

MelMACCS Models Document

(MELCOR to MACCS Interface Description)

Prepared by

Katherine McFadden, Sigma Software L.L.C.
Nathan E. Bixler, Sandia National Laboratories

1.0 MelMACCS Description

MELCOR (Gauntt et al., 2000) creates a “results” or plot file, often identified by the file extension “.ptf”, which contains a large amount of calculated information, including information needed to perform a MACCS analysis (Chanin and Young, 1998). This file can be very large (on the order of hundreds of megabytes or even a few gigabytes).

Beginning with MELCOR developmental version 1.8.5-RH, certain additional MACCS-specific data can be optionally written to the MELCOR plot file that is needed by the MelMACCS interface utility.

Starting with MELCOR 1.8.6 YQ, releases of Cs_2MoO_4 are normally written (by default) to the MELCOR plot file. MelMACCS processes these release data.

With version MELCOR 2.1.X, support for multiple rings (to model spent fuel pools for one application) was added. This modification to the plot file resulted in modifications to MelMACCS.

2.0 Calculation of MACCS variables from MELCOR variables

Following is a description of the mapping of variables from a MELCOR plot file to the MACCS input file. MelMACCS was developed to solicit input required for this mapping from the user. MelMACCS is written in the form of a wizard, which leads the user step-by-step through the decisions needed to generate the required MACCS input data.

Not all MACCS variables are directly obtained from a MELCOR plot file. However, the variables not in a MELCOR plot file are either calculated from other values in the plot file or are requested in the MelMACCS interface. All variables from MELCOR, either obtained directly or calculated, correspond to the ATMOS portion of MACCS input.

2.1 Variables Related to Chemical Group Selection

The MelMACCS user has the option of choosing which chemical groups to include in a release. The user should be aware that the MELCOR User's Guide (Gauntt et al., 2000) uses the terminology chemical class while the MACCS2 User's Guide (Chanin and Young, 1998) uses the terminology chemical group. In this document, the MACCS convention is used, i.e., chemical group is used to refer to a set of chemical elements that are treated as being the same.

2.1.1 Number of Chemical Groups, MAXGRP

The chemical group names used in WinMACCS are not used by MACCS. In WinMACCS, GRPNAM is a required variable used only for labeling. The MACCS variable MAXGRP refers to the number of chemical groups.

Within MelMACCS, all chemical groups on the plot file are accessible, namely MELCOR plot variables MACCS-CHEMICAL-GROUP(i) where i is an integer. The user selects the chemical groups to be considered when creating the MelMACCS output file.

MelMACCS considers all chemical groups listed on the .ptf file. If the chemical group has an entry in the MelMACCS.ini file under the section titled CHEM-TO-ISO and the chemical group is not specifically excluded in a section titled EXCLUDE-GROUPS then that chemical group is displayed in the MelMACCS interface with the following additional restrictions:

- The MELCOR plot file references this chemical group.
- The chemical group is not included in the list titled COMPOUND-GROUPS in the MelMACCS.ini file. Two groups are normally included, CsI and CsM, which

stand for cesium iodide and cesium molybdate. Compound groups are treated in a special way, as described later in this document.

This EXCLUDE-GROUPS list can include groups that are not shown in the MelMACCS user interface. For example, if the user doesn't want CsI to be considered when evaluating release fractions, then it should be added to the EXCLUDE-GROUPS list. Including groups on the EXCLUDE-GROUPS list that are not on the .ptf file is legal. See Appendix C for more information regarding the MelMACCS.ini file.

MelMACCS supports sets of chemical groups in multiple MELCOR rings. If the multiple ring feature is used in MELCOR, the number of chemical groups is expanded on the MELCOR plot file, with the same set of chemical groups in each ring.

All chemical groups shown in the MelMACCS interface are written to the MACCS file. However, only the chemical groups selected by the user are assigned nonzero release fractions.

Example: In MelMACCS, the user has selected chemical groups Xe, Cs, Ba, I, Te, Mo, Ce and La. However, all chemical classes listed in the user interface are included.

* Chemical names as exported from MELCOR file

ISGRPNAM001 Xe
ISGRPNAM002 Cs
ISGRPNAM003 Ba
ISGRPNAM004 I
ISGRPNAM005 Te
ISGRPNAM006 Ru
ISGRPNAM007 Mo
ISGRPNAM008 Ce
ISGRPNAM009 La

*

* Number of Chemical classes

ISMAXGRP001 9

2.1.2 Deposition flags, DRYDEP and WETDEP

Within MACCS, the dry deposition and wet deposition flags are specified for every chemical group. These flags are set to ".true." for all groups, with one exception. The first entry, representing the "Xe" chemical group, is set to ".FALSE." because the noble gases are inert and do not deposit.

Example: The first line refers to the chemical group "Xe".

```

* DryDeposition WetDeposition
ISDEPFLA001 .FALSE. .FALSE.
ISDEPFLA002 .TRUE. .TRUE.
ISDEPFLA003 .TRUE. .TRUE.
ISDEPFLA004 .TRUE. .TRUE.
ISDEPFLA005 .TRUE. .TRUE.
ISDEPFLA006 .TRUE. .TRUE.
ISDEPFLA007 .TRUE. .TRUE.
ISDEPFLA008 .TRUE. .TRUE.
ISDEPFLA009 .TRUE. .TRUE.

```

2.2 Variables Related to Particle Size Distribution

2.2.1 NPSGRP, Number of Particle Size Groups

MACCS variable NPSGRP, the number of particle size groups, is read from the MELCOR plot file, and corresponds to variable MACCS-NPSGRP(0).

Example:

```

* Number of particle size groups
DDNPSGRP001 10

```

2.2.2 Dry Deposition Velocity, VDEPOS

There are two supported models for this calculation. The model choice is driven by MelMACCS user input. The following two sections describe the models.

2.2.2.1 Dry Deposition Velocity Based on Gravitational Settling

The following formulae are used to calculate the settling velocity for the particle of geometric diameter d_g (meters).

ρ Density	density of particle (kg/m ³), read from the MELCOR parameter MACCS-RHONOM
$g = 9.8$	acceleration of gravity (m ² /s)
$\lambda = 0.069 \cdot 10^{-6}$	mean free path of air at 298 K (m)
$f_{slip} = 1.257$	slip factor
$\mu = 1.8 \cdot 10^{-5}$	viscosity of air at 298 K (N·s/m ²)
$\chi = 1$	dynamic shape factor

v_d dry deposition velocity (m/s), which defines the MACCS input parameter, VDEPOS(p), where p is the index representing the particle size bin

Variable C_m is the Cunningham slip correction factor, or particle mobility factor, and is calculated as follows:

$$C_m = 1 + \frac{2\lambda}{d_g} \left[f_{slip} + .4e^{-1.1d_g/2\lambda} \right]$$

where d_g is the geometric diameter read from the MELCOR plot file variable MACCS-PSIZE(p) for each particle size and p is the particle size index

Finally, the dry deposition velocity for particle p is calculated as follows:

$$v_d = (d_g)^2 (pDensity) g C_m / (18\mu\chi)$$

Example: Note there are ten velocities reported, one for each particle size group included in the MELCOR calculation.

