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MelMACCS User Guide – Version 4.0.0

Accident Consequence Modeling and Analysis Group, Sandia National Laboratories

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico
87185 and Livermore,
California 94550

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ABSTRACT

The MelMACCS User Guide is intended to assist analysts in how to use the MelMACCS application to create an interface file that can be used in a MACCS calculation. MelMACCS combines MELCOR results, in the form of a MELCOR plot file, with user input. This information is used to create a MelMACCS output file that is in a format compatible with MACCS. It can then be imported as an input file in WinMACCS and used for MACCS calculations.

ACKNOWLEDGEMENTS

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ACRONYMS AND DEFINITIONS

Abbreviation	Definition
BWR	Boiling Water Reactor
DOS	Disk Operating System
ISLOCA	Interfacing Systems Loss-Of-Coolant Accident
LTSBO	Long-Term Station Blackout
LCF	Latent Cancer Fatality
NRC	U.S. Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratories
PWR	Pressurized Water Reactor
SNL	Sandia National Laboratories
SGTR	Steam Generator Tube Rupture
SOARCA	State-of-the-Art Reactor Consequence Analyses
STSBO	Short-Term Station Blackout

1. INTRODUCTION

MelMACCS is a preprocessor code that was created to provide an interface utility between MELCOR and MACCS. This document provides directions on how to use MelMACCS 4.0.0 in order to create a MACCS source-term file from a MELCOR plot file. The standard method of processing a MelMACCS output in MACCS is to use the WinMACCS interface (Bixler et al., 2015) either using the import file option or the cyclical file set option, which can be used to process multiple MelMACCS output files.

Section 2 provides an overview of the MelMACCS 4.0.0 interface and describes the MelMACCS data files as well as how to run MelMACCS 4.0.0 in batch mode and on Linux. Section 3 of this document describes how to use MelMACCS 4.0.0 in interactive mode and contains the model description. Section 4 provides an overview of the MelMACCS output file. Lastly, Section 5 describes how to use a MelMACCS source term file without using the WinMACCS interface.

1.1. MELCOR Background

MELCOR is a computer code developed by Sandia National Laboratories (SNL) for the purpose of modeling the progression of severe accidents in nuclear reactors. The following information was obtained from Volume 1 of the MELCOR Computer Code Manual, SAND2017-0455 O (Humphries et al., 2017), which may be referenced for additional detail.

MELCOR is comprised of an executive driver and a set of unified code packages to represent the complex and coupled phenomena occurring both within the reactor core and external to the vessel during the accident. This structure allows MELCOR to be capable of modeling a broad spectrum of severe accident phenomena to include:

- thermal-hydraulic response of the primary reactor coolant system, the reactor cavity, the containment, and the confinement buildings,
- core uncovering (loss of coolant), fuel heat up, cladding oxidation, fuel degradation (loss of rod geometry), and core material melting and relocation,
- heat up of reactor vessel lower head from relocated fuel materials and the thermal and mechanical loading and failure of the vessel lower head, and transfer of core materials to the reactor vessel cavity,
- core-concrete attack and ensuing aerosol generation,
- in-vessel and ex-vessel hydrogen production, transport, and combustion,
- fission product release (aerosol and vapor), transport, and deposition,
- behavior of radioactive aerosols in the reactor containment building, including scrubbing in water pools, and aerosol mechanics in the containment atmosphere such as particle agglomeration and gravitational settling, and,
- impact of engineered safety features on thermal-hydraulic and radionuclide behavior

One of the code packages within MELCOR is the flow package, which is responsible for calculating flow rates of gases and liquid water through paths that connect control volumes within MELCOR. Flow paths to the environment, and thus applicable to consequence analysis, may be specified using the flow package. Multiple release paths to the environment may be specified in the flow package, which provide the information needed by MACCS on fluid flow and radionuclide transport. These outputs are described in Table 1-1 below.

Table 1-1 MACCS control function arguments from MELCOR

MELCOR Output	Description
MACCS-RHONOM	Nominal aerosol density used to relate diameter and mass. (units = kg/m^3)
MACCS-PLTEMP(MACCSname)	Fluid temperature associated with release path MACCSname (units = K)
MACCS-PLHEAT(MACCSname)	Enthalpy associated with release path NameFP. (units = J)
MACCS-PLMFLO(MACCSname)	Cumulative fluid mass flow associated with release path MACCSname. (units = kg)
MACCS-PLMWT(MACCSname)	Fluid molecular weight associated with release path MACCSname. (units = kg/mole)
MACCS-M-RE(MACCSname,NameCLS,ii)	Released radioactive mass for RN class NameCLS in size group (section) ii associated with release path MACCSname. Vapor is in size group 0. (units = kg)
MACCS-M-RE(MACCSname,NameCLS,AER)	Released radioactive aerosol mass for RN class NameCLS. (units = kg)
MACCS-M-RE(MACCSname,NameCLS,TOT)	Total released radioactive mass for RN class NameCLS, including aerosol and vapor. (units = kg)

1.2. General Source Term Guidance/Warnings

When using source term data for MACCS analyses it is always important to double check the information for any possible errors. Below are some warnings that MelMACCS/MACCS users should consider when performing their analyses.

- In some instances, MELCOR users may specify internal MACCS flow paths to track movements of radionuclides within the modeled buildings (i.e., the reactor, containment, reactor building, etc.). These flow paths should not be included in the source term to the environment, and it is the responsibility of the MELCOR analyst to mark these flow paths with a DF identifier so that they are not processed in MelMACCS. MelMACCS and MACCS users should disregard these internal MELCOR flow paths and coordinate with the MELCOR analyst to ensure they are not a part of the MelMACCS processing.
- MelMACCS users should be aware of any oscillation in the released masses. Any instance of negative mass numbers should prompt users to consult with the MELCOR analyst to determine if any errors were made during the plot file generation.

- MelMACCS users should be aware of any non-realistic sensible heat values. Negative sensible heat values are not allowed in MACCS and could possibly be due to an error in the source term. Users should work with the MELCOR analyst to determine what might be producing these negative values.
- In some instances, MELCOR user may specify flow paths that have aerosols remaining in the gas phase due to insufficient time/conditions for complete condensation. MelMACCS users should be aware that previous versions of MelMACCS did not include the gas phase contribution of aerosols to the aerosol size distribution calculations. MelMACCS 4.0 accounts for the gas phase contribution to the aerosol size distribution by adding the gas phase amount to the largest particle size bin. This was implemented to ensure that the aerosols remaining in the gas phase are accounted for in the aerosol size distribution calculations. This can result in differences in aerosol size distributions between MelMACCS 4.0 and previous versions.

2. GETTING STARTED

2.1. Overview of User Interface

MelMACCS 4.0.0 is started by selecting the MelMACCS symbol from the Windows Start Menu. This application leads the user through a series of forms in order to create a MELCOR/MACCS interface file, also referred to as a MelMACCS output file or a MACCS source-term input file.

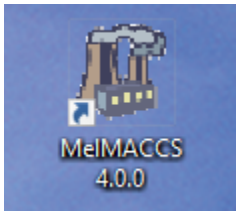


Figure 2-1 MelMACCS Windows desktop icon

2.1.1. *Creating a Project*

The first display that opens when the user starts MelMACCS 4.0.0 prompts the user to choose one of two options, either create a new project or open an existing project. When the option to open an existing project is selected, the user is asked to locate the project file for the project they wish to open. MelMACCS project files have a .mel extension. A demo project file is supplied with the MelMACCS 4.0.0 installation. This file can be found in either the Program Files installation directory or the local user document area in the MelMACCS_Docs folder. However, if the user already has a MelMACCS_Docs folder from a previous MelMACCS version, the demo project file will only be located in the Program Files installation directory. The user must delete or rename the MelMACCS_Docs folder before installing MelMACCS 4.0.0 for the demo project file to be automatically placed in the user document area.

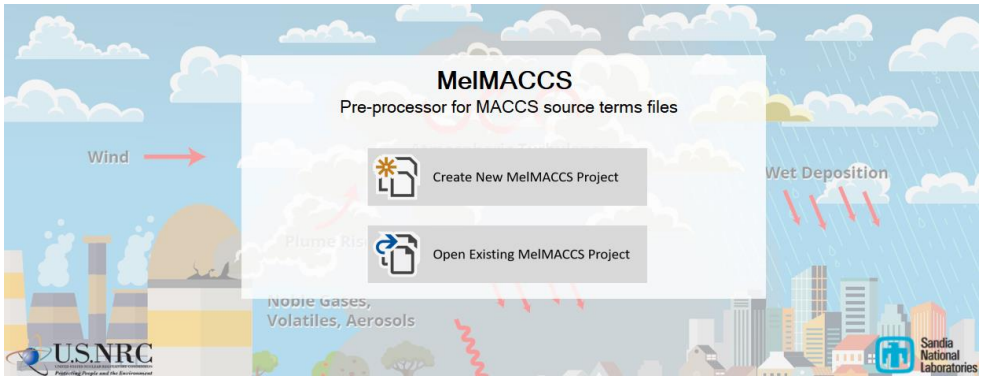


Figure 2-2 Selecting a MelMACCS project

Version upgrading: MelMACCS 4.0.0 has a project file that holds the settings used in processing a specific project. Previous versions of MelMACCS had no projects or project files. As this is new for version 4.0.0 there is no automatic conversion from unreleased MelMACCS 4.0.0 versions (MelMACCS 4.0.0-beta) to the released MelMACCS version (MelMACCS 4.0.0). **When upgrading to the released version the user must create new projects for the settings to work correctly.** Future released versions of MelMACCS will have the ability to open and upgrade previous projects.

2.1.2. *Opening a MELCOR Plot File*

Once the project is selected or created, users must choose the MELCOR plot file they wish to convert. The Open MELCOR Plot File button is clicked to choose a MELCOR plot file. The user chooses the MELCOR plot file and clicks open. The MELCOR plot file is a binary file that commonly has a .ptf extension and more information on the format of this file can be found in Appendix D. A demo plot file is also supplied with the MelMACCS 4.0.0 installation. This file can be found in either the Program Files installation directory or the local user document area in the MelMACCS_Docs folder. However, if the user already has a MelMACCS_Docs folder from a previous MelMACCS version, the demo plot file will only be located in the Program Files installation directory. The user must delete or rename the MelMACCS_Docs folder before installing MelMACCS 4.0.0 for the demo plot file to be automatically placed in the user document area.

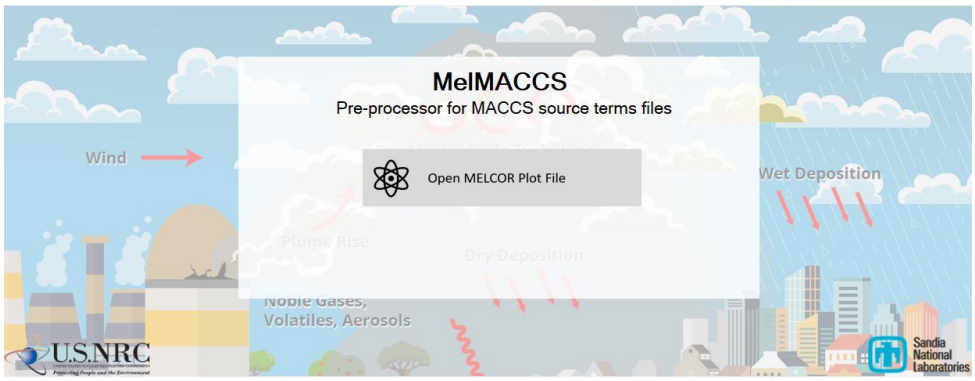


Figure 2-3 Selecting a plot file

After the user selects a MELCOR plot file to use, a progress bar will display as seen in Figure 2-4 while MelMACCS reads the plot file. When MelMACCS is done reading the file, the message next to the progress bar will say "File Read Complete". The message window below the progress bar also provides the directory for the plot file that was opened.

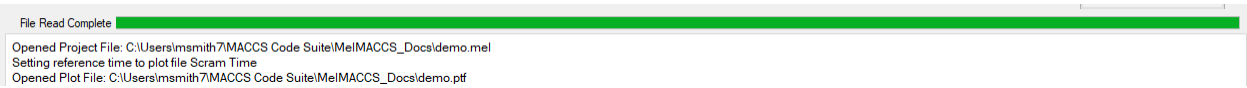


Figure 2-4 Progress bar and message window display

Warning: MelMACCS 4.0.0 is designed to have a specific project file (.mel) that corresponds to the MELCOR plot file (.ptf). MELCOR plot files may have different numbers of rings and releases. To work correctly the MelMACCS project file should have the same number and names of rings and releases as the plot file. A new project will have the same number and names of rings and releases as the plot file. For existing projects there can be a mismatch of the project and plot files. This could happen if a user ran a batch job with a project file that does not match the plot file used or if a user opened a project and then opened a plot file that does not match the project. If MelMACCS determines that the project file and the plot file do not have the same number and names of rings and releases it will use parameters that it can from the project file and create new parameters with default values for parameters that are based on the number of rings or releases. MelMACCS will print out a warning when this happens.

2.1.3. *MelMACCS Project Window Overview*

Once MelMACCS finishes reading the user-specified plot file, a display such as the one shown in Figure 2-5 below opens.

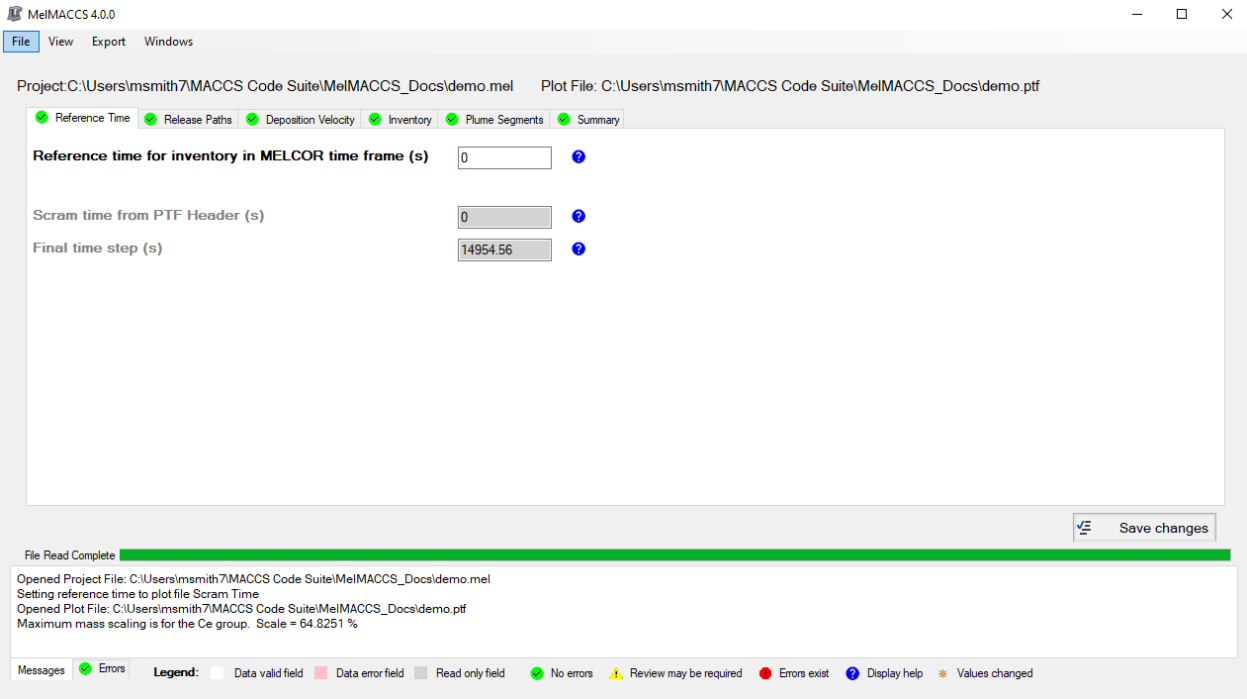


Figure 2-5 MelMACCS project window

The caption at the top of the window indicates the version on MelMACCS being used and the directories shown under the main menu options indicate the location of the project file and plot file.

The MelMACCS main menu contains the following options:

- *File* allows users to create a new project, open an existing project, or save the project currently open along with some additional functions.
- *View* displays a pop-up window with the plot file header information.
- *Export* allows users to export the plot file to a text file or to Excel. Users can also create the MACCS input file from here.
- *Windows* displays a pop-up window with information about MelMACCS 4.0.0

The message window at the bottom of the window displays whether or not the MelMACCS data files were successfully read and provides any additional information that may be beneficial to the user when working through the project.

The messages window also has an error tab which describes to the user the nature of any errors currently in the project. Users are signaled that there is an error with the help of the legend shown in Figure 2-6 below

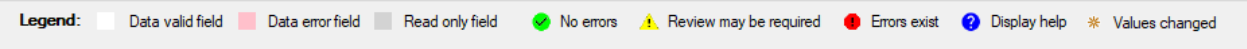


Figure 2-6 MelMACCS legend

- A white field indicates that this field can be edited by the user.
- A red field indicates that there is an error with that specific data field.
- A grey field indicates that the field is read only, and the user cannot edit this value. The information in these data fields come directly from the MELCOR plot file.
- A green circle with a check mark indicates that all information entered on the specific form passes and no errors are present
- A yellow triangle with an exclamation point indicates that review of the specific form may be required
- A red octagon with an exclamation point indicates there is an error, and a description of the error can be found in the "Errors" tab
- A gold asterisk symbol indicates a parameter on the form has been changed and the project needs to be saved.
- The blue circle with a question mark next to each parameter displays a help window to provide more information to the user.

