes and/or spray trains are present in the same control volume. For this reason, the user is strongly urged to avoid multiple droplet sizes and multiple spray trains in any control volumes where radionuclide washout calculations are to be performed.

(1) DIAMO - Initial diameter for this droplet type from this source. The value of DIAMO must be greater than zero.
(type = real, default = none, units = m)

(2) DRFREQ - Relative frequency in source for this droplet type. The value of each frequency must be between 0.0 and 1.0 and the frequencies of all droplets from a source must sum to 1.
(type = integer, default = none, units = none)

2.1.2 Spray Junction Data

Spray droplets reaching the bottom of a control volume may be carried over to other control volumes. The fraction of these droplets entering each subsequent control volume is specified by the user. If the sum of the specified fractions for a given 'from' volume is CAROVR, then CAROVR must be no greater than one. If CAROVR is less than one, and the "from" control volume is not in the list of control volumes emptying into the sum (see Section 2.1.3), then a fraction (1 – CAROVR) of the droplets is placed into the pool of the "from" volume. Spray droplets from a given spray source may pass through no more than 20 spray junctions.

SPRJUNmm – Spray Junction Volumes, Transmission Factors
01 ≤ mm ≤ 99, mm is the user-defined spray junction number (may be any value—contgiuous numbers are not necessary).
Optional

(1) KCVFM - "From" control volume number for this junction
(type = integer, default = none)

(2) KCVTO - "To" control volume number for this junction
(type = integer, default = none)

(3) FRSPTI - Fraction of spray droplets reaching bottom of "from" volume that are to be transported into "to" volume. Must be between 0 and 1.
(type = real, default = none, units = none)

2.1.3 Spray Sump Data

The user may optionally define the control volume that contains the sump. The sump is a pool into which spray droplets will be deposited if the droplets reach the bottom of user-selected control volumes and are not carried over into other control volumes. The user may define a list of control volumes from which droplets will enter the sump. If the sum of the transmission factors for a volume in that list is CAROVR, then a fraction (1 – CAROVR) of the droplets reaching the bottom of the volume is placed into the sump. At present, no more than one sump may be defined.

SPRSUMP0 – Spray Sump Control Volume
Optional

(1) MCVSUM - Number of the control volume containing the sump.
(type = integer, default = none)

SPRSUMPn – Control Volumes which Empty Sprays into Sump
$1 \leq n \leq 9$, n is used for ordering input.
Optional

These records are required if any spray droplets are to fall into the sump.

(1) ICVISM - Number of a control volume through which spray droplets may fall into sump. Up to 10 control volumes may be entered on a record. These control volume numbers must have already been input on either spray source or spray junction records.
(type = integer, default = none)

2.2 MELCOR Input

There is at present no MELCOR input to the containment sprays package.

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the MELCOR EXEC Users' Guide.

3.1 SPR Sensitivity Coefficients

The sensitivity coefficients for the containment sprays package have identifier numbers from 3000 through 3099.

3000 – Correlation Coefficients for Terminal Droplet Velocity and Reynolds Number

This correlation is used for velocity and Reynolds number calculations. Three correlations are considered to take into account different expressions for the drag coefficient based on the Reynolds number.

$$
\begin{aligned}
C_d &= C3000(1)\mathrm{Re}^{C3000(2)} && \text{for} && \mathrm{Re} < C3000(4) \\
&= C3000(5)\mathrm{Re}^{C3000(6)} && \text{for } C3000(4) < && \mathrm{Re} < C3000(8) \\
&= C3000(9) && \text{for } C3000(8) < && \mathrm{Re}
\end{aligned}
$$

The elements of sensitivity coefficient array 3000 are not independent. The following relationships should be observed:

$$C3000(3) = 2.0 + C3000(2)$$

$$C3000(7) = 2.0 + C3000(6)$$

$$C3000(4) = [C3000(1) / C3000(5)] ** \{1 / [C3000(6) - C3000(2)]\}$$

$$C3000(8) = [C3000(5) / C3000(9)] ** \{-1 / C3000(6)\}$$

(1) - Multiplier for low Reynolds number
(default = 27.0, units = none, equiv = DIVVEL)

(2) - Exponent for low Reynolds number
(default = -0.84, units = none, equiv = EXDVVL)

(3) - 2 + C3000(2)
(default = 1.16, units = none, equiv = INEXVL)

(4) - Breakpoint between low and medium Reynolds correlations
(default = 77.737154, units = none, equiv = FRBKRY)

(5) - Multiplier for medium Reynolds number
(default = 0.271, units = none, equiv = DVVEL2)

(6) - Exponent for medium Reynolds number
(default = 0.217, units = none, equiv = EDVVL2)

(7) - 2 + C3000(6)
(default = 2.217, units = none, equiv = IEXVL2)

(8) - Breakpoint between medium and high Reynolds correlations
(default = 10006.443, units = none, equiv = SCBKRY)

(9) - Drag coefficient at high Reynolds numbers
(default = 2.00, units = none, equiv = DVVEL3)

3001 – Correlation Coefficients for Mass Transfer

This correlation is used to calculate the mass derivative. It uses the mass transfer correlation described in the SPR Package Reference Manual.

$$F(\mathrm{Re}, Sc) = C3001(3) + C3001(4)\mathrm{Re}^{C3001(5)}\, Sc^{C3001(6)}$$

C3001(1) is the leading multiplier in the correlation and must be negative, and C3001(2) should not be changed.

(1) - Leading multiplier for derivative of mass with respect to time equation (default = -2.0, units = none, equiv = MLDMDT)

(2) - Additive factor in log expression (default = 1.0, units = none, equiv = LGDMDT)

(3) - Additive factor in Reynolds-Schmidt number combination (default = 1.0, units = none, equiv = ADRYSC)

(4) - Multiplicative factor in Reynolds-Schmidt number combination (default = 0.25, units = none, equiv = MLRYSC)

(5) - Exponent for Reynolds number (default = 0.5, units = none, equiv = EXREYN)

(6) - Exponent for Schmidt number (default = 0.3333, units = none, equiv = EXSCHM)

4. Plot Variables and Control Function Arguments

The Containment Sprays package's variables that may be used for plot variables and control function arguments are described below. The control function arguments are denoted by a 'c.' The plot variable arguments are denoted by a 'p.' The 'c' or 'p' characters are inside slashes '/' following the variable name.