DDVDEPOS001 1.19543E-06
 DDVDEPOS002 2.867143E-06
 DDVDEPOS003 7.561476E-06
 DDVDEPOS004 2.178411E-05
 DDVDEPOS005 6.726576E-05
 DDVDEPOS006 2.177996E-04
 DDVDEPOS007 7.263037E-04
 DDVDEPOS008 2.464056E-03
 DDVDEPOS009 8.440862E-03
 DDVDEPOS010 2.906963E-02

2.2.2.2 Dry Deposition Velocity Based on Expert Elicitation Data

Dry deposition velocities in MACCS are treated as being dependent on aerosol size, but as being independent of wind conditions and surface roughness. In an evaluation of expert elicitation data (Bixler et al., 2013), both wind speed and surface roughness were considered as variables. The experts provided data for two wind speeds, 2 and 5 m/s, and for three surface types with representative surface roughness, corresponding to prairie, forest, and urban terrains.

The approach used in this model is to retain important dependencies so that the user can decide what is most appropriate for their specific situation. This model accounts for

particle size, wind speed, surface roughness, and degree of belief. Because only particle size can be accounted for in the current MACCS dry deposition model, the user is required to choose representative values of wind speed, surface roughness, and quantile.

Dry deposition velocity is represented with the following equation:

$$\ln(v_d) = a + b(\ln(d_p)) + c(\ln(d_p))^2 + d(\ln(d_p))^3 + e(z_0) + f(z_0)^2 + g(v)$$

where

v_d = deposition velocity (cm/s)

d_p = aerodynamic particle diameter (μm) with recommended limits [0.05, 20].

z_0 = surface roughness (m) with limits [0.01, 0.2]

v = wind speed (m/s) with limits [0.5, 10].

The regression coefficients, a, b, c, d, e, f and g, are read from the file MelMACCS.ini in the DRY-DEPOSITION-COEFF data block. If the quantile selected by the user is not in the table, then linear interpolation is used to calculate the regression coefficients. Note that v_d is in units of cm/s in the above equation, so the units must be converted to m/s when evaluating the MACCS parameter VDEPOS(p).

The aerodynamic particle diameter, d_p , is calculated from the following equation:

$$d_p = \sqrt{\frac{\text{pDensity}}{1000}} \cdot d_g \cdot 10^6$$

If the version of the MELCOR plot file does not have the variable MACCS-RHONOM, the value 1000 is used as a default. Additionally, d_p is not allowed to be less than 0.05 μm . If d_p is less than 0.05 μm , it is reset to 0.05 μm .

If d_p is greater than or equal to the user input parameter, Cutoff Aerodynamic Diameter, the calculation is switched to use gravitational settling. If the value calculated using gravitational settling is less than the velocity calculated using the expert data at the cutoff diameter, the velocity calculated uses the expert data at the cutoff diameter.

2.2.3 Particle Size Distributions, PSDIST

MACCS requires the fraction of each chemical group associated with each particle size group. These fractions (which define the distribution of particle sizes for a given chemical group) are applied uniformly to all plume segments.

To estimate this, MelMACCS considers the time from the accident initiation time (Reference time for inventory in the MELCOR time frame, a MelMACCS input variable) to the last time recorded on the MELCOR plot file. ~~All~~Only MELCOR releases associated with selected plume segments are considered in the calculation, ~~even if the user does not select any plume segments from one or more release paths.~~ All chemical groups are considered. If a given chemical group has a zero initial mass, then a uniform particle size distribution is used for that group. If multiple rings are specified for the MACCS parameters on the plot file, only the releases associated with selected plume segments and relevant to the current ring are considered in the calculation.

The cumulative mass released at each time step is recorded in the MELCOR time-dependent variable MACCS-R-M-RE-C.n, where R is the release path ID, C is the chemical group ID, and n is the particle-size index.

MelMACCS calculates $T(C)$, the difference of MACCS-R-M-RE-C.n from the last time recorded on the MELCOR plot file to the accident initiation time, for chemical C, summed over all relevant MELCOR release paths, over all particle sizes. In other words, $T(C)$ is the total mass released for chemical group C summed over all MELCOR release paths associated with paths from which plume segments have been selected.

The mass related to the CsI release is also added to the releases of the constituent chemical groups, cesium (Cs) and iodine (I). The fractional constants used to distribute the mass into the chemical groups Cs and I are defined in the MelMACCS.ini file. Similarly, the mass related to Cs_2MoO_4 is split into Cs and Mo components and added to the total mass for chemical group cesium (Cs) and molybdenum (Mo) if these chemical groups are included in the calculation.

CsI or Cs_2MoO_4 releases can be excluded from a calculation by including the CsI and CsM groups in the EXCLUDE-GROUP section of the MelMACCS.usr file. If this is done, then the masses of Cs and I in the CsI group, and Cs and Mo in the CsM groups are not included when calculating the particle size distributions or release fractions.

MelMACCS calculates $T(C,p)$ = mass of released chemical group C for particle size p. From this, the particle size distribution is calculated as follows:

$$PSDIST(C, p) = T(C, p) / T(C) \text{ for } T(C) \neq 0$$
$$PSDIST(C, p) = 1. / NPSGRP \text{ for } T(C) = 0$$

Example:

Each input line shown below represents a chemical group. Values on each line correspond to particle size groups. In the following example, line one corresponds to chemical group number one, Xe. Since Xe (representing the noble gases) is a gas, its distribution within the particle size groups does not make physical sense. A uniform distribution is assigned in order to meet MACCS requirements. Because both deposition flags are set to .FALSE. for the Xe group, the particle size distribution is irrelevant.

```
RDPSDIST001 1.E-01 1.E-01 1.E-01 1.E-01 1.E-01 1.E-01 1.E-01 1.E-01 1.E-01 1.E-01
RDPSDIST002 2.5294E-02 1.5853E-01 3.1973E-01 3.1403E-01 1.5661E-01 2.1291E-02 2.1824E-03
4.4071E-04 1.3022E-04 1.7683E-03
```

2.3 Variables related to Plume Segment Selection

2.3.1 NUMREL, Number of Plume Segments

The MACCS variable NUMREL, the number of plume segments, is determined by counting the number of plume intervals selected by the MelMACCS user. Only plume intervals in which all time points within the interval are greater than or equal to the accident initiation time are allowed. The accident initiation time is a MelMACCS variable that can be modified from its default value, usually zero, within the MelMACCS interface. For example, if the user chooses time intervals [0,500] and [500,1000] and the accident initiation time is set to be 450 s, then NUMREL is set to one and only the interval [500,1000] is the only valid plume segment in the MelMACCS source term file.

Example:

* Number of releases selected by user
RDNUMREL001 2

2.3.2 Representative Position within Plume Segment, REFTIM

The value of zero for the first plume segment and 0.5 for the remaining plumes is always used. These values are consistent with the sample problems released with MACCS version 1.12. To maximize the dose estimate for the initial plume segment, where the relative timing of evacuation is critical, a value of zero is used. The values of 0.5 used for the later plumes are intended to be best estimate.

Example:

* Representative location of plume segment. 0. = leading edge, .5 = midpoint, 1. = trailing edge
RDREFTIM001 0.
RDREFTIM002 0.5

2.3.3 Plume Duration, PLUDUR

The plume duration is calculated for each plume segment selected. The plume duration is the difference between the end and the beginning of the time interval for that plume segment. If the user-selected time interval is $[T_1, T_2]$, then the plume duration is $T_2 - T_1$.

Example: In this example, the user selected time intervals are [4956.476, 8573.763] and [8573.763, 12344.56].

* Plume Duration

RDPLUDUR001 3.617287E+03

RDPLUDUR002 3.770797E+03

2.3.4 Plume Segment of Maximum Risk, MAXRIS

The MACCS variable MAXRIS specifies which plume segment is to be considered risk dominant. The selection of this plume is usually based on its potential for causing early fatalities. The user is required to select the plume of maximum risk in the MelMACCS interface.

