Simulating Molten Fuel-Moderator Interactions with the Code MC3D

J. Licht
Atomic Energy of Canada Limited, Chalk River, Ontario, Canada

Abstract

The code MC3D was used to simulate a set of molten fuel-moderator interactions experiments associated with a single channel pressure tube failure. The code CATHENA was used to determine the discharge characteristics and input parameters for the water and steam at the location of the pressure tube failure. Despite some of the limitations of the code MC3D, simulations of the pressure pulses generated from the break qualitatively agreed with the experimentally measured values.

1. Introduction

One of the very low probability design basis accident scenarios postulated for CANDU reactors is a single channel blockage event that can lead to fuel melting and pressure tube failure. The molten fuel will be ejected into the D_2O moderator, resulting in a molten fuel-moderator interaction (MFMI). A key parameter of interest is the pressure wave generated by the MFMI at the vessel wall.

The MFMI may be classified into one of two limiting situations: forced interactions or free interactions.

Forced interactions are characterized by rapid quenching of finely fragmented melt particles giving rise to modest pressure pulses that can be sustained by the calandria vessel wall. The current understanding is that such an event occurs due to the fuel becoming finely fragmented as it is discharged from the pressure tube. This makes the fuel surface area large and the heat transfer relatively efficient as the melt is quenched in a multiphase mixture of steam, melt fragments and water droplets. This situation creates local pressures in the mixing zone which are lower than the driving pressure initiated from the pressure tube (i.e., 10 MPa).

A free interaction is not as precisely defined, but considered to be a steam explosion; i.e., a low velocity melt ejection that accumulates outside of the channel as a coarse melt-water-steam mixture with minimal pressurization during a latent mixing period, followed by triggering and propagation of a steam explosion, generating local pressures well in excess of the driving pressure.

An experimental program conducted at Atomic Energy of Canada Limited (AECL) at Chalk River Laboratories showed that for pressurized ejection of molten corium, the dominant mode is forced interaction [1, 2]. MFMI can be considered a subset of fuel-coolant interactions (FCI) that are currently being investigated internationally through projects like SERENA (Steam Explosion REsolution for Nuclear Applications). The goal of SERENA is to assess the capabilities of current computer codes in predicting FCI's in water reactor applications and to identify code deficiencies for improvement.

This paper presents preliminary results of MFMI simulations using the code designated MC3D and comparing the simulation results to data obtained from the experimental program conducted at AECL.

2. Background

2.1 Experimental facility

The purpose of the MFMI tests was to melt corium (fuel) inside an instrumented pressure tube and eject the ~2400°C melt at a pressure of ~10 MPa pressure into ~68°C water through a rupture, initiated at an axially machined defect in the pressure tube, to confirm that forced interaction is the dominant mode of interaction between molten corium and water. The mode of interaction was determined from the measured dynamic pressure transients and the size distribution of the melt particles recovered from the water tank.

Figure 1 shows a 3D rendering of the experimental apparatus and its major components as described in the following sections.

