MELCOR 2.1 Leak Path Factor Assessments and Guidance

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MELCOR 2.1 is the current version of MELCOR developed at Sandia National Laboratories (SNL) for the Nuclear Regulatory Commission (NRC). Starting with version 2.0 and beyond, MELCOR is developed in the FORTRAN 95 programming language. In addition, MELCOR 1.8.5, which is listed in the current Department of Energy (DOE) Toolbox Tool Codes for leak path factor (LPF) calculations, is no longer developed or maintained for code issues. SNL will continue to develop and assess the MELCOR 2.1 code while improving code numerics and performance. We recommend adopting MELCOR 2.1 or later versions for LPF calculations to take advantage of new code development efforts.

Starting in MELCOR 2.0, the input format has changed dramatically. To help this transition, an input deck converter is available for translating inputs from MELCOR 1.8.6 to 2.1. The use of the converter and guidance/limitation of MELCOR 2.1 features for LPF applications will be provided as an appendix in the planned release of the Volume III (Demonstration Problems) of the MELCOR manuals. A summary of the guidance/limitations is given in this paper.

Finally, this paper discusses the assessment of MELCOR 2.1 using the sample problems as described in the current DOE MELCOR Computer Code Application Guidance for LPF in Documented Safety Analysis (2004). The results of the comparison among MELCOR 1.8.5, 1.8.6 and 2.1 by using these sample problems show no significant difference. Additional assessments on MELCOR 2.1 features for the LPF applications were also performed and described in this paper.

Introduction

MELCOR is being developed by SNL for modeling nuclear reactor severe accidents and funded by the NRC. However, MELCOR code has been used in the LPF analysis at the DOE nuclear and nonnuclear facilities for many years [1-5]. Unlike many safety analysis codes that are specifically designed only for nuclear reactor applications, MELCOR is a modular computer code which allows users to select specific packages for their specific applications (i.e., LPF calculations), without any issue. In fact the current DOE Toolbox Tool specification designates MELCOR to be used in performing LPF calculations [3]. However, the MELCOR version listed in the Toolbox Tool central registry is 1.8.5, which is no longer supported by SNL (i.e., no new model development, testing or issue correction). In addition, many of the safety analysts in the DOE safety basis have used MELCOR 1.8.6 (also currently unsupported by SNL) with an independent verification and validation procedure to comply with the DOE quality assurance program for many years. To minimize the effectiveness and conserve resources, SNL has decided only to support MELCOR 2.0 and beyond.

Code Version Difference

Starting with Version 2.0 and beyond, MELCOR is developed in FORTRAN 95. The use of FORTRAN 95 allows MELCOR to continue its development in the future in terms of extensibility and maintainability. All previous versions of MELCOR were developed in FORTRAN 77 (obsolete), which

is no longer supported by many FORTRAN compilers currently available today. Most of our development work is done in Visual Studio ™ and Intel Fortran compiler ™ in the Windows ™ environment.

Another major difference between Version 2.0 and 1.8.6 is the code architecture, even though most of the 1.8.6 algorithms were kept intact. The original Version 2.0 was developed using the object-oriented approach in terms of input and calculated variables (using different levels: program [MELGEN, MELCOR], package [CVH, FL, etc.], and object [CV_ID, etc.] levels) and storage spaces (dynamically allocated memory). Thus this difference contributes the input format change between these two versions. Version 1.8.6 and previous versions used numbers as the unique identification for input card or a set of cards. Figure 1 shows difference comparison of input format between the two versions. As shown in this figure, 2.1 uses the "block input" format, which requires a "INPUT" card for the designation of a package input, then followed by "_ID" Therefore, the input format starting in Version 2.0 is called "block input".

```
* Comments common to MELGEN and MELCOR
*
*EOR* MELGEN
TITLE          Test
RUNONLY        NM
RESTARTFILE    tmirest
OUTPUTFILE     tmioutg
DIAGFILE       tmidiagg
DTTIME         0.1
CRTOUT
R*I*F          cvhinput
FL00100  cv101-cv102   101 102  1.5  1.5
...
FL00200  cv103-cv104   103 104  1.22 1.22
...
...

R*I*F          hsinput
R*I*F          rninput
R*I*F          otherinput
;
*
*EOR* MELCOR
TITLE          Test
RUNONLY        NM
RESTARTFILE    tmirest
OUTPUTFILE     tmiout
DIAGFILE       tmidiag
MESSAGEFILE    tmimes
PLOTFILE       tmiplot
CPULEFT        30.0
CPULIM         36000.0
CRTOUT
NOCOPY
RESTART        0
TIME1            0.0    5.0   0.0001   500.0   2.0   500.0
TIME2          1000.0   10.0   0.0001  1000.0   5.0  1000.0
TEND           6000.0
R*I*F          scinput
PLOT000        RN1-ADEP-1-10-1.30001
PLOTabc.......RN1-ADEP-1-9-1.30001
...
PLOTxyz        RN1-ADEP-1-10-1.30001
.
```

