

Lessons from Assessment of Analytical Problems with MELCOR 2.2

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1. Introduction

Proper validation of physical models of a computer code is essential to provide developers the guidance in developing algorithms and numerical methods for describing physical processes. Such validation usually takes place by assessing the models against available test data or analytic test cases [1]. Moreover, validation exercises help code users obtain knowledge of the internal models and their applications to real-world, including the code capabilities and limitations. In this way the exercises can contribute to reduce user effects which have been often identified in benchmark exercises such as International Standard Problems (ISPs) proposed by the OECD Nuclear Energy Agency (NEA).

The main sources of code user effects on the predicted code results are system nodalization, code options and physical model parameters, input parameters for system characteristics and system components, specification of initial and boundary conditions, specification of state and transport properties, time steps, and code input errors [2]. Even though code user effects on the predicted system behavior cannot be completely avoided, there are some suggestions for reducing them. They are, for instance, user training, improved user guidelines, user discipline, quality assurance, code improvement, and graphical user interfaces [2]. Especially, in order to ensure reliable results from our confirmatory analysis using the MELCOR code, we consider that adequate training and discipline are important [3, 4].

From this motive, we assessed five test cases with analytical solutions, developed by the Sandia National Laboratories, available to benchmark the following phenomena:

1. Saturated liquid depressurization,
2. Adiabatic flow of hydrogen,
3. Transient heat flow in a semi-infinite solid with convective boundary conditions,
4. Cooling of rectangular and annular heat structures in a fluid,
5. Self-initialization of steady-state radial temperature distributions in annular structures.

These are simple, fast-running cases that provide a test of nodalization and time-step dependence [1]. Our assessment was performed with the latest version of MELCOR (V2.2) and modified input decks, which were originally developed for MELCOR 1.6.0 validation

carried out by the SNL (Sandia National Laboratories) in 1980's [5]. The results and lessons from this assessment are described below.

2. Assessment of Analytical Problems

In this section the problem description on the five test cases, assessment results and comparison to the analytical solutions, and lessons from these assessments are described.

2.1 Saturated Liquid Depressurization

The analysis of severe accidents involves predicting the depressurization of the reactor vessel into its containment, as shown in Fig. 1. For some accident sequences, the reactor vessel contains significant quantities of high-pressure, high-temperature water, which will undergo rapid flashing during depressurization. The ability of MELCOR to adequately represent the outcome of such a depressurization has been tested, focusing on the CVH (Control Volume Hydrodynamic), FL (Flow Path), HS (Heat Structure) packages [1, 5]. The analytical solution for the final system state is obtained in terms of specific internal energies of liquid and steam, and steam quality at equilibrium, which depend on pressure and temperature. The initial conditions are described in Table I.

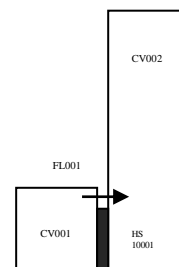


Fig. 1. Saturated liquid depressurization problem model.

Table I: The Initial Conditions and the System

| Parameter | Volume 1 | Volume 2 |
|-----------------|----------|----------|
| Pressure (MPa) | 7.999 | 0.01 |
| Temperature (K) | 568.23 | 568.23 |
| Water Mass (kg) | 72240 | 0.0 |
| Steam Mass (kg) | 0.0 | 152.57 |
| Void Fraction | 0.0 | 1.0 |

The calculated pressures and temperatures of the two volumes are shown in Figs. 2(a) and (b). Compared to the analytic solutions, they differed by only 0.0003MPa and 0.004K, respectively, as shown in Table II.

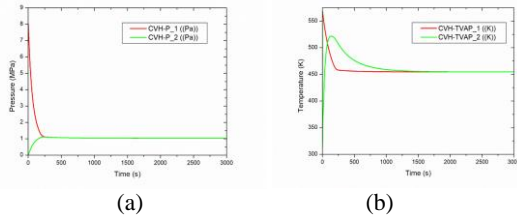


Fig. 2. The calculated pressures (a) and temperatures (b) of the two volumes.

Table II: Comparison of calculated results to analytic solution

| Case | Pressure (MPa) | Temperature (K) | Quality |
|------------|----------------|-----------------|---------|
| Analytic | 1.037 | 454.7 | 0.297 |
| MELCOR 2.2 | 1.03733 | 454.696 | 0.29737 |

There were several lessons from this assessment:

- “Separate pool and atmosphere input” option is recommended for normal applications, applying the CV_THERM record which consolidates the state definition inputs into a single user defined table.
- If there is only one fluid field (pool or atmosphere) in a control volume, equilibrium thermodynamics is used.
- When there is heat transfer between control volumes, in addition to that through the flow paths, heat structure must be modeled.
- The default HS heat transfer coefficients (“CalcCoefHS” option) are too small to correctly simulate this phenomenon.
- “Quality” could be approximated by dividing the mass of vapor in both volumes by total water mass in the pool and the atmosphere of the volumes.

