International Conference
Nuclear Energy for New Europe 2007
Portorož /Slovenia /September 10-13
port2007@ijs.si
www.nss.si/port2007
+386 1 588 5247, fax +386 1 588 5376
PORT2007, Nuclear Society of Slovenia, Jamova 39, SI-1000 Ljubljana, Slovenia

Simulation of Steam Explosion Experiment TROI-13 with MC3D

Mitja Uršič, Nicolas Marmin, Matjaž Leskovar
Jožef Stefan Institute
Jamova 39, SI-1000 Ljubljana, Slovenia
mitja.ursic@ijs.si

ABSTRACT

A steam explosion is an important nuclear safety issue in case of a severe reactor accident because it could induce dynamic loading on surrounding structures, leading potentially to an early release of radioactive material into the environment.

Studies of the steam explosion consequences have to be based on experimental research programs like TROI (Test for Real cOrium Interaction with water) and FCI (fuel coolant interaction) codes like MC3D. In this work the TROI-13 FCI experiment was analysed with the MC3D code. The TROI-13 experiment resulted in a spontaneous steam explosion.

The premixing simulation was performed to determine the initial conditions for the steam explosion. A number of steam explosion simulations were performed, changing the mass of melt droplets and position of triggering. The results showed that there is an important influence of the participating mass of melt droplets on the pressure impulse. To determine the participating mass, the processes of melt droplets creation and droplets solidification should be properly taken into account.

1 INTRODUCTION

A steam explosion may develop when the molten core (corium) interacts with the coolant (water). During this process the thermal energy of corium is intensively transferred to water. The time scale of heat transfer from melt to water is shorter than the time scale for pressure relief. The water vaporizes at high pressure and expands, doing work on its surroundings. Although the steam explosion has probably a low probability of occurrence, it is an important nuclear safety issue in case of a severe reactor accident. The expansion caused by the very high pressure could induce dynamic loading on surrounding structures including safety relevant components of the plant. A potential catastrophic consequence of dynamic loadings is an early loss of containment integrity, leading to an early release of radioactive material into the environment. [1, 2]

The prediction of steam explosion consequences and the understanding of the steam explosion event have to be based on experiments and models. Experiments provide experimental data to investigate the fundamental issues of steam explosions, to enable the evaluation of structural loadings and to improve the severe accident management. Experimental data are also used for FCI computer models verification. Models are used for modelling of the different steam explosion phases: premixing (fragmentation of corium when mixing with water), triggering of the explosion, propagation (thermal energy of the melt is converted into thermal energy of the coolant) and expansion (thermal energy of the coolant is converted into mechanical energy). Modelling improves understanding of the steam explosion

event and also highlights some issues that are either not well understood or require further experimental investigation and verification. [3, 4]

TROI is one of the research programs, which was established to provide experimental data to investigate the fundamental issues of steam explosions, to enable the evaluation of structural loadings and to improve the severe accident management. The program started in 1997 at KAERI (Korea Atomic Energy Research Institute). The TROI facility has a 3D geometry and so is an extension of 1D experiments to more realistic conditions. Among several experiments performed in the TROI programme, the TROI-13 FCI experiment was chosen for the simulation. Namely, in the TROI-13 experiment, an eutectic corium composition was used and the experiment resulted in a spontaneous steam explosion. The TROI-13 experiment was simulated and analysed with the computer code MC3D version 3.5 patch 3. MC3D is being developed by IRSN and CEA, France. MC3D is built mainly for the evaluation of the complex phenomenon of FCI. MC3D has two main applications, which are being developed for premixing and steam explosion calculations. The premixing application describes the jet break-up from the jet into melt droplets (order of cm in diameter), coalescence of melt droplets to the jet, coarse melt droplets break-up and fine fragmentation of melt drops into fine fragments (less than 100 μm in diameter). The steam explosion application deals with fine fragmentation of melt drops and heat exchange between the produced fragments and the coolant. [1, 5, 6, 7]

In the paper, the description of the TROI facility and the main TROI-13 experimental results are first provided. Next, the simulation results of the performed MC3D calculations of steam explosion TROI-13 experiment are being presented and discussed in comparison with the experimental measurements. Finally, conclusion remarks are provided.