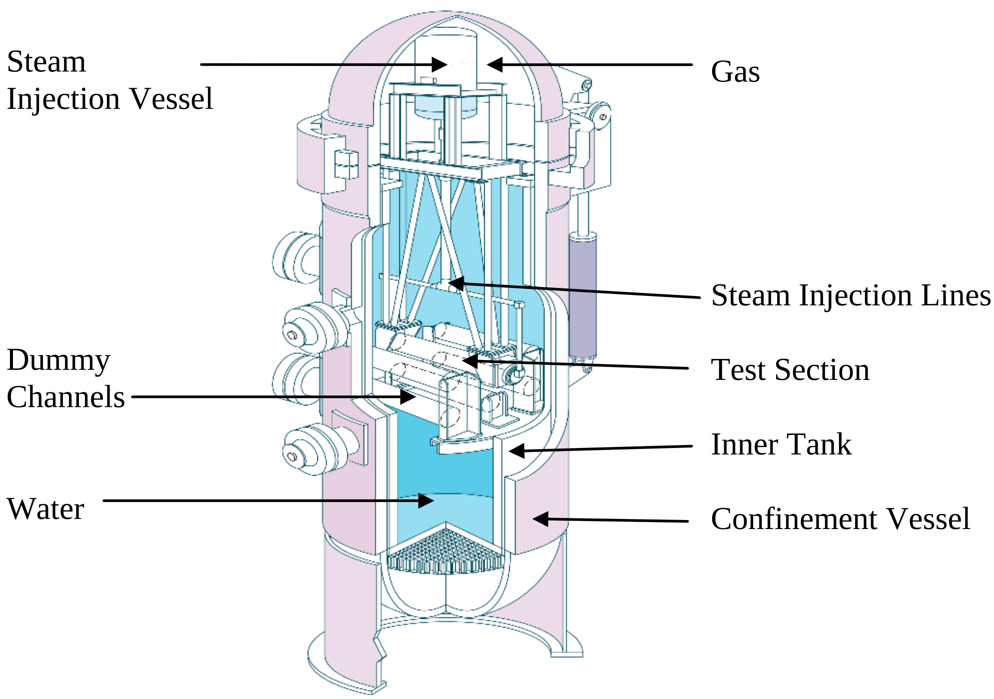

Figure 1 Drawing of the confinement vessel, inner tank, steam injection vessel and the test section.

2.1.1 Confinement vessel

The experiment was conducted inside a carbon steal confinement vessel purged with helium to provide containment of the radiological debris and to provide a safety barrier for projectiles generated from the rupture and/or molten-corium moderator interaction. The confinement vessel had an inner diameter of 1.5 m and a height of 5.0 m. A hinged lid that opens to the full vessel diameter and five access ports provide access to the vessel interior. The confinement vessel gases are evacuated and back filled with helium prior to the experiment.

Energy absorbing material at the bottom of the confinement vessel absorbs the pressure pulse from the pressure-tube rupture and the corium/water interaction and distributes the load evenly over the bottom head of the vessel.

2.1.2 Inner tank

The stainless steel inner tank had an inner diameter of 1.25 m, thickness of 6.35 cm, and a height of 2.9 m. The steam injection vessel and test section are mounted to the top of the inner tank. The test section is located at a height of 1.4 m relative to the bottom of the inner tank. The tank is filled, to a height of 2.8 m, with ~68°C distilled water simulating the CANDU moderator conditions. The test section was located 1.4 m from the bottom of the inner tank and 1.4 m below the surface of the water. For some of the experiments, additional dummy tubes were placed on the side and below the test section forming a 2 by 3 matrix of channels, as illustrated in Figure 1.

The inner tank was instrumented with dynamic pressure transducers intended to measure the pressure pulse generated by the pressure tube rupture and molten fuel moderator interaction. The pressure transducer located at the bottom of the inner tank (PDE-1) and another 0.95 m from the bottom and 0.175 m from the axis (PDE-2, located on a bar) are utilized in the comparisons between experiment and simulation.

2.1.3 Test section

The test section was a horizontally positioned 1.14 m long CANDU-6 pressure tube filled with a thermite mixture that has a similar composition as CANDU corium ($0.73UO_2/0.11Zr/0.06ZrO_2/0.1Cr$ wt%). The pressure tube was insulated from the thermite with Zircar and tantalum cylinders. The pressure tube ends were sealed with end hubs that attach to the steam injection vessel and support structure. The test section itself was insulated from the water with a quartz tube. This was done to limit heat transfer between the pressure tube and ~68°C water prior to melt ejection. The annulus was filled with low pressure CO_2 (180 kPa). The bottom of the pressure tube had a pre-machined groove located on the outside surface to ensure a predictable rupture at a defined location.

2.1.4 Steam injection vessel

The steam injection vessel was used to supply steam to the pressure tube, simulating the coolant flow to the channel following pressure-tube rupture via the non-blocked end of a pressure tube in a reactor. The steam injection vessel had a total volume of 23 L and was separated from the test section by the steam injection lines and the steam injection ball valves. The steam injection lines and gas space in the test section were initially filled with helium.