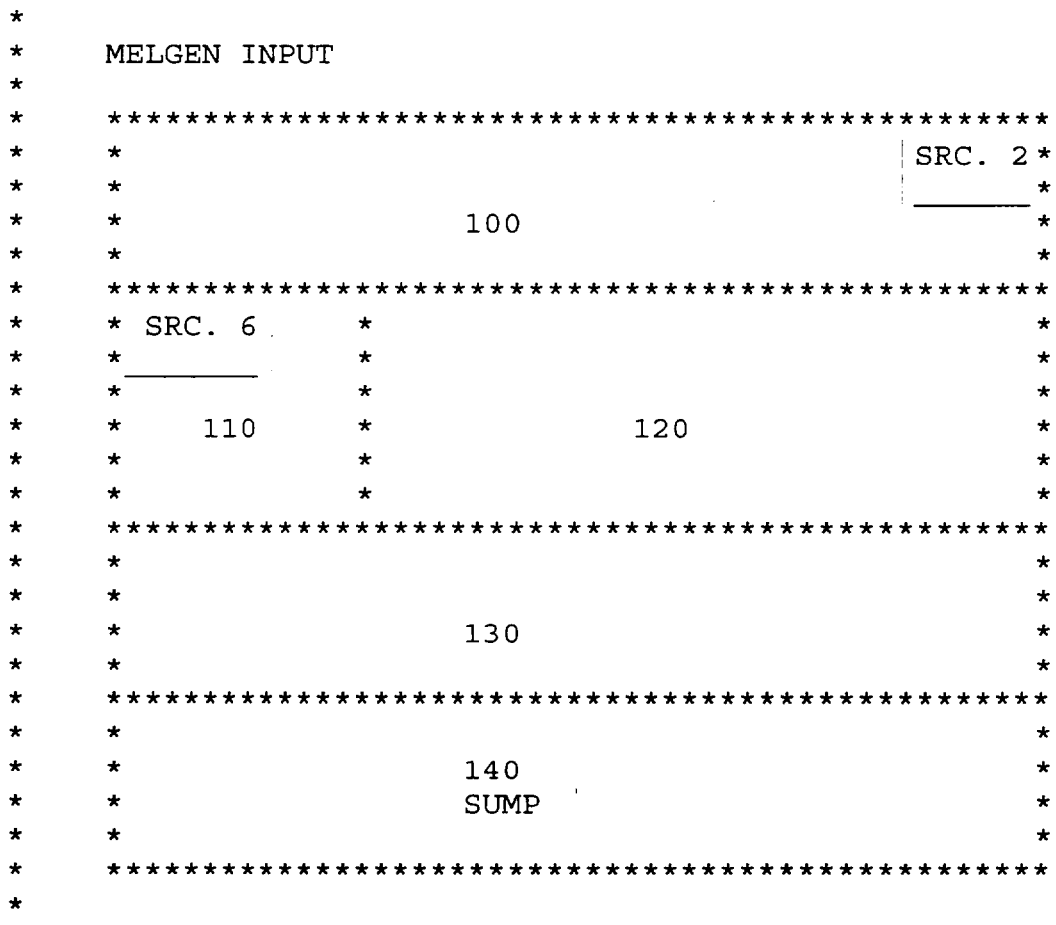
SPR-TP.n	/cp/	Temperature of spray droplets from source n (units = K)
SPR-FL.n	/cp/	Flow rate of spray droplets from source n (units = m^3/s)
SPR-HTTRAN.j	/cp/	Rate of heat transfer from sprays to steam in control volume j (units = W)
SPR-MSTRAN.j	/cp/	Rate of mass transfer from sprays to steam in volume j (units = kg/s)
SPR-SUMPHT.j	/cp/	Rate of heat transfer from sprays to pool in sump control volume j (units = W)
SPR-SUMPMS.j	/cp/	Rate of mass transfer from sprays to pool in sump control volume j (units = kg/s)

5. Example Input

5.1 Sample Problem Description

Containment is nodalized into 5 control volumes, numbered 100, 110, 120, 130, and 140. Two spray sources with different characteristics are defined. Source 2, in volume 100, has three droplet sizes and source 6, in volume 110, has two droplet sizes. Seventy percent of the droplets leaving volume 100 fall into volume 120, with the rest falling into volume 110. All droplets leaving volumes 110 and 120 fall into volume 130. Volume 140 is designated as the sump and all droplets leaving volume 130 are to enter the sump volume.

5.2 Sample Problem MELGEN User Input



```
*          SUMP INFO
*
*          SUMP CONTROL VOLUME
SPRSUMP0            140
*          CONTROL VOLUME OVER SUMP
SPRSUMP1       130
*
*          SPRAY JUNCTION DATA
*
*          FROM VOL   TO VOL     TRAN FAC
SPRJUN05     100         110         0.3
SPRJUN15     100         120         0.7
SPRJUN25     110         130         1.0
SPRJUN35     120         130         1.0
*
*          SPRAY SOURCE DATA
*
*                         SOURCE 2
*          NAME           VOL   ELEV       ON/OFF CF
SPRSR0200 MAINSPRAY       10    10.0       -1
*
*               TEMP   FLOW   TEMPERATURE CF     FLOW CF
SPRSR0201       300.    2.5   -1                 -1
*
*          THREE DROPLET SIZES
*           DIAM       REL. FREQ.
SPRSR0202   1.0E-3          0.6
SPRSR0203   .5E-3           0.3
SPRSR0204   .25E-3          0.1
*
*                         SOURCE 6
*           NAME          VOL         ELEV       ON/OFF CF
SPRSR0600   BACKUPSPRAY   110         10.0       -1
*
*           TEMP      FLOW    TEMPERATURE CF     FLOW CF
SPRSR0601   320.      1.3     -1                 -1
*
*                     TWO DROPLET SIZES
*                     DIAM       REL. FREQ.
SPRSR0602             0.75E-3          0.75
SPRSR0603             0.66E-3          0.25
*
```

5.3 Inventory-Limited Spray Sample Input

It is often necessary to simulate situations where the inventory of spray source water is limited. For example, if the spray source water is taken from a tank, the sprays must be