Example:

* Risk dominant plume segment

RDMAXRIS001 2

2.3.5 Start Time of Plume Segment, PDELAY

The start times for plume segments are relative to the accident start time input by the MelMACCS user. If the user selected time interval in the MELCOR reference frame is $[T_1, T_2]$ and the accident start time is T_3 , where $T_3 < T_1$, then PDELAY is $T_1 - T_3$.

Example: In this example, the user selected the same two plume segments as in Subsection 2.3.3.

* Start Time of Release

RDPDELAY001 4956.476

RDPDELAY002 8573.763

2.3.6 Plume Segment Height, PLHITE

Each MELCOR release path has a corresponding height read from the plot file variable MACCS-PHITE(R), where R is the release path. The plume height is estimated for each

release path associated with the set of plume segments. This height is adjusted by subtracting the MELCOR height associated with ground level (grade), which is a MelMACCS user input. This value can be overwritten by the MelMACCS user for each release path. This feature was added to accommodate situations where the MELCOR analyst defines a flow path that terminates below ground level.

Example: In this example, the user selected two plume segments. Each plume segment was selected from a different release. MelMACCS has a separate graphics window for each release path, so the user selected the release from two separate graphics windows.

* Initial plume height
RDPLHITE001 0.E+00
RDPLHITE002 10.E+00

2.3.7 Building Wake Calculations, BUILDH, SIGYINIT, SIGZINIT

The values for BUILDH, SIGYINIT, and SIGZINIT, are manually entered into the MelMACCS interface.

Example:

* Height of the facility building (m)
WEBUILDH001 1.E+00
WEBUILDH002 1.E+00
*
* Initial Sigma-Y width of plume (m)
SIGYINIT001 1.E-01
SIGYINIT002 1.E-01
*
* Initial Sigma-Z height of plume (m)
SIGZINIT001 1.E-01
SIGZINIT002 1.E-01

2.3.8 Sensible Heat, PLHEAT

MELCOR supplies the time-cumulative fluid enthalpy in Joules (J), relative to an ambient temperature of 300 K associated with each release path. The variable name in the time dependent blocks is MACCS-R-PLHEAT.0 where R is the release path.

$H(R,t)$ is the value of variable MACCS-R-PLHEAT.0 at time t .

$PLHEAT = (H(R,T_2) - H(R,T_1)) / (T_2 - T_1)$ is the MACCS parameter for rate of release of sensible heat in units of W calculated for the plume segment $[T_1, T_2]$, where the

MelMACCS user selected plume segment time interval $[T_1, T_2]$ for MELCOR release path R.

Example:

* Rate of release of sensible heat in Watts (or J/s)

RDPLHEAT001 1.235826E+06

RDPLHEAT002 3.375748E+06

2.3.9 Average Plume Flow Rate, PLMFLA

MELCOR supplies a cumulative fluid mass flow for each release path in moles, PLMFLO, and an average molecular weight in kg/mole, PLMWT, for each time step.

If the user chooses a plume segment interval $[T_1, T_2]$ for MELCOR release path R, MelMACCS calculates a plume flow during time step t_i as follows:

$$Flow_i = (PLMFLO(i) - PLMFLO(i-1)) \cdot (PLMWT(i) + PLMWT(i-1)) / 2$$

where PLMFLO and PLMWT correspond to the MELCOR variables MACCS-R-PLMFLO.0 and MACCS-R-PLMWT.0 and R is the release path number.

The calculated flow is in units of kg. The average flow rate over the interval $[T_1, T_2]$ is calculated by averaging the flow rates for each time step t_0, t_1, \dots, t_m within the interval $[T_1, T_2]$, where time $t_0 = T_1$ and $t_m = T_2$, as follows:

$$\frac{1}{T_2 - T_1} \left[\sum_{i=1}^m Flow_i \right]$$

Example: for each of the two selected plumes in this example, the average plume mass flow rate was calculated.

* Mass Flow Rate (kg/s)

RDPLMFLA001 3.7333E+00

RDPLMFLA002 4.5358E+00

2.3.10 Plume Gas Density, PLMDEN

For each time step and release path, MELCOR supplies a molecular weight in kg/mole, PLMWT (corresponding to variable MACCS-R-PLMWT.0, where R is the release path), a fluid temperature in degrees K, PLTEMP (corresponding to variable MACCS-R-PLTEMP.0, where R is the release path) and a cumulative fluid mass flow for each

release path in moles, PLMFLO (corresponding to variable MACCS-R-PLMFLO.0, where R is the release path).

An average gas density over all time steps in the interval is estimated as follows:

$p_0 = 1.013$ is the ambient pressure in bar.

$r_u = .00008314$ is the universal gas constant in bar-m³/mol-K.

The average density at a given time step i is calculated using the following factor:

$$F_i = PLMWT(i) / PLTEMP(i)$$

The average value of the density in the interval $[T_1, T_2]$ containing the discrete time sequence $t_0, t_1, t_2, \dots, t_m$ where $T_1 = t_0$ and $T_2 = t_m$ is calculated from the following factor:

$$F_{average} = (1 / (PLMFLO(T_2) - PLMFLO(T_1))) \frac{1}{2} \sum_{i=1}^m (F_i + F_{i-1}) (PLMFLO(t_i) - PLMFLO(t_{i-1}))$$

If the temperature, PLTEMP at time t_0 , is equal to zero, the calculation is adjusted to consider the time sequence $t_k, t_{k+1}, t_{k+2}, \dots, t_m$ where t_k corresponds to the first time in the sequence $t_0, t_1, t_2, \dots, t_m$ when the corresponding temperature is nonzero.

The gas density, PLMDEN, can then be expressed as follows:

$$PLMDEN = F_{average} \left(\frac{p_0}{r_u} \right).$$

If the temperature recorded on the plot file is zero, then the gas density, PLMDEN, returned is zero. This should only happen when the flow over the interval $[T_1, T_2]$ is zero.

Example: The gas density is calculated for each plume segment selected by the user.

* Gas Density (kg/m3)

RDPLMDEN001 4.4156E-01

RDPLMDEN002 5.5859E-01

2.3.11 Release Fraction, RELFRC

Release fractions are calculated for each chemical group and plume segment.

$Mass_{C,R}(t)$ is the sum of time dependent variables MACCS-R-M-RE-C.n at time t , for chemical group C, and for release R, summed over all particle sizes, n.

Masses for compound chemical groups are added to the elemental chemical groups, as described in Section 2.1.1, before release fractions are calculated. This is also true for the core inventory masses described in the following paragraph.

$CMass_C$ is the initial core mass for chemical group C. The value is taken from the MELCOR parameter MACCS-INITIAL-MASS(C) on the plot file. The fractional release for each chemical class and plume segment is calculated from the following expression:

$$(Mass_{C,R}(T_2) - Mass_{C,R}(T_1)) / CMass_C$$

Within the MelMACCS interface, the cumulative individual fractional release, $Mass_{C,R}(t) / CMass_C$, is plotted as a function of time. This plot is created to help the user define plume segments.

Release fractions are set to zero for any chemical groups the user has not chosen and for chemical groups with zero for the initial core inventory.

Example:

```
*      Xe  Cs
RDRELFRC001 1.7274E-02 6.0151E-06
RDRELFRC002 8.0438E-01 2.429E-01
```

2.4 Variables Related to Radionuclides

MELCOR treats chemical groups or classes of isotopes with similar chemical properties rather than individual isotopes. The mass of each chemical group in the core inventory is written onto the plot file in variable MACCS-INITIAL-MASS(C) for chemical group C. The chemical groups are composed of the elements shown in the following table. This table is included in MelMACCS.ini (see Appendix B). This table is taken from the MELCOR users guide, NUREG/CR-6119.