2.1.5 General test procedure

Programmable logic controllers were used to control the series of events that led to the ejection of molten corium. First, the confinement tank was evacuated and then filled with helium to reduce the oxygen concentration. The inner tank was then filled with water that was initially ~90°C. The water in the steam injection vessel was heated to its saturation temperature (~310°C). Next, the

~2400°C molten corium was generated by sending current through the igniter wire and sparkler located within the thermite. Upon successful ignition, the ball valves interconnecting the pressure tube and steam injection vessel were then opened, providing ~17 L of steam at ~10 MPa to the pressure tube, increasing the test section pressure and causing it to rupture. Measurements of the recorded and saved transient included static and dynamic pressures, temperatures, and acceleration. Post test analysis included examination of the test section and measurements of corium particle size and composition.

2.1.6 Experimental Results

Prior to the corium ejection tests, two base-line reference tests, with no molten material present, were completed to characterize the pressure pulse and subsequent vessel response following rupture of the pressure tube at ~10 MPa. These tests are referred to as the Non-Corium Commissioning tests and are labeled as NC1 and NC2 in this paper. The test procedure for the non-corium tests were similar to the corium tests, except that the pressure tube was filled with helium instead of thermite. One experiment with 5 kg of thermite in the test section was selected for modeling. This test is labeled as 5kg. Details of these experiments can be found in [1, 2] and a summary of the initial conditions, pulse magnitudes, and their response times are given in Table 1.

Table 1 Important information for the first and second non corium test (NC1 and NC2) [1] and the 5 kg test [2].

Test Label	Driving Material	Driving Temperature at time of Rupture (°C)	Driving Pressure at time of Rupture (MPa)	Moderator Temperature at time of Rupture (°C)	PCB-1 Response Times (s)	PCB-2 Magnitude (MPa)
NC1	Water	315	12.2	~68	0.003, 0.015, 0.023	3.5
NC2	Water	314	14.6	~68	NA	5.5-7.0
5kg	Water / corium	310	11.5	~68	0.003, 0.01, 0.0165	4.0

2.2 MC3D

MC3D V3.6 is a program for the calculation of different types of multiphase multicomponent flows. It has been built with the FCI calculations in mind. Other FCI programs exist and a comparative review of the similarities and differences of these codes was given by Meignen [3].

MC3D has two applications, PREMIXING and EXPLOSION, that when combined together simulate the injection and interaction of the molten fuel with the subcooled moderator and determines the pressure wave, as well as other thermophysical parameters, generated by the interaction [4, 5]. Only the EXPLOSION application is used in this work.

The EXPLOSION application has five constituents named liquid (LIQ), steam (VAP), non-condensable gases (MEL), fuel drops (GOU), and fuel fragments (FRA). The terms in parentheses are the variable names in the code. Each component has its own continuity equation, but there are only four momentum and energy equations since gases are handled as one. There is also one volume balance equation. The main variables are five volume fractions, four velocity vectors, four enthalpies, and one pressure.

The heat and mass transfer in the EXPLOSION application of MC3D utilizes the non-equilibrium approach (as opposed to a micro-interaction approach) where the fragments give off their heat to the surrounding environment, through heating or vaporization, over a finite time determined by the local conditions and assumptions. The micro-interaction approach assumes a homogenous mixture.

The fragmentation of large drops into smaller fragments can be accommodated by either the thermal or hydrodynamic phenomena. The thermal fragmentation is due to instabilities of the vapour film around the drops whereas the hydrodynamic fragmentation is due to velocity differences between the drops and surrounding medium.

3. MC3D modelling assumptions for the MFMI experiment

3.1 Geometry

Of the two options available, a Cylindrical coordinate system was chosen. Each option (Cylindrical or Cartesian) had limitations in correctly modelling the actual geometry since a full 3D model is required (although the code is named MC3D, it is not currently able to handle a full 3D simulation). The Cartesian coordinate system allowed for modelling the test section and dummy channels, but the surrounding walls could not be modelled as cylindrical. This deficiency prevented comparison of the reflected pressure waves in the experiment, which is an important factor in comparing numerical to experimental results.