shut off when the tank runs dry. The following control functions simulate this situation. They assume that control function 100 has already been formulated to represent the demanded spray volumetric flow rate. The remaining input integrates the spray flow rate and shuts off the sprays when the total spray flow reaches 1000.0 m^3.

```
*
* CF 100 (NOT SHOWN) IS DEMANDED SPRAY VOLUMETRIC FLOW RATE
*
* THIS CONTROL FUNCTION INTEGRATES THE DEMANDED FLOW RATE
*
CF10100   TOTAL      INTEG      2     1.0   0.0
CF10101   0.0
CF10110   1.0        0.0        CFVALU.100
CF10111   1.0        0.0        TIME
*
* THIS CONTROL FUNCTION GIVES ( 1000 M**3 - INTEGRAL FLOW ), SO
* IT IS NEGATIVE IF MORE THAN 1000 M**3 HAS BEEN DEMANDED.  THEN
* IT TAKES THE 'SIGN' FUNCTION OF THE DIFFERENCE, GIVING A VALUE
* +1 IF INTEGRAL IS LESS THAN 1000 M**3, AND -1 IF GREATER.  THE
* VALUE IS THEN LIMITED TO BE BETWEEN 0.0 AND 1.0.  THUS, THE
* RESULT OF THIS CONTROL FUNCTION IS:
* 0.0     IF INTEGRAL IS GREATER THAN 1000 M**3 (FLOW IMPOSSIBLE)
* 1.0     IF INTEGRAL IS LESS THAN 1000 M**3 (FLOW IS POSSIBLE)
*
CF10200   MULTIPLIER     SIGNI      1     1.0   0.0
CF10201    1.0
CF10202    3          0.0        1.0
CF10210   -1.0        1000.0     CFVALU.101
*
* NOW MULTIPLY DEMANDED SOURCE BY FLOW POSSIBLE MULTIPLIER (ABOVE)
CF10300   SPSOURCE   MULTIPLY   2     1.0   0.0
CF10310   1.0   0.0  CFVALU.100
CF10311   1.0   0.0  CFVALU.102
*
* THIS CONTROL FUNCTION (103) MUST BE REFERENCED ON SPRAY PACKAGE
* RECORD SPRSRNN01 AND REPRESENTS THE ACTUAL VOLUMETRIC FLOW RATE
* TO BE SENT TO THE SPRAYS
```

6. Example Output

In the following output listings, the term "volume weighted frequency" is defined as the sum over all droplet sizes of the droplet frequency multiplied by the cube of the droplet diameter. The sign convention is positive for heat and mass transfer from the spray droplets to the control volume.

6.1 MELGEN Output

```
***** CON SPRAY SETUP EDIT *****

TOTAL NUMBER OF CON SPRAY SOURCES    =   2
TOTAL NUMBER OF CON SPRAY VOLUMES    =   4
TOTAL NUMBER OF CON SPRAY JUNCTIONS  =   4

EDIT OF CON SPRAY SOURCE NUMBER     2
CON SPRAY NAME = MAINSPRAY
SPRAY SOURCE CONTROL VOLUME = 100
SPRAY SOURCE SPRAY VOLUME INDEX =   1
SPRAY SOURCE VOLUME SUMP INDEX =    0
SPRAY SOURCE ELEVATION = 0.10000D+02
SPRAY SOURCE CONTROL FUNCTION =     -1

DROPLET TEMPERATURE =     0.30000D+03
DROPLET TEMPERATURE CONTROL FUNCTION =  -1
DROPLET FLOW RATE = 0.25000D+01
DROPLET FLOW RATE CONTROL FUNCTION =     -1
VOLUME WEIGHTED FREQUENCY =    0.63906D-09
DATA FOR THE   3 DROPLET GROUPS IN THIS SOURCE
**** DROPLET GROUP 1 ****
INITIAL DROPLET DIAMETER =     0.10000D-02
DROPLET FREQUENCY = 0.60000D+00
DROPLET FLOW RATE = 0.44828D+10
INITIAL DROPLET MASS =    0.52133D-06
**** DROPLET GROUP 2 ****
INITIAL DROPLET DIAMETER =     0.50000D-03
DROPLET FREQUENCY =       0.30000D+00
DROPLET FLOW RATE =       0.22414D+10
INITIAL DROPLET MASS =    0.65166D-07
**** DROPLET GROUP 3 ****
INITIAL DROPLET DIAMETER =     0.25000D-03
DROPLET FREQUENCY =       0.10000D+00
DROPLET FLOW RATE =       0.74713D+09
INITIAL DROPLET MASS =       0.81457D-08

EDIT OF JUNCTION DATA FOR THE 4 JUNCTIONS
IN THE FLOW PATH FOR THIS SOURCE
JUNCTION 1 FROM SPRAY VOL 1 TO SPRAY VOL 2 TRAN FAC 0.30000D+00
JUNCTION 2 FROM SPRAY VOL 2 TO SPRAY VOL 4 TRAN FAC 0.10000D+01
JUNCTION 3 FROM SPRAY VOL 1 TO SPRAY VOL 3 TRAN FAC 0.70000D+00
JUNCTION 4 FROM SPRAY VOL 3 TO SPRAY VOL 4 TRAN FAC 0.10000D+01

EDIT OF CON SPRAY SOURCE NUMBER     6
CON SPRAY NAME = BACKUPSPRAY
```

```
SPRAY SOURCE CONTROL VOLUME = 110
SPRAY SOURCE SPRAY VOLUME INDEX =  2
SPRAY SOURCE VOLUME SUMP INDEX =   0
SPRAY SOURCE ELEVATION = 0.10000D+02
SPRAY SOURCE CONTROL FUNCTION =    -1
DROPLET TEMPERATURE =    0.32000D+03
DROPLET TEMPERATURE CONTROL FUNCTION =  -1
DROPLET FLOW RATE = 0.13000D+01
DROPLET FLOW RATE CONTROL FUNCTION =    -1
VOLUME WEIGHTED FREQUENCY =   0.38828D-09
DATA FOR THE 2 DROPLET GROUPS IN THIS SOURCE
**** DROPLET GROUP 1 ****
INITIAL DROPLET DIAMETER =    0.75000D-03
DROPLET FREQUENCY = 0.75000D+00
DROPLET FLOW RATE = 0.47958D+10
INITIAL DROPLET MASS =   0.21842D-06
**** DROPLET GROUP 2 ****
INITIAL DROPLET DIAMETER =    0.66000D-03
DROPLET FREQUENCY = 0.25000D+00
DROPLET FLOW RATE = 0.15986D+10
INITIAL DROPLET MASS =   0.14885D-06

EDIT OF JUNCTION DATA FOR THE 1 JUNCTIONS
IN THE FLOW PATH FOR THIS SOURCE

JUNCTION 1 FROM SPRAY VOL 2 TO SPRAY VOL 4 TRAN FAC 0.10000D+01

EDIT OF CON SPRAY JUNCTION NUMBER  5
'FROM' CONTROL VOLUME NUMBER =     100
'TO' CONTROL VOLUME NUMBER =  110
TRANSMISION FACTOR =     0.30000D+00

EDIT OF CON SPRAY JUNCTION NUMBER  15
'FROM' CONTROL VOLUME NUMBER =     100
'TO' CONTROL VOLUME NUMBER =  120
TRANSMISSION FACTOR =    0.70000D+00

EDIT OF CON SPRAY JUNCTION NUMBER  25
'FROM' CONTROL VOLUME NUMBER =     110
'TO' CONTROL VOLUME NUMBER =  130
TRANSMISSION FACTOR =    0.10000D+01

EDIT OF CON SPRAY JUNCTION NUMBER  35
'FROM' CONTROL VOLUME NUMBER =     120
'TO' CONTROL VOLUME NUMBER =  130
TRANSMISSION FACTOR =    0.10000D+01
```

```
EDIT OF SPRAY VOLUME AND CONTROL VOLUME TABLE

SPRAY VOLUME    CONTROL VOLUME CARRY-OVER FRACTION SUMP INDEX
1               100            0.100D+01           0
2               110            0.100D+01           0
3               120            0.100D+01           0
4               130            0.000D+00           1

EDIT OF CONTROL VOLUMES CONNECTED TO SUMP CONTROL VOLUME = 140

130
```