2 TROI

2.1 TROI facility and test procedure

As shown on Figure 1, the TROI facility consists of a furnace vessel, a pressure vessel and a sliding valve. The furnace vessel contains a cold crucible (copper tubes), release assembly (plug and puncher) and instrumentation for transient pressure (FSVP001) and melt temperature (pyrometer). The melt is prepared in the cold crucible. The sliding valve is opened after the melting is completed. The melt with a temperature higher than 3000 K is being released when the plug is removed and the puncher breaks the 2-3 mm thick crust formed at the bottom of the melt. The puncher actuation time is the starting time for the dynamic data acquisition system and camera. The melt is delivered into the pressure vessel, which contains the test section and the instrumentation for the measurement of coolant temperature (IVT101 - IVT104), dynamic pressure in the coolant (IVDP101 – IVDP104), dynamic load at the bottom of the test section (IVDL101), atmosphere temperature (PVT001 – PVT005), transient pressure (PVSP004 – PVSP005), dynamic pressure (PVDP004 – PVDP005), gas sampling (GAS004 – GAS005) and visualization (cameras). The melt is poured into the water inside the test section, which is 150 cm high and has an inner diameter 60 cm. Due to FCI a steam explosion may occur. [5, 6]

2.2 TROI-13 experiment

The TROI-13 experiment was one of the various experiments performed in the TROI facility. The corium composition used in the experiment was 70w% (mass fraction) of UO_2 and 30w% of ZrO_2. The corium (13.7 kg) was heated to a temperature near 3500 K. 7.735 kg of the melt corium was poured into the test vessel filled up to 67 cm with water at a temperature 292 K. The initial pressure in air was 0.108 MPa. The free fall of the melt corium

was 3.8 m. The free volume of the pressure vessel was 8.032 m^3. In the experiment a spontaneous steam explosion occurred around 0.092 s after the melted corium (jet) hit the surface of the water. Results of measurements are presented on Table 1 and Figure 2. [6]

In Table 1 some results of different TROI experiments are given. All experiments have a similar experimental set-up as the TROI-13 experiment. Some important information could be inferred from Table 1 and reference [6]. First the amount of fragments smaller than 0.425 mm ($p_{<0.425mm}$) become important in the case of steam explosion. For that reason fine droplet fragmentation was not taken into account in the premixing simulation of TROI-13 experiment. Next a SDM (mean Sauter diameter is defined as the diameter of a sphere that has the same volume/surface area ratio as a particle of interest) of less than 1 mm could be expected in the case of steam explosions. Furthermore the SDM around 2 mm could be expected in the premixing phase. In case of the TROI-11 experiment the SDM is overestimated because a lot of UO_2 pellets in their original shape were observed in the test vessel. This indicates that the mixture had not been fully melted in TROI-11. Finally coalescence of the melt droplets was low (no information about observed cake was given).

Figure 2 gives the dynamic pressure history measured inside test vessel in the TROI-13 experiment. Steam explosion started at about 1220 ms. A pressure peak of 7 MPa and duration of 1 ms was measured at 1224 ms. Also the dynamic load was measured at the bottom of test vessel. The pressure impulse was 250 kN high and 15 ms long.