Class	Description	Member Elements
-------	-------------	-----------------

Xe	Noble Gases	He, Ne, Ar, Kr, Xe, Rn, H, N
Cs	Alkali Metals	Li, Na, K, Rb, Cs, Fr, Cu
Ba	Alkaline Earths	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
I	Halogens	F, Cl, Br, I, At
Te	Chalcogens	O, S, Se, Te, Po
Ru	Platinoids	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
Mo	Early Transition Elements	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
Ce	Tetravalent	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
La	Trivalents	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
U	Uranium	U
Cd	More Volatile Main Group	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
Sn	Less Volatile Main Group	Ga, Ge, In, Sn, Ag

MACCS normally considers a subset of all the isotopes that exist in an operating reactor based on their potential contribution to doses and health effects, as described in Chanin and Young, 1998. The isotopes to treat depend on the specific problem. The list of isotopes can be redefined in the MelMACCS user file, MelMACCS.usr.

2.4.1 The Isotopes and their Chemical Groups, NUMISO, NUCNAM and IGROUP

MACCS variable NUMISO, the number of isotopes, is determined by the number of isotopes listed in the MelMACCS.usr file in the data block section MACCS-ISOTOPES. For each chemical group, only the associated elements, as read from the MelMACCS.ini file in data block section CHEM-TO-ISO, are considered. For example, considering the iodine group, the isotopes of elements F, Cl, Br, I, and At are considered. From all the isotopes associated with these elements, only the isotopes that are listed in the MelMACCS.usr file in data block section MACCS-ISOTOPES are treated in a subsequent MACCS calculation. In the above example, only radionuclides I-131, I-132, I-133, I-134 and I-135 are included from the chemical group iodine. See Appendix C for more information.

Example: All isotopes are included, independent of the user's selection of chemical groups. However, initial activities are set to zero for excluded chemical groups.

* Number of radionuclides belonging to chemical classes

ISNUMISO001 69

*

* Data in MelMACCS.ini are used to map radionuclide to the corresponding chemical class

ISOTPGRP001 Kr-85 1

ISOTPGRP002 Kr-85m 1
ISOTPGRP003 Kr-87 1
ISOTPGRP004 Kr-88 1
ISOTPGRP005 Xe-133 1
ISOTPGRP006 Xe-135 1
ISOTPGRP007 Xe-135m 1
ISOTPGRP008 Cs-134 2
ISOTPGRP009 Cs-136 2
ISOTPGRP010 Cs-137 2
ISOTPGRP011 Rb-86 2
ISOTPGRP012 Rb-88 2
ISOTPGRP013 Ba-139 3
ISOTPGRP014 Ba-140 3
ISOTPGRP015 Sr-89 3
ISOTPGRP016 Sr-90 3
ISOTPGRP017 Sr-91 3
ISOTPGRP018 Sr-92 3
ISOTPGRP019 Ba-137m 3
ISOTPGRP020 I-131 4
ISOTPGRP021 I-132 4
ISOTPGRP022 I-133 4
ISOTPGRP023 I-134 4
ISOTPGRP024 I-135 4
ISOTPGRP025 Te-127 5
ISOTPGRP026 Te-127m 5
ISOTPGRP027 Te-129 5
ISOTPGRP028 Te-129m 5
ISOTPGRP029 Te-131m 5
ISOTPGRP030 Te-132 5
ISOTPGRP031 Te-131 5
ISOTPGRP032 Rh-105 6
ISOTPGRP033 Ru-103 6
ISOTPGRP034 Ru-105 6
ISOTPGRP035 Ru-106 6
ISOTPGRP036 Rh-103m 6
ISOTPGRP037 Rh-106 6
ISOTPGRP038 Nb-95 7
ISOTPGRP039 Co-58 7
ISOTPGRP040 Co-60 7
ISOTPGRP041 Mo-99 7
ISOTPGRP042 Tc-99m 7
ISOTPGRP043 Nb-97 7
ISOTPGRP044 Nb-97m 7
ISOTPGRP045 Ce-141 8
ISOTPGRP046 Ce-143 8
ISOTPGRP047 Ce-144 8
ISOTPGRP048 Np-239 8
ISOTPGRP049 Pu-238 8
ISOTPGRP050 Pu-239 8
ISOTPGRP051 Pu-240 8

ISOTPGRP052 Pu-241 8
ISOTPGRP053 Zr-95 8
ISOTPGRP054 Zr-97 8
ISOTPGRP055 Am-241 9
ISOTPGRP056 Cm-242 9
ISOTPGRP057 Cm-244 9
ISOTPGRP058 La-140 9
ISOTPGRP059 La-141 9
ISOTPGRP060 La-142 9
ISOTPGRP061 Nd-147 9
ISOTPGRP062 Pr-143 9
ISOTPGRP063 Y-90 9
ISOTPGRP064 Y-91 9
ISOTPGRP065 Y-92 9
ISOTPGRP066 Y-93 9
ISOTPGRP067 Y-91m 9
ISOTPGRP068 Pr-144 9
ISOTPGRP069 Pr-144m 9

2.4.2 Inventory Scaling Factor, CORSCA

This variable is included because the core inventory is included in the export file. CORSCA can be used to scale the inventory of all the radionuclides defined in the MACCS model. This variable is set to the user-selected value in the MelMACCS interface.

Example:

* Scaling Factor to adjust core inventory for power level
RDCORSCA001 1.0

2.4.3 Core inventory, CORINV

ORIGEN is used to construct the mapping of the inventory by chemical group used in MELCOR to the activities of isotopes needed by MACCS. The end result of this calculation is a value for the activity of important radionuclides in the core, based on assumptions documented in Appendix D. Though several inventories are provided, the user can provide their own inventory files. The activities and masses of the radionuclides are categorized in ORIGEN as follows:

- Activation products created from impurities and structural materials
- Actinides created from fuel isotopes
- Fission products created by nuclear fission

These categories are preserved within the MelMACCS.inv file. The activities used for the core inventory calculations are the sum over all three of these categories.

MelMACCS includes four default inventories. One is based on a low burn-up, 33 MWd/kg batch average at the end of the 3rd cycle), two high burn-up and one medium burn-up inventories are included. The two high burn-up inventories are based on a 65 MWd/kg peak fuel rod with the choices of a PWR plant, based on Sequoyah, and BWR plant, based on Peach Bottom. A medium burn-up inventory, based on Peach Bottom with 49 MWd/kg for the peak fuel rod is also supported. The medium burn-up inventory assumes that the accident occurs mid cycle.

From these quantities, the MACCS core inventory was calculated as follows:

$Mass_{\alpha}$ is the combined mass over all three categories of radionuclide α in g

$Activity_{\alpha}$ is the activity over all three categories of radionuclide α in Bq

$ChemicalMass_C = \sum Mass_{\alpha} / 1000$. in units of kg, where the sum is taken over all radionuclides in the ORIGEN results that belong to chemical group C, where the inclusion of the radionuclide within chemical group C is determined by the CHEM-TO-ISO data section in the MelMACCS.ini file. This sum includes radionuclides that are not treated by MACCS. Division by 1000 converts the chemical mass from grams to kilograms.