6.2 MELCOR Output

```
****************************************
*   CONTAINMENT SPRAY PACKAGE EDIT     *
****************************************

CONTAINMENT SPRAY SOURCES

SOURCE     CONTROL VOL     DROP TEMP TEMP DROP FLOW RATE FLOW
NO. NAME        NO.             K    CON FUN   M**3/SEC  CON FUN

2 MAINSPRAY     100  3.00000E+02     -1   2.50000E+00     -1
6 BACKUPSPRAY   110  3.20000E+02     -1   1.30000E+00     -1

NO. DROP SIZES STATUS
3          ON
2          ON

DROPLET DISTRIBUTIONS FOR SOURCE 2

GROUP  DIAMETER      REL. FREQ.      FLOW RATE       DROPLET MASS
NO.       M                        DROPS/SEC            KG

1     1.0000E-03     6.0000E-01     4.4828E+09     5.2133E-07
2     5.0000E-04     3.0000E-01     2.2414E+09     6.5166E-08
3     2.5000E-04     1.0000E-01     7.4713E+08     8.1457E-09

DROPLET DISTRIBUTIONS FOR SOURCE 6

GROUP  DIAMETER      REL. FREQ.      FLOW RATE       DROPLET MASS
NO.       M                        DROPS/SEC            KG

1     7.5000E-04     7.5000E-01     4.7958E+09     2.1842E-07
2     6.6000E-04     2.5000E-01     1.5986E+09     1.4885E-07
```

```
SPRAY JUNCTION DATA FOR SOURCE 2

JUNCTION NO.    FROM VOLUME     TO VOLUME TRANSMISSION FACTOR

5               100             110       3.00000E-01
25              110             130       1.00000E+00
15              100             120       7.00000E-01
35              120             130       1.00000E+00

SPRAY JUNCTION DATA FOR SOURCE 6

JUNCTION NO.    FROM VOLUME     TO VOLUME TRANSMISSION FACTOR

25              110             130       1.00000E+00

SPRAY HEAT AND MASS TRANSFER DATA

CONTROL VOL     HEAT TRAN RATE       MASS TRAN RATE
NO.                   W                    KG/S

100             -8.92000E+08         -3.02538E+02
110             -3.25078E+08         -8.97975E+01
120              1.03529E+07          2.46219E+01
130              2.58977E+07          6.15919E+01

SPRAY DROPLETS LEAVING THESE CONTROL VOLUMES WILL ENTER SUMP
VOLUME 140

130

SPRAY SUMP HEAT AND MASS TRANSFER DATA

CONTROL VOL     HEAT TRAN RATE       MASS TRAN RATE
NO.                   W                    KG/S

140             1.76877E+09          4.08073E+03

END OF EDIT FOR SPR
```

7. Diagnostics and Error Messages

A diagnostic message is printed whenever the differential equation solver is having difficulty integrating the droplet mass equation as the droplet falls through a control volume. This can occur when the problem is determined to be stiff.

A diagnostic message is printed if a droplet enters a control volume in which the saturation temperature corresponding to total pressure is lower than the temperature of the spray

droplet. In that case, the heat and mass transfer rates are not calculated, though calculation of the fall of the droplet will continue.

A diagnostic message is printed if the code is not able to determine the equilibrium temperature of the spray droplet in the steam environment.

Tabular Function (TF) Package
Users' Guide

The Tabular Function (TF) package allows the user to input one-dimensional tables, specify boundary conditions at the end points of the table and use the tables from any portion of the code.

The Users' Guide gives a description of the TF package input, with some examples.

Contents

1. Introduction

The Tabular Function (TF) package allows the user to define one-dimensional tables of (x,y) data pairs for arbitrary independent and dependent variables and to specify extrapolation conditions at the end points of these tables. These tables may then be accessed from other packages in MELCOR as specified by the user via input to those packages. Common uses of tabular functions in MELCOR include specifying decay heat power, control volume mass/energy sources, and flow path velocities as functions of time; defining material properties as functions of temperature; and specifying heat structure boundary conditions (heat transfer coefficient, heat flux, or surface temperature) as functions of time or temperature. Also, user-defined control functions may access tabular functions to specify functional relationships between arbitrary pairs of variables.

Tabular function tables are defined by entering data pairs for the independent and dependent variables. The value of the tabular function (i.e., the y-value for a given x-value) is generated by linear interpolation between the data pairs. The interpolated value is then multiplied by a factor specified by the user and added to another user-specified constant. The minimum number of data pairs defined by the user is one; the maximum is presently limited to a thousand. (For very large tables, the External Data File package can be used; see the EDF Package Users' Guide.)

In most situations input data pairs are sorted so that the independent variables are monotonically increasing. However, step functions can be included in a table by entering two or more values of the independent variable which are equal. In this case, the values are not automatically sorted and entering a decreasing sequence of the independent variable is treated as a fatal error. If a step function is entered and a value is requested which is exactly equal to the step position, the last value entered is returned.

Three options for extrapolation conditions at the upper and lower boundaries of the table are available:

(1) The domain of the function can be extended indefinitely with the function value set equal to the value at the boundary and held constant (the default).

(2) The domain of the function can be extended indefinitely with the two data pairs at the boundary used to linearly extrapolate the table.

(3) The domain of the function can be limited to that spanned by the data pairs' independent variables. If the independent variable is outside the domain of definition, then a fatal error flag is set, and the value is set equal to the boundary value.

Different options may be applied at each end of a table.

2. MELGEN User Input

The user must input two or more records to define a tabular function. The records and their fields are required unless otherwise stated. The records are:

TFnnn00 – Tabular Function Parameter Record
001 ≤ nnn ≤ 999, nnn is the tabular function number.
Required

This record defines the tabular function name, number of data pairs, additive and multiplicative constant. The number of tabular function pairs entered on this record is compared to the number of pairs read in for this tabular function. If they do not agree, then an error occurs. The value of the tabular function is equal to

$$TFVALU = TFSCAL * f(x) + TFADCN$$

where f(x) is the interpolated value of the data pairs. If TFADCN is not defined on the record, then a default value of zero is used.

