

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.

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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

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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	Trivalent	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 ₂ O	H ₂ O
15	Concrete	---	---
16	Cesium iodide	Csl- --	Csl- --

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

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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 RNCLSNXX 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 RNgAPIj00 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,

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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 diffusio-phoresis, 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 RNRCTIYY 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

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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 B₂O₃.
(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)

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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 ≤ XX ≤ 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)

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- (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 ₂ O)	(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 ≤ XX ≤ 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 (Csl)	2 (Cs) and 4 (I)
13 (Al)	15 (concrete)	26 (I)	None
		27 (Xe)	None

Csl (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 ≤ jj ≤ 99, jj is the user-specified cavity number

01 ≤ XX ≤ 99, XX is a sequencing parameter

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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 $NINP \leq 0$, 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 $NINP \leq 0$, 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 total 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)

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...

...

(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

$000 \leq XXX \leq 999$, 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

$000 \leq XXX \leq 999$, 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 ≤ XXX ≤ 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)

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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 ratio 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 Csl 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 Csl).
 (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 RNCFXML 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/m³)

RNACOEFL 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 RNACOEFL record, the RNCFXML 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 RNCFXML 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 ≤ XXX ≤ 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)

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- (4) RHOG - Nominal density used in generation of aerosol coefficients.
(type = real, default = none, units = kg/m³)

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 = m²/s³)

- (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 Csl (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

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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 ≤ XXX ≤ 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 = m²)

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

$000 \leq XXX \leq 999$, 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|

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- (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)GEO MM	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)

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= 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

$000 \leq XXX \leq 999$, 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 = $\text{MIN}(\text{VOLUME}^{1/3}, \text{CVARA}^{1/2})$, 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

$000 \leq XXX \leq 999$

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)

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- (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 ≤ XXX ≤ 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 RNDHSSXXX 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 = m²)
- (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

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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 \equiv (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)

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- (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

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- (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/m² 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/m² 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/m³)
- (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

$00 \leq II \leq 99$, II is the reaction number

$00 \leq YY \leq 99$, 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

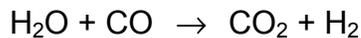
- (1) ICLAST - The *to* reacting classes
(type = integer, default = none, units = none)
- (2) FRACT - The mole fraction for this class based on a stoichiometric reaction
(type = real, default = 0.0, units = none)

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 $A + B \rightarrow C + D$, 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



The mass fraction input would be 0.89 (wt of O divided by wt of H₂O), 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 ≤ II ≤ 99, II is the transfer number

00 ≤ YY ≤ 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.

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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) ISTAT - 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 if 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 ≤ xx ≤ 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 Csl class is ON, as iodine released in the Csl 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 ≤ xx ≤ 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.

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- (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 selects 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.

RNDOSxxxxy – 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

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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 to 13 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

$$\min [1.0, \text{Atmosphere_density} \times \text{CVPATH} / \text{C7002}(1)],$$

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/m², 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

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		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

$$\text{Release Rate (fraction / min)} = A \exp (BT)$$

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

$$\text{Release Rate (fraction / min)} = k_o \exp(-Q / RT)$$

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 $1.987\text{E-}3$ 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**

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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:

$$\text{Release Rate}(k) = \text{Release Rate}(\text{Cs}) \times \text{C7103}(k)$$

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

$$\text{Release Rate} = \text{Release Rate (CORSOR or CORSOR-M)}$$

$$\times (S/V)_{\text{structure}} / (S/V)_{\text{base}}$$

where the $(S/V)_{\text{base}}$ 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 than 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

$$D = D_0 \times \text{EXP}(-Q / RT)$$

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 $D \times \text{TIME} / A^2$ where A is the equivalent sphere radius for the fuel grain.