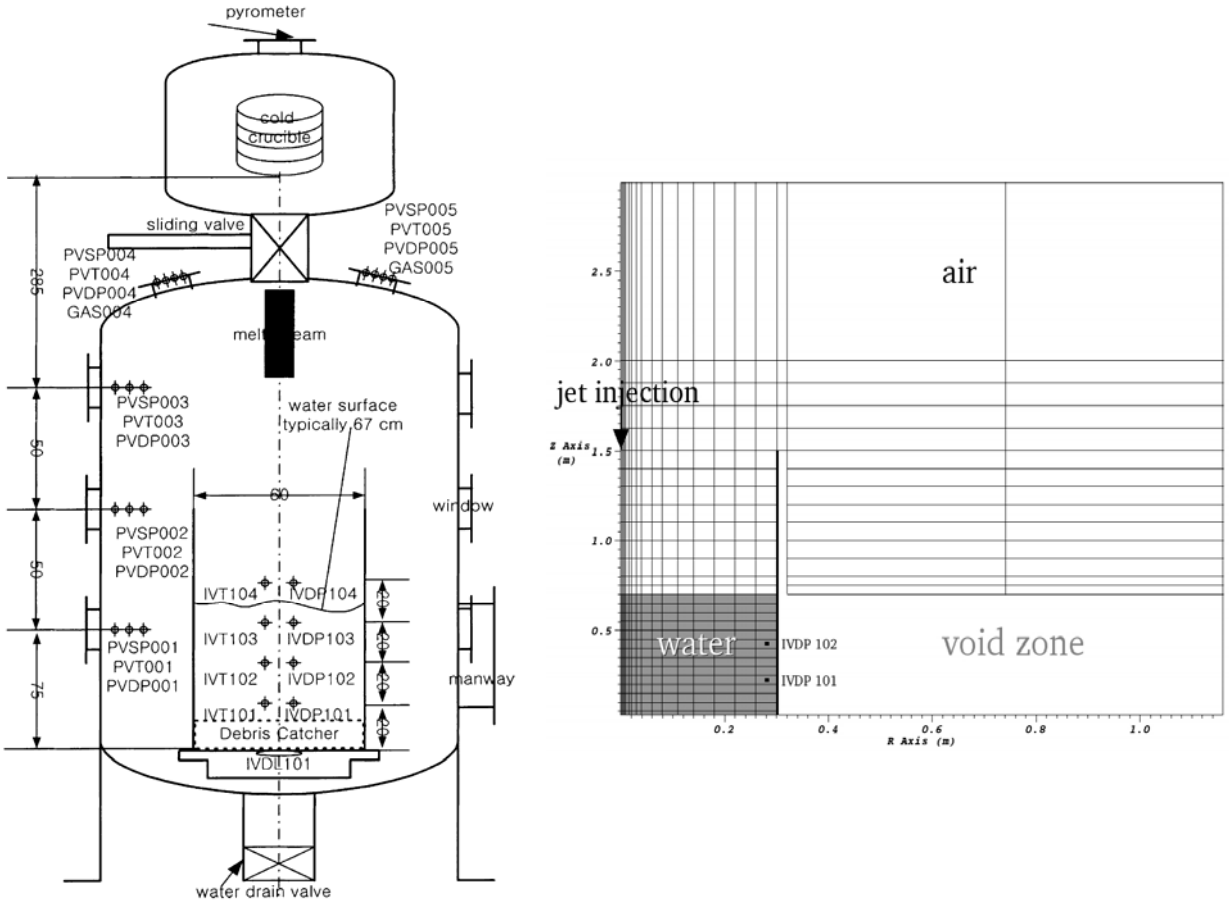

Figure 1**:** Schematic diagram of TROI facility with units in cm is shown on left [6]. On right the mesh representation of the TROI-13 experiment used for MC3D simulations is shown. On the bottom of the test section a 0.03 m thick debris catcher is placed. The jet was injected at height 1.75 m with velocity 7.35 m/s and diameter of 2 cm. Level of the water was 0.7 m.

Table 1: Results from TROI FCI experiments [6]. Abbreviation are: SDM is the mean Sauter diameter of the experimental measured debris, $p_{<0.425mm}$ is the mass fraction of debris particles whose size was lower than the sieve size of 0.425 mm and SE indicates whether a spontaneous steam explosion occurred or not.

Result	*Unit*	*TROI-9*	*TROI-10*	*TROI-11*	*TROI-12*	*TROI-13*	*TROI-14*
SDM	mm	1.87	1.08	2.99	0.68	0.71	0.81
$p_{<0.425mm}$	%	2.3	8.7	0.5	20.9	18.9	15.7
SE	N/A	No	Yes	No	Yes	Yes	Yes