MELCOR 1.8.6

```
! Comments common to MELGEN and MELCOR
!
MEG_DIAGFILE    tmidiagg
MEL_DIAGFILE    tmidiag
MEG_OUTPUTFILE  tmioutg
MEL_OUTPUTFILE  tmiout
MEG_RESTARTFILE tmirest
MEL_RESTARTFILE tmirest    NCYCLE     0
PLOTFILE        tmiplot.ptf
MESSAGEFILE     tmimes
Program MELGEN
!* Block: EXEC data ************************************
EXEC_INPUT
EXEC_TITLE  "Test" ! Title of the calculation
EXEC_RUNONLY NM
EXEC_DTTIME  0.1

!* END EXEC ********************************************
INCLUDE cvhinput
FL_INPUT
FL_ID    'cv101-cv102'       1
!
FL_FT    '101'    '102'    1.5     1.5
...
FL_ID    'cv103-cv104'       2
!
FL_FT    '103'    '104'    1.22    1.22
...
...

INCLUDE hsinput
INCLUDE rninput
INCLUDE otherinput
...
END Program MELGEN data
!
Program MELCOR
!* Block: MEX (Exec) data ***************************
EXEC_INPUT
EXEC_TITLE   "Test" ! Title of the calculation
EXEC_RUNONLY NM
EXEC_TIME  2 !  NUMBER TIME DTMAX DTMIN DTEDT DTPLT DTRST DCRST
                 1    0.0   5.0 0.0001 500.0  2.0 500.0  0.1E+11
                 2  1000.0 10.0 0.0001 1000.0 5.0 1000.0 0.1E+11
EXEC_CPULEFT   30.0
EXEC_CPULIM    36000.0
EXEC_TEND      6000.0
EXEC_NOCOPY
EXEC_PLOT  3
     1 RN1-ADEP(HS30001,LHS,U02,TOT)
     2 RN1-ADEP(HS30001,LHS,LA,TOT)
     3 RN1-ADEP(HS30001,LHS,U02,TOT)
!* END MEX (Exec) ****************************
INCLUDE scinput
END Program MELCOR data
```

MELCOR 2.1

Figure 1 Difference in Input Format between MELCOR 1.8.6 and MELCOR 2.1

To help the user transition to this new format, a converter allows the conversion from an input developed in version 1.8.6 (or 1.8.5 deck without COR input) to version 2.x, SNAP, which stands for Symbolic Nuclear Analysis Package developed by Applied Programming Technology, Inc. for the NRC (see Figure 2). There is a plug-in of SNAP for MELCOR specified. SNAP can also be used for post-processing and visualization (see Figure 2). Editing tools from SNAP can also provide additional simulation needs.