The core inventory is calculated for each radionuclide α that belongs to the MACCS variable NUCNAM as follows:

$$CoreInventory_{\alpha} = Activity_{\alpha} / ChemicalMass_C * MelcorMass_C$$

where $MelcorMass_C$ is the value of MELCOR parameter MACCS-INITIAL-MASS(C), where C is the chemical group to which radionuclide α belongs. Zero is reported for entries in the core inventory for radionuclides in chemical groups that were not included or that have zero in the core inventory.

Example (data are reported in Bq):

RDCORINV001 I-131 3.437425E+18
RDCORINV002 I-132 4.938601E+18
RDCORINV003 I-133 6.864887E+18
RDCORINV004 I-134 7.502555E+18
RDCORINV005 I-135 6.426491E+18
RDCORINV006 Te-127 3.874595E+17
RDCORINV007 Te-127m 4.797917E+16
RDCORINV008 Te-129 1.133504E+18
RDCORINV009 Te-129m 1.696226E+17

RDCORINV010 Te-131m 5.10681E+17
RDCORINV011 Te-132 4.908715E+18

References

Gauntt, R.O., R.K. Cole, C.M. Erickson, R.G. Gido, R.D. Gasser, S.B. Rodriguez, M.F. Young, 2000, MELCOR Computer Code Manuals, Primer and User's Guide, Version 1.8.5, NUREG/CR-6119, Vol. 1, Rev. 2, SAND2000-2417/1, US Nuclear Regulatory Commission, Washington, DC.

Chanin, D., and M.L. Young, 1998, Code Manual for MACCS2, User's Guide, NUREG/CR-6613, Vol. 1, SAND97-0594, US Nuclear Regulatory Commission, Washington, DC.

Ostemeyer, R. M., 1985, An Approach to Treating Radionuclide Decay Heating for Use in the MELCOR Code System, Sandia National Laboratories, NUREG/CR-4169, SAND84-1404, US Nuclear Regulatory Commission, Washington, DC.

Bixler, N.E., E. Clauss, C.W. Morrow, J.A. Mitchell, C. Navarro, and J. Barr, 2013, Synthesis of Distributions Representing Important Non-Site-Specific Parameters in Off-Site Consequence Analysis, NUREG/CR-7161, SAND2010-3380P, US Nuclear Regulatory Commission, Washington, DC.

Bixler, N.E., 2007, Evaluation of Differences Between Isotopic Levels in Low- and High-Burnup Fuels, Letter report to the US NRC (contract DEAC04-94AL85000), Sandia National Laboratories, April 18.

Bixler, N., R. Gauntt, J. Jones, and M. Leonard, 2013, State-of-the-Art Reactor Consequence Analysis Project Vol. 1: Peach Bottom Integrated Analysis, NUREG/CR-7110, Rev. 1, US Nuclear Regulatory Commission, Washington, DC.

Ilas, G., and I.C. Gauld, 2005, Light-Water Reactor Source Terms for Accident Analysis with MELCOR, Letter report to the US NRC (contract JCN Y6517), Oak Ridge National Laboratories, June 29.

Appendix A – Format of a MELCOR plot file

The following section presents an overview of the structure of a MELCOR plot file. The plot file is a binary file created with FORTRAN code. Some blocks of data are encoded as real numbers, some blocks are character strings, and some blocks are long integers. This file can be read by a FORTRAN program without considering extra binary-encoded information. However other compilers, such as Visual Basic or a FORTRAN compiler different than the one used to create the binary file, may require detailed information regarding the binary structure of the file.

Character strings are preceded and followed by the number of characters they contain. For example, if the string “Hello World” is on the plot file, it is preceded by the number 11 and followed by the number 11. These numbers are encoded as 4-byte integers.

The file is divided into blocks. The first block is a header. Following this are the time-independent data blocks. Following these are the time-dependent data blocks. Each of these blocks is associated with a MELCOR time step.

In some cases, there are time-dependent data blocks where the recorded time is the same as for the previous block. This can occur when time-step size is very small. The actual times internal to MELCOR are distinct, but because of the precision of the data written to the file, the recorded times are identical.

Blocks of data start with the characters “./” and two additional characters. The block type indicators are as follows:

“./*/” is the main header. This is a header block.

“./SP” is the beginning of a special data block. This is also a header block.

“./TR” is the beginning of a special block of time data. This is a time-dependent data block.

The following is the description of a sample main header.

Type	Number Bytes	Sample Value	Meaning
Long	4	4	Number of characters that follow
String	4	./*/	Flag indicating beginning of header
Long	4	4	Number of characters that precede
Long	4	4	Number of characters that

			follow
String	4	“TITL”	Key word indicating plot title
Long	4	4	Number of characters that precede
Long	4	110	Number of characters that follow
String		“RBKJCYMRF/11/18/02 /09:33:09 /DEMO, Version 1.8.5”	Number of bytes is value of previous field (in this example, 110) The first 7 characters of this string form a unique job id generated from the date and time. Alternatively, this ID could have been supplied by the user. The next two characters are the code version, ‘RF’ in this example. This is followed by the date and time of the run, /11/18/02 /09:33:09 / in this example. 'DEMO, Version 1.8.5' is user supplied title information
Long	4	110	Number of characters that precede
Long	4	4	Number of characters that follow
String	4	./*/	Flag indicating end of header
Long	4	4	Number of characters that precede
Long	4	4	Number of characters that follow
String	4	“KEY “	Flag indicating beginning of Key section of plot file
Long	4	4	Number of characters that precede
Long	4	8	Number of bytes in next block
Long	4	953	nKeys , number of time dependent variables
Long	4	5951	nValues, Size of time dependent block
Long	4	8	Number of bytes in previous block
Long	4	22872	Number of bytes in next block (24* nKeys)

String	24* nKeys	“CVH-RHO.1”	An array of variable names, VarNames(). Total number of names is m_nKeys (or 24* 953 bytes in this example). Each name is 24 characters long.
Long	4	22872	Number of bytes in previous block
Long	4	3812	Number of bytes in next block (4*nKeys)
Long	4*nKeys	44	An array of pointers into the time dependent block, Index(). Say Index(5) = 44 and Index(6) = 56. Then, data values 44 through 55 in the data block correspond to VarNames(5)
Long	4	3812	Number of bytes in previous block
Long	4	15248	Number of bytes in next block (16*nKeys)
String	16*nKeys	“KG/M**3”	Units corresponding to variables. M_units(5) corresponds to varname(5)
Long	4	15248	Number of bytes in previous block
Long	4	23804	Number of bytes in next block (4 * nValues)
Long	4*nValues		An array of ID's, nid(). See explanation below for usage
Long	4	23804	Number of bytes in previous block

Usage of an array of ID's, Nid: Each Variable name, VarNames(), is concatenated with a value of Nid to create a complete variable name.

Example: VarNames(i) corresponds to the index Index(i). Suppose Index(i) = K. The next data block begins at Index(i+1) = J. Then Nid(K) thru Nid(J-1) are postfix indices for variable names for the data in this block.

Example: suppose VarNames(38) = " MACCS-51-M-RE-01" and Index(38) = 49 and Index(39) = 60. This means that in the time dependent data block, entries 49 through 59 correspond to variable 38, or to MACCS-51-M-RE-01. The values of nid(49) to nid(59)

are written to the plot file, and are set to values 10, 0, 1, 2, 3, 4, 5, 6, 7, 8 and 9. Concatenating VarNames(38) with these values, we get the following variables and their corresponding locations on the MELCOR plot file.