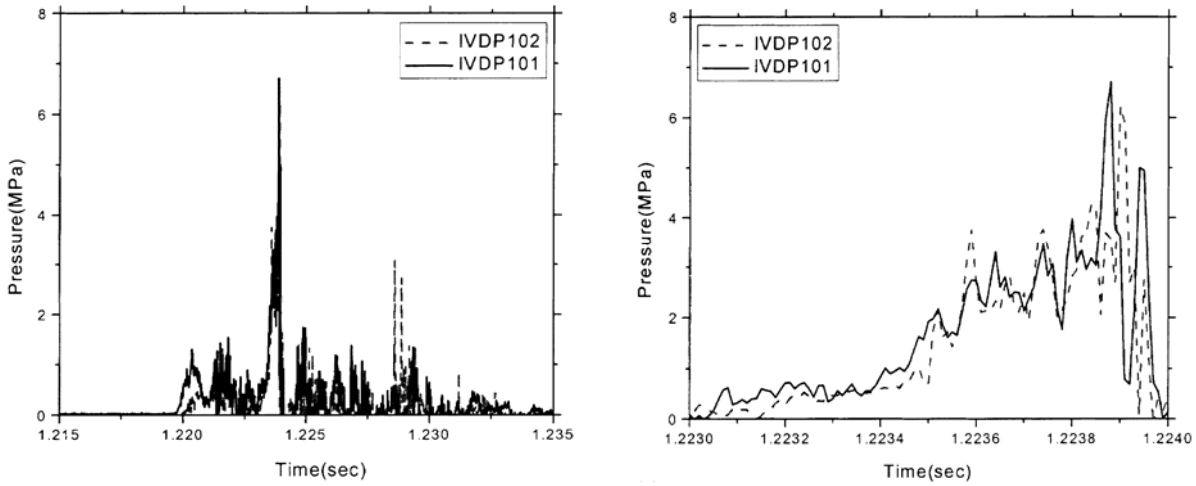

Figure 2**:** Experimental measurements of dynamic pressure inside test vessel (left). On the right enlarged result is given. [6]

3 SIMULATION OF EXPERIMENT TROI-13 WITH MC3D

3.1 Premixing simulation

The simulation of the premixing phase is important to determine the initial conditions for the explosion application. On figure 1 the mesh used for the TROI-13 premixing experiment simulation is given. Data necessary for the simulation were gained or estimated based on ref. [6]. Estimation was important due to the lack of the premixing experimental results.

The MC3D premixing application description of the melt is made with three fields, describing the continuous fuel, the melt droplets and the fragments. The continuous field is used to describe the jet. The second field corresponds to the drops describing droplets issued from the jet fragmentation. The last field, which is not taken into account in the TROI-13 premixing simulation (see Section 2.2), is used to describe the fuel fragments issuing from drop fine fragmentation. The relations of jet fragmentation and coalescence are used to describe the mass transportation between the continuous fuel and droplets field. Droplet fragmentation inside the droplet field is driven by the coarse melt drop break-up process.

Although default or recommended values were used as far as possible in the premixing simulation with MC3D code, information from [6,8,9] were used to study and estimate some simulation parameters which could have an influence on the mechanisms of jet break-up, coalescence process, melt droplets coarse break-up and solidifications effects of the melt droplets. The amount of melt droplets is important because they drive the heat transfer and also represent the source for fine fragmentation during the explosion.

Both, the jet fragmentation and coalescence processes in water depend on material properties of the melted corium. The temperature of the injected jet (T_{jet}) was first taken into

account. As it could be seen from [6] the results of T_{jet} measurements were not reliable. Also the position of jet injection in the simulation was lower than it was in the experiment. Finally the temperature of 3300 K was chosen based on ref. [9]. Next the temperature ($T_{sol\text{-}liq}$) to avoid strong compaction of the solid corium droplets (coalescence) was considered. $T_{sol\text{-}liq}$ represents the threshold temperature for the solid aspect of the drop. The MC3D code compares the drop mean temperature with $T_{sol\text{-}liq}$. Below $T_{sol\text{-}liq}$ the droplet is treated as solid and no coalescence is allowed. $T_{sol\text{-}liq}$ could be equal to solid temperature only if the melt inside the droplet is well mixed. If no mixing occurs then the heat could be transferred only by conduction and a profile as given in ref. [8] could occur. Because the MC3D code does not take into account a temperature profile and it is believed that mixing inside the melt drop is not ideal, the $T_{sol\text{-}liq}$ temperature higher then the default solid temperature (2800 K) should be used. Finally, the liquidus temperature (2820 K) was chosen for $T_{sol\text{-}liq}$.

The coarse drop break-up model used in the MC3D code is based on the coarse fragmentation by Rayleigh-Taylor instabilities and depends on the Weber's number (We). If the We of the droplet is above the critical value (We_{crit}) hydrodynamic fragmentation of the droplet could occur. Below We_{crit} internal forces inside the droplet cannot overcome the cohesive forces of droplet surface tension and coarse droplet break-up stops. Due to the uncertainties in the correlation [7] the default value We_{crit}=12 was kept despite the fact that at coarse droplet break-up also droplets with We< We_{crit} are formed. The correlation used in MC3D should hold for We above 350. For We below 350 two additional damping functions were introduced. The first damping function f_1 is for We below 20 and the second f_2 for We below 350. A sensitivity study was performed to evaluate the influence of damping functions on the premixing results (Figure 3).