(1) TFNAME - User-specified tabular function name.
(type = character*16, default = none)

(2) NTFPAR - Number of tabular function data pairs.
(type = integer, default = none, units = none)

(3) TFSCAL - Multiplicative scale factor.
(type = real, default = none, units = none)

(4) TFADCN - Additive constant. This field is optional.
(type = real, default = 0, units = none)

TFnnn01 – Boundary Condition Record
001 ≤ nnn ≤ 999, nnn is the tabular function number.
Optional

The tabular function may be extended beyond its endpoints by extending the function indefinitely and holding the value constant at the endpoint, linearly extrapolating the value from the endpoint and the value nearest the endpoint, or returning an error if a value outside the domain of definition is requested. The upper and lower boundary switches may be individually set as follows:

= 0, Extend the domain indefinitely and hold constant at the boundary value (the default).

= 1, Extend the domain indefinitely and linearly extrapolate the two data pairs at the boundary.

= 2, Running off the domain of the tabular function is prohibited.

(1) NTFBDL - Lower boundary condition switch.
(type = integer, default = 0, units = none)

(2) NTFBDU - Upper boundary condition switch.
(type = integer, default = 0, units = none)

TFnnnkk – Data Pairs
001 ≤ nnn ≤ 999, nnn is the tabular function number.
10 ≤ kk ≤ 99, kk is used for ordering the input.
Required

The tabular function is defined by data pairs. The first number in a pair is the independent variable, the second number is the dependent variable. There may be an arbitrary number of pairs on a record, but a pair may not be split across a record.

(1) X - The first element (independent variable) in a data pair.
(type = real, default = none, dimension = none, units = as appropriate for the tabular function data)

(2) Y - The second element (dependent variable) in a data pair.
(type = real, default = none, units = as appropriate for the tabular function data)

3. MELCOR User Input

At present the TF package data cannot be changed in MELCOR user input.

4. Example Input

The following input records define four tabular functions. The first has four data pairs and the second has only one (constant function). The last two are step functions with a control function that could be used with a valve junction to open and close the valve. For more information on control functions, see the CF Package Users' Guide.

```
TF00100    ' Bills function'    4     1.
TF00110    0.    1.    5.    100.5     * first two data pairs
TF00111    100.8      55.              * third data pair
```

```
TF00120   5000.      90.993          * fourth data pair
*
*
TF10000   'Sams constant function' 1    1.   0.
TF10010   0.   1.
*
* Note the next two functions illustrate two different
* ways of constructing a step function.
* These tabular functions with the control function can be
* used as a valve to control opening and closing.
*
CF20000   'valve control'     HYST 1    1.   0.
CF20001   0.0
CF20003   -201       * open TF
CF20004   -202       * close TF
CF20010   1.0  0.0  cvh-p.210 * look at pressure in cvh volume 210
*
TF20100   'valve open'   2    1.   0.
TF20101   0    0     * this is the default
TF20110   7.07E6     0.    * closed until p increases to 7.07 MPa
TF20111   7.07E6     1.    * full open
*
TF20200   'valve close'  4    1.   0.
TF20201   2    2
TF20210   -1.E20     0.
TF20211   6.7E6      0.    * opened until p decreases to 6.7 MPa
TF20212   6.7E6      1.    * full close
TF20213   1.E20      1.
```

Transfer Process (TP) Package
Users' Guide

The Transfer Process (TP) package provides a standard interface for a MELCOR package to send mass and its associated enthalpy to one or more other packages. The identities of materials may change across the TP package.

This document provides a short description of the TP package, including the default identity translation matrix and the user input requirements for MELGEN and MELCOR, respectively, with some examples.

Contents

1. Introduction

The TP package provides a standard interface for a physics package to transfer mass and energy to one or more other packages. In other words, the TP package essentially functions as a sophisticated bookkeeper for inter-package mass and energy transfers. (The CVH package provides its own utility interface for control volume fluid mass and energy transfers involving other packages; the TP package is not involved.)

There are two types of transfer processes: *in* and *out*. An *in* transfer process sends information to the TP package where it is stored. On request, the TP package retrieves the information, processes it, and sends it to a calling *out* transfer process. User input defines the relationships between the *in* and *out* transfer processes. Currently, required input to the TP package is prescribed by the COR, CAV, and RN packages, and optionally by the FDI, HS, and SPR packages. (See the corresponding users' guides for details.) Eventually, much of this transfer of information will be made transparent to the user and obviate the need for TP input.

Masses may change identities across the TP package. This capability was originally intended for such uses as conversion of the materials called steel and steel oxide in the Core package into the materials called iron, chromium, nickel, and carbon and their oxides in the Cavity package. This particular use has been eliminated by inclusion of the material composition information (specified via Core package input) in a separate TP interface array that is used directly by the Cavity package to break the steel and steel oxide into their constituent components. This will allow definition of time-dependent steel compositions sometime in the future. The material conversion feature of the TP package is now used only to handle imperfect interfaces between packages or between a package and an external data file.

The user must specify a translation matrix to relate materials in the *out* process to those in the *in* process through the matrix equation.

$$\textit{mass out} = \textit{translation matrix} \times \textit{mass in}$$

The total mass of a material is conserved only if the elements in all translation matrix columns for the material sum to one. Thus, it is possible for mass to be retained or created by the TP package, which might be necessary because of imperfect interfaces between packages. For example, if the Core package ejects B_4C and the Cavity package does not recognize that material (as is currently the case), it must be retained by the TP package by using the translation matrix to eliminate the B_4C from the output masses:

Any mass retained or created by the TP package is printed in MELCOR output in terms of the *in* process masses.