The Cylindrical coordinate system required an approximation of the test section. It was modelled as a partial sphere with flat bottom representing the injection site. This shape is not thought to play a significant role in the results. Because of the use of the Cylindrical coordinate system, it was not possible to create the dummy channels. However, the dummy channel effect on the pressure wave was investigated in the Cartesian coordinate system. It was found that the dummy channels did not play a significant role in dynamic pressure wave in MC3D.

The inner tank was modelled with an inner radius of 0.625 m. The center of the test section was positioned 1.4 m from the bottom of the tank. The water-air interface was located 2.8 m from the bottom of the tank. The gas column above the water was chosen to be 2.2 m high to simulate the amount of gas space inside the confinement tank.

3.2 Constituents

Fuel - The molten material was selected as user defined. The properties of the corium in the MFMI experiment are not specifically known. Instead, the material properties were taken from those used in modelling the KROTOS experiments, which can be considered similar. The only property that was changed was the solid/liquid temperatures, which were chosen to be $2630^{o}K$ and $2650^{o}K$, respectively; to match the melting temperature values determined from melt tests of the MFMI corium.

Liquid - The option named WATER was used to represent the moderator, as recommended in the MC3D user manual [6]. For simplicity, vapour is used as the cover gas in the confinement vessel.

Non-Condensable gases - The non-condensable gas produced from the molten fuel moderator interaction is hydrogen. More specifically, the hydrogen is generated from the oxidation of the zirconium in the molten fuel.

3.3 Meshing

The fixed grid had 38 nodes in the radial direction (R) and 115 nodes in the axial direction (Z) (Figure 2). The axial and radial nodeing was positioned such that the resolution was higher near the location of the pressure tube. The azimuthal direction also required input. This was chosen as 1 cell to represent the full 360 degrees (as recommended in the MC3D user manual [6]). Evaluation of the mesh sensitivity was not performed in this work. Meshing resolution was based on meshing schemes presented in the literature [7].

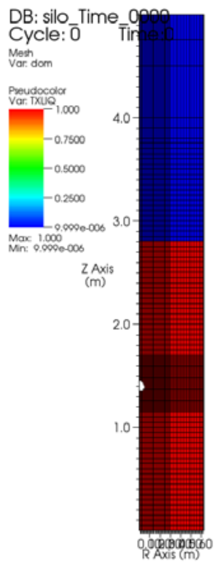

Figure 2 Grid of MFMI simulation.

3.4 Initial and boundary conditions

For the initial conditions, the hydrostatic pressure was set to 10^5 Pa and the domain temperature was set to 341^oK.

All four domain-edges were considered rigid boundaries, meaning that the perpendicular velocity was set equal to zero. The cell faces on the pressure tube were also considered rigid.

The bottom three cell faces of the pressure tube were the injection sites. The faces required inputs of the material being injected, the volume fraction, the velocity, the temperature, and the pressure. This input boundary condition is discussed in the next section.

3.5 CATHENA simulations

CATHENA (Canadian Algorithm for THermalhydraulic Network Analysis) is a thermalhydraulics code developed by AECL [8]. CATHENA was used to model the input parameters required for MC3D. These input parameters were void fraction, pressure, liquid velocity, vapour velocity, liquid temperature and vapour temperature, all as a function of time. The geometry modeled in CATHENA included the steam injection vessel, test section, and interconnected piping. The first CATHENA input file for each test condition was run using the boundary condition from Table 1 to develop the steady state conditions. These steady state conditions were then used in the second input file which included a break discharge model intended to simulate the failure of the pressure tube. The break in the pressure tube was assumed to be instantaneous and the discharge coefficient was set to a value of 1.0. The output results from CATHENA were then discretized and input into the MC3D boundary conditions.