2.2. MelMACCS Data/Information Files

Along with the MELCOR plot file and the project file (.mel), three data files are needed to successfully use MelMACCS. These files include the user settings file, MelMACCS.usr, the configuration file, MelMACCS.ini, and the user defined inventory files (.inv). With the exception of the MELCOR plot file, the format of data files read by MelMACCS all follow the same language rules. This format supports editing in an ASCII text editor, such as Microsoft Notepad or Notepad++. Microsoft Word™ and Microsoft Word Pad™ can add extra invisible formatting characters that are not compatible with MelMACCS, so these editors should not be used to modify these files. Additionally, new lines in the MelMACCS data files are indicated by the Windows standard carriage return (ASCII 13) and line feed (ASCII 10) characters.

The following components are found in a MelMACCS data file:

- A comment is indicated by an asterisk, "*", in column one. Comments can occur anywhere in the file.
- Comments following data in a data line are not supported. Place all comments on their own line beginning with an asterisk in column one.
- A keyword starts with a slash, "/", in column one, followed by a keyword followed by value(s) associated with that keyword. The number of values required depends on the keyword.
- Values are separated on data or keyword lines using white space such as spaces or tabs.
- A data block begins with a keyword line. This is followed by a series of data lines. The end of the data block is indicated by the following character sequence starting in column one, "/END".
- Some keyword lines are not associated with a data block.

- Blank lines are permitted in the file. Blank lines can occur anywhere.
- If a value is a string containing spaces, it must be enclosed by the double quote characters (" ").
- White space can be any number of spaces, tabs, or otherwise unreadable characters. More precisely, characters with an ASCII code less than or equal to 32 are considered white space.

2.2.1. *Project (.mel) Files*

As stated previously, the .mel files are the project files. These files are created when a user saves their project in the user interface. The settings within these files can be updated through the user interface or users can manually edit these files if wanting to run MelMACCS in batch mode.

An example project file and its contents can be seen in Appendix B.

2.2.2. *MelMACCS.usr File*

The file MelMACCS.usr contains settings that are editable by the user. Each user has their 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 Section 2.2.4.

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

- **EXCLUDE-GROUPS –** contains a list of the chemical groups that are not automatically selected by default when displaying the 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 that follows later.

  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

2.2.3. *MelMACCS.ini File*

MelMACCS.ini contains settings the user should not normally need to change. This file is in the Program Files installation directory. However, a copy of MelMACCS.ini is copied from the installation folder to the local user document area in the MelMACCS_Docs folder.

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
```

2.2.4. *MelMACCS.inv File*

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 Curies 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
```

2.3. Running MelMACCS in Batch Mode

MelMACCS can be run from a command prompt window (cmd.exe) or from a batch file (.bat file). The parameter values are read from a MelMACCS project file (.mel extension). A sample project file, demo.mel, based on the sample plot file demo.ptf, is provided with MelMACCS. The format of this file is shown in Appendix B.

The format of a command is as follows:
BatchMelMACCS.exe projectfile -i melcorplotfile -o maccsfile [-a]

The following is an example of a line to run MelMACCS in batch mode:

BatchMelMACCS.exe demo.mel -i "D:\demo.ptf" -o MACCSInterface.inp -a

There are three files specified. **If full paths are not specified, then it is assumed that the files are in the directory the batch is run from**. File paths and names should be delimited by quotes when there are embedded spaces in the file names.

The meanings of the arguments are as follows:

- BatchMelMACCS.exe: This executable is located in the Program Files directory under the "MelMACCS 4.0.0" folder. **If the user is not running from the directory in which the executable is located, it is important that the full path of the executable is specified in the command shown above.**

- MelMACCS project file: This must be the first argument. This file is in JSON format and contains all information that would normally be entered by the user. All values specified in the project file are loaded into the interface.

- MELCOR plot file: The plot file is specified with the entry, "-i melcorplotfile". The plot file normally ends with a. ptf extension. If missing, an error is shown in the command window and log file.

- MelMACCS output file: The output file is specified in the entry, "-o maccsname". This entry defines the MACCS interface file that MelMACCS creates. **It is recommended that this file be saved in the designated MelMACCS_Docs folder. This output file CAN NOT be saved under the Program Files directory where BatchMelMACCS.exe is located.**

- If the -a option is set, MelMACCS will process all rings in the plot file and create an output for each ring. The respective output files will be names maccsfile.inp1, maccsfile.inp2, etc. for each ring

It is expected that users might run batch mode in three possible ways:

1. Using multiple project (.mel) files with different parameter values in them on a single plot (.ptf) file.
2. Using a single project (.mel) file on multiple plot (.ptf) files that have the same rings and releases.
3. Using a single project (.mel) file on multiple plot (.ptf) files that may not have the same rings and releases. This may give unintended results if there is a mismatch of the project and plot files.

2.4. Using MelMACCS on Linux

MelMACCS 4.0.0 is a C# WinForms program built using the Microsoft .Net Framework 4.8. It may be run on Linux by using the Mono software platform (https://www.mono-project.com/). Mono is no longer actively supported; hence it is recommended to use MelMACCS on Windows.

MelMACCS 4.0.0 running on Linux has been tested on Linux Ubuntu 21.04, running on a virtual machine. It is expected to work on other Linux distributions as well. When running MelMACCS 4.0.0 on Linux the user will notice some differences that are mostly cosmetic. The most notable of these is the standard file browser dialog does not have some of the icons on its buttons, such as the up-directory button. The button is still there but with no icon. This is a known bug but, as there is no active development in Mono, it cannot be addressed at this time. The batch version of MelMACCS 4.0.0 (BatchMelMACCS.exe) also runs on Linux.

2.4.1. *Installing MelMACCS on Linux*

The first step to install MelMACCS 4.0.0 on Linux is to install Mono using the download and instructions for your Linux distribution that may be found (when this document was written) at: https://www.mono-project.com/download/stable/#download-lin .

Then the user should unpack the MelMACCS for Linux compressed distribution file to a directory of their choice that they have access to on their Linux machine. The files in this compressed MelMACCS distribution file are identical to the files that would be found in the /Program Files/MelMACCS[Version] directory when MelMACCS is installed on Windows using the MelMACCS Windows installer.

2.4.2. *Running MelMACCS on Linux*

MelMACCS 4.0.0 may be run on Linux by opening a Terminal, changing the current directory to where MelMACCS 4.0.0 installed (or using the full path for the executable) and typing in:

Mono GUI_MelMACCS.exe

The MelMACCS 4.0.0 user interface should be displayed and work the same as on windows.
The batch version of MelMACCS 4.0.0 (BatchMelMACCS.exe) may be run with the command:

Mono BatchMelMACCS.exe projectfile -i melcorplotfile -o maccsfile

It is important to note that because Linux files have only the line feed character, files created on a Linux system may not be compatible with MelMACCS on a Window™ system unless the unix2dos command is run over the file to convert it to Window™ / DOS™ format. However, the MelMACCS.ini, MelMACCS.usr, and MelMACCS.inv files seem to be capable of being used with or without carriage returns. Additionally, the project file is saved in the format specified for the operating system and project files saved on Windows can be opened in Linux. The MELCOR plot files are binary files and do not need any conversions between operating systems.

3. MELMACCS USER GUIDE AND MODEL DESCRIPTION

The following section describes how source term information from a MELCOR plot file is converted into a MACCS input file. MelMACCS was developed to solicit input required for this mapping from the user. MelMACCS is written to lead 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.

A summary of how to create a MACC input file from a MELCOR plot file can be seen in the MelMACCS process flowchart shown in Appendix A.

3.1. Entering the Reference Time

The first form, the Reference Time form, contains the user inputted reference time and the scram time and final time step which is read from the MELCOR plot file. The scram time is read into MelMACCS using the MELCOR-SCRAM_Time variable but it does not appear in all ptf files. If this variable is not present MelMACCS assigns a value of 0 s by default.

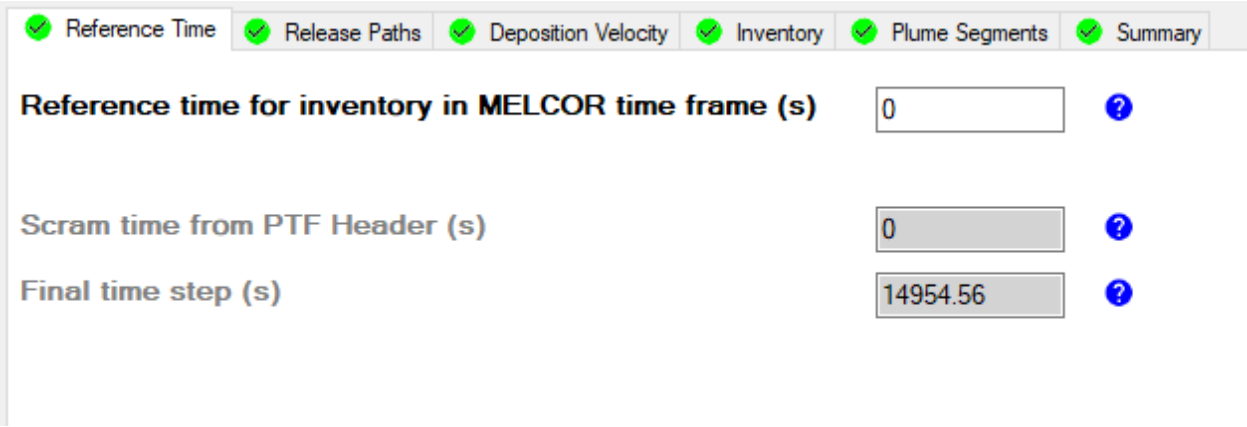


Figure 3-1 Reference Time form

The default value of the MelMACCS variable labeled "*Reference time for inventory in MELCOR time frame (s)*" corresponds to a MELCOR input variable indicating the reactor scram time. Typically, MELCOR input is set up so that reactor scram occurs at time zero, but this need not be the case. If either this value is missing from the plot file or if the value on the plot file is less than the time of the first data block written to the plot file, the value is set to zero.

This time is used to adjust the time of plume releases saved in the MelMACCS output file which corresponds to the PDELAY variable in MACCS. For example, if the value of the time of accident initiation is input to be 100 s and the user selects a plume segment that starts at MELCOR time 300 s in a *Plume Segment* form, the starting time for the plume written to the MACCS Input file is 300 -100

= 200 s. The primary significance of this parameter is to control the start of radionuclide decay in the MACCS calculation.

3.2. Entering the Release Path Information

The grid shown on the next form (labeled as "Release Paths") contains the release path identification number, the release path height, the adjusted release height based on subtracting the user entered value labeled "*Height of ground level in MELCOR model*" from the release path height read from the MELCOR plot file, the building height, the building width, the building length, the building angle, and the initial plume dimensions.

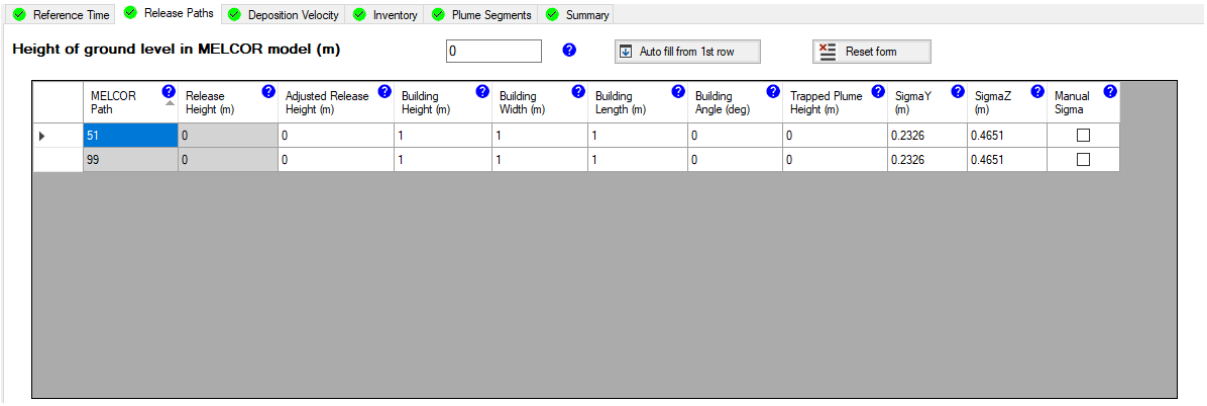


Figure 3-2 Release Path form

The release path identification number and release path height information come directly from the MELCOR plot file. The rest of the parameters are entered in by the user. Clicking the button labeled "*Reset form*" will reset the table and text entry field back to their default values. The values will not be reset to zero. If a row in the grid is defined, clicking the button labeled "*Auto fill from 1st row*" copies the row to vacant entries in subsequent rows until a completed row is encountered. The row that is copied is the last defined row.

3.2.1. *Ground Height Relative to MELCOR and Adjusted Release Height*

The text box labeled "*Height of ground level in MELCOR model (m)*" is the ground height in the MELCOR reference frame. Heights in MELCOR are relative to some fixed reference height that may not always be ground elevation. Therefore, in order to adjust the MELCOR release height for the MACCS analysis (which uses ground elevation as its fixed reference height), MelMACCS users may provide a reference height to represent the ground height relative to MELCOR. For example, as shown in Figure 3-3, the fixed reference height in MELCOR is set to be 10 m below ground level. Therefore, MelMACCS users would specify the height of ground level in the MELCOR model as -10 m. This will consequently adjust the release path height from 20 m to 30 m. This feature is especially useful if the MELCOR release height is a negative number. If no adjustment is necessary, the default reference height is set to 0. Based on the specified reference height, the "*Adjusted Release Height (m)*" box will update accordingly for each release path.

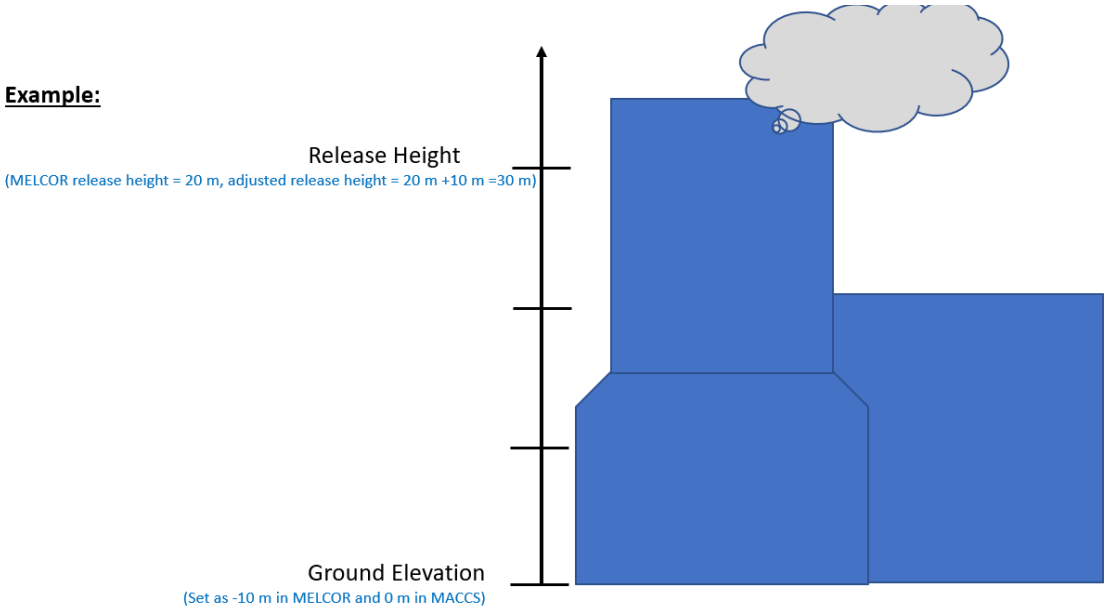


Figure 3-3 Adjusting the MELCOR release height example

3.2.2. *Building Dimensions*

For each plume segment, MACCS requires the dimensions of the building where the release occurred to be defined. The required dimensions are building height, building width, building length, and the building angle from north. More information on the required building dimensions is shown in Table 3-1 below.

Table 3-1 Building dimension inputs and acceptable ranges

Variable	Corresponding MACCS Variable	Acceptable Range
Building height	BUILDH	0 to 1000 m
Building width	BUILDW	1 to 1000 m
Building length	BUILDL	1 to 1000 m
Building angle	BUILDA	-180 to 180 deg

This information is used to evaluate whether a buoyant plume is entrained in the building wake. These values are not always trivial to select, especially when dealing with multiple buildings in the same location. If the release occurs at multiple buildings, different releases or release paths may have different building parameters. Representative values are required for MACCS and can be changed in MACCS after the fact if needed. Fortunately, these values only influence the plume concentrations at relatively short distances and generally have modest influence at distances of several kilometers downwind.

3.2.3. *Trapped Plume Height*

For each plume segment, MACCS also requires a specified trapped plume release height that is used to determine plume trapping/downwash when either of the Briggs trapping and downwash models are selected in MACCS. Using these models, if the plume is determined to be trapped in the building wake this value is used in MACCS calculations instead of the plume release height which is determined by the adjusted path height parameter. It is recommended that this value be set to zero but can be set to another value as needed or subsequently changed in MACCS.