2.2 Adiabatic flow of hydrogen

Two control volumes are pressurized with hydrogen such that the pressure in volume 1 is greater than that in volume 2. At time zero, a flow path is opened between the two control volumes, and hydrogen from the higher-pressure control volume expands into the lower-pressure control volume until the two pressures equilibrate. The initial conditions, control volume sizes, and flow path parameters were varied over a wide range to provide a thorough test of the MELCOR packages [1, 5]. In our study, however, only flow path area was varied, as shown in Table III.

Table III: The Initial Conditions for the Hydrogen Adiabatic Expansion

| Case | Vol.1 (M ³) | Vol.2 (M ³) | T(1, 2) (K) | P(1) (Pa) | P(2) (Pa) | Flow area(m ²) | Loss coeff. |
|------|-------------------------|-------------------------|-------------|-----------|-----------|----------------------------|-------------|
| 1 | 1000 | 1000 | 300 | 2.0E5 | 1.0E5 | 0.05 | 2.0 |
| 2 | 1000 | 1000 | 300 | 2.0E5 | 1.0E5 | 50 | 2.0 |

Assuming adiabatic flow and treating hydrogen as an ideal gas, analytic expressions for the control-volume temperatures and pressures, as transient functions of the mass transferred, were made. Comparison of MELCOR calculations to a closed-form analytical solution shows good agreement between them as shown in Figs. 3(a) and (b).

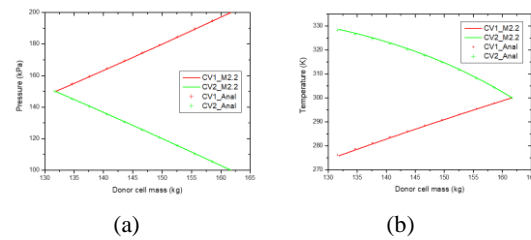


Fig. 3. The calculated pressures (a) and temperatures (b) of the two volumes vs. donor cell mass.

The slight differences arose in part due to temperature dependent heat capacities in MELCOR, and partly due to the time-step selection. The results were sensitive to flow area, given the time step of 0.01 s (The area of 0.05 m² was changed to 50 m²). The calculations with the time step equal to or smaller than 0.001 s gave an accurate prediction of the exact solution.

2.3 Transient Heat Flow in a Semi-Infinite Heat Structure Test

This problem simulates the conduction heat transfer in thick walls, for instance, the containment walls during a severe accident. This analysis demonstrates the accuracy of the MELCOR heat conduction models, and provides guidelines for node spacing and time step sizes for concrete containment walls. Transient heat flow in a semi-infinite solid with convective boundary conditions was modeled in MELCOR using a finite slab heat structure of sufficient thickness to approximate a semi-infinite solid. The specifications for this simulation is described in Table IV [1, 5].

- A 10m-thick heat structure with logarithmic node spacing was assumed.
- The smallest node spacing was on the left side of the heat structure, which is adjacent to a very large control volume.
- On the left side of the heat structure, a convective heat transfer boundary condition was specified with a heat transfer coefficient of 10W/m²-K.
- An adiabatic boundary condition was specified for the right side of the heat slab.

Table IV: Specifications for Semi-Infinite Heat Conduction Analyses

| Initial Temp. (K) | Fluid Temp. (K) | Material | Density (kg/m ³) | Specific Heat (J/kg-K) | Thermal Conduct. (W/m-K) |
|-------------------|-----------------|----------|------------------------------|------------------------|--------------------------|
| 300 | 450 | concrete | 2300 | 650 | 1.6 |

These node structures were designed to include 69, 35, 18, 11, 8, and 5 nodes up to one meter. Nodes between 0.0 and 0.001m were equally spaced, whereas nodes between 0.001 and 10m were logarithmically spaced. The base case calculation with 69 nodes and a 10 second time step size was selected to give an accurate prediction of the exact solution (Fig. 4). Realistic severe accident assessments are likely to use at most the 18 nodes and 30 second time step size case for estimating the heat transfer into the containment walls (Fig. 5(a) and (b)) [1, 5].

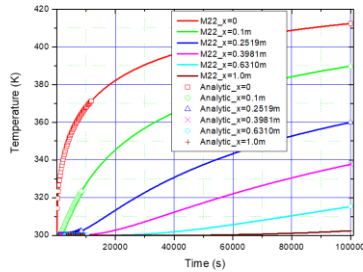


Fig. 4. Temperature distribution with 69 nodes in the first meter.