Variable Name	Pointer to value in time dependent plot block
MACCS-51-M-RE-01.10	49
MACCS-51-M-RE-01.0	50
Etc...	...
MACCS-51-M-RE-01.9	59

After this initial header, there are a sequence of “./SP” records preceding the time dependent, or “./TR” records. This is special time independent data or a special data block. These are formatted as follows:

Type	Number Bytes	Sample Value	Meaning
Long	4	4	Number of characters that follow
String	4	“./SP/”	Indicates the beginning of a special, time independent, data block
Long	4	4	Number of characters that precede
Long	4	72	Number of characters that follow
String	Variable	“MACCS-NPSGRP((0))1.0000000E+01”	Number of bytes is value of previous field (in this example, 72)
Long	4	72	Number of characters that precede

Following the “./SP” data blocks, there are a sequence of “./TR” records. These are time dependent records, and are repeated for each time step written to the MELCOR plot file.

Type	Number Bytes	Sample Value	Meaning
Long	4	4	Number of characters that follow
String	4	“./TR/”	Indicates the beginning of a special, time independent, data block
Long	4	4	Number of characters that

			precede
Double	8		RtimeNotUsed
Single	4	2	ProblemTime in seconds
Single	4	1	Dt, time step size
Single	4	.350385	Cpu, processing time used by computer
Long	4	2	Ncycle
Single	NValues*4		Data block. Indices into block are calculated using arrays VarNames(), Index() and nid() as read from the main header.

Appendix B. MelMACCS/ MELCOR Interface Requirements

The MELCOR plot file contains two main classes of data. One class of data is time independent. These data are constant for the duration of the accident simulation. They consist of both variable names and constant values. When it is desired to create MACCS information from a MELCOR analysis, the MELCOR user must request that MACCS interface data are written to the plot file via MELGEN input, as documented in the MELCOR user's guide and the MelMACCS User's guide.

B.1 Time independent data written to the MELCOR plot file

The following section presents a summary of the MACCS-related information encoded in the MELCOR binary plot file.

The information indicating that CsI and CsM are compounds, and the fraction of the elements Cs, I, and Mo in the respective releases are read from the MelMACCS.ini file. This means that if it is necessary to add a new compound to the MELCOR plot file, MelMACCS does not need to be modified. Only the MelMACCS.ini file needs to be modified.

Time Independent Variable Name	Value in sample plot file	Description
MELCOR-VERSION(0)	2.1.1234	Version number of MELCOR. Last group of digits in version indicate SVN number.
MELCOR-SCRAM_TIME(0)	0.5	Indicates time of reactor shut down in seconds. This reflects MELCOR input variable DCH_SHT. This is an optional entry to the plot file
MACCS-NPSGRP(0)	1.00000E+01	Number of particle size groups. In MACCS 3.8, the upper bound is 20. MACCS variable NPSGRP is set to this number.
MACCS-PSIZE(1)	1.15002E-07	The geometric size of particle group in meters
MACCS-PSIZE(2)	2.14092E-07	
MACCS-PSIZE(3)	3.98564E-07	
MACCS-PSIZE(4)	7.41986E-07	
MACCS-PSIZE(5)	1.38131E-06	
MACCS-PSIZE(6)	2.57152E-06	
MACCS-PSIZE(7)	4.78725E-06	
MACCS-PSIZE(8)	8.91217E-06	
MACCS-PSIZE(9)	1.65913E-05	
MACCS-PSIZE(10)	3.08871E-05	
MACCS-NUMRING(0)	2	Number of rings. If this isn't present, assume one ring.
MACCS-RINGNAM(1)	Spent Fuel Pool	Name of ring. Entry for each ring. Required for each

		Aring if MACCS-NUMRINGS specified. These input entries are optional.
MACCS-RINGNAM(2)	Spent Fuel Pool B	
MACCS-MAXGRP(0)	34	Number of chemical groups. This is the total number of chemical groups over all batches.
MACCS-CHEMICAL-GROUP(1)	Xe	MACCS-CHEMICAL-GROUP(i) is name of chemical group i.
MACCS-CHEMICAL-GROUP(2)	Cs	
MACCS-CHEMICAL-GROUP(3)	Ba	
MACCS-CHEMICAL-GROUP(4)	I	
MACCS-CHEMICAL-GROUP(5)	Te	
MACCS-CHEMICAL-GROUP(6)	Ru	
MACCS-CHEMICAL-GROUP(7)	Mo	
MACCS-CHEMICAL-GROUP(8)	Ce	
MACCS-CHEMICAL-GROUP(9)	La	
MACCS-CHEMICAL-GROUP(10)	U	
MACCS-CHEMICAL-GROUP(11)	Cd	
MACCS-CHEMICAL-GROUP(12)	Sn	
MACCS-CHEMICAL-GROUP(13)	B	By default setting, the MelMACCS.usr file excludes this group in the EXCLUDE-GROUPS section, hence does not import data for this group. This can be changed by the user.
MACCS-CHEMICAL-GROUP(14)	H2O	This is not considered by MelMACCS because the MelMACCS.ini file has no entries for H2O in the CHEM-TO-ISO section.
MACCS-CHEMICAL-GROUP(15)	Cnct	This is not considered by MelMACCS because the MelMACCS.ini file has no entries for Cnct in the CHEM-TO-ISO section.
MACCS-CHEMICAL-GROUP(16)	CsI	Cesium Iodide is not used directly by MACCS. Released CsI is split into Cs and I masses and is used to calculate the total fractional releases of Cs and I. The initial mass of CsI is assumed to have already been added to initial masses of the Cs and I groups, so it is not used.
MACCS-CHEMICAL-GROUP(17)	CsM	Cesium Molybdate, Cs ₂ MoO ₄ , is not used directly by MACCS. The initial mass is added to the masses of Cs and Mo by MELCOR. Treatment of releases is similar to CsI, the release is split into the Cs and Mo groups. Note: prior to MELCOR 2.x chemical group entries 18 to 23 were included but not used. Now, only the relevant chemical groups have entries.
MACCS-CHEMICAL-GROUP(18)	Xe	This is the beginning of a sample batch 2

MACCS-CHEMICAL-GROUP(19)	Cs	
MACCS-CHEMICAL-GROUP(20)	Ba	
MACCS-CHEMICAL-GROUP(21)	I	
MACCS-CHEMICAL-GROUP(22)	Te	
MACCS-CHEMICAL-GROUP(23)	Ru	
MACCS-CHEMICAL-GROUP(24)	Mo	
MACCS-CHEMICAL-GROUP(25)	Ce	
MACCS-CHEMICAL-GROUP(26)	La	
MACCS-CHEMICAL-GROUP(27)	U	
MACCS-CHEMICAL-GROUP(28)	Cd	
MACCS-CHEMICAL-GROUP(29)	Sn	
MACCS-CHEMICAL-GROUP(30)	B	
MACCS-CHEMICAL-GROUP(31)	H2O	
MACCS-CHEMICAL-GROUP(32)	Cnct	
MACCS-CHEMICAL-GROUP(33)	CsI	
MACCS-CHEMICAL-GROUP(34)	CsM	
MACCS-INITIAL-MASS(1)	5.56451E+02	Initial mass of MACCS-CHEMICAL-GROUP(i) in the core (kg).
MACCS-INITIAL-MASS(2)	3.22020E+02	
MACCS-INITIAL-MASS(3)	2.49029E+02	
MACCS-INITIAL-MASS(4)	2.51176E+01	
MACCS-INITIAL-MASS(5)	4.89470E+01	
MACCS-INITIAL-MASS(6)	3.68391E+02	
MACCS-INITIAL-MASS(7)	4.20773E+02	
MACCS-INITIAL-MASS(8)	7.12738E+02	
MACCS-INITIAL-MASS(9)	6.85259E+02	
MACCS-INITIAL-MASS(10)	1.65847E+05	
MACCS-INITIAL-MASS(11)	1.68781E+00	
MACCS-INITIAL-MASS(12)	1.03046E+01	
MACCS-INITIAL-MASS(13)	0.00000E+00	
MACCS-INITIAL-MASS(14)	0.00000E+00	
MACCS-INITIAL-MASS(15)	0.00000E+00	
MACCS-INITIAL-MASS(16)	0.00000E+00	
MACCS-INITIAL-MASS(17)	1.20000E-09	Note: if this corresponds to Cesium Molybdate the initial mass of Cs due to this compound and Mo has already been added to the Cs and Mo chemical groups. CsI has been treated similarly with respect to the Cs and I chemical groups. This mass is not used by MelMACCS.
MACCS-INITIAL-MASS(18)	1.20000E-09	
MACCS-INITIAL-MASS(19)	1.20000E-09	