3.2.4. *Sigma Y and Sigma Z*

Initial plume dimensions, Sigma Y and Sigma Z, are also needed by MACCS. These values represent the standard deviation of the Gaussian plume in the crosswind and vertical dimensions, respectively. The MACCS User's Guide recommends values as follows (Leute et al., 2021):

$$\sigma_y = \frac{W}{4.3} \quad \textbf{(1)}$$

$$\sigma_z = \frac{H}{2.15} \quad \textbf{(2)}$$

Where:

- σ_y is the initial crosswind plume dimension
- σ_z is the initial vertical plume dimension
- W is the building width
- H is the building height

When the user enters the building height and width on this form, the initial plume dimensions will be automatically calculated using the equations specified above. However, if the user wishes to use another method for determining these dimensions, the user can select the "*Manual Sigma*" box and manually enter their chosen values for each release path.

3.3. Specifying the Deposition Velocity

This form allows selection of the method used to calculate the MACCS variable VDEPOS. This variable describes the set of deposition velocities used to determine the relative dry deposition of the particles. There are two model choices. The first is based on gravitational settling. The default model is based on a correlation of expert elicitation data (Bixler et al., 2013).

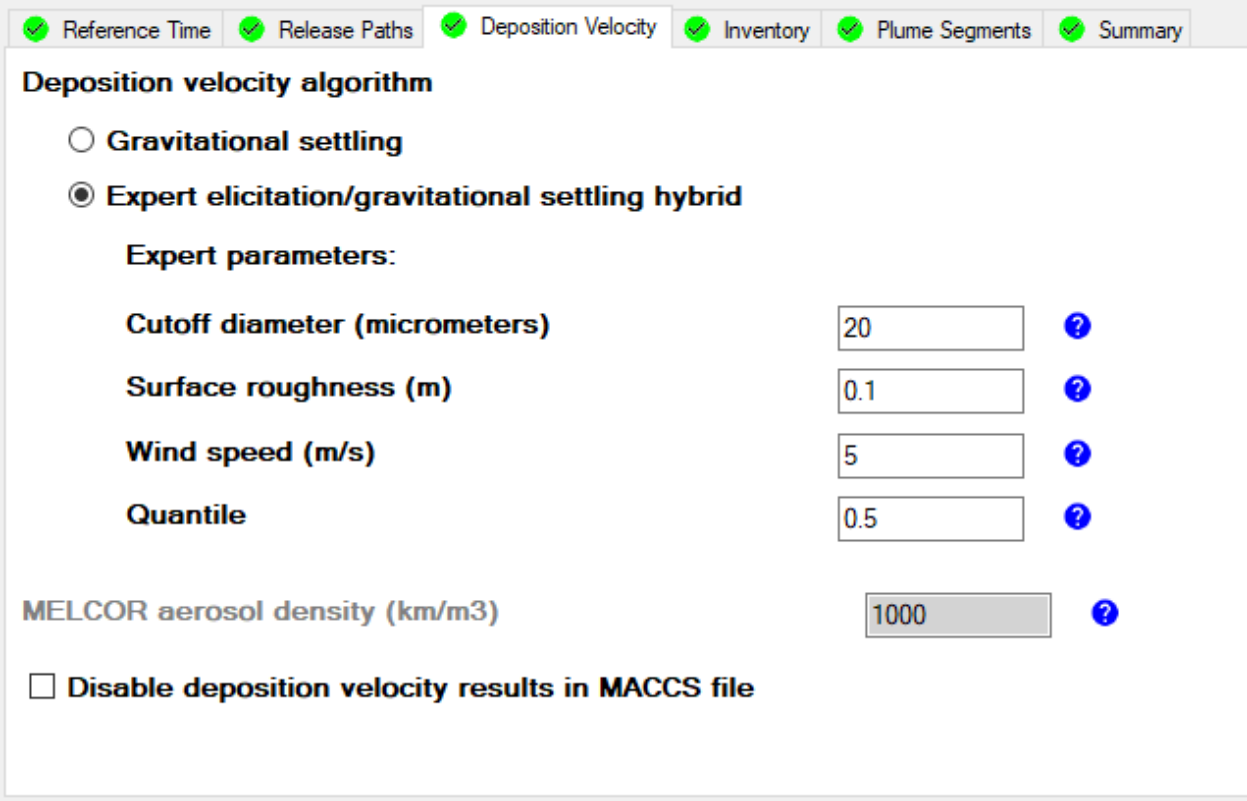


Figure 3-4 Deposition Velocity form

When the expert elicitation option is chosen, additional inputs are required as follows:

- *Cutoff Aerodynamic Diameter*: This is the point at which the deposition velocity calculation is switched from the expert elicitation correlation to gravitational settling. The default and recommended value is 20 μm. An exception to this rule is made when the gravitational settling result for a particle diameter is less than the value calculated using the expert elicitation correlation for the cutoff diameter, in which case the velocity calculated for the cutoff diameter using the expert correlation is used.

- *Surface Roughness*: This is a measure of the terrain roughness, which is the terrain's ability to generate turbulence and enhanced vertical mixing, and it has the potential to affect both the vertical dispersion and dry deposition velocities of aerosol particles. The default value is set to 0.1 m. The range of this value is from 0.001 m to 10 m. Figure 3-5 below describes the estimated surface roughness for different terrain types.

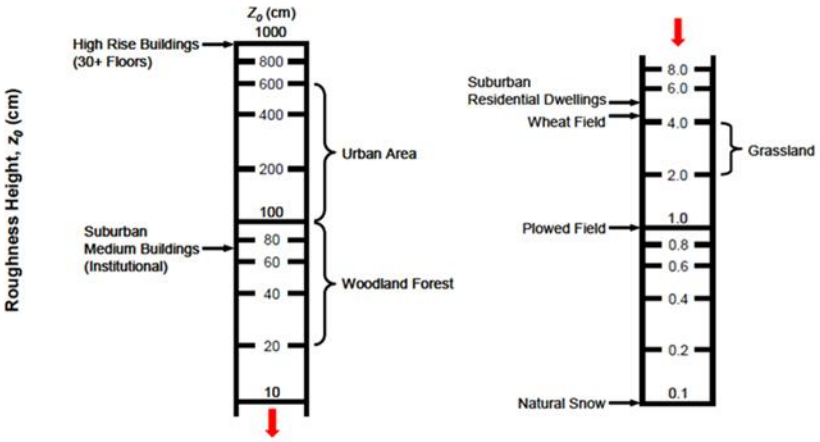


Figure 3-5 Approximate surface roughness lengths (Leute et al., 2021)

- *Wind Speed*: The default wind speed is 5 m/s. The range of values are 0.5 to 10 m/s.

- *Quantile*: This is a measure of degree of belief in deposition velocity, as expressed by a group of experts. A value of 0 represents the smallest value that the experts thought to be possible; a value of 0.5 represents the best guess; a value of 1 represents the highest value that the experts thought to be possible. This value is 0.5 by default.

Two of these parameters, wind speed and surface roughness, must be specified as representative values over the grid and for all weather trials. Surface roughness often varies over the grid. Wind speed varies from hour to hour and weather trial to weather trial. As a result, a reasonable, representative value needs to be chosen considering the expected variability at a site.

The *MELCOR Aerosol Density* is read from the MELCOR plot file using the variable MACCS-RHONOM. If this value is not included on the plot file, a value of 1000 kg/m^3 is used as a default.

If the check box titled *"Disable deposition velocity results in MACCS file"* is checked, the deposition velocity is still calculated, but the values are written to the MelMACCS output file as comments meaning both WinMACCS and MACCS ignore these cards and deposition velocities must be specified separately. This option is useful for uncertainty analyses for which deposition velocity is treated as an uncertain input.

For example, the input image containing the deposition velocity is disabled in the following line because it starts with the * character:
*DDVDEPOS001 8.7563E-04

If the check box is not selected, then the input image containing the deposition velocity is enabled, as shown in the line below:
DDVDEPOS001 8.7563E-04

3.3.1. *Dry Deposition Velocity Based on Gravitational Settling*

The following formulae are used to calculate the settling velocity for the released particles.

$$C_m = 1 + \frac{2\lambda}{d_g}\left[f_{Slip} + .4e^{-1.1d_g/2\lambda}\right] \quad \textbf{(3)}$$

Where:

- C_m is the Cunningham slip correction factor, or particle mobility factor
- 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
- λ is the mean free path of air at 298 K and is set to $0.069 \cdot 10^{-6}$ (m)
- f_{Slip} is the slip factor and is set to 1.257

$$v_d = (d_g)^2 (pDensity) g C_m / (18\mu\chi) \quad \textbf{(4)}$$

Where:

- v_d is the dry deposition velocity (m/s), which defines the MACCS input parameter, VDEPOS(p), where p is the index representing the particle size bin
- $pDensity$ is the density of particle (kg/m^3), read from the MELCOR parameter MACCS-RHONOM
- g is the acceleration of gravity (9.8 m^2/s)
- μ is the viscosity of air at 298 K ($1.8 \cdot 10^{-5}$ N·s/m^2)
- χ is the dynamic shape factor which is equal to 1

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

3.3.2. *Dry Deposition Velocity Based on Expert Elicitation Data*

Dry deposition velocities in MACCS are treated as being dependent on aerosol size and independent of wind conditions and surface roughness. In an evaluaton 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:

$$\ln(v_d) = a + b(\ln(d_p)) + c(ln(d_p))^2 + d(ln(d_p))^3 + e(z_0) + f(z_0)^2 + g(v) \quad \textbf{(5)}$$

Where:

- v_d is the deposition velocity (cm/s)
- d_p is aerodynamic particle diameter (μm)
- z_0 is the user specified surface roughness
- v is the user specified wind speed (m/s)

After a re-evaluation of the expert elicitation data (Bixler et al., 2013), Equation 5 above was updated and the dry deposition velocity is now represented by the following equation:

$$\ln(v_d) = a + b(\ln(d_p)) + c(ln(d_p))^2 + d(ln(d_p))^3 + e(z_0) + g(v) \quad \textbf{(6)}$$

Since the only change was the removal of the $f(z_0)^2$ term in the equation, this was remedied in MelMACCS by assigning the f regression coefficient a value of 0 for all quantiles. The regression coefficients, a, b, c, d, e, f, and g shown in Table 3-2 below, 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.

Table 3-2 Values of regression coefficients in Equation 6

Quantile	a	b	c	d	e	f	g
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
0.05	-5.582	1.121	0.284	-0.048	0.754	0.000	0.160
0.10	-5.075	1.033	0.282	-0.042	0.764	0.000	0.155
0.25	-4.334	0.981	0.256	-0.050	0.902	0.000	0.178
0.50	-3.964	0.992	0.190	-0.072	1.061	0.000	0.169
0.75	-1.889	0.843	0.204	-0.045	1.403	0.000	0.170
0.90	-1.446	0.950	0.259	-0.041	2.430	0.000	0.218
0.95	-0.857	1.002	0.272	-0.041	2.625	0.000	0.230
0.99	0.408	0.934	0.266	-0.032	2.357	0.000	0.216
1.00	1.507	0.976	0.242	-0.042	2.049	0.000	0.191

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:

$$d_p = \sqrt{\frac{\text{pDensity}}{1000}} \cdot d_g \cdot 10^6 \quad \textbf{(7)}$$

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 0.05μm, a value of 0.05μm is used in the calculation.

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

3.4. Entering the Options that Affect the Core Inventory

The next form allows the user to specify the set of chemical groups to be included, the core inventory, and the ring (if the MELCOR plot file contains release data for more than one radioactive source).

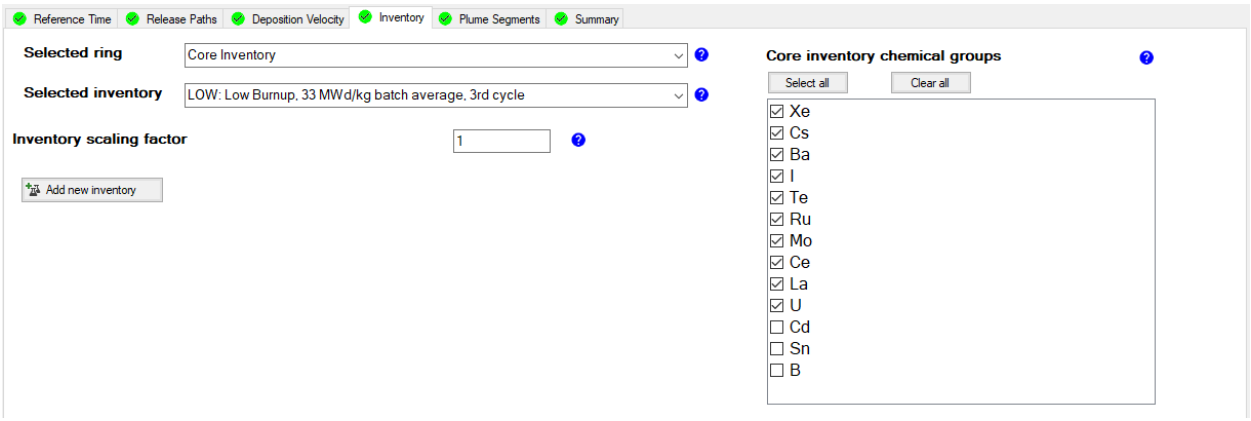


Figure 3-6 Inventory form

3.4.1. *Ring Number*

MELCOR can be run with multiple rings, but in most cases a single ring is present on the MELCOR plot file.

Multiple rings are especially useful for spent fuel pool modeling, where different rings can represent fuel of different ages. MelMACCS processes multi-ring release fractions when they are present in the MELCOR plot file. When this is done, each ring has a set of initial masses and released masses on the

plot file. The same set of chemical groups is common for all rings. Because the rings may represent fuel of different ages, each ring may be associated with a different inventory. When the MELCOR plot file only contains a single ring, the selection has already been made and the user does not need to do anything further. If the plot file does have multiple rings the user will need to manually select which ring they choose to use and either update the project and create a MelMACCS output file for each ring or create a designated project for each ring separately. If running MelMACCS in batch mode, the user can choose to run all rings at once (see Section 2.3 for more information)

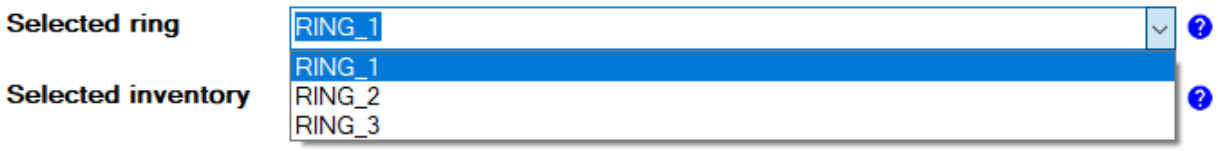


Figure 3-7 Inventory ring selection

3.4.2. *Inventory selection*

Next, the user must select the inventory that is closest to the inventory modeled by MELCOR. A description field is shown in the user interface to describe each inventory. Ideally, the same ORIGEN calculation is used to define the MELCOR inputs and to create an inventory for MelMACCS. This is done by creating one or more inventory files.

The inventory list shows the core inventories read from the MelMACCS.inv file found in the installation folder and additional inventory files created or added by the user. User-defined inventory files are placed in the MelMACCS_Docs\Inventories folder. Under Windows 10, the inventory folder is C:\Users\username\MelMACCS_Docs\Inventories. Note this file path may be different for international Windows layouts.

Each available inventory is displayed in the user interface as shown.

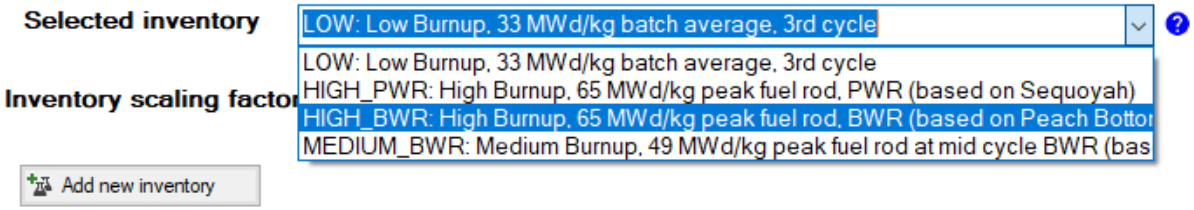


Figure 3-8 Selecting inventory type

MelMACCS includes four default inventories. They are based on one low burn-up, two high burn-up and one medium burn-up inventories. The low burn-up inventory is based on a 33 MWd/kg batch average at the end of the 3rd cycle. 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.

New inventory files can be added by clicking the button labeled *Add new inventory*. When a new inventory file is added, a copy of that file is placed in the MelMACCS_Docs\Inventories folder. The

next time MelMACCS starts, the new inventory file is automatically loaded. Users can also choose to manually place the inventory file in the MelMACCS_Docs\Inventories folder. Using either option, inventories will remain in that folder and loaded in MelMACCS unless the inventory file is removed from that folder.

3.4.2.1. Default Inventory Data

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.