On Figure 3 (left) the results of simulated SDM are given. The comparison of simulation results to conclusions made in Section 2.2 indicates that the use of both damping functions ($f_1 \cdot f_2$) overestimate SDM (simulated SDM was around 3.5 mm instead of expected 2 mm). The SDM was strongly underestimated due to the overestimation of the coarse break-up process if both damping functions were suppressed (1). By suppressing only the f_2 damping function SDM is still underestimated (f_1). The SDM values for f_1 were around 1.5 mm in the area where coalescence was still not dominant. Therefore simulated SDM was comparable to expected 2 mm (conclusions in Section 2.2). The final decrease of SDM to around 1 mm was due to the coalescence of larger melt droplets at the end of premixing phase.

Figure 3 (right) gives the fraction of melt droplets with regard to the total injected jet mass. Although it was expected to reach lower coalescence with the increased $T_{sol\text{-}liq}$ and by selecting the lower T_{jet} it can be seen from Figure 3 (right), that coalescence in the performed simulation still remains important once the jet reaches the bottom of the test vessel at around 0.25 s. Because the steam explosion occurred before the coalescence could take an important role, no other parameters influencing the coalescence were changed in the premixing simulation. As seen on Figure 3 (left) the suppression of damping functions strongly influences the SDM and consequently the coalescence. The reduction of coalescence at smaller melt droplets could be explained with more extensive droplets freezing. The coalescence was overestimated if compared to the conclusions in Section 2.2 (low coalescence was expected) in all simulated cases. One way to improve the coalescence behaviour in future is to improve the model of melt droplet solidification. The jet fragmentation rate was set to default values and it did not depend on the use of damping functions. There were no experimental data available to evaluate the use of the jet fragmentation model.

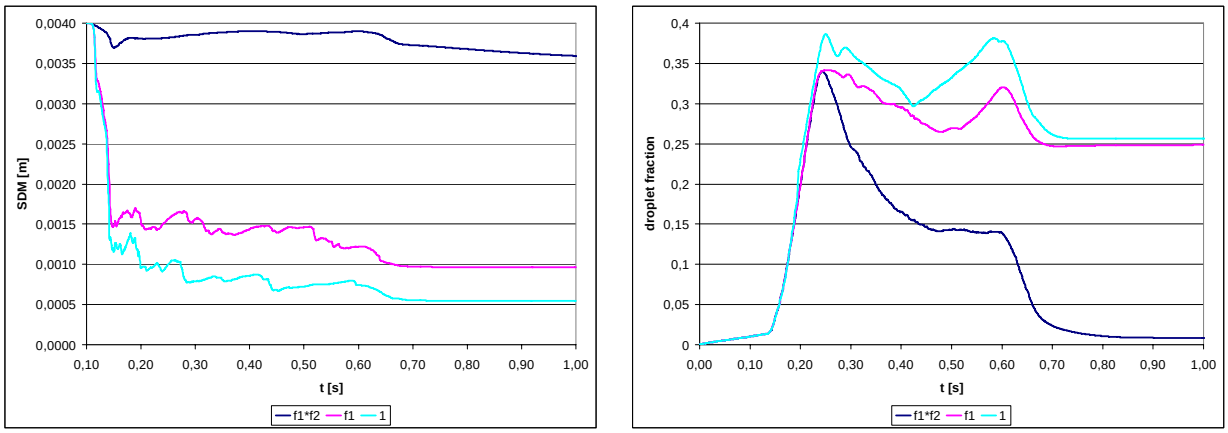

Figure 3**:** The mean Sauter diameter (SDM) history (left) and the melt droplets fraction history (right) for TROI-13 premixing simulation. $f_1 \cdot f_2$ indicates the use of both damping functions, f_1 the use of the first damping function and 1 the use of no damping functions.

3.2 Initial conditions for explosion simulation

The initial conditions inside the test vessel for the steam explosion simulation were chosen based on the TROI-13 experiment premixing simulation when f_2 damping function was suppressed (f_1). The premixing results (f_1) underestimate SDM and overestimate coalescence. The steam explosion was triggered at premixing time 0.25 s. The time was chosen based on the information that the steam explosion occurred around 0.092 s after the jet entered into water (corresponds to premixing time 0.23 s) and based on the high probability that the steam explosion was triggered by the contact of the melt with the bottom of test vessel (premixing time 0.25 s) [6].