4. Results and Discussion

Comparisons were made between simulations and results for pressure transducers PDE-1 and PDE-2. The pressure transducer PDE-1 was located at the bottom of the inner tank and PDE-2 was located on a bar 0.95 m from the bottom of the tank and 0.175 m from the axis. In particular, PDE-1 and PDE-2 simulations were evaluated for the magnitudes in pressure pulses and timing of the reflected waves. Simulations and results for the first and second non-corium and 5 kg tests are given in this section.

A comparison of the dynamic pressure measured and simulated at PDE-1 and PDE-2 for the first non-corium commissioning test is shown in Figure 3 and Figure 4, respectively. The experiment shows that the pressure transducer PDE-1 measured a maximum pressure pulse of ~5 MPa with three distinct pressure pulses within the first 0.03 s. Despite MC3D not being able to complete its calculation, the results show that it did not capture the pulse frequency correctly. The reflected waves are generated by the pressure wave travelling inside the confinement vessel and through the moderator and cover gas. It was expected that the frequency would not be captured exactly because of small differences in geometry and because of the approximation in the code that the cover gas was vapour instead of helium. However, the speed of sound in helium is much faster than in vapour, meaning the results are opposite of what was expected. The reason for this is explained in the next paragraph. The magnitude of the first simulated pulse appears to have two parts. The first part is very sharp spike in pressure reaching 3 MPa, while the rest of the pulse has a peak of ~1.5 MPa. The pressure transducer PDE-2 measured a large single pulse of ~4 MPa followed by only one small reflected wave at 0.015 s. MC3D shows a smaller magnitude in pressure pulse of ~1 MPa with a similar discrepancy in the timing of reflected pressure waves.

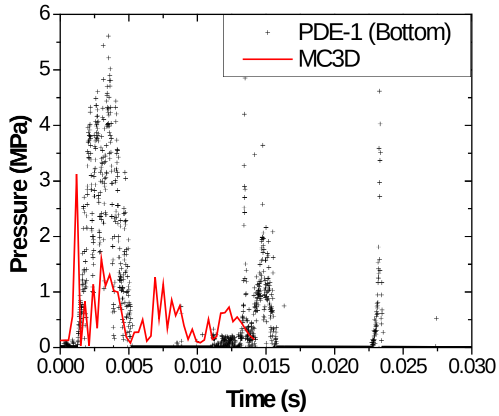

Figure 3 Comparison of the dynamic pressure measured and simulated at the location of PDE-1 for NC1.

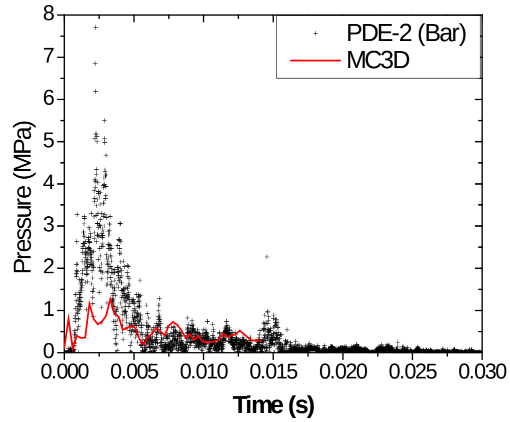

Figure 4 Comparison of the dynamic pressure measured and simulated at the location of PDE-2 for NC1.

A comparison of the dynamic pressure measured and simulated at PDE-1 and PDE-2 for the second non-corium commissioning test is shown in Figure 5 and Figure 6, respectively. PDE-1 failed in this experiment and did not provide any data for comparison. The simulation shown in Figure 5 is similar to that of Figure 3 except that the higher test section pressure resulted in an overall increase in the pressure wave magnitude. Again, MC3D was not able to complete its calculations due to an error generated during the calculation. The pressure transducer PDE-2 measured a large single pulse of ~6 MPa followed by a distinct reflected wave at 0.005 s before the pressure dropped to values below 1 MPa. MC3D predicts a much smaller pulse magnitude ~1.5 MPa and disagreement in the timing of the reflected wave. This time however, the reflected waves in the experiment have a smaller period than what was calculated, which was what was expected. The timing of the measured pulses of the NC2 test was significantly different then the first test. The timing of the pulses in the NC2 test is consistent with what was expected. This may indicate that the confinement vessel may not have been adequately purged with Helium in the NC1 test. The pressure pulses were more consistent with air as the cover gas.