UO_2		1	0	0	0	0	0		UO_2
Zr		0	1	0	0	0	0		Zr
Steel	=	0	0	1	0	0	0	X	Steel
ZrO_2		0	0	0	1	0	0		ZrO_2
St. Ox.		0	0	0	0	1	0		St. Ox.
									B_4C

The translation matrix may also be used to accommodate *in* processes defined by external data files that do not have the precise format expected by the *out* process. For example, a 7-group (Reactor Safety Study, WASH-1400) source of fission products could be partitioned into the default 15 groups expected by the RN package through an appropriate translation matrix with 15 rows and 7 columns:

Noble gases		1	0	0	0	0	0	0		Noble Gases
Alk. Metals		0	0	1	0	0	0	0		Halogens
Alk. Earths		0	0	0	1	0	0	0		Alk. Metals
Halogens		0	1	0	0	0	0	0		Alk. Earths
Chalcogens		0	0	0	0	.967	0	0	X	Te Group
Platinoids		0	0	0	0	0	.53	0		Trans. Metals
Trans. Metals		0	0	0	0	0	.47	.002		Lanthanides
Tetravalents	=	0	0	0	0	0	0	.702		
Trivalents		0	0	0	0	0	0	.296		
Uranium		0	0	1	0	0	0	0		
As, Sb		0	0	0	0	.033	0	0		
Sn, Ag		0	0	0	0	0	0	0		
Boron		0	0	0	0	0	0	0		
Water		0	0	0	0	0	0	0		
Concrete		0	0	0	0	0	0	0		

The total enthalpy of materials transferred from one package to another via the TP package may not be conserved, either because masses may not be conserved or because of differences in equation-of-state representations between the two packages. The *out* package that receives masses also receives thermodynamic variables to calculate the enthalpy of the masses it has just received and transmits that information back to the TP package. For example, the Core package may use temperature for the thermodynamic variable and calculate an enthalpy of 2 MJ for a mass. The Cavity package may receive the mass and temperature but calculate an enthalpy of 2.7 MJ. The Cavity package transmits the 2.7 MJ value back to the TP package, which will log an enthalpy difference of 0.7 MJ. The enthalpy differences are also printed in MELCOR output.

If the equations of state for a material are the same for two packages except for a difference in reference point, there will be no real energy error if temperature is used as the thermodynamic variable. If the equations of state are not the same, there is an energy discrepancy that cannot be resolved (without choosing one equation or the other as "right"),

and there will be either an energy error if temperature is held constant during the transfer or a temperature jump if energy is held constant during the transfer. For the former case, the energy error will be on the order of the uncertainty in the equation of state (hence the difference in state formulations) as long as the temperature at which material is transferred is not on one side of a phase transition for one equation and on the other side of the phase transition for the other equation. MELCOR currently uses this approach to avoid step changes in temperature during debris ejection from the core to the cavity.

2. Default Translation Matrices

The commonly used identity translation matrix is available for use as default matrix number 1. It is square and all its elements are zero except for ones along the diagonal. This matrix preserves all characteristics of the incoming material when it is passed to the *out* transfer process.

3. MELGEN User Input

The user defines the *in* and *out* transfer processes and the matrices that convert the *in* materials to the *out* materials. Every *in* process must be associated with at least one *out* process. Every translation matrix must be associated with at least one *out* process.

The following input descriptions are generic in nature. Several MELCOR packages (the COR, FDI, CAV, and RN packages) have specific requirements for TP package input. Details regarding the specific input required for these packages may be found in their respective users' guides.

TPINnnn00 – *In* Transfer Process

001 ≤ nnn ≤ 999, nnn is the transfer process number.
Required

This record defines an *in* transfer process, the number of masses in and the number of thermodynamic variables in. Enthalpy calculated using the thermodynamic variables is also transferred, but is itself not one of those variables.

(1) NMSIN - Number of masses in.
(type = integer, default = none, units = none)

(2) NTHRM - Number of thermodynamic variables.
(type = integer, default = none, units = none)

TPINnnn01 – Connection to External Data File

001 ≤ nnn ≤ 999, nnn is the transfer process number.

Optional

This record allows association of an *in* transfer process with an external data file. (See the External Data File (EDF) Package Users' Guide.) It may be used to write out a history of the *in* process; this allows data from one MELCOR run to be saved for later use. Conversely, it may be used to read in such a history, and to generate appropriate mass transfers from it; this allows data from a previous MELCOR run (or those from another simulation code) to be used to generate sources of debris or radionuclides as though they had been received through an *in* transfer process.

If a file is written, each record will contain NMSIN cumulative masses, the cumulative enthalpy, and NTHRM thermodynamic variables (i.e., NMSIN + NTHRM + 1 EDF channels). The masses and the thermodynamic variables will be in the order defined by the package which will use this *in* process. See the description of NTPCOR on input record COR00004, or of NFDTPI on input record FDInn00 for debris transfers.

Note that a second transfer process for associated radionuclides will ordinarily be defined, with a user number exactly 500 greater than that for the debris. It will have NMSIN = NUMCLS (described for input record RN1001) and NTHRM = 1. Each record in the file will contain NUMCLS + 2 channels (dependent variables) since a cumulative enthalpy will also be written.

If a file is read, it is assumed to have the same format, although differences in the number and order of masses from the MELCOR transfer process it replaces may be accommodated through proper definition of the translation matrix using TPMnnnkkkk input.

(1) DIRECT - Direction of connection. This may be either 'WRITE' to write a history file or 'READ' to read a file.
(type = character*5, default = none, units = none)

(2) IP2EDF - User number of associated EDF file.
If DIRECT = 'WRITE', this must be the number of a valid "PUSH" file containing exactly NMSIN + 1 + NTHRM channels.

If DIRECT = 'READ', this must be the number of a valid "READ" file containing at least NMSIN + 1 + NTHRM channels, of which the first NMSIN + 1 + NTHRM will be used.

See the EDF Users' Guide for further input requirements, including file names and record frequency for output files.

TPOTnnn00 – *Out* Transfer Process Record
001 ≤ nnn ≤ 999, nnn is the transfer process number.
Required

This record defines an *out* transfer process, the number of masses passed back to the calling subroutine and the associated *in* transfer process number.

(1) NMSOT - Number of masses associated with this *out* transfer process.
(type = integer, default = none, units = none)

(2) NPOTOI - Associated *in* transfer process number.
(type = integer, default = none, units = none)

(3) OUTMTX - Associated translation matrix.
In process masses are multiplied by a translation matrix to generate the *out* process masses. Each *out* transfer process has a translation matrix associated with it. OUTMTX must be specified in the form of KEYWORD.IOTMTX, where KEYWORD must be the character string DEF or UIN, and where IOTMTX is the number of the translation matrix used for this *out* transfer process. DEF is used to specify a default translation matrix (see Section 2). Currently, only DEF.1, the identity matrix, is available. UIN is used if the user defines a translation matrix via user input. For example, UIN.200 would specify user-defined matrix 200. Refer to the TPMnnnkkkk input records described below.
(type = character, default = none, units = none)

TPMnnn0000 – Translation Matrix
001 ≤ nnn ≤ 999, nnn is the translation matrix number.
Optional

This record defines a translation matrix. It defines the number of rows and columns of the matrix. All nonzero elements of the matrix must be defined using input record TPMnnnkkkk below.