The mesh used for the premixing simulation was also used for the steam explosion simulation (Figure 1). For the initial conditions the area of water inside the test vessel was divided into three zones (interaction zone, trigger zone and bulk zone). From premixing results it was estimated that the interaction zone extends from the water surface (0.70 m) to the bottom of the test vessel (0.03 m) and has a radius of 4 cm. A homogenous distribution of melt droplets, vapour and water was set. The volume fraction of melt droplets in the interaction zone was determined based on the mass of the jet entered in the water at time 0.25 s (~1.9 kg). The volume fraction of droplets participating in the steam explosion was varied in the performed simulations. Based on the premixing simulation the temperature and diameter of melt droplets were set to 3150 K and 1.6 mm (Figure 3 (left)). The volume fraction and the temperature of vapour inside the interaction zone were set to values estimated from premixing results (fraction 0.43 and temperature 2760 K). Since the sum of the volume fractions is 1, the volume fraction of water inside the interaction zone had to be adjusted. The water temperature in the interaction zone was set to 310 K and was also estimated from premixing results. The trigger of the steam explosion was modelled with a trigger zone inside the interaction zone. A 1 MPa triggering pressure cell was positioned at the centre axis. The triggering pressure was chosen based on a sensitivity study where the influence of the triggering pressure on the steam explosion results was investigated. The position of the trigger zone in horizontal direction was varied. In the trigger zone the volume fraction of melt droplets from the interaction zone was divided between volume fractions of melt fragments and melt droplets. Other parameters were kept same as in the interaction zone. In the bulk zone only water and vapour were present. The volume fraction of vapour in bulk zone was estimated from premixing results and was set to 0.01. The temperature of water and vapour there was set to the initial temperature of water (292 K). In the simulation also the increase of the water level due to the presence of the jet and vapour was taken into account based on premixing results.

3.3 Results of explosion simulation

The main results of the steam explosion simulations are given on Figure 4 and should be compared with experimental results on Figure 2. The results are given for different positions of the trigger zone. In the simulations the steam explosion was triggered between the bottom (0.03 m) and near-mid (0.4 m) part of the test vessel. The mass of melt droplets participating in the steam explosion was set to fractions 40%, 60%, 80% and 100% of the total jet mass entered in water at triggering time. The pressure was tracked at the positions of pressure detectors IVDP101 and IVDP102 (Figure 1). From the results it can be seen that the mass of droplets has an influence on the height and the position of the pressure peak. With larger melt mass more thermal energy of melt drops is available, resulting generally in higher pressure peaks and larger pressure impulses. Also at higher melt droplets mass the pressure peak was developed earlier.

Further results from Figure 4 are discussed in more details. In the case of triggering the steam explosion at position 0.03 m and 0.1 m the calculated pressure peak height becomes comparable to experimental measurements when assuring that the mass fraction of melt droplet participating in the explosion is 80%. For triggering of the steam explosion at position 0.2 m the calculated pressure peak height becomes comparable to experimental measurements when assuring that the mass fraction of melt droplet participating in the explosion is between 60% and 80%. Next the simulation was performed when the steam explosion was triggered at position 0.3 m. The calculated pressure peak height becomes comparable to experimental measurements when assuring that the mass fraction of melt droplet participating in the explosion is between 40% and 60%. Finally the simulation was performed when the steam explosion was triggered at position 0.4 m. The calculated pressure peak heights are not comparable to experimental measurements. In all discussed pressure peaks the width of the peak was similar to the width of the experimental peak (around 1 ms).

The simulated pressure peak become comparable with measured data if around 60 – 80% of the injected jet mass presented as melt droplets was taken into account in the steam explosion which was triggered at or near the bottom of test vessel. This is in agreement with premixing simulation results where initially 77% of the jet mass in water at triggering time was broken-up into melt droplets. Also the simulated mass of droplets involved in the steam explosion was comparable with the measured mass of fine fragments in Table 1. A possible reasons why the entire melt droplet mass does not participate in the steam explosion is droplet solidification. It is assumed that at triggering time an amount of droplets is already partially frozen and that this crust formation limits fine fragmentation of melt droplets [8]. Further investigations are needed.