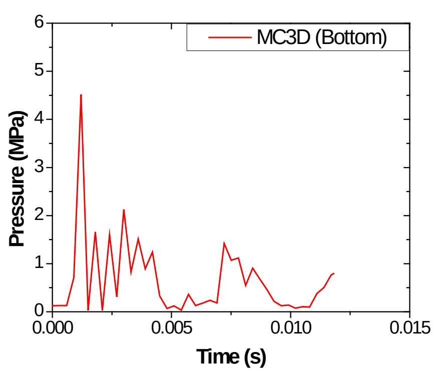

Figure 5 Dynamic pressure simulated at the location of PDE-1 for NC2.

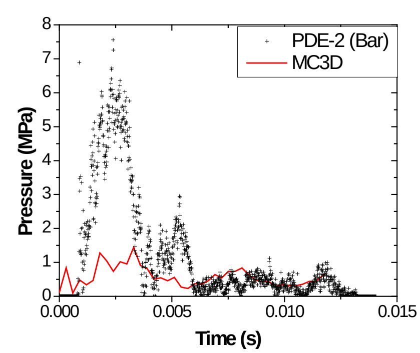

Figure 6 Comparison of the dynamic pressure measured and simulated at the location of PDE-2 for NC2.

Two cases were run in MC3D for the 5 kg commissioning test. The first was done using the assumption that water was the only material ejected from the pressure tube. In the second case, the melt and water are ejected with the assumptions of a dispersed discharge model. This discharge model assumes that the acoustic pressure waves in the channel, caused by the rupture of the pressure tube, cause the molten material and steam to form a homogeneous mixture that exits the channel at a common velocity. It was also assumed that the melt does not play a significant role in the ejection. With these assumptions, the CATHENA results are used for the boundary conditions, but with one modification. The melt particles are assumed to be injected at the same conditions as the liquid water. The last parameter to choose is the volume fraction of the melt. No experimental information for this parameter is available and a parametric study would normally be required. However, another investigation of the same experiments was performed by Diab [9] and that work included a parametric study of this parameter. A volume fraction of the melt equal to 8% of the total volume was used based on Diab's work. The volume fractions of the liquid and vapour calculated by CATHENA were adjusted accordingly. The two calculations are used to show the difference in results with the addition of molten material.

A comparison of the dynamic pressure measured and simulated at PDE-1 and PDE-2 for the 5 kg commissioning test is shown in Figure 7 and Figure 8, respectively. PDE-1 measured six pressure pulses within 0.03 s, with the maximum pulse pressure being ~2.3 MPa. The results for both calculations show a slightly faster pressure pulse frequency. The magnitudes of the reflected pressure waves are in good agreement. However, the initial pulse in the two simulations is quite different from each other and from the measured pulse. The simulation with water-only has one initial spike in the first pulse that reaches 4.2 MPa. The simulation with water and corium melt has two spikes, the first is 4.6 MPa and the second 6.8 MPa. PDE-2 measured a pressure pulse of ~4 MPa with several fluctuation occurring before the pressure dropped off to ~0.0 MPa. In Figure 8, it can be seen that the two simulations are quite similar with the exception being that the water and melt case had a slightly higher peak pressure. Both the simulation and measurements show pressure oscillations until 0.02 s before smoothly declining to 0.0 MPa.

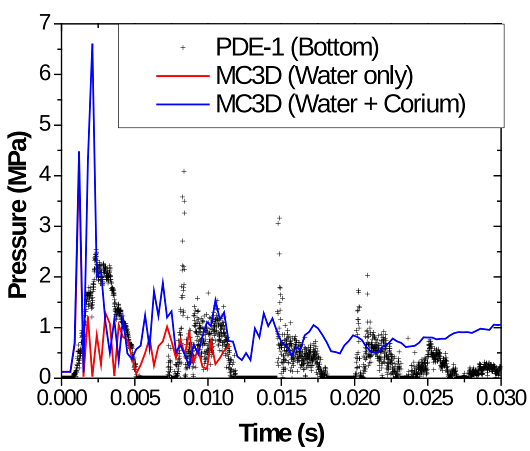

Figure 7 Comparison of the dynamic pressure measured and simulated at the location of PDE-1 for 5 kg.