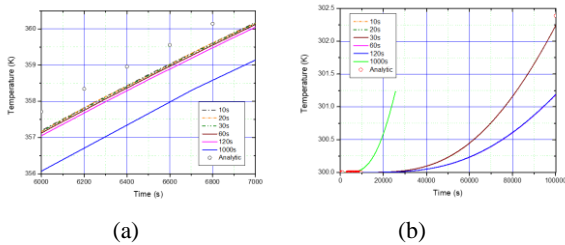


Fig. 5. Temperature at the surface (a) and at 1 m (b) vs. time for different time steps.

2.4 Cooling of Heat Structures in a Fluid

MELCOR calculations were performed for the cooling of two heat structures in a fluid, and the results were compared to an exact, analytic solution. Both rectangular and cylindrical geometries were tested. This problem primarily tests the implementation of the internal heat conduction methodology in the absence of internal or surface power sources. These structures, initially at 1,000K, were immersed in a fluid at 500K. Table V shows values of the various thermal properties of the material in these structures, as well as other parameters used in these calculations [1, 5].

Table V: Specifications for Heat Structure Cooling Analyses

| Parameter | Value |
|-----------|-------|
|-----------|-------|

| | |
|-----------------------------------|-------------------------|
| Thermal conductivity | 50.0 W/m-k |
| Density | 1.0 kg/m ³ |
| Specific heat capacity | 1500.0 J/kg-K |
| Surface heat transfer coefficient | 50.0W/m ² -K |
| Structure initial temperature | 1000.0 K |
| Fluid temperature | 500.0 K |
| Rectangular slab thickness | 0.1 m |
| Rectangular slab surface area | 1.0m ² |
| Cylindrical slab radius | 0.1m |
| Cylindrical slab height | 1.0m |

Excellent agreement was achieved between the MELCOR results and the analytic solution as shown in Fig. 6. Both structures are cooled as expected and have surface temperatures at the end of the 10s period that are nearly equal to the fluid temperature, held fixed at 500.0K.

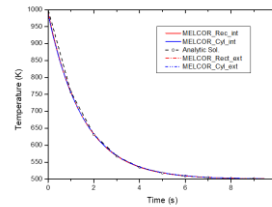


Fig. 6. Surface temperature of rectangular and cylindrical structures vs. time.

2.5 Radial Conduction in Annular Structures

MELCOR 2.2 estimations of the steady-state and transient temperature distributions resulting from radial heat conduction in annular structures were compared to the results obtained from exact analytic solutions. The MELCOR model consists of a hollow, cylindrical heat structure, with boundary conditions specified on the inside and outside surfaces. Two cases were considered, with dimensions and initial and boundary conditions as specified in Table VI. The first case tests the heat structure temperature self-initialization logic in MELCOR, whereas the second case test is initialized with a uniform temperature across the annulus that is then driven by heat transfer to the steady-state temperature profile [1, 5].

Table VI: Specifications for Annular, Radial Heat Conduction Analyses

| Case | Type | Left/Inside | | Right/Outside | | Radius | |
|------|--------|-------------|-------------------------|---------------|-------------------------|-----------|-----------|
| | | T (K) | h (W/m ² -K) | T (K) | h (W/m ² -K) | Inner (m) | Outer (m) |
| 1 | Steady | 600 | 1000 | 550 | 5.0 | 3.1856 | 3.3412 |
| 2 | Trans. | 600 | 1000 | 550 | 5.0 | 3.1856 | 3.3412 |

The agreement between the MELCOR/MELCOR results and the analytic solutions was good as shown in Fig. 7 (b). The MELCOR steady option leads to an identical temperature profile through the heat structure.

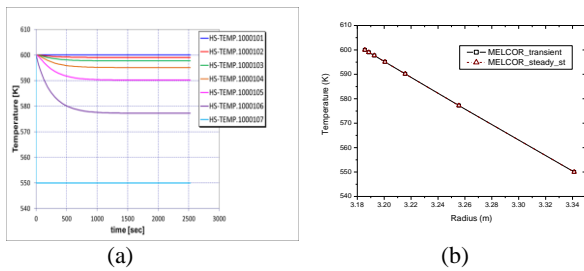


Fig. 7. Temperature profile for radial heat conduction in annular structures.

3. Conclusions

As part of training and discipline of the MELCOR users to reduce user effects on the predicted code results, five test cases with analytical solutions, including saturated liquid depressurization, were assessed with MELCOR 2.2. The input decks were based on those for MELCOR 1.6 validation. The results show reasonable agreement between the MELCOR results and the analytic solutions. Lessons were obtained about the modeling method as well as the appropriate node spacing and time step size, and HS heat transfer coefficients for simulation of a severe accident.

Acknowledgments

This work was supported by the Nuclear Safety Research Program through the Korea Foundation Of Nuclear Safety (KoFONS) using financial resources granted by Nuclear Safety and Security Commission (NSSC), Republic of Korea (No. 1805001).

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