(1) NROW - Number of rows.
(type = integer, default = none, units = none)

(2) NCOL - Number of columns.
(type = integer, default = none, units = none)

TPMnnnkkkk – Define Translation Matrix
001 ≤ nnn ≤ 999, nnn is the translation matrix number.
0001 ≤ kkkk ≤ ZZZZ, kkkk is a collocation field

Optional

This record defines the nonzero elements of a translation matrix. The input is in the form of data pairs. The first element of the data pair is of the form NROW/NCOL where NROW is the row number and NCOL is the column number of the translation matrix. The second number is a real number that is the value of the NROW-th, NCOL-th element of the matrix. An arbitrary number of data pairs may be defined on a single record but a data pair may not be split across two records. If an element of the matrix is defined more than once, then the last value is retained.

(1) NROW/
NCOL - Character string with NROW equal the row number and NCOL equal to the column number. For example 3/5 is the third row and fifth column.
(type = character, default = none, units = none)

(2) VALUE - Value of the NROW-th row and NCOL-th column in the matrix.
(type = real, default = 0, units = none)

4. MELCOR User Input

For a given *out* transfer process, the user may redefine the associated *in* transfer process number and translation matrix. The elements of a translation matrix may be redefined. No new *in* transfer processes, *out* transfer processes, or translation matrices may be defined in MELCOR. Every *in* process must be associated with at least one *out* process.

TPOTnnn00 – *Out* Transfer Process Record
$001 \leq nnn \leq 999$, nnn is the transfer process number.
Optional

For an existing *out* transfer process, this record may redefine the associated *in* transfer process number, and the associated translation matrix.

(1) NMSOT - Number of masses associated with this *out* transfer process. This may not be changed in MELCOR.
(type = integer, default = none, units = none)

(2) NPOTOI - Associated *in* transfer process number.
(type = integer, default = none, units = none)

(3) OUTMTX - Associated translation matrix.
In process masses are multiplied by a translation matrix to generate the *out* process masses. Each *out* transfer process has

a translation matrix associated with it. OUTMTX must be specified in the form of KEYWORD.IOTMTX, where KEYWORD must be the character string DEF or UIN, and where IOTMTX is the number of the translation matrix used for this *out* transfer process. DEF is used to specify a default translation matrix (see Section 2). Currently, only DEF.1, the identity matrix, is available. UIN is used if the user defines a translation matrix via user input. For example, UIN.200 would specify user-defined matrix 200. Refer to the TPMnnnkkkk input records described below. Any redefinition of translation matrices must be done so that the number of rows and columns do not change, whether default or user-defined matrices are used.
(type = character, default = none, units = none)

TPMnnn0000 – Translation Matrix

001 ≤ nnn ≤ 999, nnn is the translation matrix number.
Optional

This record defines the size of a translation matrix, and may be input in MELCOR for a matrix already defined in MELGEN. However, the number of rows and columns of a matrix cannot be changed in MELCOR. If this record is input without any TPMnnnkkkk records, all elements of matrix nnn are set to zero, and all information will be lost.

(1) NROW - Number of rows.
(type = integer, default = none, units = none)

(2) NCOL - Number of columns.
(type = integer, default = none, units = none)

TPMnnnkkkk – Define Translation Matrix

001 ≤ nnn ≤ 999, nnn is the translation matrix number.
0001 ≤ kkkk ≤ ZZZZ, kkkk is a collocation field.
Optional

This record defines the nonzero elements of a translation matrix that has been defined in MELGEN. If any TPMnnnkkkk records are input, all elements of matrix nnn not defined in TPMnnnkkkk records are set to zero. The input is in the form of data pairs. The first element of the data pair is of the form NROW/NCOL, where NROW is the row number and NCOL is the column number of the translation matrix. The second number is a real number that is the value of the NROW-th, NCOL-th element of the matrix. An arbitrary number of data pairs may be defined on a single record but a data pair may not be split across two records. If an element of the matrix is defined more than once, then the last value is retained.

(1) NROW/ NCOL - Character string with NROW equal the row number and NCOL equal to the column number. For example 3/5 is the third row and fifth column.
(type = character, default = none, units = none)

(2) VALUE - Value of the NROW-th row and NCOL-th column in the matrix.
(type = real, default = 0.0, units = none)

5. Example Input

5.1 Example 1

Example 1 below provides input to define two *in* transfer processes, three *out* transfer processes, and two translation matrices. The first *in* transfer process has three masses in and one thermodynamic variable. The second *in* transfer process has four masses and two thermodynamics variables. The first *out* transfer process is associated with the first *in* transfer process, has three masses out and uses the default identity translation matrix. The second and third *out* transfer process are associated with the second *in* transfer process. Note that the sum of the fourth column of the two matrices do not add to one, so the total mass in will not be equal to the total mass out.

```
TPIN10100  3  1    * MASSES THERMO
TPIN10200  4  2    * MASSES THERMO
*
TPOT20100  3  101  DEF.1     * MASSES, IN PROCESS, DEFAULT MATRIX 1
TPOT20200  6  102  UIN.100   * MASSES, IN PROCESS, USER MATRIX 100
TPOT20300  4  102  UIN.101   * MASSES, IN PROCESS, USER MATRIX 101
*
*               | .8   0    0    0 |
*               | .1   0    0    0 |
* MATRIX 100:   |.08   0    0    0 |
*               |.02   0    0    0 |
*               | 0    1    0    0 |
*               | 0    0    1    0 |

TPM1000000    6 4                        * 6X4 MATRIX
TPM1000001    1/1  .8                    * ROW 1, COLUMN 1
TPM1000002    2/1  .1                    * ROW 2, COLUMN 1
TPM1000003    3/1  .08                   * ROW 3, COLUMN 1
TPM1000004    4/1  .02                   * ROW 4, COLUMN 1
TPM1000005           5/2  1.             * ROW 5, COLUMN 2
TPM1000006                   6/3  1.  * ROW 6, COLUMN 3
*
```

```
*                |  0    0    0    0  |
* MATRIX 101:    |  0    0    0    0  |
*                |  0    0    0    0  |
*                |  0    0    0   .9  |
*
TPM1010000 4 4                          * 4X4 MATRIX
TPM1010001 4/4    .9                    * DEFINE NONZERO ELEMENTS
```