Assessments

Assessments for MELCOR 2.x code are planned to be completed this summer, with the release of the Volume III (Demonstration Problems) of the MELCOR manuals. Appendix A of Volume III is designated for the non-reactor applications, which includes detailed LPF assessments and guidance. A

brief LPF assessment in terms of verifications is provided in this paper based on the MELCOR assessment final report by DOE [3] and the LPF assessments done by Los Alamos National Laboratory [2]. Table 1 shows the comparison of the results among using MELCOR 1.8.5, 1.8.6 and 2.1 for the MELCOR assessment final report [3]. Note that some discrepancies have been identified in Ref [5] from the MELCOR assessment final report [3]. These discrepancies are not repeated here. As shown in Table 1, MELCOR 2.1 results agree well with MELCOR 1.8.6 and 1.8.5. Additional assessment is performed for a LPF calculation of a fire scenario in a complex facility as described in LA-UR-03-7945[2]. As shown in Table 2, MELCOR results are described from different MELCOR versions and the referenced MELCOR results reported in LA-UR-03-7945[2]. As shown in this table, the reference MELCOR calculations use 1.8.5 version that yield slightly higher results than the results from the various versions done by SNL, except the cases when smoke aerosols are modeled. In these smoke cases, unlike the referenced results, all code versions predict that LPF decreases as the amount of smoke aerosols increases due to the agglomeration. These differences with the referenced results are unexplained. In comparing among different versions of MELCOR, all versions predict similar results as shown in Table 2, except Case5 for the 1.8.5 version.

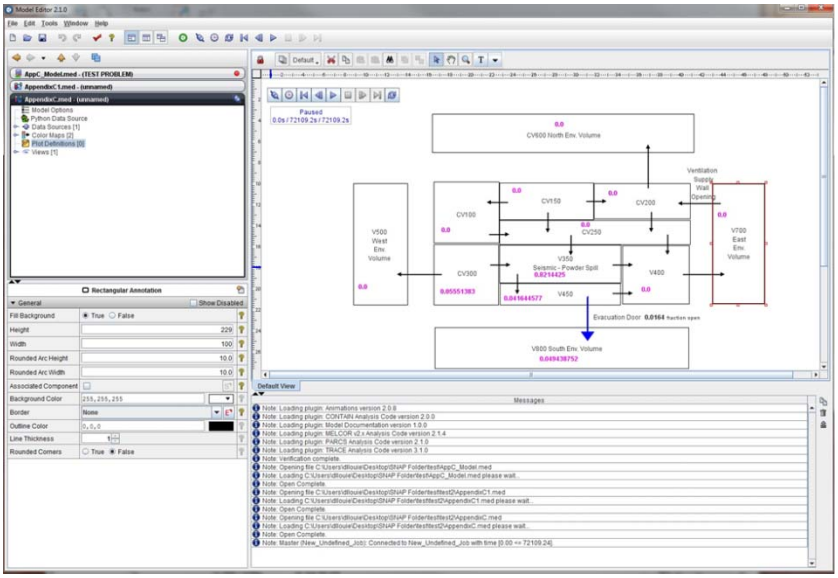

Figure 2. Typical SNAP Simulation

Table 1. MELCOR LPF Results (%)* from Test Problems in MELCOR Guidance Report [3]

Test Problem	Reference Value from interpolated from (figures) in Guidance Report	1.8.5	1.8.6	2.1
Appendix C	~8.1 (7-6)	8.13	8.10	8.09
Appendix D	~0.39 (7-12)	0.39	0.39	0.39
Appendix E	~26.3 (7-18)	26.66	26.64	26.63
Appendix F	~0.43 (7-21)	0.43	0.43	0.43
Appendix G				
1000 g	~11.58 (7-26)	10.42	10.39	10.38
100g	~12.03 (7-26)	10.79	10.75	10.74
10g	~12.09 (7-26)	10.83	10.79	10.78
1g	~12.09 (7-26)	10.83	10.79	10.78

*1.8.5 is calculated using the official release version RL, 1.8.6 is calculated using the official release version YV 3404, and 2.1 is calculated using revision 1570.