3.4.2.2. Calculating MACCS Core Inventory

The ORIGEN output categories described in the section above are preserved within the MelMACCS.inv file. The activities used for the core inventory calculations are the sum over all three of these categories. The MACCS core inventory is calculated as follows:

First, the chemical mass, in units of kg, is calculated 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.

$$ChemicalMass_C = \sum Mass_\alpha / 1000. \quad \textbf{(8)}$$

Where:

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

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

$$CoreInventory_\propto = \frac{MelcorMass_C}{ChemicalMass_C} * Activity_\propto \quad \textbf{(9)}$$

Where:

- $Activity_\propto$ is the activity over all three categories of radionuclide α in Bq
- $MelcorMass_C$ 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

It is important to note that Equation 8 above applies a mass scaling factor to the inventory when the mass for each chemical group in the inventory file does not match with the initial masses specified for each MELCOR chemical class. This is an automatic calculation happening behind the scenes in MelMACCS and it is especially useful when using an inventory file that is not representative of a full core inventory. When applying this mass scaling factor MelMACCS will output a maximum error message in the messages window to give an indication of the relative difference between the chosen

inventory file and the initial masses specified in the MELCOR plot file. An example of this message can be seen below:

Maximum mass scaling is for the Ce group. Scale=64.8251%

Users should consider this when choosing what inventory file to use as well as when deciding to apply an inventory scaling factor which is described in the next section.

3.4.3. *Inventory scaling factor*

The default value of the inventory scaling factor is 1.0, which is usually the desired value, but this value can be changed and defines the value of the MACCS parameter, 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

This parameter is useful when the MELCOR calculation has been done for a reactor that is similar, but different in size and power rating, then the reactor that is to be evaluated with MACCS.

Figure 3-9 Specifying the inventory scaling factor

3.4.4. *Chemical Groups*

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 (Humphries et al., 2017) uses the terminology chemical class while the MACCS User's Guide (Leute et al., 2021) uses the terminology chemical group. In this document, the MACCS convention is used with chemical group referring to a set of chemical elements that are treated as being the same.

MELCOR treats chemical groups or classes of isotopes with similar chemical properties rather than individual isotopes. The first 13 MELCOR radionuclide classes are the default classes. These broadly represent the same 13 chemical groups in MACCS shown in the following table, which is taken from the MACCS radionuclide screening report, SAND2021-11703 (Andrews et al., 2021). 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 and MelMACCS automatically collects the MELCOR masses from the default 13 MELCOR radionuclide classes to compute the radionuclide inventories of the 13 MACCS chemical groups (see the discussion in Section 3.4.2.2). The chemical groups are composed of the elements and includes all of the chemical groups currently used within MACCS.

Other radionuclide classes in MELCOR may be with respect to important chemical compounds (e.g., CsI, CsMoO4) or bulk materials (e.g., concrete, water). Bulk materials are not considered by MelMACCS because the MelMACCS.ini file has no entries for them in the CHEM-TO-ISO section. Additionally, the chemical compounds CsI and CsMoO4 are split into separate masses for Cs/I and Cs/Mo respectively and are used to calculate the total fractional releases of Cs, I and Mo. The initial mass of both compounds are assumed to have already been added to initial masses of the Cs, I, and Mo groups, so they are not used in MelMACCS.

Table 3-3 Chemical groups currently used in MACCS

Group	Description	Member Elements
1	Noble Gases	He, Ne, Ar, Kr, Xe, Rn, H, N
2	Alkali Metals	Li, Na, K, Rb, Cs, Fr, Cu
3	Alkaline Earths	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	Halogens	F, Cl, Br, I, At
5	Chalcogens	O, S, Se, Te, Po
6	Platinoids	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	Early Transition Elements	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	Tetravalents	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	Trivalents	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10	Uranium Group	U
11	Cadmium Group	Cd, Hg, Zn, As, Sb, Pb, TI, Bi
12	Tin Group	Ga, Ge, In, Sn, Ag
13	Boron Group	B, Si, P

Select the chemical groups that are to be included in the MACCS analysis using the check boxes. By default, all chemical groups not listed in the /EXCLUDE-GROUPS section in the MelMACCS.usr file are checked. Excluded chemical groups must be manually checked if they are to be included the MACCS analysis.

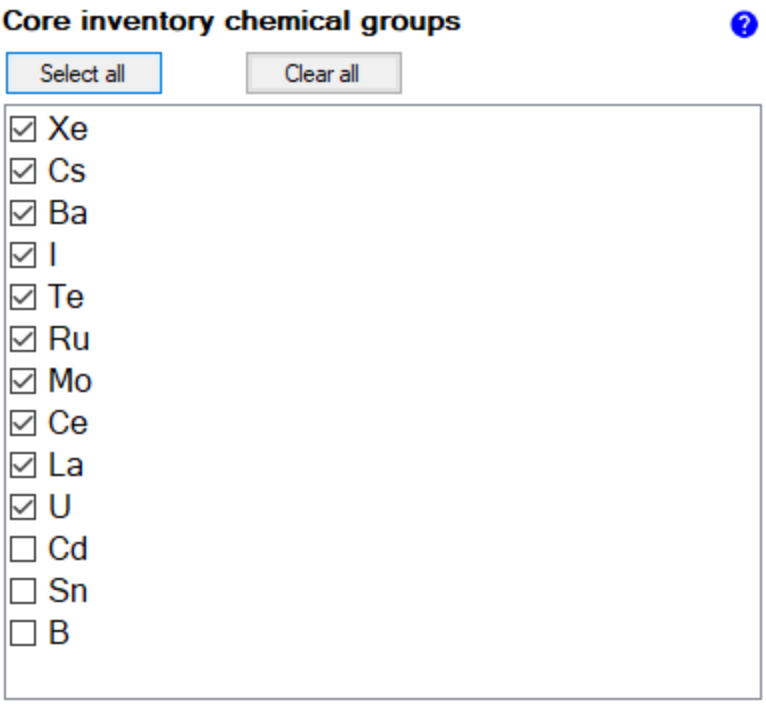


Figure 3-10 Selecting chemical groups to include

If the user wishes for a new chemical group to be accepted by MelMACCS, the MelMACCS.ini file needs to be edited. Each chemical group is associated with a set of elements. The association corresponding to the MelMACCS.ini file is in a section labeled /CHEM-TO-ISO. This is necessary to calculate the core inventory by isotope. This is especially useful for advanced reactor applications as the MELCOR analyst may change or add chemical classes to better fit the behavior of new reactor designs. Before running MelMACCS the user should work with the MELCOR analyst and verify that the MelMACCS initialization file has the instructions to distribute radionuclides to the correct chemical groups in relation to the specific MELCOR classes used.

3.4.5. *Isotopes*

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.

Nonetheless, the 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 G 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

3.5. Plume Segment Information

The next form specifies the plume segment and release path information.

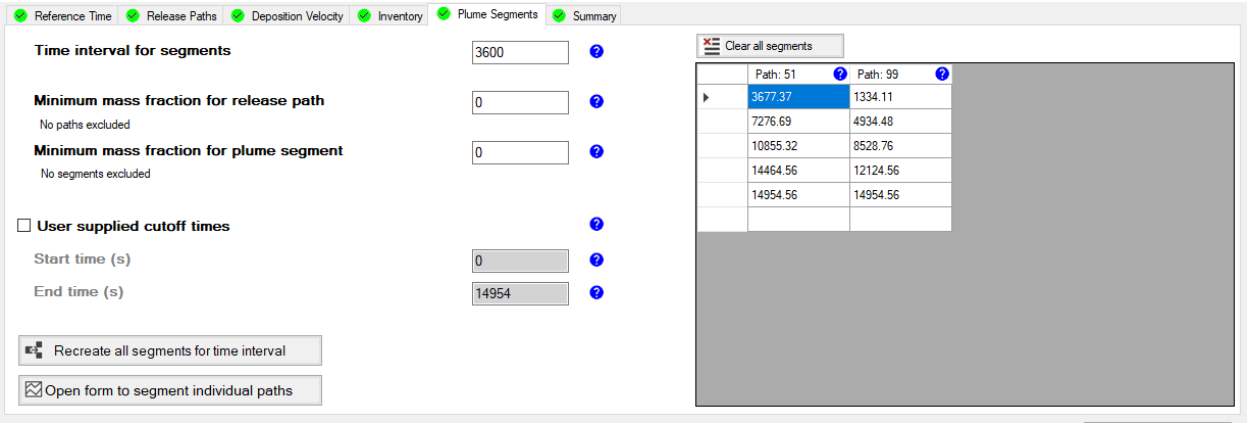


Figure 3-11 Plume Segments form

3.5.1. *Mass Threshold Fractions*

The two threshold values on this form allow for insignificant release paths and plume segments to be excluded from consideration. There are two threshold values that can be entered to allow this filtering as follows:

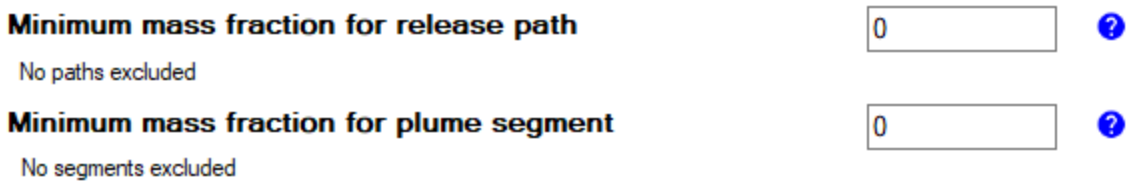


Figure 3-12 Specifying mass threshold fractions

When zero is entered for *Minimum mass fraction for release path,* every non-zero release path is active. Otherwise, only paths with a release fraction equal to or exceeding the threshold are active.

When zero is entered for *Minimum mass fraction for plume segment*, then all non-zero plume segments are recorded on the *Summary* form.

When a positive value is entered for *Minimum mass fraction for plume segment*, each release fraction for each chemical group of the candidate plume segment is tested against a threshold value determined by the fraction entered on this form. If this plume segment has at least one release fraction from a chemical group that is equal to or greater than the threshold, it is recorded on the *Summary* form.

3.5.2. *Creating segments from a chosen time interval*

The first option for creating plume segments is to create them from a chosen time interval. This option will break up each path identified to exceed the threshold using the user specific value. If the user wishes to use this option, they must enter their specified time interval in the *Time interval for segments* text box and the select the *Recreate all segments for time interval* button at the bottom of the form. Once this is done the segments for each path shown in the table on the right will update accordingly. It is important to note that the recorded times in MELCOR will not always be able to fit the time intervals specified in MelMACCS. Therefore, when specifying a time interval, MelMACCS will use times recorded in the plot file that are as close as possible to the user specified value.

Figure 3-13 Creating plume segments form time interval

3.5.3. *Creating segments from the table or chart*

The second option for creating plume segments is to either create them using the table to the right on this form or through the use of charts. This allows users to choose different time intervals for various release paths.

When using the table option, users must manually enter the chosen time intervals for each release path. As discussed in the previous section, user specified times might not match the recorded times in the plot file so MelMACCS will find the closest recorded time and report that. For example, if a user enters 3000 for one of the times in the table and the closest MELCOR time value is 3000.58, MelMACCS will automatically update the field to show 3000.58.

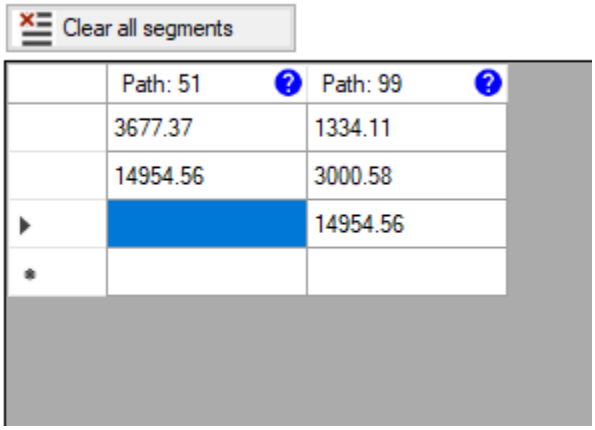


Figure 3-14 Plume segment table

If users wish to use the chart option, they must select the *Open form to segment individual paths* button. This will open up a second window displaying the charts for each of the release paths separated by tabs.

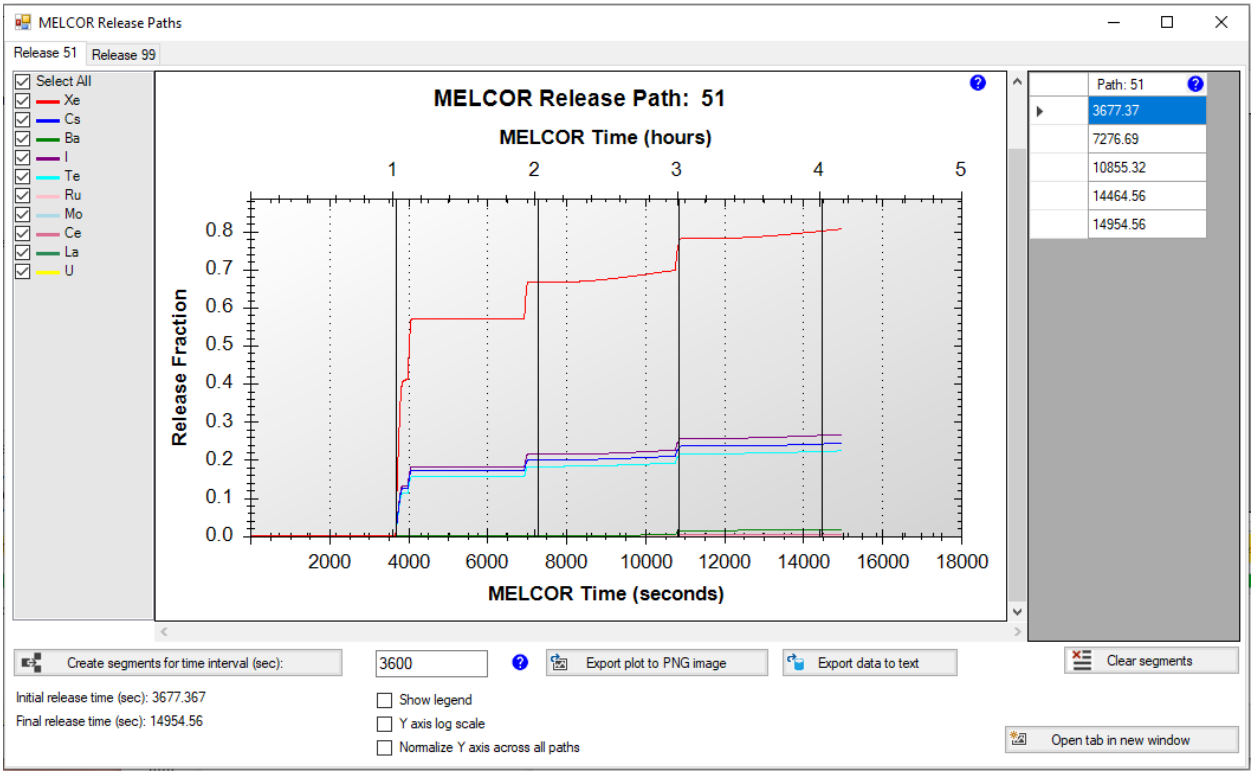


Figure 3-15 Plume segment plot window

From here, the following options are available:

- A dashed, vertical line tracks the mouse movement as the mouse moves across a plot. The time and release fraction corresponding to the location of the mouse is displayed next to the

cursor. Clicking on the plot records a time in the plume segment table to the right. A series of n recorded times, t_1, $t_2 \ldots t_n$ corresponds to plume segments $[t_1,t_2]$, $[t_2,t_3]$, …, $[t_{n-1},t_n]$.

- A time can also be recorded by typing a value in the plume segment table.

- A single selected time can be deleted by clicking the time in the table and pressing the *Delete* key on the keyboard. All user recorded times are deleted if the button *Clear segments* is clicked. The time of the first and last mass released is retained.

- A sequence of times is inserted by typing in a time interval and clicking the *Create segments for time interval (sec)* button. To use this feature, at least two times must be recorded. Insertion is between the first and last recorded times at the interval indicated. The last interval is usually shorter than the selected time interval.

- To display the legend of chemical groups on the plot, users can check the *Show legend* box. This is recommended if exporting the plot to a PNG.

- Y-axis scale can be changed from linear to log by checking the *Y axis log scale* box. Users also have the option to normalize the Y-axis across all paths.

- The plot can be exported to a PNG image by clicking *Export plot to PNG image* button. The MELCOR data within the plot can also be exported as text by clicking the *Export data to text.*

- Clicking the *Open tab in new window* button separates the various release paths into their own pop-up windows.

The time preceding the first nonzero flow greater than or equal to the reference time and the time corresponding to the last nonzero flow are automatically recorded, although these can be manually deleted. These times mark the logical beginning and end of a set of plume segments for this release path.

The time corresponding to the first nonzero flow is recorded on the bottom left of the graphics window adjacent to the label *Initial release time (sec)* and similarly for the *Final release time (sec).*

The plot legend shows the chemical groups chosen in the Inventory form. The legend entries can be unchecked in the legend, which causes the corresponding release fraction curve to become invisible in the plot. This option is used to help identify the data series in the plot. This option does not modify the chemical group information saved in the MelMACCS output file.

3.5.4. *Release Boundaries for All Paths*

The default release or time boundaries for each path is set to have the lower bound as zero and the upper bound equal to the final time step read from the MELCOR plot file. However, users have the option to choose their own time boundaries. This can be done by checking the *User supplied cutoff times* box and then manually entering the chosen times for both the lower and upper bound.

Figure 3-16 User supplied plume segment time boundaries

3.6. Navigating the Summary Form

The last form, the summary form, contains a summary of the source term release information that will be added to the MACCS compatible input file. This form contains the start time, duration, release height, adjusted release height, heat, flow rate, gas density and release fractions for each release path defined from the previous form. It is important to note that the segments shown in this form and in the output file are ordered by time.