MACCS-INITIAL-MASS(20)	1.20000E-09	
MACCS-INITIAL-MASS(21)	1.20000E-09	
MACCS-INITIAL-MASS(22)	1.20000E-09	
MACCS-INITIAL-MASS(23)	1.20000E-09	
...		
MACCS-INITIAL-MASS(34)	1.20000E-09	
MACCS-NPATH(0)	2.00000E+00	Number of release paths.
MACCS-RELEASE-PATH(1)	5.10000E+01	MELCOR ID of release path.
MACCS-FLNUM(51)	3.99000E+02	MELCOR ID of flow number. There is a one-to-one correspondence between a release path ID and a flow number ID. MACCS-FLNUM(k) reference k is the release path ID.
MACCS-PHITE(51)	0.00000E+00	MACCS-PHITE(k) is the height in m of release path k.
MACCS-RELEASE-PATH(2)	9.90000E+01	
MACCS-FLNUM(99)	3.98000E+02	
MACCS-PHITE(99)	0.00000E+00	
MACCS-RHONUM	1.00000E+03	MACCS-RHONUM is the nominal density of aerosols (kg/m**3).

B.2 Time Dependent Data Written to the MELCOR Plot File

The second class of data written to the MELCOR plot file is a sequence of data blocks at each time step, as requested by the MELCOR user. If there are two time blocks with identical recorded times, MelMACCS saves the data associated with the first time block recorded.

Sample Variable Name	Example Description	Description
MACCS-51-M-RE-01.0	Release path ID 51, Chemical ID 1, particle size 0. Corresponds to XE (value of time independent variable MACCS-CHEMICAL-GROUP(1)). In the above example, this variable is repeated for each release (2), for each chemical (32), for each particle size group (11). Thus, there are 704 entries related to fractional release for each time step recorded.	Cumulative mass of release. Particle size 0 has no corresponding particle in MACCS, and represents a vapor. These variables are repeated for each release, for each chemical and for each particle size group. Only the mass of the radioactive portion released is reported. This is significant when considering the mass of Cs ₂ MoO ₄ released. Units are in kg.
MACCS-51-PLTEMP.0	Temperature for release path 51	Fluid temperature associated with release path in degrees K.
MACCS-51-PLHEAT.0	Sensible heat for release path 51	Cumulative fluid sensible heat associated with a release path relative to an ambient temperature of 300K. Units are in J.
MACCS-51-PLMFLO.0	Fluid mass flow for release path 51	Cumulative fluid mass flow for each release path. Units are in moles.
MACCS-51-PLMWT.0	Fluid molecular weight for release path 51	Fluid molecular weight for each release path. Units are kg/mole.

Appendix C – MelMACCS information files, MelMACCS.ini, MelMACCS.usr, and MelMACCS.inv

These three files and their formats are described below. Each of these files uses the following conventions:

- An asterisk in column 1 indicates that the line is a comment and is ignored by MelMACCS. These lines can appear anywhere in this file.
- This file contains comments and data blocks. Data blocks begin with a backslash, “/”, in column one and are followed by a keyword and optional parameters (depending on the keyword) separated by white space.
- Data blocks contain data relevant to the block type (i.e., the keyword previously indicated) separated by white space.
- White space is defined as any sequence of ASCII characters where the coded value of each character is less than or equal to 32. This includes TAB characters.
- Data blocks end with the characters “/END” starting in column one.

C.1 MelMACCS.usr

The file MelMACCS.usr contains settings that are editable by the user. Each user has his or her own copy of this file to modify. A copy of MelMACCS.usr is copied from the installation folder to the local user document area in the MelMACCS_Docs folder.

The following keywords are supported:

- **DEFAULT-DIR** - the default project file directory. If this is not specified or is not used, the local user document area in the MelMACCS_Docs folder is used. If this folder does not exist, MelMACCS creates it. A folder called "Inventories" is created in this folder if one does not exist.

The user can create additional inventory files and copy them to the Inventories folder. These file names are shown in MelMACCS to allow the selection of these additional inventories. The format must be the same as that of the MelMACCS.inv file described in this Appendix.

Example:

```
/DEFAULT-DIR "C:\MelMACCS Project"
```

- **EXCLUDE-GROUPS** – contains a list of chemical groups to exclude from consideration when displaying chemical groups in the user interface. This list may also include CsI and CsM; however, these are never shown in the user interface. If

CsI or CsM is on this list, then the masses of Cs and I in the CsI group, or Cs and Mo in the CsM groups are not included when calculating masses to determine the particle size distribution or the release fraction.

Example:

```
/EXCLUDE-GROUPS  
B  
Sn  
Cd  
U  
/END
```

- **MACCS-ISOTOPES** - Isotopes supported in MACCS. Only data related to these isotopes in the /CORE data blocks are written to the MelMACCS source-term file.

Isotope names consist of an element name (case nonspecific) followed by a dash (“-”) followed by the atomic weight of the isotope. These names are matched to values in the CHEM-TO-ISO data block to find the related chemical group associated with the element. In the example below, Np-239 is associated with the Ce chemical group as shown in the chemical to isotope association list in the **CHEM-TO-ISO** block example shown below.

Example:

```
/MACCS-ISOTOPES  
*RadioNuclide  
...  
Ce-143  
Ce-144  
Np-239  
Pu-238  
Pu-239  
...  
/END
```

- **MACCS-PSEUDOSTABLE-ISOTOPES** – Pseudostable isotopes supported by MACCS. These isotopes are considered to terminate a decay chain and are not treated in dose calculations.

The pseudostable isotope names that follow consist of the element name followed by a dash (“-”) followed by the atomic weight of the isotope. MelMACCS writes this list of pseudostable isotopes to the source-term file without performing any validation of the isotope names.

/MACCS-PSEUDOSTABLE-ISOTOPES

* pseudostable isotope and potential decay products do not contribute to doses

I-129

Xe-131m

Xe-133m

Cs-135

Sm-147

U-234

U-235

U-236

U-237

Np-237

Rb-87

Zr-93

Nb-93m

Nb-95m

Tc-99

Pm-147

/END

C.2 MelMACCS.ini

MelMACCS.ini contains settings the user should not normally need to change. This file is in the Program Files installation directory.

The following keywords are supported:

- **DRY-DEPOSITION-COEFF** - contains values of regression coefficients to optionally calculate the MACCS dry deposition velocity based on expert elicitation data. Column one contains the quantile level indicating degree of belief. Remaining entries two through eight contain the coefficients used for each term in the equation, a, b, c, d, e, f and g.