Table 2. MELCOR Results on Example 3 of LA-UR-03-7945 [2]

Case	Crack Width (mm)	Wind Speed (mph)	Smoke Generated by Fire (kg)	HEPA Collect Efficiency (%)	MELCOR LPF Results (fraction)*			
					1.8.5 Reference**	1.8.5	1.8.6	2.1
1	0.5	30	None	99.98	3.9×10^{-3}	3.0×10^{-3}	3.0×10^{-3}	3.0×10^{-3}
2	1	30	None	99.98	9.3×10^{-3}	7.5×10^{-3}	7.5×10^{-3}	7.4×10^{-3}
3	2	30	None	99.98	2.0×10^{-2}	1.7×10^{-2}	1.7×10^{-2}	1.7×10^{-2}
4	5	1	None	99.98	5.1×10^{-2}	4.5×10^{-2}	4.4×10^{-2}	4.4×10^{-2}
5	0.5	10	None	99.98	2.8×10^{-7}	1.2×10^{-7}	2.3×10^{-7}	2.3×10^{-7}
6	0.5	20	None	99.98	1.1×10^{-4}	7.2×10^{-5}	7.6×10^{-5}	7.4×10^{-5}
7	0.5	30	None	99.98	1.0×10^{-3}	9.6×10^{-4}	9.6×10^{-4}	9.3×10^{-4}
8	0.5	30	10	99.98	2.6×10^{-5}	2.8×10^{-3}	2.8×10^{-3}	2.7×10^{-3}
9	0.5	30	25	99.98	1.1×10^{-5}	2.5×10^{-3}	2.5×10^{-3}	2.4×10^{-3}
10	0.5	30	50	99.98	3.9×10^{-3}	2.1×10^{-3}	2.1×10^{-3}	2.0×10^{-3}
11	0.5	30	None	99.95	3.9×10^{-3}	3.0×10^{-3}	3.0×10^{-3}	3.0×10^{-3}

*1.8.5 values are using the official release version RL, 186 values are calculated using the official release version YV 3404, and 2.1 values are calculated using official release version RL NL 4261.
**1.8.5 reported values from Table 4-2 of LA-UR-03-7945 [2].

Features Useful for LPF Analyses

SNL has made a decision to only develop new models in MELCOR 2.0 and beyond to conserve resources and man power. Table 3 describes the MELCOR packages and models that may be of interest to the safety basis community for use in the LPF analyses. As shown Table 3, there are a number of packages that should be included in the LPF calculation. RN, CVH, and FL packages are the major packages utilized by the LPF problem, since the RN package tracks the radionuclides and aerosol, and both CVH and FL define the thermal conditions of the problem. FL is also used to track the release of the radionuclide and aerosol to the environment. Also shown in this table is the number of models available for use in the LPF calculations. Significant improvement in the aerosol deposition model has been done in MELCOR, namely the ability to disable the aerosol deposition model, and model the turbulent deposition in pipes and ducts, including bends (see Table 3 for the model limitation).

To support sensitivity studies, a new pre-processing feature of MELCOR 2.x is the common block, identified in Table 3. This minimizes the needs of additional input files to conduct these types of studies. As shown in Figure 2, the SNAP interface can be used to allow visualization of the MELCOR results, permitting a better understanding of the results, instead of reading through outputs or plots. Interactive calculations using the SNAP interface can be possible, and changing MELCOR parameters on the fly is extremely useful for some applications.

Future Developments

SNL recommends the following future enhancements for MELCOR. Examples of interest to the safety basis communities include: (a) hot gas layer modeling for simulating fire scenarios; and (b) other combustibles of solid, liquid and gas (including user-defined combustible), in addition to the current hydrogen and carbon monoxide models).

Conclusions

MELCOR 2.x represents the latest version of MELCOR, which should be used by the safety basis community for the LPF applications. Assessments of this current code version show results that are consistent with MELCOR 1.8.5, the current DOE Toolbox code. With the enhancements to be included in this code version and beyond, the safety analyst should be benefited.