5.2 Example 2

Example 2 provides sample input for the COR, FDI, CAV, and TP packages for a typical plant calculation. To help make sense of this input, let 1 = COR, 2 = FDI, 3 = CAV, and 9 = TP in the various *in* and *out* transfer process numbers, so that all *out* transfer process numbers begin with 9 (or 59 for 3-digit RN TP numbers) and all *in* transfer process numbers end with 9. For example, TP #29 is an *in* transfer process describing masses passed in to TP from FDI.

```
* COR, FDI, AND CAV PACKAGE INPUT
* NO INPUT REQUIRED FOR RN PACKAGE
*          COR'IN'TP
COR00004   19
*          NCV     NCAV      FDI'IN'TP     FDI'OUT'TP
FDI0500    500     10        29            92
*          CAV'OUT'TP
CAV10TP    93
*
* 'IN' TRANSFER PROCESS FOR COR PACKAGE
*             NMSIN          NTHRM
TPIN01900     6              9
* 'OUT' TRANSFER PROCESS FOR FDI PACKAGE
*             NMSOT          NPOTOI   IOTMTX
TPOT09200     5              19       UIN.506
* 'IN' TRANSFER PROCESS FOR FDI PACKAGE
*             NMSIN          NTHRM
TPIN02900     5              9
* 'OUT' TRANSFER PROCESS FOR CAV PACKAGE
*             NMSOT          NPOTOI   IOTMTX
TPOT09300     5              29       DEF.1
*
* COR-FDI TRANSLATION MATRIX
* *** NOTE *** CONTROL POISON MASS IS NOT CONSERVED
*             NROW           NCOL
TPM5060000    5              6
*             NROW/NCOL      VALUE
TPM5060001    1/1            1.0      * UO2 MASS
TPM5060002    2/2            1.0      * ZR MASS
TPM5060003    3/3            1.0      * STEEL MASS
```

```
TPM5060004    4/4            1.0      * ZRO2 MASS
TPM5060005    5/5            1.0      * STEEL OXIDE MASS
*
* TRANSFER PROCESSES FOR RADIONUCLIDE TRANSFER
* RN TP NUMBERS MUST BE COR, FDI, CAV TP NUMBERS + 500
TPIN51900  15      1
TPIN52900  15      1
TPOT59200  15      519       DEF.1
TPOT59300  15      529       DEF.1
```

5.3 Example 3

Example 3 provides sample input to split ejected core debris into two separate reactor cavities for molten core-concrete interactions. Seventy-five percent of the debris is discharged to cavity 2, and the remainder is discharged to cavity 3. The numbering scheme for transfer process numbers is similar to that for Example 2, with 1 = COR, 2 = CAV2, 3 = CAV3, and 9 = TP.

```
* COR AND CAV PACKAGE INPUT
*          COR'IN'TP
COR00004   19
*          CAV2'OUT'TP
CAV02TP    92
*          CAV3'OUT'TP
CAV03TP    93
*
* 'IN' TRANSFER PROCESS FOR COR PACKAGE
*          NMSIN  NTHRM
TPIN01900  6      9
* 'OUT' TRANSFER PROCESSES FOR CAV PACKAGE
*          NMSOT  NPOTOI    IOTMTX
TPOT09200  5      19        UIN.2
TPOT09300  5      19        UIN.3
*
* COR-CAV TRANSLATION MATRICES
* 0.75 TO CAVITY 2, 0.25 TO CAVITY 3
* *** NOTE *** CONTROL POISON MASS IS NOT CONSERVED
*          NROW   NCOL
TPM0020000 5      6
*           NROW/NCOL       VALUE
TPM0020001 1/1              0.75     * UO2 MASS
TPM0020002 2/2              0.75     * ZR MASS
TPM0020003 3/3              0.75     * STEEL MASS
TPM0020004 4/4              0.75     * ZRO2 MASS
TPM0020005 5/5              0.75     * STEEL OXIDE MASS
*
*          NROW   NCOL
```

```
TPM0030000 5      6
*          NROW/NCOL       VALUE
TPM0030001 1/1             0.25     * UO2 MASS
TPM0030002 2/2             0.25     * ZR MASS
TPM0030003 3/3             0.25     * STEEL MASS
TPM0030004 4/4             0.25     * ZRO2 MASS
TPM0030005 5/5             0.25     * STEEL OXIDE MASS
*
* TRANSFER PROCESSES FOR RADIONUCLIDE TRANSFER
* RN TP NUMBERS MUST BE COR AND CAV TP NUMBERS + 500
TPIN51900  15     1
TPOT59200  15     519      UIN.12
TPOT59300  15     519      UIN.13

* MATRIX 12 IS 15 X 15 IDENTITY MATRIX TIMES 0.75
*          NROW   NCOL
TPM0120000 15     15
*          NROW/NCOL       VALUE
TPM0120001 1/1             0.75
TPM0120002 2/2             0.75
TPM0120003 3/3             0.75
TPM0120004 4/4             0.75
TPM0120005 5/5             0.75
TPM0120006 6/6             0.75
TPM0120007 7/7             0.75
TPM0120008 8/8             0.75
TPM0120009 9/9             0.75
TPM0120010 10/10           0.75
TPM0120011 11/11           0.75
TPM0120012 12/12           0.75
TPM0120013 13/13           0.75
TPM0120014 14/14           0.75
TPM0120015 15/15           0.75
*
* MATRIX 13 IS 15 X 15 IDENTITY MATRIX TIMES 0.25
*          NROW   NCOL
TPM0130000 15     15
*          NROW/NCOL       VALUE
TPM0130001 1/1             0.25
TPM0130002 2/2             0.25
TPM0130003 3/3             0.25
TPM0130004 4/4             0.25
TPM0130005 5/5             0.25
TPM0130006 6/6             0.25
TPM0130007 7/7             0.25
TPM0130008 8/8             0.25
TPM0130009 9/9             0.25
```

```
TPM0130010  10/10           0.25
TPM0130011  11/11           0.25
TPM0130012  12/12           0.25
TPM0130013  13/13           0.25
TPM0130014  14/14           0.25
TPM0130015  15/15           0.25
```

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SUPPLEMENTARY NOTES

11. ABSTRACT *(200 words or less)*

MELCOR is a fully integrated, engineering-level computer code that models the progression of severe accidents in light water reactor nuclear power plants. MELCOR is being developed at Sandia National Laboratories for the U.S. Nuclear Regulatory Commission as a second-generation plant risk assessment tool and the successor to the Source Term Code Package. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. These include thermal-hydraulic response in the reactor coolant system, reactor cavity, containment, and confinement buildings; core heatup, degradation, and relocation; core-concrete attack; hydrogen production, transport, and combustion; fission product release and transport behavior. This publication of the MELCOR computer code manuals corresponds to MELCOR 1.8.5. Volume 1 contains a primer that describes MELCOR's phenomenological scope, organization (by package), and documentation. The remainder of Volume 1 contains the MELCOR User's Guides, which provide the input instructions and guidelines for each package. Volume 2 contains the MELCOR Reference Manuals, which describe the phenomenological models that have been implemented in each package.

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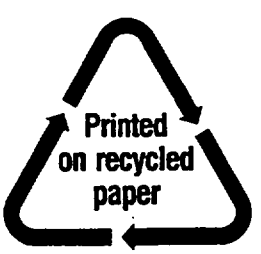

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