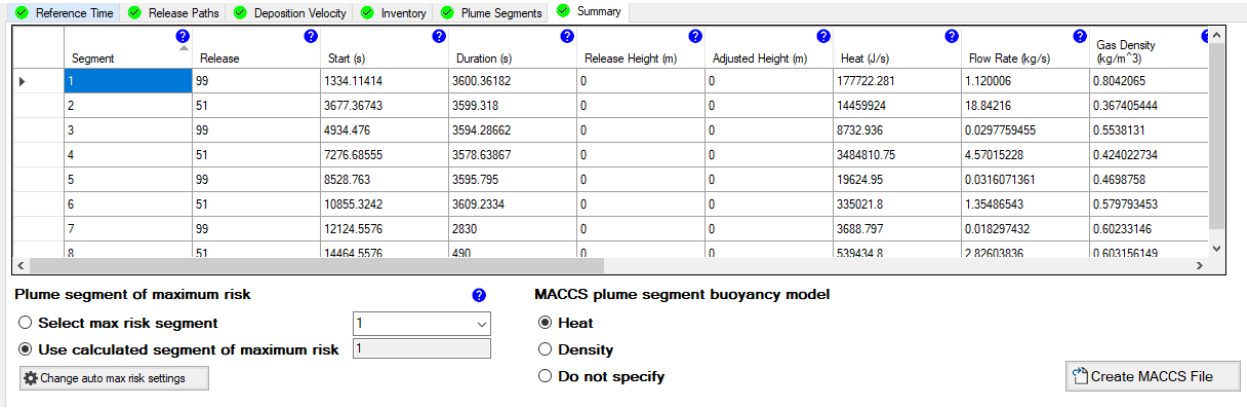


Figure 3-17 Summary form

3.6.1. *Number of Plume Segments, NUMREL*

The first column describes the MACCS variable NUMREL, which is the number of plume segments. This 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 reference time are allowed. The reference 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.

3.6.2. *Start Time of Plume Segment, PDELAY*

The start times for plume segments are relative to the time intervals chosen on the Plume Segments form. However, if a reference time other than zero is entered by the MelMACCS user, the start time of release changes which is reflected by the MACCS variable PDELAY. If the user selected time interval in the MELCOR reference frame is [T_1, T_2] and the reference time is T_3, where $T_3<T_1$, then PDELAY is T_1-T_3 and this adjustment is shown in the output file.

* Start Time of Release

RDPDELAY001 1.3341E+03

RDPDELAY002 3.6774E+03

3.6.3. *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.

* Plume Duration

RDPLUDUR001 3.617287E+03

RDPLUDUR002 3.770797E+03

Warning: MACCS does not allow plume durations to be less than 60 sec. The user must be aware of this and choose appropriate time intervals in MelMACCS that avoid this.

3.6.4. *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. Both the release height read from the plot file and the user adjusted height is shown on this form for each plume segment and release path.

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

3.6.5. *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. The rate of sensible heat in units of W for each plume segment shown on this form is calculated using the following equation.

$$PLHEAT = (H(R,T_2) - H(R,T_1))/(T_2 - T_1) \quad \textbf{(10)}$$

Where:

- $H(R,t)$ is the value of variable MACCS-R-PLHEAT.0 at time t
- $[T_1, T_2]$ is the MelMACCS user selected plume segment time interval 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

Please note negative sensible heat values are not allowed in MACCS and should be investigated as explained in Section 1.2. If negative values are present in the summary form MelMACCS will return a warning message similar to the example shown below.

Warning: Negative heat value: -6.09616607915235 calculated for segment path: 11 start time: 11140.04 There may be errors in the plot file and this may cause errors when running MACCS.

3.6.6. *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:

$$Flow_i = \left(PLMFLO(i) - PLMFLO(i-1)\right) \cdot \left(PLMWT(i) + PLMWT(i-1)\right)/2 \quad \textbf{(11)}$$

Where:

- PLMFLO and PLMWT correspond to the MELCOR variables MACCS-R-PLMFLO.0 and MACCS-R-PLMWT.0 respectively with R being the specific 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 $t_0, t_1, ..., t_m$ within the interval $[T_1, T_2]$, where time $t_0 = T_1$ and $t_m = T_2$, as follows:

$$\frac{1}{T_2 - T_1}\left[\sum_{i=1}^{m} Flow_i\right] \quad \textbf{(12)}$$

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

3.6.7. *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:

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

$$F_i = PLMWT(i) / PLTEMP(i) \quad \textbf{(13)}$$

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

$$F_{average} = (1/(PLMFLO(T_2) - PLMFLO(T_1)))\frac{1}{2}\sum_{i=1}^{m}(F_i + F_{i-1})(PLMFLO(t_i) - PLMFLO(t_{i-1})) \quad \textbf{(14)}$$

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

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

$$PLMDEN = F_{average}\left(p_0 / r_u\right) \quad \textbf{(15)}$$

Where:

- $p_0 = 1.013$ is the ambient pressure in bar.
- $r_u = .00008314$ is the universal gas constant in bar-m^3/mol-K.

.

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

3.6.8. *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 3.4.4, 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:

$$(Mass_{C,R}(T_2) - Mass_{C,R}(T_1))/CMass_C \quad \textbf{(16)}$$

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 as explained in Section 3.5.3.

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
```

3.6.9. *Specifying Plume of Maximum Risk, MAXRIS*

Within this form the user must also determine the MACCS variable MAXRIS which 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. The user can either manually choose the risk dominant plume or choose for MelMACCS to calculate it which will determine the risk dominant plume using the Equation 17 below.

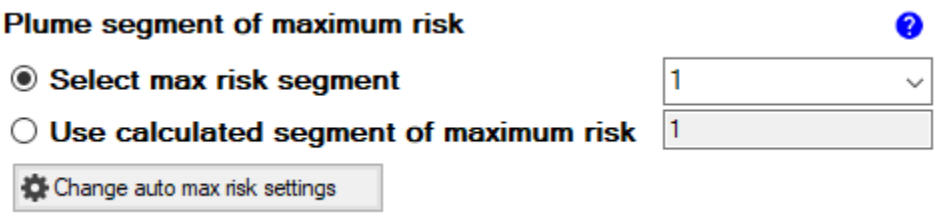


Figure 3-18 Options for specifying plume segment of maximum risk

There are two primary aspects of selecting a plume of maximum risk:

1. The doses that are potentially induced by the plume segment. Clearly, a plume segment is more important when its activity levels are high so that it contributes significantly to the exposure pathways and produces a large dose to a phantom individual.
2. The timing of the plume segment. A plume segment is more important when it occurs early so that the nearby population has not evacuated. Large doses to a phantom become relatively unimportant when there are no actual members of the public to receive the dose.

Furthermore, a plume segment that is released a long time after reactor shutdown may contain very little of an isotope with a short half-life, so the importance of each chemical group contains an inherent time dependence.

One of the difficulties in assessing the importance of a plume segment for producing doses is that each chemical group contributes differently to the exposure pathways that can create a dose to an individual. A general method for determining a plume segment of maximum risk should account for a weighted sum of the released activity rates, accounting for the relative importance of each chemical group. Since it may not be possible to determine a priori the appropriate weighting factors for each of the chemical groups, a flexible algorithm is preferred.

To account for the importance of the rate of release of activity, a simple strategy seems reasonable for ranking the plume segments. The most important plume segment is that one determined by the following equation:

$$I = \max_{i=1,N} \sum_{j=1}^{J} A_{ij} w_j / \Delta t_i \qquad \textbf{(17)}$$

Where:

- i is the plume segment number
- I is the number of plume segment with maximum risk
- N is the final plume segment considered in the evaluation
- j is the chemical group number
- J is the number of chemical groups
- A_{ij} is the activity released in plume segment i for chemical group j (Bq), not accounting for any radioactive decay or ingrowth following reactor shutdown
- w_j is the user-specified weighting factor for chemical group j
- Δt_i is the duration of plume segment i (s)

To account for the fact that earlier releases are more important than later ones, the user prescribes a cutoff time, T, beyond which plume segments are not considered. This time is a duration that starts with the initial time of the first plume segment. In the equation above, N is the last plume segment that starts before the user-prescribed cutoff time, T.

As described above, this algorithm is a simple approximation to the much more complicated reality. The real situation is that the dose induced by a plume segment depends on the activity released during the plume segment, the timing of the plume segment, and the population exposed to the plume segment. A more realistic treatment would account for the time dependence of radioactive decay and ingrowth for each chemical group, the time dependence of evacuation and relocation, whether a chemical group deposits or not, the dose conversion factors of the radionuclides in a chemical group and the possible dose pathways to which it contributes, etc. An algorithm that accounts for these effects would be far too complex to implement. Instead, a flexible algorithm in which the user prescribes a set of weighting factors for the chemical groups is a reasonable compromise. The weighting factors should characterize a specific type of accident, the type of risk to be evaluated, e.g., latent cancer fatality risk versus early fatality risk, and other unique aspects of the problem to be solved. At zeroth order, weighting factors drawn from the sensitivity analysis performed for the Surry SOARCA uncertainty analysis provides a reasonable set of defaults for these weighting factors, assuming latent cancer fatality risk is the dominant health effect. Those weighting factors are shown in Table 3-4 below.

Table 3-4 Chemical group weighting factors

Chemical Group Number, j	Chemical Group Name	Weighting Factor, w_j
1	Xe/Kr	0.000
2	Cs	0.847
3	Ba/Sr	0.000
4	I	0.000
5	Te	0.010
6	Ru	0.113
7	Mo	0.029
8	Ce	0.000
9	La	0.000

The weighting factors in the table have the meaning of the relative LCF risk induced per unit activity released. These values are similar, but not identically equal to, the population dose received per unit activity released. The specific values in the table are for Surry and are for the population within 50 miles averaged over one year of weather. These values represent default values that the user can choose to use. However, the user also has the availability to change these weighting factors to better suit their specific project. For example, some users may place higher priority on early fatality risk when determining the plume segment of maximum risk and these values should be updated to reflect that.

3.7. Specifying the MACCS Plume Segment Buoyancy Model

Along with the plume segment parameters summary, the user must also select a MACCS model to specify the plume segment parameters. The model is chosen for the MACCS plume buoyancy calculation. Each of the parameters, namely heat, flow and density, for each plume segment, are calculated by MelMACCS and are written to the output file. When this file is read into WinMACCS,

the parameters imported are dependent on the model setting defined here. If *Heat* is selected, the heat values are imported into WinMACCS. If *Density* is selected, the flow rate and gas density values are imported into WinMACCS. If *Do not specify model* is selected, the parameters used by WinMACCS are dependent on the buoyancy model defined on the *Plume/Source* tab on the WinMACCS *Project Properties* form. Selecting *Do not specify model* offers the most flexibility.

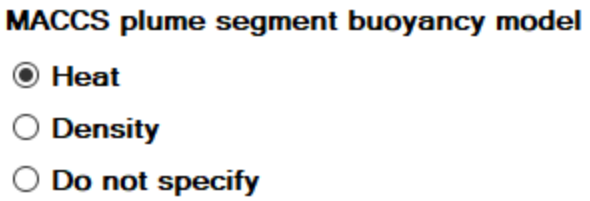


Figure 3-19 Selecting the MACCS plume segment buoyancy model

3.8. Creating the MelMACCS Output File

After all release paths have been considered, clicking the *Create MACCS File* button creates the MelMACCS output file. The folder and name of the output file is then entered.

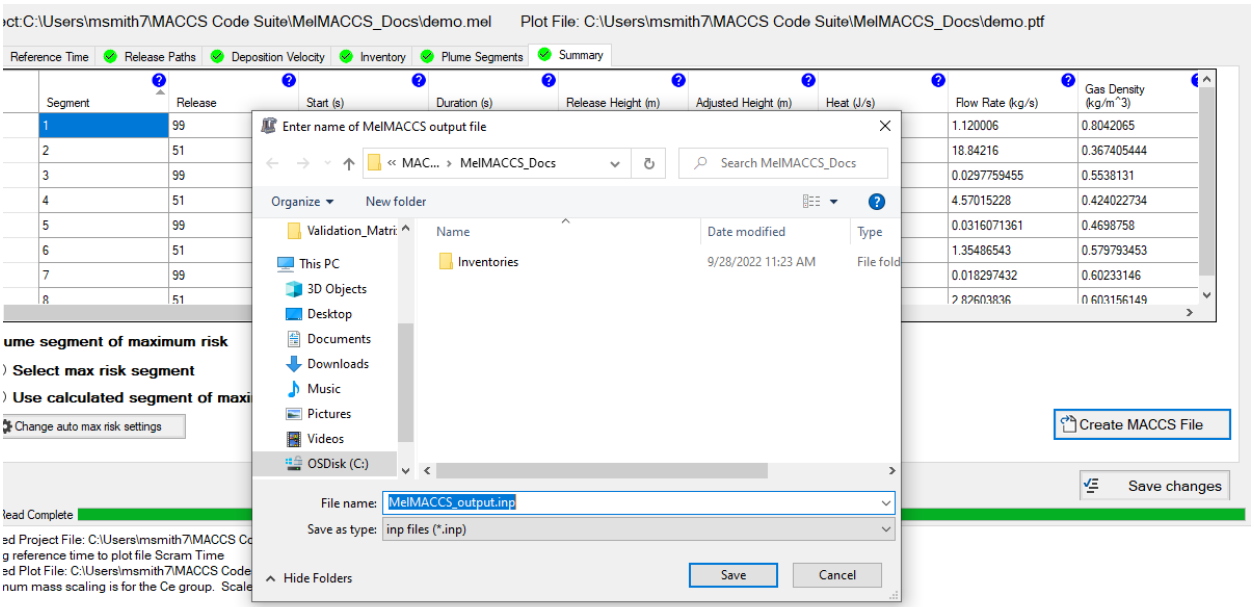


Figure 3-20 Creating the MelMACCS output file

4. OVERVIEW OF THE MELMACCS OUTPUT FILE/MACCS INPUT FILE

Once the user creates the MelMACCS output file that is also the MACCS compatible input file. The file will consist of all parameters and information specified in Section 3 above. An example of this .inp file can be found in Appendix C.

In addition to this information, two additional parameters are included within the file that are not shown in the user interface. These parameters are the representative position within the plume segment and the particle size distributions. More information on these two parameters is described in the subsequent subsections below.

4.1.1. *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 4.1. 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

4.1.2. Particle Size Distributions, PDIST

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 which is the reference time for inventory in the MELCOR time frame (see Section 3.2) to the last time recorded on the MELCOR plot file. Only MELCOR releases associated with selected plume segments are considered in the calculation. 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:

$$PSDIST(C,p) = T(C,p)/T(C) \text{ for } T(C) \neq 0 \quad \textbf{(18)}$$

$$PSDIST(C,p) = 1./NPSGRP \text{ for } T(C) = 0 \quad \textbf{(19)}$$

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

5. CREATING A COMPLETE MACCS INPUT FILE

The MelMACCS output file created contains MACCS input cards that define the source term. This is not a complete MACCS ATMOS input file. A MelMACCS output file can easily be used in WinMACCS by either importing the MelMACCS output file into WinMACCS or linking the MelMACCS output file(s) to WinMACCS using the cyclical option to allow for MACCS to run successive simulations with multiple MelMACCS output files. More information on how to use the cyclical option in WinMACCS is described in Section 9 of the MACCS 4.0 User's Guide (Leute et al., 2021)

If not running WinMACCS, one technique that can be used to incorporate the source-term information into an existing MACCS input file is to copy the contents of the MelMACCS output file and paste it at the end of an existing ATMOS input file. This works because MACCS uses the last data values encountered in the input file. The user needs to be cautious if there are fewer values for a given MACCS variable in the MELMACCS interface file than are in the exiting MACCS input deck. For example, if the number of plume segments, chemical groups, radionuclides, pseudostable radionuclides, or particle size groups is less than the original set in the MACCS ATMOS file, this file will be in error.

To merge a MelMACCS output file with an existing MACCS ATMOS input file

- Open the MelMACCS output file in Notepad or another ASCII text editor. Select the contents of this file and copy to the windows clipboard (using the Copy function from the Edit menu).

- Open an existing MACCS ATMOS input file in a text editor. Paste the contents of the clipboard into an ATMOS file immediately preceding the first line consisting of a "." in column one. The amended file is a valid ATMOS file that can be run using MACCS.

A new input variable, GRPNAM, is included in the MACCS cards, one vector entry for each chemical group. This is required by WinMACCS, but at this time MACCS does not recognize this card and ignores it. If the output from MelMACCS is imported into WinMACCS, these cards should not be removed.

6. REFERENCES

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.

Chanin, D., M. L. Young, J. Randall, and K. Jamali, 1998, "Code Manual for MACCS2: Volume 1, User's Guide," NUREG/CR-6613, SAND97-0594, US Nuclear Regulatory Commission, Washington, DC.

Bixler, N.E., F. Walton, R. Haaker, K. McFadden and J. Barr, 2015, "MELCOR Accident Consequence Code System (MACCS) User's Guide and Reference Manual" to be published as a NUREG/CR report, US Nuclear Regulatory Commission, Washington, DC.

Gauntt, R.O., R.K. Cole, C.M. Erickson, R.G. Gido, R.D. Gasser, S.B. Rodriguez and 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.

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., 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.

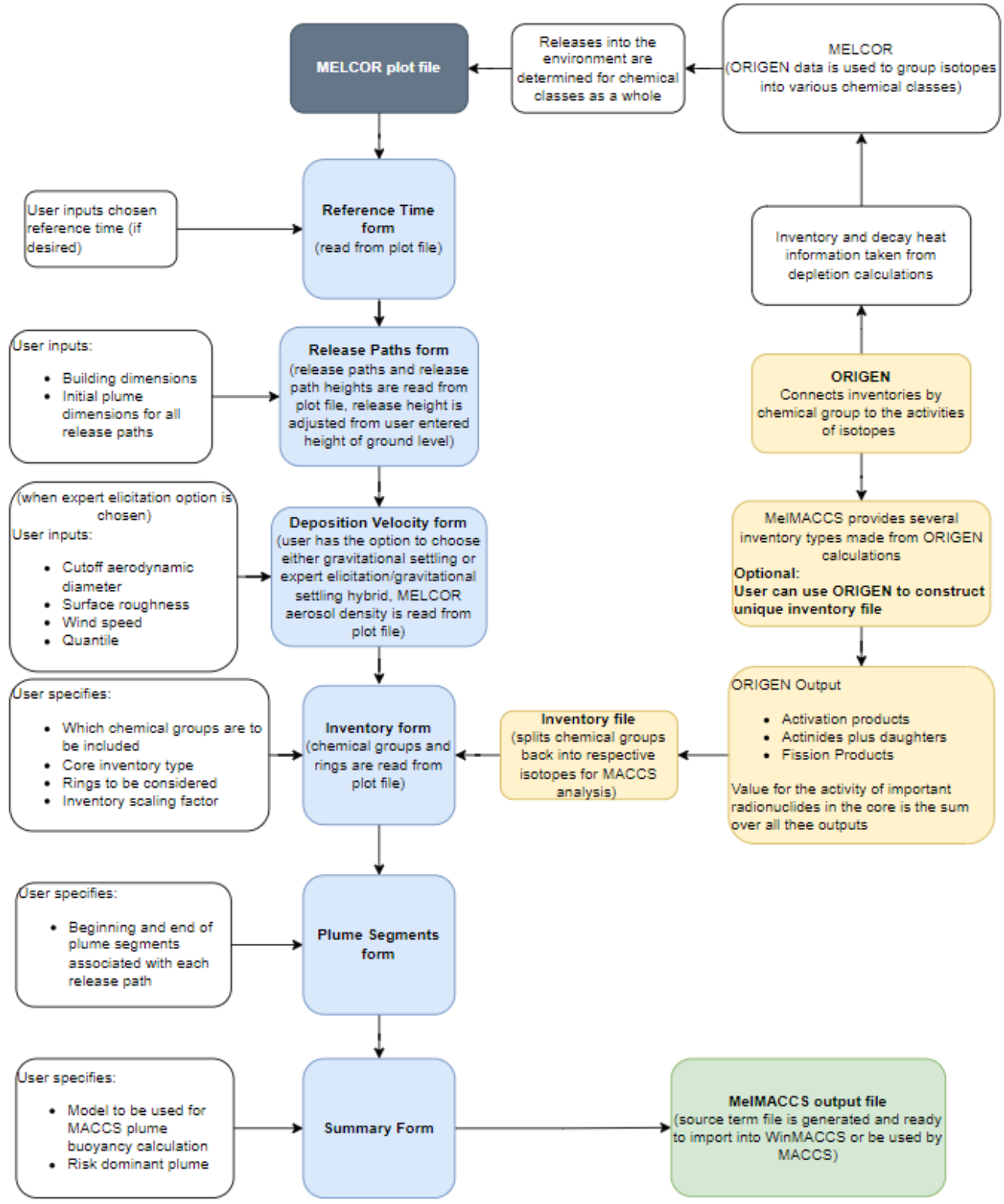
Humphries, L.L., B.A. Beeny, F. Gelbrad, D.L. Louie and J. Phillips, 2017, "MELCOR Computer Code Manuals, Vol. 1: Primer and User's Guide," Version 2.2.9541, SAND2017-0455 O, Sandia National Laboratories, Albuquerque, NM.

Leute, J., F. Walton, R. Mitchell and L. Eubanks, 2021, "MACCS (MELCOR Accident Consequence Code System) User Guide – Version 4.0," SAND2021-8998, Sandia National Laboratories, Albuquerque, NM.

Andrews, N.C., M. Higgins, A. Taconi and J. Leute, 2021, "Preliminary Radioisotope Screening for Off-site Consequence Assessment of Advanced Non-LWR Systems," SAND2021-11703, Sandia National Laboratories, Albuquerque, NM.

McFadden, K. and N.E. Bixler, 2015, "MelMACCS Version 2.0.2 User's Guide," Sandia National Laboratories, Albuquerque, NM.

APPENDIX A. MELMACCS PROCESS FLOWCHART



APPENDIX B. EXAMPLE PROJECT FILE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    "value": 0.0,
    "min": 0.0,
    "max": 14954.5576,
    "units": "seconds",
    "name": "Reference time for inventory in MELCOR time frame (s)",
    "tooltip": [
      "The MelMACCS reference time controls the start of radionuclide decay by shifting PDELAY ",
      "and defines how the lower time bounds are determined for a path."
    ]
  },
  "scramTime": {
    "description": "Scram time from PTF Header (s)",
    "value": 0.0,
    "min": 0.0,
    "max": 3.40282347E+38,
    "units": "seconds",
    "name": "Scram time from PTF Header (s)",
    "tooltip": [
      "Scram time is a MELCOR input variable.",
      "Typically, this should correspond to the MelMACCS reference time, but this is not consistently the case.",
      "The primary significance of this parameter is to control the start of radionuclide decay in the MACCS calculation.",
      "A scram time of zero corresponds to a MelMACCS reference time of zero. This is a read only field."
    ]
  },
  "finalTimeStep": {
    "description": "Final time step from MELCOR file (s)",
    "value": 14954.5576,
    "min": 0.0,
    "max": 3.40282347E+38,
    "units": "seconds",
    "name": "Final time step (s)",
    "tooltip": [
      "This is the value of the final time step read from the MELCOR file. This is a read only field."
    ]
  },
  "groundHeight": {
    "description": "Ground height relative to height recorded on Melcor plot file (m)",
    "value": 0.0,
    "min": -1000.0,
```

```
   "max": 1000.0,
   "units": "meters",
   "name": "Height of ground level in MELCOR model (m)",
   "tooltip": [
    "This height is used to calculate the value of PLHITE, the plume segment height, in the
MelMACCS output file.",
    "For example, if a MELCOR release path height of -10 m corresponds to a MACCS model
height of 30 m,",
    "this variable should be -40 m where 30 m =  -10 m - (-40 m)."
   ]
  },
  "buildingParameters": {
   "51": {
    "description": "Parameters associated with each Melcor release path",
    "pathIndex": {
     "description": "Release path from the MELCOR",
     "value": 0,
     "min": 0,
     "max": 2147483647,
     "units": "",
     "name": "Release path from the MELCOR",
     "tooltip": [
      "Release path from the MELCOR. This is a read only field."
     ]
    },
    "heightAdjusted": {
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     "value": false,
     "units": "",
     "name": "Adjusted release height entered",
     "tooltip": [
      "Adjusted release height calculated, true is user defined"
     ]
    },
    "melcorPathHeight": {
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     "value": 0.0,
     "min": 0.0,
     "max": 3.40282347E+38,
     "units": "meters",
     "name": "Release height from MELCOR (m)",
     "tooltip": [
      "Release height from MELCOR (m). This is a read only field."
     ]
    },
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     "value": 0.0,
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  "tooltip": [
   "Adjusted release height"
  ]
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  "min": 0.0,
  "max": 1000.0,
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  "tooltip": [
   "Height of building where release occurs"
  ]
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  "min": 1.0,
  "max": 1000.0,
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  ]
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  "min": 1.0,
  "max": 1000.0,
  "units": "meters",
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  "tooltip": [
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  ]
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  "value": 0.0,
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  "max": 180.0,
  "units": "degrees",
  "name": "Building angle",
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  "tooltip": [
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  ]
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  "value": 0.0,
  "min": 0.0,
  "max": 1000.0,
  "units": "meters",
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  "tooltip": [
    "Trapped plume (near building) height (m)"
  ]
},
"sigmaY": {
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  "value": 0.2326,
  "min": 0.1,
  "max": 1000.0,
  "units": "meters",
  "name": "Initial sigma-y",
  "tooltip": [
    "This is auto-calculated each time building width changes by the equation:",
    "SigmaY = buildingWidth/4.3",
    "After calculated it may be edited by the user"
  ]
},
"sigmaZ": {
  "description": "Initial sigma-z (m)",
  "value": 0.4651,
  "min": 0.1,
  "max": 1000.0,
  "units": "meters",
  "name": "Initial sigma-z",
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    "SigmaZ = buildingHeight/2.15",
    "After calculated it may be edited by the user"
  ]
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  "value": false,
  "units": "",
  "name": "Manual sigma values used",
  "tooltip": [
    "Manual sigma values used",
```

```
        "If true, values entered by the user for sigmaY and sigmaZ are used",
        "If false, values for sigmaY and sigmaZ are calculated from buildingWidth and
buildingHeight"
       ]
      }
    },
    "99": {
      "description": "Parameters associated with each Melcor release path",
      "pathIndex": {
        "description": "Release path from the MELCOR",
        "value": 0,
        "min": 0,
        "max": 2147483647,
        "units": "",
        "name": "Release path from the MELCOR",
        "tooltip": [
          "Release path from the MELCOR. This is a read only field."
        ]
      },
      "heightAdjusted": {
        "description": "Adjusted release height entered, true is user defined",
        "value": false,
        "units": "",
        "name": "Adjusted release height entered",
        "tooltip": [
          "Adjusted release height calculated, true is user defined"
        ]
      },
      "melcorPathHeight": {
        "description": "Release height from MELCOR (m)",
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        "min": 0.0,
        "max": 3.40282347E+38,
        "units": "meters",
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          "Release height from MELCOR (m). This is a read only field."
        ]
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        "min": 0.0,
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        "name": "Adjusted release height",
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          "Adjusted release height"
```

```
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},
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  "value": 1.0,
  "min": 0.0,
  "max": 1000.0,
  "units": "meters",
  "name": "Height of building where release occurs",
  "tooltip": [
    "Height of building where release occurs"
  ]
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  "description": "Width of building (m)",
  "value": 1.0,
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  "units": "meters",
  "name": "Building width",
  "tooltip": [
    "Building width"
  ]
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  "max": 1000.0,
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  ]
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"buildingAngle": {
  "description": "Building angle to North (degrees)",
  "value": 0.0,
  "min": -180.0,
  "max": 180.0,
  "units": "degrees",
  "name": "Building angle",
  "tooltip": [
    "Building angle to North (degrees)"
  ]
},
"trappedPlumeHeight": {
  "description": "Trapped plume (near building) height (m)",
```