Example:

/DRY-DEPOSITION-COEFF

0.00	-6.569	1.578	-0.068	0.015	0.439	0.000	0.071
------	--------	-------	--------	-------	-------	-------	-------

0.01	-6.225	1.448	0.183	-0.057	0.766	0.000	0.086
------	--------	-------	-------	--------	-------	-------	-------

...

/END

- **COMPOUND-GROUPS** – Some chemical groups on the MELCOR plot file represent chemical compounds rather than chemical (elemental) groups. The mass release from these compounds can be added to the chemical groups if specified on these lines. The first entry on a line is the compound name as read from the MELCOR plot file from a time-independent entry MACCS-CHEMICAL-

GROUP. For example, MACCS-CHEMICAL-GROUP(17) is assigned the value CsM. The second entry on a line is the chemical group that is used by MelMACCS to add the mass for the compound. The third entry is the fraction of the mass from the compound that is added to the chemical group specified in the second entry on this line (this is a molar fraction).

Example:

```
/COMPOUND-GROUPS
CSI  I  0.488444
CSI  Cs 0.511556
CSM  Cs 0.73478922
CSM  Mo 0.26521078
/END
```

- **CHEM-DECAY** - Each parent group contains a radionuclide with a decay product in the child chemical group. The first entry on a line is the parent chemical group, the second entry is the child chemical group.

Example: Radionuclides in the Ba chemical group (elements Be, Mg, Ca, Sr, Ba, Ra, Es, Fm) have daughter products that are in the chemical groups listed below. Only the specific isotopes associated with this chemical group in the MACCS need to be considered when developing this list.

```
/CHEM-DECAY
*Parent Child
...
Ba      Te
Ba      I
Ba      Xe
Ba      La
Ba      Ce
Ba      Mo
...
/END
```

- **CHEM-TO-ISO** - defines an association between chemical groups and elements. This is necessary to define core inventory and release fractions, since MELCOR does not supply data in terms of elements or isotopes, but in terms of chemical groups. This list was derived from the MELCOR input manual, NUREG/CR-6119, Rev 2, page DCH-RM-8.

The data in this block consist of the chemical group name followed by an element that belongs to that chemical group. These chemical group names are compared

with the chemical group names recorded in the MELCOR plot file. These group names are not case sensitive.

Example: The following shows that all isotopes of the element Np are associated with the chemical group Ce.

```
/CHEM-TO-ISO
*Name Isotope Element
...
*Alkaline Earths
*Tetravalent
Ce      Ti
Ce      Zr
Ce      Hf
Ce      Ce
Ce      Th
Ce      Pa
Ce      Np
Ce      Pu
Ce      C
*Trivalents
La      Al
La      Sc
...
/END
```

C.3 MelMACCS.inv

MelMACCS.inv contains four default inventories that are distributed with MelMACCS. The user should not change this file. It is located in the Program Files installation directory.

Additional inventories can be defined using this same format. These additional inventory files need to be put in the project Inventories folder to be recognized by MelMACCS.

- **CORE-LABEL** – defines keywords and labels used to identify different reactor inventories. On each line, the first column is the key word and the second column is a more descriptive label. The keyword is used to associate data with the reactor core in the CORE sections of the MelMACCS.inv file.

Example:

```
/CORE-LABEL
LOW      "Low Burnup, 33 MWd/kg batch average, 3rd cycle"
HIGH_PWR "High Burnup, 65 MWd/kg peak fuel rod, PWR (based on Sequoyah)"
HIGH_BWR "High Burnup, 65 MWd/kg peak fuel rod, BWR (based on Peach Bottom)"
```

MEDIUM_BWR "Medium Burnup, 49 MWd/kg peak fuel rod at mid cycle BWR (based on Peach Bottom)"
/END

- **CORE-DESC PARAM1** – allows an optional extended description of the core inventory.

PARAM1 identifies the reactor inventory. This is a keyword that matches one of the keywords in the CORE-LABEL section.

The description following this line is shown in the MelMACCS user interface when the specific inventory is selected.

Example:

/CORE-DESC LOW

The inventory results were created by an Origin run simulating

The third cycle of a 33 MWd/kg batch average.

Starting with MelMACCS 2.0 these, extended descriptions are supported.

The number of lines entered in this section is unlimited.

This description is optional

/END

- **CORE PARAM1 PARAM2 PARAM3** - defines activity and/or mass information regarding the state of the reactor core in terms of isotopes.

PARAM1 identifies the reactor inventory. This is a keyword that matches one of the keywords in the CORE-LABEL section.

PARAM2 indicates whether the values are activities (keyword ACTIVITY) or masses (keyword MASS).

PARAM3 indicates whether the data that follow are from the actinide and daughter products category (ACTINIDE), from the fission products category (FISSION), or due to activation of impurities or structural materials (ACTIVATION) of an ORIGEN output.

PARAM3 is not used by MelMACCS at this time. All activity is treated equally when mapped to MACCS variables.

If PARAM2 is the keyword ACTIVITY, then the data in this block consist of activities as measured in Curries of the various radionuclides. If Param2 is the keyword MASS, then the data are masses measured in grams.

The data block contains the following items on each line:

- The element name associated with the radionuclide. Starting with MelMACCS version 2.0.1, this is case insensitive. Before 2.0.1, all elements need to be all in upper case.
- The atomic mass of the radionuclide
- The associated value (in grams or curies depending on the value of PARAM2 above)

The data included were from a set of ORIGEN calculations. It is interesting to note that not all radionuclides are present in all categories.

Example:

/CORE LOW MASS ACTIVATION

H 1 9.584E-03

H 3 2.718E-02

HE 3 2.358E-04

...

/END

Appendix D – Isotopic Inventory

The data for the isotopic inventory for the two high-burnup cores were supplied by Oak Ridge National Laboratory (ORNL) from a sequence of ORIGEN calculations (Ilas and Gauld, 2005, Bixler, 2007). ORNL performed a set of ORIGEN calculations for Sequoyah, a four-loop Westinghouse PWR with an ice-condenser containment, and for Peach Bottom, a GE BWR Type 4 with a Mark I containment. These calculations realistically account for both radial and axial peaking factors. Furthermore, they considered burnups at the current limit authorized by the NRC, 65 MWd/kgU for the peak fuel rod.

The data for the medium burnup reactor modeling were supplied by the NRC for Peach Bottom and are the values used in SOARCA (Bixler et al., 2013). A set of ORIGEN calculations were based on actual refueling practices at the plant circa 2005.

The data for the isotopic inventory of the low burnup reactor modeling were supplied by Sandia National Laboratories, as documented in Ostemeyer (1985).

The output from ORIGEN is organized in groups as follows:

- Activation Products. This group contains the activity due to activation of impurities in the fuel and any structural materials included in the calculation.
- Actinides plus Daughters. This group contains the activity due to neutron absorption by uranium isotopes in the fuel.
- Fission Products. This group contains activity due to fissions and radioactive decay of these fission products.

Additional data were supplied for the core in the same type of grouping, namely activation, actinides plus daughters and fission products. Data were grouped in both isotope and chemical categories. For each of these categories, the output report contained results reported by mass (in grams), activity (in curies) and thermal power (in watts).

All of the ORIGEN calculations used to construct the inventory data account for batches of fuel corresponding to first, second, and third cycle. Some of the calculations also account for specific refueling patterns and radial and axial peaking factors. The high burnup inventories were calculated for end of cycle, i.e., just before refueling. The medium burnup inventory is at the middle of a fuel cycle, i.e., midway between the last and next refueling outages. The low burnup is at end of fuel cycle but reflects a relatively low operating power level. All inventories are averaged over the entire core.