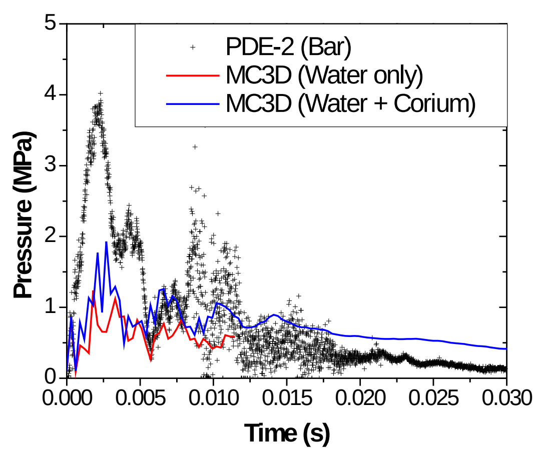

Figure 8 Comparison of the dynamic pressure measured and simulated at the location of PDE-2 for 5 kg.

5. Conclusion

MC3D V3.6 is a program for the calculation of different types of multiphase multi-component flows with an emphasis on FCI's. One of the significant differences between the MFMI experimental program and others is that the MFMI is high pressure driven discharge where as the others are low pressure or gravity driven. MC3D is very well developed for the low pressure or gravity driven flows since this is its main focus. Many difficulties were encountered in the MFMI simulations because of the inability to properly specify discharge parameters. This information must be provided in the MC3D input file. CATHENA is capable of calculating this information, but only for a steam/water discharge. In general, MC3D simulations of the experimental results with corium captured the qualitative characteristics. The simulated pressure magnitudes were mostly lower at the bar than what was measured in the experiment. More consistency would be gained if it were possible to better define the boundary conditions at the location of the break.

6. References

[1] T. Nitheanandan, G. Kyle, D.B. Sanderson and A.J. White, "Molten Fuel Moderator Interaction Experiments for PHWR's", Proceedings of the 2005 International Congress on Advances in Nuclear Power Plants, Seoul, Korea, 2005 May 15-19.

[2] T. Nitheanandan, G. Kyle, R. O'Conner, and D.B. Sanderson, "The Results From the First High-Pressure Melt Ejection Test Completed in the Molten Fuel Moderator Interaction Facility at Chalk River Laboratories", Proceedings of the 2006 International Congress on Advances in Nuclear Power Plants, Reno, Nevada, 2006 June 4-8.

[3] R. Meignen and D. Magallon, "Comparative Review of FCI Computer Models Used in the OECD-SERENA Program", Proc. ICAPP '05. Seoul, Korea, 2005 May 15-19, Paper 5087.

[4] R. Meignen, "MC3D V3.6 Description of the Physical Models of the PREMIXING Application", ISRN Report, DSR/SAGR/67, 2009.

[5] R. Meignen, "MC3D V3.6 Description of the Physical Models of the EXPLOSION Application", ISRN Report, DSR/SAGR/68, 2009.

[6] S. Picchi, M. Elmo, R. Meignen and J. Lamome, "MC3D V3.6 User's Guide", ISRN Report, DSR/SAGR/65, 2009.

[7] M. Leskovar, "Simulation of First SERENA KROTOS Steam Explosion Experiment", Proceedings of the 2009 International Congress on Advances in Nuclear Power Plants, Tokyo, Japan, 2009 May 10-14.

[8] B.N. Hanna, Nuclear Engineering & Design, 180, pp. 113-131, 1998

[9] A.K. Diab, "Modeling of Molten-Fuel-Moderator Interactions", Thesis, UW-Madison, Wisconsin, USA, 2007.