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      "value": 0.0,
      "min": 0.0,
      "max": 1000.0,
      "units": "meters",
      "name": "Trapped plume height",
      "tooltip": [
        "Trapped plume (near building) height (m)"
      ]
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    "sigmaY": {
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      "value": 0.2326,
      "min": 0.1,
      "max": 1000.0,
      "units": "meters",
      "name": "Initial sigma-y",
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        "This is auto-calculated each time building width changes by the equation:",
        "SigmaY = buildingWidth/4.3",
        "After calculated it may be edited by the user"
      ]
    },
    "sigmaZ": {
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        "This is auto-calculated each time building height changes by the equation:",
        "SigmaZ = buildingHeight/2.15",
        "After calculated it may be edited by the user"
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    "manualSigma": {
      "description": "Manual sigma values used",
      "value": false,
      "units": "",
      "name": "Manual sigma values used",
      "tooltip": [
        "Manual sigma values used",
        "If true, values entered by the user for sigmaY and sigmaZ are used",
        "If false, values for sigmaY and sigmaZ are calculated from buildingWidth and
buildingHeight"
      ]
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  },
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    "value": "EXPERT",
    "units": "",
    "name": "Deposition velocity algorithm",
    "tooltip": [
      "This indicates the method used to estimate deposition velocity.",
      "Possible values are EXPERT and SETTLING."
    ]
  },
  "disableDepositionVelocity": {
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    "value": false,
    "units": "",
    "name": "Disable deposition velocity",
    "tooltip": [
      "True means the deposition velocity information is written to the MelMACCS output file as
comments."
    ]
  },
  "cutoffDiameter": {
    "description": "Cutoff diameter. Only relevant for DeposVelocity.EXPERT, Aerodynamic
Diameter (micrometers)",
    "value": 20.0,
    "min": 0.0,
    "max": 3.40282347E+38,
    "units": "micrometers",
    "name": "Cutoff diameter (micrometers)",
    "tooltip": [
      "Cutoff diameter (micrometers), Threshold particle size(micrometers) for which below this size",
      "EXPERT is used to calculate deposition velocity, otherwise GRAVITY is used."
    ]
  },
  "surfaceRoughness": {
    "description": "Only relevant for DeposVelocity.EXPERT, Surface roughness (m)",
    "value": 0.1,
    "min": 0.001,
    "max": 10.0,
    "units": "meters",
    "name": "Surface roughness (m)",
    "tooltip": [
      "This is a measure of the terrain roughness, which is the terrain's ability to generate turbulence
and enhanced vertical mixing, ",
      "and it has the potential to affect both the vertical dispersion and dry deposition velocities of
aerosol particles."
    ]
  },
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    "min": 0.5,
    "max": 10.0,
    "units": "m/s",
    "name": "Wind speed (m/s)",
    "tooltip": [
      "Only relevant for DeposVelocity.EXPERT, Wind speed (m/s)."
    ]
  },
  "quantile": {
    "description": "Only relevant for DeposVelocity.EXPERT, higher number increases deposition
velocity",
    "value": 0.5,
    "min": 0.0,
    "max": 1.0,
    "units": "",
    "name": "Quantile",
    "tooltip": [
      "Quantile (for expert data interpolation).",
      "This is a measure of degree of belief in deposition velocity. ",
      "A value of 0 represents the smallest value that the experts thought to be possible; ",
      "a value of 0.5 represents the best guess; ",
      "a value of 1 represents the highest value that the experts thought to be possible."
    ]
  },
  "melcorAerosolDensity": {
    "description": "MELCOR aerosol density (km/m3)",
    "value": 1000.0,
    "min": 0.0,
    "max": 1000.0,
    "units": "km/m3",
    "name": "MELCOR aerosol density (km/m3)",
    "tooltip": [
      "MELCOR aerosol density (km/m3). This is a read only field."
    ]
  },
  "chemicalGroups": {
    "description": "Chemical group names match with names in the Melcor plot file.",
    "value": [
      "Xe",
      "Cs",
      "Ba",
      "I",
      "Te",
      "Ru",
      "Mo",
```

```
      "Ce",
      "La",
      "U"
    ],
    "units": "",
    "name": "Chemical groups to be included in core inventory",
    "tooltip": [
      "Chemical group names match with names in the Melcor plot file.",
      "At least one group must be selected."
    ]
  },
  "ringToProcess": {
    "description": "Ring to process",
    "value": 1,
    "min": 1,
    "max": 1,
    "units": "",
    "name": "Ring to process",
    "tooltip": [
      "The current ring to process."
    ]
  },
  "inventoryName": {
    "description": "Inventory name",
    "value": "LOW",
    "units": "",
    "name": "Inventory name",
    "tooltip": [
      "The inventory name to use."
    ]
  },
  "inventoryScalingFactor": {
    "description": "Inventory scaling factor",
    "value": 1.0,
    "min": 2.7E-10,
    "max": 1E+16,
    "units": "",
    "name": "Inventory scaling factor",
    "tooltip": [
      "This value is used to scale the inventory of all the radionuclides defined in the MACCS model.",
      "This parameter is useful when the MELCOR calculation has been done for a reactor that is
similar, ",
      "but different in size and power rating, then the reactor that is to be evaluated with MACCS."
    ]
  },
  "globalMaxRisk": {
    "description": "Global default value for plume of maximum risk",
    "value": 1,
```

```
    "min": 0,
    "max": 2147483647,
    "units": "",
    "name": "Global Max Risk",
    "tooltip": [
      "Global default value for plume of maximum risk."
    ]
  },
  "releasePathThreshold": {
    "description": "Threshold fraction of a chemical group for a single release (plume segment)",
    "value": 0.0,
    "min": 0.0,
    "max": 1.0,
    "units": "",
    "name": "Minimum mass fraction for release path",
    "tooltip": [
      "Value is the threshold fraction of the mass release of a chemical group for a given release path
to the total mass release for that same  chemical group",
      "summed over all release paths. If any chemical group release in the release path  is equal to or
exceeds this fraction,",
      "then the window for that release path is displayed. Release paths with mass releases that fall
below this threshold for every chemical group",
      "are not available for further processing."
    ]
  },
  "releaseSegmentThreshold": {
    "description": "Threshold fraction of mass release for a chemical group for a given path",
    "value": 0.0,
    "min": 0.0,
    "max": 1.0,
    "units": "",
    "name": "Minimum mass fraction for plume segment",
    "tooltip": [
      "Value is the threshold fraction of the mass release of a chemical group for a given plume
segment ",
      "to the total mass release for that same chemical group",
      "summed over all release paths. If any chemical group release in the plume segment exceeds this
fraction, ",
      "then the segment is saved when Apply is clicked. ",
      "Segments with mass releases that fall below this threshold for every chemical group are not
saved."
    ]
  },
  "userSuppliedBounds": {
    "description": "User supplies the lower and upper cutoff times for plume segments for all paths",
    "value": false,
    "units": "",
    "name": "User supplied cutoff times for all paths",
```