- (1) - low burn-up value of D₀
(default = 5.E-8, units = m²/s, equiv = none)
- (2) - high burn-up value of D₀
(default = 2.5E-7, units = m²/s, equiv = none)
- (3) - burn-up value at which value of D₀ changes
(default = 3.E4, units = MWD/MTU, equiv = none)

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- (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:

$$\text{SFACT}(k) = \text{C7107}(3,k) \times \text{EXP}(\text{C7107}(4,k) \times \text{MIN}(\text{TEMP}, \text{C7107}(5,k)))$$

when the oxide mass fraction is below C7107(6,k) the class k scaling factor is given by:

$$\text{SFACT}(k) = \text{C7107}(7,k)$$

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	0.015992 3	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 Csl, 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 UO₂ 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		

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		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 ₂ O ₃	69.622	B ₂ O ₃	69.622
14	H ₂ O	18.016	H ₂ O	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

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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

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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,

$$\text{fraction_of_class_i_relocated} = \text{C7136(i)} \times \text{fraction_of_film_relocated}.$$

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
 $\text{Departure_diameter} = 0.0208 \times \text{C7140(2)} \times \sqrt{(\sigma / g)}$
(default = 10.0, units = degrees, equiv = none)
- (3) - Coefficient of bubble coalescence and breakup.
 $n_{\text{bub}}/t = \text{C7140(3)} \times r_{\text{bub}}^3 \times n_{\text{bub}}^2 + \text{nucleation} - \text{rise}$
(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 = m²/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.

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- (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-AI 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

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$$D_g^3 = 1.5 v_n D_o^2 (\sigma / \rho_l g)^{1/2}$$

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 $i = \text{MVENT}$.

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 noncondensable 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 ratio 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

$$V_r = C7153(1) (\sigma / \rho_l)^{1/4} \text{ (cm/s) for } d_{vm} \leq 0.5 \text{ cm}$$

$$V_r = C7153(3) V_r(d_{vm} = 0.5 \text{ cm}) d_{vm}^{C7153(4)} \text{ (cm/s) otherwise}$$

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

$$\bar{V}_s = \text{MIN} \{ 0.5 [V_s(x=0) + V_s(x=h_p)] C7154(5) \}$$

where

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$$V_s(x) = \{[(Q_s + C7154(1)]/C7154(2)]^{C7154(3)} [1 - C7154(4)x]\}(\text{cm/s})$$

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/cm², 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

$$Stk_i = \frac{\rho_i V_e d_i^2}{9 \mu D_o}$$

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

$$\alpha_i = C7155(1) \cdot C7155(2)^{C7155(3)\sqrt{Stk_i}} \text{ if } \sqrt{Stk_i} \leq C7155(4)$$

$$\alpha_i = C7155(5) \cdot C7155(6)^{C7155(7)\sqrt{Stk_i}} \text{ otherwise}$$

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

$$I_{\text{sol}}[T^{\circ}\text{C}] = I_{\text{sol}}[\text{C7156(9)}][1 + \text{C7156(8)}\{T - \text{C7156(9)}\}] \quad (\text{sol} = \text{CsOH or CsI})$$

$$I_{\text{CsOH}}[\text{C7156(9)}] = \text{C7156(6)} + \text{C7156(7)}[n_{\text{CsOH}}/n_{\text{T}}]$$

$$I_{\text{CsI}}[\text{C7156(9)}] = \text{C7156(1)} + \text{C7156(2)}[n_{\text{CsI}}/n_{\text{T}}] \quad \text{for } n_{\text{CsI}}/n_{\text{T}} \leq \text{C7156(3)}$$

$$I_{\text{CsI}}[\text{C7156(9)}] = \text{C7156(4)} + \text{C7156(5)}[n_{\text{CsI}}/n_{\text{T}}] \quad \text{otherwise}$$

$$I_{\text{sol}}[T^{\circ}\text{C}] = \text{C7156(10)} \quad \text{for all other solutes in the droplet}$$

where $n_{\text{T}} = n_{\text{CsOH}} + n_{\text{CsI}} + n_{\text{sol}} + n_{\text{w}}$ 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