Table 3. MELCOR Packages and Models Useful for LPF Analyses

Package	**Description/Comments**
EXEC	Main control of various processing tasks and control of the overall calculation sequence. Sensitivity coefficients of many package models can be redefined in MELGEN or changed at any restart via MELCOR input. Common block feature, which is designated in the input as starting with "(((name block" and ending with "))" can be used to allow a single input file to simulate a number of different runs. The name block can be included during execution of the MELGEN/MELCOR calculations or included in the beginning of the input file. The use of the common blocks is extremely useful for sensitivity studies.
NCG	NCG package is used to define the gases in the control volumes.
CVH/FL	Use time-independent volume for the environment, which prevent aerosols from being drawn back into the facility. A large environment volume ($10^{10}m^3$) may be too large, since its energy and mass may dilute any actual mass and energy errors in the problem. Therefore, it is recommended to use a reasonable size volume. MELCOR 1.8.6 users may find it difficult to use the new CVH inputs to define the thermodynamic condition of the volume. To ease this problem, an alternative input, CV_THERM, restores some features as in MELCOR 1.8.6 version. In addition, FL_MACCS input in FL package serves as the designated data set that can be provided for the consequence code MACCS, since MACCS requires data on fluid flows and radionuclide transport to the environment.
HS	This package allows the model of heat transfer surfaces in the facility as well as for any aerosol deposition or condensation of the water.
RN	This package is the most important package for the LPF analysis, because this package tracks and models much of the physics for the aerosols and radionuclides modeled. A new input, RN1_VISUAL enables the extraction of aerosol information (such as aerosol section and deposition masses) as a function of time to store in files for post-processing, using "ResultsViewer" to display graphically.
CF/TF	Both the control function (CF) and tabular function (TF) packages provide a way to control the problem as well as to read and write data for the problems.
EDF	This package stands for the external data file, which provides a way to read or write a large amount of data that can be input to MELCOR, or that MELCOR can write out for plotting or inputs to other applications.
Models	**Description/Comments**
Counter-current flow model	A new stratified counter current flow of gases in a flow path was developed (see FL package input – FL_CCF). User input is available to allow coupling of flows in two paths through momentum exchange, using Epstein-Kenton correlations.
Critical Flow	CVH package provides an option to select the critical flow in the atmosphere, when two-phase flow may be important. This input card, CVH_ATMCS, is provided. Additionally, the user can print out the sound speed of the flow using CVH_CSTBL.
Aerosol deposition model deactivation flag	RN1_ADFG input in the RN package permits disabling a particular aerosol deposition models – such as gravitational, diffusive or thermophoresis aerosol settling model. This allows the users to determine which deposition model has the effect on the results.
Turbulent Aerosol Deposition	RN1_TURB input in the RN package allows the modeling of the turbulent aerosol deposition in pipe or duct which contains gas flows in the turbulent regime. Deposition in bends, venturi and contraction of the pipe or duct transitions can also be captured. Because many of the benchmarks done for this model are from the reactor applications, cautions should be placed when applying this model for the LPF application.
Filters	Filter models within the RN2 inputs in the RN package are flexible enough to permit the user to model a variety of aerosol or vapor filters in deposition, flow and degradation phenomena, because many of the filter inputs can be modeled using control function logic.
Sprays	The SPR package was developed for the containment spray in the reactor containment. Because of the generality of the spray inputs, this spray model can be used to simulate the fire sprinkler system to reduce the thermal condition of control volumes and can be used to scrub radionuclides/aerosols to minimize the LPF value.

References

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[2] H. Jordan and M.T. Leonard, Attenuation of Airborne Source Terms in Leak Paths, LA-UR-03-7945, Los Alamos National Laboratory, October 2003.

[3] MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis – final report, U.S. Department of Energy, May 2004.

[4] P. McClure, "In-Facility Transport Modeling (Leak Path Factor Determination)," LA-UR-05-2879 (Presentation), Los Alamos National Laboratory, EFCPG SAWG 2007 Workshop, Idaho Falls, ID, May 2007.

[5] T. Sanchez, et.al, "Experiences and Lessons Learned During Verification and Validation of the MELCOR Code," Presentation, OMICRON Safety and Risk Technologies, Inc., EFCOG SAWG 2007 Workshop, Idaho Falls, ID May 19-24, 2007.