```
   "tooltip": [
     "If true, then the user supplies the lower and upper cutoff times for plume segments for all
paths"
   ]
  },
  "lowerBound": {
   "description": "Smallest time for a release point when userSuppliedBounds = true",
   "value": 0.0,
   "min": 0.0,
   "max": 14954.5576,
   "units": "s",
   "name": "Start time (s)",
   "tooltip": [
     "Smallest time for a release point when userSuppliedBounds = true."
   ]
  },
  "upperBound": {
   "description": "Largest time for a release point when userSuppliedBounds = true",
   "value": 14954.0,
   "min": 0.0,
   "max": 14954.5576,
   "units": "s",
   "name": "End time (s)",
   "tooltip": [
     "Largest time for a release point when userSuppliedBounds = true."
   ]
  },
  "globalApplyInterval": {
   "description": "Apply time interval between bounds for all paths if true, use times in list if false",
   "value": true,
   "units": "",
   "name": "Apply time interval",
   "tooltip": [
     "Apply time interval between bounds for all paths if true, use times in list if false"
   ]
  },
  "globalInterval": {
   "description": "Time interval for all paths to insert segments.",
   "value": 3600.0,
   "min": 0.0,
   "max": 3.40282347E+38,
   "units": "s",
   "name": "Time interval for segments",
   "tooltip": [
     "Time interval to insert segments for all paths."
   ]
  },
  "cutoffTime": {
```

```
  "description": "Cutoff time for max risk algorithm.",
  "value": 13621.0,
  "min": 0.0,
  "max": 13621.0,
  "units": "s",
  "name": "Cutoff time",
  "tooltip": [
   "To account for the fact that earlier releases are more important than later ones,",
   "a cutoff time is used beyond which plume segments are not considered.",
   "This time is a duration that starts with the initial time of the first plume segment."
  ]
 },
 "ring": {
  "description": {
   "description": "Parameters associated with each Melcor ring",
   "value": "",
   "units": "",
   "name": "Parameters associated with each Melcor ring",
   "tooltip": [
    "Parameters associated with each Melcor ring."
   ]
  },
  "releases": {
   "51": {
    "description": "ReleaseParam defines the method for determining the plume boundaries",
    "intPathID": 51,
    "applyInterval": {
     "description": "Apply time interval between bounds if true, use times in list if false",
     "value": true,
     "units": "",
     "name": "Apply time interval",
     "tooltip": [
      "Apply time interval between bounds if true, use times in list if false."
     ]
    },
    "interval": {
     "description": "Time interval to insert segments for this path only.",
     "value": 3600.0,
     "min": 0.0,
     "max": 3.40282347E+38,
     "units": "seconds",
     "name": "",
     "tooltip": [
      "Time interval to insert segments for this path only."
     ]
    },
    "times": {
     "description": "List of times (s) defining absolute insertion points to define plume segments",
```

```
    "value": [
      3677.36743,
      7276.68555,
      10855.3242,
      14464.5576
    ],
    "min": 3677.36743,
    "max": 14954.5576,
    "units": "",
    "name": "Plume segment times list for Path: 51",
    "tooltip": [
      "List of times (s) defining absolute insertion points to define plume segments."
    ]
  }
},
"99": {
  "description": "ReleaseParam defines the method for determining the plume boundaries",
  "intPathID": 99,
  "applyInterval": {
    "description": "Apply time interval between bounds if true, use times in list if false",
    "value": true,
    "units": "",
    "name": "Apply time interval",
    "tooltip": [
      "Apply time interval between bounds if true, use times in list if false."
    ]
  },
  "interval": {
    "description": "Time interval to insert segments for this path only.",
    "value": 3600.0,
    "min": 0.0,
    "max": 3.40282347E+38,
    "units": "seconds",
    "name": "",
    "tooltip": [
      "Time interval to insert segments for this path only."
    ]
  },
  "times": {
    "description": "List of times (s) defining absolute insertion points to define plume segments",
    "value": [
      1334.11414,
      4934.476,
      8528.763,
      12124.5576
    ],
    "min": 1334.11414,
    "max": 14954.5576,
```

```
      "units": "",
      "name": "Plume segment times list for Path: 99",
      "tooltip": [
       "List of times (s) defining absolute insertion points to define plume segments."
      ]
     }
    }
   },
   "maxRiskSegment": {
    "description": "Plume segment of maximum risk",
    "value": 1,
    "min": 0,
    "max": 8,
    "units": "",
    "name": "Plume segment of maximum risk",
    "tooltip": [
     "Plume segment of maximum risk. "
    ]
   },
   "autoCalculatedMaxRiskSegment": {
    "description": "Use automatically calculated plume segment of maximum risk",
    "value": 1,
    "min": 0,
    "max": 2147483647,
    "units": "",
    "name": "Use calculated segment of maximum risk",
    "tooltip": [
     "Use automatically calculated plume segment of maximum risk."
    ]
   }
  },
  "plumeSegmentBouyancyModel": {
   "description": "Plume segment buoyancy model",
   "value": "NONE",
   "units": "",
   "name": "Plume segment buoyancy model",
   "tooltip": [
    "Specifies the plume buoyancy model to be used in MACCS.",
    "Possible values are NONE, HEAT, and DENSITY."
   ]
  },
  "autoCalculateMaxRiskSegment": {
   "description": "Automatically calculate max risk segment",
   "value": true,
   "units": "",
   "name": "Automatically calculate max risk segment",
   "tooltip": [
    "Automatically calculate max risk segment if true."
```

```
  ]
 },
 "chemGroupWeightingFactors": {
  "description": "Dictionary<string, float> of chemical group weighting factors used for the
calculate max risk segment algorithm",
  "value": {
   "Xe": 0.0,
   "Cs": 0.847,
   "Ba": 0.0,
   "I": 0.0,
   "Te": 0.01,
   "Ru": 0.113,
   "Mo": 0.029,
   "Ce": 0.0,
   "La": 0.0,
   "U": 0.0,
   "Cd": 0.0,
   "Sn": 0.0,
   "B": 0.0
  },
  "min": 0.0,
  "max": 1.0,
  "units": "",
  "name": "Chemical group weighting factors",
  "tooltip": [
   "Dictionary<string, float> of chemical group weighting factors used for the calculate max risk
segment algorithm."
  ]
 },
 "projectFile": {
  "description": "Name of project file",
  "value": "C:\\Users\\msmith7\\MACCS Code Suite\\MelMACCS_Docs\\demo.mel",
  "units": "",
  "name": "Name of project file",
  "tooltip": [
   "Name of project file."
  ]
 },
 "plotFile": {
  "description": "Path and name of plot file",
  "value": "C:\\Program Files\\MACCS Code Suite\\MelMACCS_Docs\\demo.ptf",
  "units": "",
  "name": "Path and name of plot file",
  "tooltip": [
   "Path and name of plot file."
  ]
 },
 "plotFileTitle": {
```

```
    "description": "Title in plot file",
    "value": "RBKJCYMRF/11/18/02 /09:33:09 /DEMO, Version 1.8.5",
    "units": "",
    "name": "Title in plot file",
    "tooltip": [
      "The title in the plot file opened.",
      "Should be unique for each plot file.",
      "Used to determine if plot file opened does not match plot file used to create project file."
    ]
  }
}
```

APPENDIX C. EXAMPLE OF MELMACCS OUTPUT FILE

* RIMELMAC lines are constructed for ease of software parsing
* The data on each line starts and ends with the MACCS string delimiter '
* The delimited data contains an optional comment followed by a space, followed by a capitalized keyword (no spaces)
* The first colon on the line will follow this keyword followed by a single space
* Value of that keyword will be all characters following in the line
*
* Quality assurance information
RIMELMAC001 'MelMACCS generated MACCS_FILE: C:\Users\msmith7\MACCS Code Suite\MelMACCS_Docs\MelMACCS_output.inp'
RIMELMAC002 'MACCS input cards generated by MelMACCS_VERSION: 4.0.0 Git SHA: de0dbe61ffc2027698c73d6007c9ae038fcf4aff Build date: 2022-09-23'
RIMELMAC003 'File CREATION_DATE: 9/26/2022 10:04:24 AM'
RIMELMAC004 'MelMACCS PROJECT_NAME: C:\Users\msmith7\MACCS Code Suite\MelMACCS_Docs\demo.mel'
RIMELMAC005 'MELCOR PTF_FILE: C:\Users\msmith7\MACCS Code Suite\MelMACCS_Docs\demo.ptf'
RIMELMAC006 'MELCOR plot file modification date PTF_DATE: 11/24/2021 4:07:18 PM'
RIMELMAC007 'MELCOR plot file title PTF_TITLE: RBKJCYMRF/11/18/02 /09:33:09 /DEMO, Version 1.8.5'
RIMELMAC008 'MELCOR_VERSION: Not_available'
RIMELMAC009 'RING_NUMBER: 1'
RIMELMAC010 'RING_DESCRIPTION: Core Inventory'
*
* C:\Users\msmith7\MACCS Code Suite\MelMACCS_Docs\MelMACCS.ini modification date: 11/24/2021 4:07:18 PM
* Inventory file:C:\Program Files\MACCS Code Suite\MelMACCS 4.0.0-beta-3\\MelMACCS.inv modification date: 2/14/2022 2:07:30 PM
* Inventory used to calculate core inventory: LOW
*
* Mass threshold fraction for path: 0
* Mass threshold fraction for plume segment: 0
*
* Maximum mass scaling is for the Ce group. Error=64.8251 %
*
* MELCOR compound chemical groups counted in MACCS chemical groups using the following fractions:
* Mass of I in CSI moved to chemical group I using mass fraction: 0.488444
* Mass of Cs in CSI moved to chemical group Cs using mass fraction: 0.511556
* Mass of Cs in CSM moved to chemical group Cs using mass fraction: 0.7347892
* Mass of Mo in CSM moved to chemical group Mo using mass fraction: 0.2652108
*
* Number of Chemical classes
ISMAXGRP001 10
*
* 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
ISGRPNAM010 U
*
* Particle size diameters equal or greater than 20 microns use gravitational deposition velocity
calculation
*
* Expert deposition velocities based on linear regression of expert elicited data
* NUREG/CR-7161, N. E.Bixler, E. Clauss and C. W. Morrow
* See MELMACCS Models Document for detail.
* The following model parameters were used:
*     Surface roughness: 0.1(m)
*     Wind speed: 5(m/s)
*     MELCOR aerosol density : 1000(kg/m**3)
*     Quantile: 0.5
*     Regression coefficients a, b, c, d, e, f, g:
* -2.964          0.992   0.19     -0.072  1.061   0         0.169
*
* Gravitational deposition velocities calculated using particle sizes from MELCOR
*     MELCOR aerosol density : 1000, slip factor of 1.257
*     Assume Mean free path of air at 298 K, .069E-6 m
*     Assume viscosity of air at 298 K, 1.8 E-5 N-s/m**2
*
* PSize: MELCOR (physical) diameter (micrometers); d_p: aerodynamic diameter used
(micrometers)
*     PSize(1): 0.11500173      d_p(1): 0.11500173      Expert elicitation
*     PSize(2): 0.21409247      d_p(2): 0.21409247      Expert elicitation
*     PSize(3): 0.39856434      d_p(3): 0.39856434      Expert elicitation
*     PSize(4): 0.7419855       d_p(4): 0.7419855       Expert elicitation
*     PSize(5): 1.3813142       d_p(5): 1.3813142       Expert elicitation
*     PSize(6): 2.5715176       d_p(6): 2.5715176       Expert elicitation
*     PSize(7): 4.7872545       d_p(7): 4.7872545       Expert elicitation
*     PSize(8): 8.9121704       d_p(8): 8.9121704       Expert elicitation
*     PSize(9): 16.591304       d_p(9): 16.591304       Expert elicitation
*     PSize(10): 30.887131      d_p(10): 30.887131      Gravitational deposition velocity
* Dry Deposition Velocity
DDVDEPOS001 7.8771E-04
DDVDEPOS002 5.9198E-04
DDVDEPOS003 6.663E-04
DDVDEPOS004 1.0126E-03
DDVDEPOS005 1.873E-03
```

DDVDEPOS006 3.8017E-03
DDVDEPOS007 7.6335E-03
DDVDEPOS008 1.3669E-02
DDVDEPOS009 1.9679E-02
DDVDEPOS010 2.9018E-02
*
* Number of particle size groups
DDNPSGRP001 10
*
* Particle size distribution
RDPSDIST001 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 1.0E+00
RDPSDIST002 1.129E-02 5.638E-02 1.0658E-01 1.3514E-01 1.2728E-01 4.1589E-02 7.6197E-03 1.2275E-03 1.5797E-04 5.1274E-01
RDPSDIST003 7.9857E-03 1.6048E-02 3.3849E-02 1.3117E-01 3.6364E-01 2.2868E-01 4.5358E-02 6.1913E-03 6.1544E-04 1.6646E-01
RDPSDIST004 1.1321E-02 5.6067E-02 1.0446E-01 1.3641E-01 1.3515E-01 4.6279E-02 8.7061E-03 1.4096E-03 1.7679E-04 5.0002E-01
RDPSDIST005 6.8327E-02 9.3548E-02 1.1538E-01 1.6186E-01 1.8644E-01 5.7278E-02 9.6038E-03 1.7392E-03 3.939E-04 3.0543E-01
RDPSDIST006 1.8336E-02 3.8278E-02 3.1691E-02 1.8878E-01 4.5005E-01 2.2044E-01 4.0307E-02 5.4172E-03 5.3697E-04 6.1676E-03
RDPSDIST007 2.0235E-02 4.1851E-02 3.2665E-02 1.9754E-01 4.5615E-01 2.0659E-01 3.3791E-02 3.9584E-03 3.5402E-04 6.8667E-03
RDPSDIST008 3.3707E-03 1.161E-02 3.1187E-02 1.4807E-01 4.4769E-01 2.9269E-01 5.7131E-02 7.46E-03 7.0751E-04 8.5752E-05
RDPSDIST009 3.3566E-03 1.1398E-02 3.0184E-02 1.4391E-01 4.4189E-01 2.9805E-01 6.1578E-02 8.6454E-03 8.6516E-04 1.3187E-04
RDPSDIST010 5.8138E-03 1.5734E-02 3.0154E-02 1.5028E-01 4.4118E-01 2.8662E-01 5.9627E-02 8.5656E-03 8.7384E-04 1.1518E-03
*
* WETDEP, DRYDEP, wet and dry deposition flags for each nuclide group
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.
ISDEPFLA010 .TRUE. .TRUE.
*
* Number of Pseudostable Radionuclides
ISNUMSTB001 16
*
* List of Pseudostable Radionuclides
ISNAMSTB001 I-129

ISNAMSTB002 Xe-131m
ISNAMSTB003 Xe-133m
ISNAMSTB004 Cs-135
ISNAMSTB005 Sm-147
ISNAMSTB006 U-234
ISNAMSTB007 U-235
ISNAMSTB008 U-236
ISNAMSTB009 U-237
ISNAMSTB010 Np-237
ISNAMSTB011 Rb-87
ISNAMSTB012 Zr-93
ISNAMSTB013 Nb-93m
ISNAMSTB014 Nb-95m
ISNAMSTB015 Tc-99
ISNAMSTB016 Pm-147
*
* Number of releases as selected by user
RDNUMREL001 8
*
* Height of the facility building (m)
WEBUILDH001 1.0E+00
WEBUILDH002 1.0E+00
WEBUILDH003 1.0E+00
WEBUILDH004 1.0E+00
WEBUILDH005 1.0E+00
WEBUILDH006 1.0E+00
WEBUILDH007 1.0E+00
WEBUILDH008 1.0E+00
*
* Width of the facility building (m)
WEBUILDW001 1.0E+00
WEBUILDW002 1.0E+00
WEBUILDW003 1.0E+00
WEBUILDW004 1.0E+00
WEBUILDW005 1.0E+00
WEBUILDW006 1.0E+00
WEBUILDW007 1.0E+00
WEBUILDW008 1.0E+00
*
* Length of the facility building (m)
WEBUILDL001 1.0E+00
WEBUILDL002 1.0E+00
WEBUILDL003 1.0E+00
WEBUILDL004 1.0E+00
WEBUILDL005 1.0E+00
WEBUILDL006 1.0E+00
WEBUILDL007 1.0E+00
WEBUILDL008 1.0E+00