Figure 5 shows the steam explosion propagation inside test vessel. The steam explosion was triggered at the bottom of the test vessel with mass fraction 80% of melt droplets in the interaction zone. The steam explosion first developed along the interaction zone and then the pressure wave propagated towards the test vessel wall (time 0.5, 1 and 1.5 ms on Figure 5). The increase of pressure near the wall was due to the superposition of the incoming and reflecting pressure (2 ms). Finally, the pressure decreased between 2.5 and 3 ms.

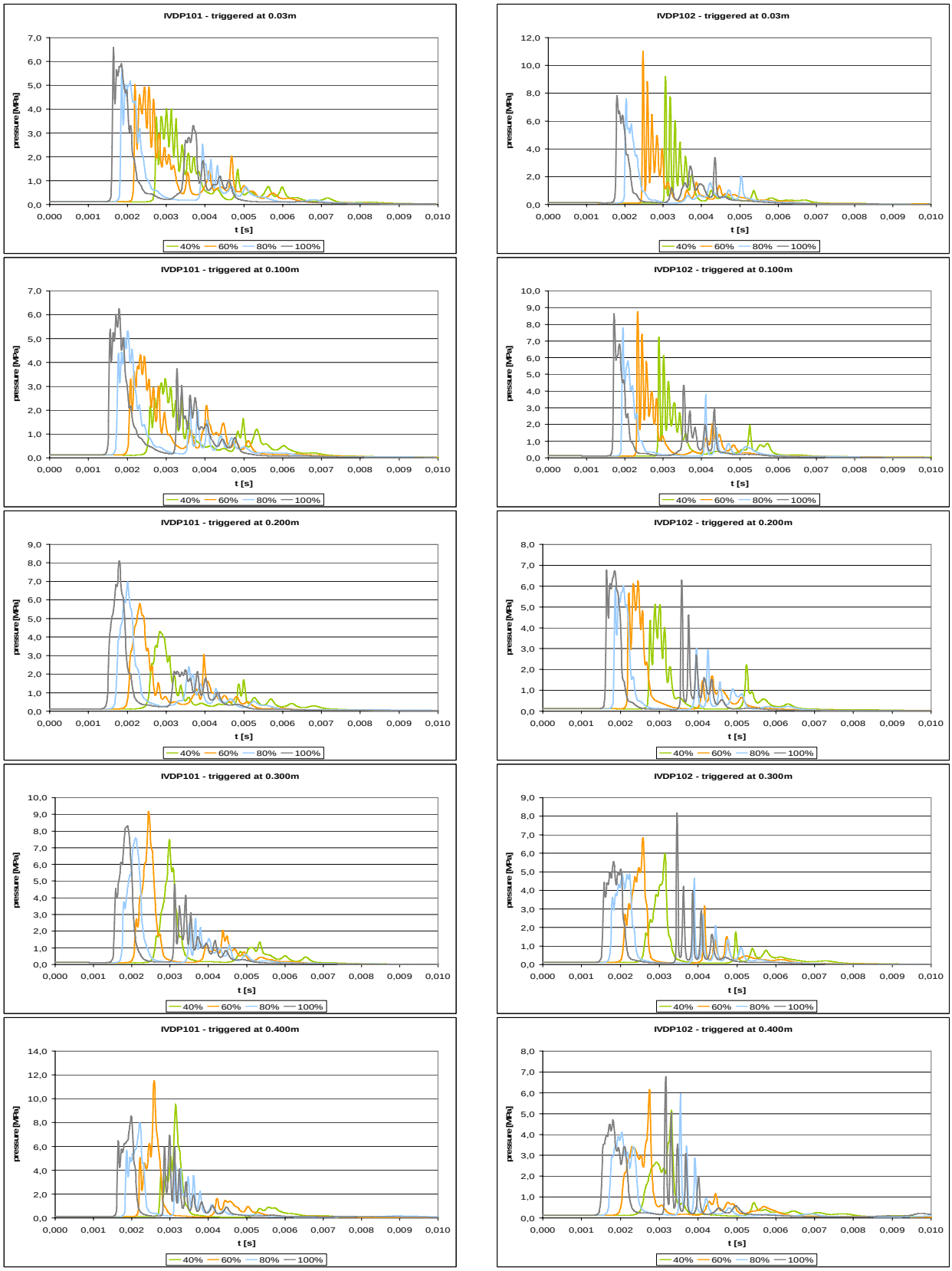

Figure 4**:** Simulated pressure histories at the position of pressure detectors IVDP101 and IVDP102 (Figure 1). Triggering was performed at positions 0.03, 0.1, 0.2, 0.3 and 0.4 m. The melt droplets mass involved in steam explosion is presented as 40%, 60%, 80% and 100% fraction of the total jet mass entered in the water at the time of steam explosion triggering. Time zero on figures represents time of steam explosion triggering.