$$f(Re) = (4 \rho_i \rho_g g d_i^3) / (3 \mu^2)$$

$$\begin{aligned} Re &= [f(Re)/C7157(2)]^{C7157(3)} \text{ if } C7157(1) < f(Re) < C7157(4) \\ &= [f(Re)/C7157(5)]^{C7157(6)} \text{ if } C7157(4) \leq f(Re) < C7157(7) \\ &= [f(Re)/C7157(8)]^{C7157(9)} \text{ if } C7157(7) \leq f(Re) < C7157(10) \\ &= [f(Re)/C7157(11)]^{C7157(12)} \text{ if } C7157(10) \leq f(Re) < C7157(13) \\ &= [f(Re)/C7157(14)]^{C7157(15)} \text{ if } C7157(13) \leq f(Re) \end{aligned}$$

For particles with a diameter less than about 70 microns, the gravitational settling velocity follows Stokes law and is given by

$$V_{g,i} = (\rho_i g S_i d_i^2) / (18\mu) \text{ if } f(Re) \leq C7157(1)$$

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)

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- (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 (CH₃I) is given by the following correlation

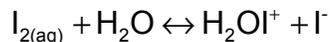
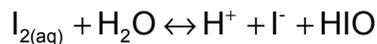
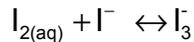
$$H_{OI} = T/10^{C7158(1)/T+C7158(2)}$$

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 I₂ scrubbing model. The reactions considered are



The equilibrium constant for the ith reaction (i = 1,..,4) is given by

$$EQK(i) = C7159(2 \cdot i - 1) \exp[C7159(2 \cdot i)/T]$$

while the equilibrium constant for the dissociation of water is given by

$$EQK(5) = C7159(9) \exp[C7159(10) / T + C7159(11) / T^2]$$

The twelfth parameter is a value of gaseous iodine concentration (moles/cm³) 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 = moles², 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 = moles², 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 = K², 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/cm³, 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

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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 $\text{CsI} \rightarrow \text{Cs}^+ + \text{I}^-$. 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 H₂O], equiv = none)
- (4,N) - Saturation solubility [kg/kg H₂O] at high temperature reference.
(default = See Table 3, units = [kg/kg H₂O], 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/m³], 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 ₂ O]	Compound Solubility At 373K [kg/kg H ₂ O]	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: UO ₂	10960	0	0	2
11. Cd	8150	0	0	2
12. Sn	6446	0	0	2
13. Boron	2520	0	0	2
14. Water: H ₂ O	1000	--	--	0
15. Concrete	2250	0	0	2
16. Csl	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) - H₂NO₃ acid deposition rate.
(default = 0.003, units = m/s, equiv = none).

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- (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/m³, 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/m³, equiv = none).

- (2) - Maximum atmosphere pressure.
(default = 1E6, units = Pa, equiv = none).
- (3) - Minimum atmosphere volume.
(default = 0.1, units = m³, 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 = m³, 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)

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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)

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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)

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RN1-IOP-cccccc.nnn	/c/	Concentration of aqueous species ccccc 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 ccccc 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)

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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 <i>from</i> volume associated with flow path NFL, ip=10*NFL+2 for the <i>to</i> 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 <i>from</i> volume associated with flow path NFL, ip=10*NFL+2 for the <i>to</i> 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 <i>from</i> volume associated with flow path NFL, ip=10*NFL+2 for the <i>to</i> volume associated with flow path NFL, and ip=10*NCAV for the pool associated with cavity NCAV.) <u>Currently, only x=4 is calculated.</u>
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 <i>from</i> volume associated with flow path NFL, ip=10*NFL+2 for the <i>to</i> 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 <i>from</i> volume associated with flow path NFL, ip=10*NFL+2 for the <i>to</i> 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 <i>from</i> 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

```


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```

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.
*
RNACOEFF    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  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
*           IFLTFF    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

```

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```
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.

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