*
* Angle, degrees from N to facility building width (degrees)
WEBUILDA001 0.0E+00
WEBUILDA002 0.0E+00
WEBUILDA003 0.0E+00
WEBUILDA004 0.0E+00
WEBUILDA005 0.0E+00
WEBUILDA006 0.0E+00
WEBUILDA007 0.0E+00
WEBUILDA008 0.0E+00
*
* Trapped plume release height (m)
RDPHTRAP001 0.0E+00
RDPHTRAP002 0.0E+00
RDPHTRAP003 0.0E+00
RDPHTRAP004 0.0E+00
RDPHTRAP005 0.0E+00
RDPHTRAP006 0.0E+00
RDPHTRAP007 0.0E+00
RDPHTRAP008 0.0E+00
*
* Initial Sigma-Y width of plume segment (m)
SIGYINIT001 2.326E-01
SIGYINIT002 2.326E-01
SIGYINIT003 2.326E-01
SIGYINIT004 2.326E-01
SIGYINIT005 2.326E-01
SIGYINIT006 2.326E-01
SIGYINIT007 2.326E-01
SIGYINIT008 2.326E-01
*
* Initial Sigma-Z height of plume segment (m)
SIGZINIT001 4.651E-01
SIGZINIT002 4.651E-01
SIGZINIT003 4.651E-01
SIGZINIT004 4.651E-01
SIGZINIT005 4.651E-01
SIGZINIT006 4.651E-01
SIGZINIT007 4.651E-01
SIGZINIT008 4.651E-01
*
* Representative location of plume segment.0. = leading edge, .5 = midpoint, 1. = trailing edge
RDREFTIM001 0.
RDREFTIM002 0.5
RDREFTIM003 0.5
RDREFTIM004 0.5
RDREFTIM005 0.5
RDREFTIM006 0.5

RDREFTIM007 0.5
RDREFTIM008 0.5
*
* plume segment duration
RDPLUDUR001 3.6004E+03
RDPLUDUR002 3.5993E+03
RDPLUDUR003 3.5943E+03
RDPLUDUR004 3.5786E+03
RDPLUDUR005 3.5958E+03
RDPLUDUR006 3.6092E+03
RDPLUDUR007 2.83E+03
RDPLUDUR008 4.9E+02
*
* MELCOR Time associated with reference time for inventory: 0 (s)
* Plume Segment 1 is associated with release path 99 at MELCOR time 1334.114 s
* Plume Segment 2 is associated with release path 51 at MELCOR time 3677.367 s
* Plume Segment 3 is associated with release path 99 at MELCOR time 4934.476 s
* Plume Segment 4 is associated with release path 51 at MELCOR time 7276.686 s
* Plume Segment 5 is associated with release path 99 at MELCOR time 8528.763 s
* Plume Segment 6 is associated with release path 51 at MELCOR time 10855.32 s
* Plume Segment 7 is associated with release path 99 at MELCOR time 12124.56 s
* Plume Segment 8 is associated with release path 51 at MELCOR time 14464.56 s
* Start Time of Release
RDPDELAY001 1.3341E+03
RDPDELAY002 3.6774E+03
RDPDELAY003 4.9345E+03
RDPDELAY004 7.2767E+03
RDPDELAY005 8.5288E+03
RDPDELAY006 1.0855E+04
RDPDELAY007 1.2125E+04
RDPDELAY008 1.4465E+04
*
* MELCOR Height associated with ground level:0 (m)
* Release path: 51 MELCOR Height: 0.0E+00 (m)
* Release path: 99 MELCOR Height: 0.0E+00 (m)
* Adjusted plume segment height
RDPLHITE001 0.0E+00
RDPLHITE002 0.0E+00
RDPLHITE003 0.0E+00
RDPLHITE004 0.0E+00
RDPLHITE005 0.0E+00
RDPLHITE006 0.0E+00
RDPLHITE007 0.0E+00
RDPLHITE008 0.0E+00
*
* Risk dominant plume segment
RDMAXRIS001 1
*

* Flag indicating plume segment buoyancy model
* RDPLMMOD001 DENSITY
*
* RDPLMMOD001 HEAT
*
* Rate of release of sensible heat in Watts (J/s)
RDPLHEAT001 1.7772E+05
RDPLHEAT002 1.446E+07
RDPLHEAT003 8.7329E+03
RDPLHEAT004 3.4848E+06
RDPLHEAT005 1.9625E+04
RDPLHEAT006 3.3502E+05
RDPLHEAT007 3.6888E+03
RDPLHEAT008 5.3943E+05
*
* Mass Flow Rate (kg/s)
RDPLMFLA001 1.12E+00
RDPLMFLA002 1.8842E+01
RDPLMFLA003 2.9776E-02
RDPLMFLA004 4.5702E+00
RDPLMFLA005 3.1607E-02
RDPLMFLA006 1.3549E+00
RDPLMFLA007 1.8297E-02
RDPLMFLA008 2.826E+00
*
* Gas Density (kg/m^3)
RDPLMDEN001 8.0421E-01
RDPLMDEN002 3.6741E-01
RDPLMDEN003 5.5381E-01
RDPLMDEN004 4.2402E-01
RDPLMDEN005 4.6988E-01
RDPLMDEN006 5.7979E-01
RDPLMDEN007 6.0233E-01
RDPLMDEN008 6.0316E-01
*
* MELCOR Chemical Classes Considered: Xe Cs Ba I Te Ru Mo Ce La U
* Release fraction and core inventory are zero for Chemical Classes:
* Xe Cs Ba I Te Ru Mo Ce La U
RDRELFRC001 1.5442E-02 5.4657E-06 1.2009E-08 5.6863E-06 5.1152E-06 3.447E-17 2.4584E-12 6.2305E-18 2.2207E-15 1.7658E-15
RDRELFRC002 6.6658E-01 1.9973E-01 8.2488E-04 2.1403E-01 1.8271E-01 3.476E-09 2.0535E-04 1.0668E-06 2.4642E-07 1.8047E-07
RDRELFRC003 8.5732E-04 2.439E-07 5.3524E-09 2.7515E-07 2.3041E-07 2.2726E-14 1.342E-09 3.833E-10 1.0443E-11 1.4149E-12
RDRELFRC004 1.1274E-01 3.5081E-02 1.3451E-02 4.145E-02 3.3012E-02 4.4924E-09 2.4019E-04 2.2437E-03 6.3599E-05 1.9206E-06
RDRELFRC005 7.6175E-04 2.3778E-07 8.7339E-08 2.817E-07 2.2226E-07 3.0138E-14 1.5986E-09 1.4426E-08 4.1171E-10 1.251E-11

RDRELFRC006 2.1451E-02 6.8301E-03 2.3666E-03 8.6943E-03 6.2397E-03 1.0059E-09 3.495E-05 4.3876E-04 1.5829E-05 5.0625E-07
RDRELFRC007 2.134E-04 6.7755E-08 2.3483E-08 8.6773E-08 6.2262E-08 1.0374E-14 3.4129E-10 4.3998E-09 1.6317E-10 5.2612E-12
RDRELFRC008 5.2577E-03 1.6519E-03 5.6559E-04 2.1484E-03 1.5363E-03 2.6519E-10 8.2281E-06 1.061E-04 4.0575E-06 1.3626E-07
*
* Scaling Factor to adjust core inventory for power level
RDCORSCA001 1
*
* Number of radionuclides belonging to chemical classes
ISNUMISO001 69
*
* Data in melmaccs.ini is used to map radionuclide to the corresponding chemical class
*
* Radionuclide and associated chemical group
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
*
* Initial Xe mass/inventory mass = 142.5916
* Initial Cs mass/inventory mass = 149.1238
* Initial Ba mass/inventory mass = 150.974
* Initial I mass/inventory mass = 130.6511
* Initial Te mass/inventory mass = 137.1912
* Initial Ru mass/inventory mass = 143.8977
* Initial Mo mass/inventory mass = 150.0607
* Initial Ce mass/inventory mass = 60.18168
* Initial La mass/inventory mass = 130.9275
* Initial U mass/inventory mass = 171.0927

*
* Initial Core Mass from MELCOR Chemical Class Xe 556.45056kg
* Initial Core Mass from MELCOR Chemical Class Cs 322.02002kg
* Initial Core Mass from MELCOR Chemical Class Ba 249.02879kg
* Initial Core Mass from MELCOR Chemical Class I 25.117559kg
* Initial Core Mass from MELCOR Chemical Class Te 48.947044kg
* Initial Core Mass from MELCOR Chemical Class Ru 368.39084kg
* Initial Core Mass from MELCOR Chemical Class Mo 420.77277kg
* Initial Core Mass from MELCOR Chemical Class Ce 712.73755kg
* Initial Core Mass from MELCOR Chemical Class La 685.25854kg
* Initial Core Mass from MELCOR Chemical Class U 165847.28kg
*
* Maximum mass scaling is for the Ce group. Error=64.8251 %
* Data in Inventory (.inv file) used to calculate core inventory (Becquerels)
RDCORINV001 Kr-85 3.6319E+16
RDCORINV002 Kr-85m 1.4978E+18
RDCORINV003 Kr-87 2.8975E+18
RDCORINV004 Kr-88 4.0814E+18
RDCORINV005 Xe-133 1.0974E+19
RDCORINV006 Xe-135 2.4538E+18
RDCORINV007 Xe-135m 2.1262E+18
RDCORINV008 Cs-134 4.7804E+17
RDCORINV009 Cs-136 2.0266E+17
RDCORINV010 Cs-137 3.9384E+17
RDCORINV011 Rb-86 7.5591E+15
RDCORINV012 Rb-88 4.3307E+18
RDCORINV013 Ba-139 1.0457E+19
RDCORINV014 Ba-140 1.015E+19
RDCORINV015 Sr-89 5.9044E+18
RDCORINV016 Sr-90 3.0008E+17
RDCORINV017 Sr-91 7.2283E+18
RDCORINV018 Sr-92 7.7646E+18
RDCORINV019 Ba-137m 3.784E+17
RDCORINV020 I-131 4.8776E+18
RDCORINV021 I-132 7.0578E+18
RDCORINV022 I-133 1.0065E+19
RDCORINV023 I-134 1.106E+19
RDCORINV024 I-135 9.3878E+18
RDCORINV025 Te-127 5.1624E+17
RDCORINV026 Te-127m 6.1776E+16
RDCORINV027 Te-129 1.5863E+18
RDCORINV028 Te-129m 2.3665E+17
RDCORINV029 Te-131m 7.34E+17
RDCORINV030 Te-132 7.3045E+18
RDCORINV031 Te-131 4.539E+18
RDCORINV032 Rh-105 4.7588E+18
RDCORINV033 Ru-103 7.9278E+18
RDCORINV034 Ru-105 5.1986E+18

RDCORINV035 Ru-106 1.8629E+18
RDCORINV036 Rh-103m 7.1398E+18
RDCORINV037 Rh-106 2.1659E+18
RDCORINV038 Nb-95 9.3444E+18
RDCORINV039 Co-58 9.4721E+13
RDCORINV040 Co-60 6.0464E+14
RDCORINV041 Mo-99 1.0517E+19
RDCORINV042 Tc-99m 9.2056E+18
RDCORINV043 Nb-97 9.6498E+18
RDCORINV044 Nb-97m 9.0724E+18
RDCORINV045 Ce-141 3.8634E+18
RDCORINV046 Ce-143 3.5694E+18
RDCORINV047 Ce-144 2.2534E+18
RDCORINV048 Np-239 4.4134E+19
RDCORINV049 Pu-238 2.5318E+15
RDCORINV050 Pu-239 6.0923E+14
RDCORINV051 Pu-240 7.1211E+14
RDCORINV052 Pu-241 1.8014E+17
RDCORINV053 Zr-95 3.8522E+18
RDCORINV054 Zr-97 3.8366E+18
RDCORINV055 Am-241 3.1638E+14
RDCORINV056 Cm-242 9.2236E+16
RDCORINV057 Cm-244 3.935E+15
RDCORINV058 La-140 9.0007E+18
RDCORINV059 La-141 8.2886E+18
RDCORINV060 La-142 8.0416E+18
RDCORINV061 Nd-147 3.3019E+18
RDCORINV062 Pr-143 7.6734E+18
RDCORINV063 Y-90 2.7274E+17
RDCORINV064 Y-91 6.4672E+18
RDCORINV065 Y-92 6.7627E+18
RDCORINV066 Y-93 7.7267E+18
RDCORINV067 Y-91m 3.6386E+18
RDCORINV068 Pr-144 4.9557E+18
RDCORINV069 Pr-144m 5.8907E+16
*
* PARENT means decay products are released at the same fraction as their parent
RDAPLFRC001 PARENT
*

APPENDIX D. 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 Values	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

Type	Number Bytes	Sample Values	Meaning
			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)

Type	Number Bytes	Sample Values	Meaning
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 pot 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

Type	Number Bytes	Sample Value	Meaning
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 E. CREATING A MELCOR PLOT FILE WITH MACCS INFORMATION

There are two major versions of MELCOR available, 1.8.6 and 2.2. Input for 2.1 and 2.2 differ from 1.8.6. Directions are included in the MELCOR user's guide (Humphries et al., 2017).

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 Cs2MoO4 are normally written (by default) to the MELCOR plot file. MelMACCS processes this 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.

E.1.1. Directions for MELCOR Version 1.8.6:

When using 1.8.6 RG, created on November 20, 2002, or later, the following input cards should be included in the MELGEN input.

> MACCSnn - MACCS Release Path Definition
> 1 <= nn <= 99 is the release path assigned by the MELCOR user.
> This input card contains one parameter as follows:
> (1) MCCSFP - MCCSFP is the number of the flow path; the sign is the sign of flow corresponding to "release".
> (type = integer, default = none, units = none)

This record allows identification of flow paths that serve as "release" paths for the consequences code, MACCS. For these paths, and these paths only, fluid and radionuclide transport data are written to the plot file.

Example: This example is consistent with DEMO(rhonom=2500, the sample MELCOR input file released with MelMACCS.

> MACCS51 399
> MACCS99 398

E.1.2. Directions for MELCOR Version 2.x:

The MELCOR version must be 2.1.1461 or later. Previous versions of 2.1 MELCOR create plot files that are not compatible with MelMACCS.

FL_MACCS – MACCS Release Paths Definition

This record allows identification of flow paths that serve as release paths for the consequences code MACCS. For these paths, and these paths only, data about fluid and radionuclide transport through the path are written to the plot file. The record can also be used simply to force such data to be

written to the plot file for other applications. However, all MACCS flow paths in a MELCOR plot file are evaluated by MelMACCS, so only the ones relevant to MACCS calculations should be defined if the plot file is to be processed with MelMACCS.

MACCSN - The number of MACCS release paths.
(type = integer, default = 0, units = dimensionless)

The following data are input as a table with length MACCSN. Variables are input in the order listed below.

Variable	Description
NFL	Table row index.
	(type = integer, default = none, units = none)
MACCSNAME	MACCS release path name (type = character*16, default = none, units = none)
MACCSNUMBER	MACCS release path (type = integer, default = none, units = none)
FPNAME	Flow path name (type = character*16, default = none, units = none)
DIRFL	Direction of flow corresponding to release. FROM TO (type = character*4, default = none, units = none)

MELCOR allows the flow path name to be any character string. However, MelMACCS requires this to be converted to an integer. This means that it is necessary to use an integer in the field FPNAME.

The field MACCSNAME is not currently used by MelMACCS.

When comparing the input format, a positive flow release path in 1.8.6 input corresponds to the keyword FROM, a negative number corresponds to the keyword TO.

Example corresponding to the same problem as referenced above in describing the sample input for 1.8.6:

FL_MACCS 2
1 'Release 51' 51 '399' FROM
2 'Release 99' 99 '398' FROM

APPENDIX F. 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.

F.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 demo 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	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)	1	Number of rings. If this isn't present, assume one ring.
MACCS-RINGNAM(1)	Core Inventory	Name of ring. Entry for each ring. Required for each ring if MACCS-NUMRINGS specified. These input entries are optional.
MACCS-MAXGRP(0)	23	Number of chemical groups. This is the total number of chemical groups over all batches.

Time Independent Variable Name	Value in demo plot file	Description
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	
MACCS-CHEMICAL-GROUP(14)	H2O	This is not considered by MelMACCS because the MelMACCS.ini file has no entries for H20 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_2MoO_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.

Time Independent Variable Name	Value in demo plot file	Description
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-NPATH(0)	2.00000E+00	Number of release paths.
MACCS-RELEASE-PATH(1)	5.10000E+01	MELCOR ID of release path.
MACCS-FLNUM(51)	3.98000E+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	

Time Independent Variable Name	Value in demo plot file	Description
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).

F.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_2MoO_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.

DISTRIBUTION

Email—Internal

Name	Org.	Sandia Email Address
David Lyle Luxat	08852	dlluxat@sandia.gov
Larry L. Humphries	08852	llhumph@sandia.gov
David Louie	08852	ddlouie@sandia.gov
Cathy Ottinger Farnum	08854	cfarnum@sandia.gov
Dan Clayton	08855	djclayt@sandia.gov
Kyle Clavier	08855	kaclavi@sandia.gov
Josh Dise	08855	jtdise@sandia.gov
Lee Eubanks	08855	lleuban@sandia.gov
John Fulton	08855	jdfulto@sandia.gov
Jennifer Leute	08855	jeleute@sandia.gov
Mariah Smith	08855	msmith7@sandia.gov
Fotini Walton	08855	fwalton@sandia.gov
Technical Library	01177	libref@sandia.gov

Email—External

Name	Company Email Address	Company Name
Jonathan Barr	Jonathan.barr@nrc.gov	US NRC
Luis Betancourt	Luis.betancourt@nrc.gov	US NRC
Keith Compton	Keith.compton@nrc.gov	US NRC
Salman Haq	Salman.haq@nrc.gov	US NRC
Alfred Hathaway	Alfred.hathaway@nrc.gov	US NRC
Carlos Navarro Alicea	Carlos.navarroalicea@nrc.gov	US NRC
Andrew Nosek	Andrew.nosek@nrc.gov	US NRC
Todd Smith	Todd.Smith@nrc.gov	US NRC
Nazila Tehrani	Nazila.tehrani@nrc.gov	US NRC

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