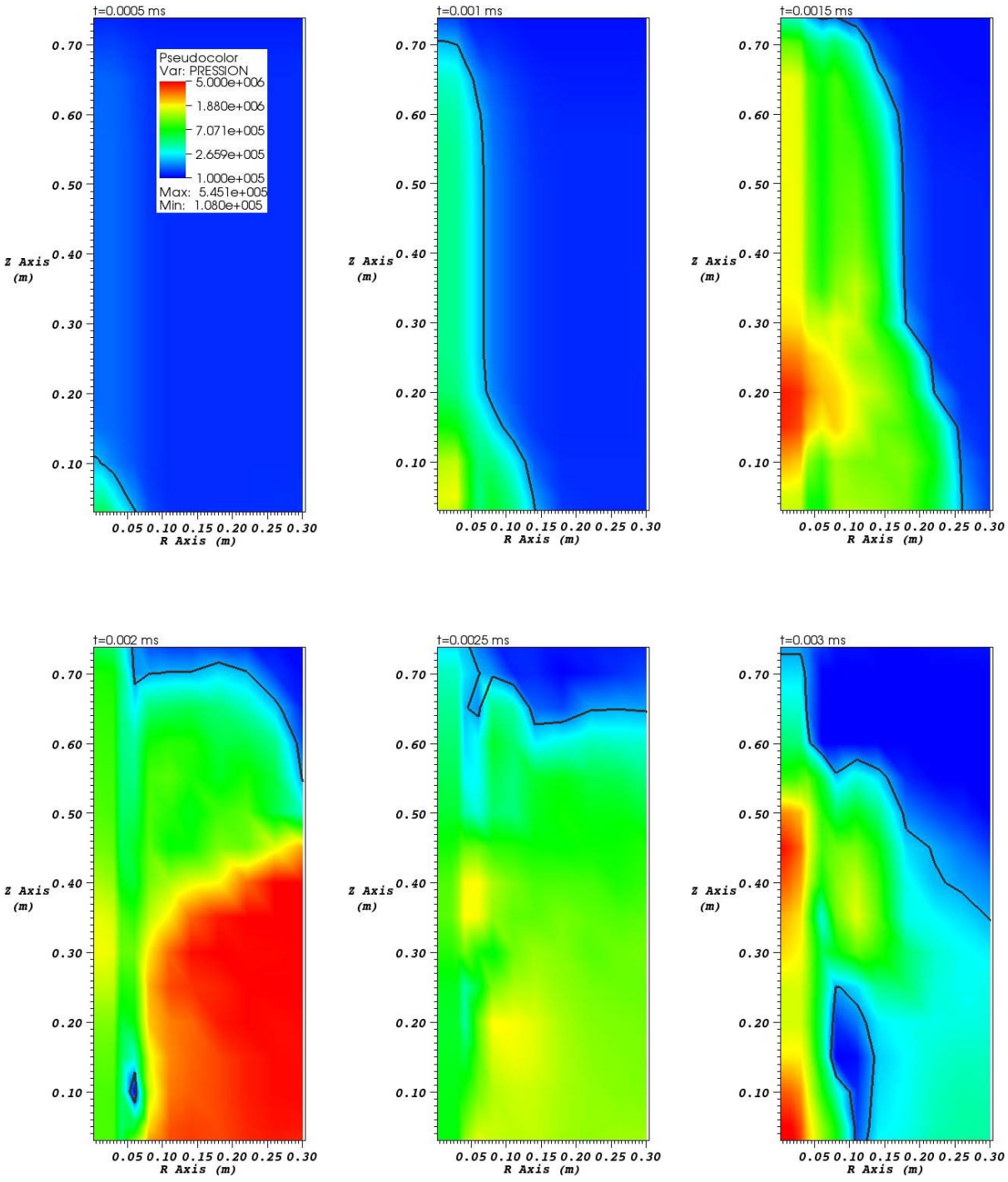

Figure 5**:** Simulated pressure in water inside the test vessel between 0.5 and 3 ms with step of 0.5 ms. The explosion was triggered at position 0.03 m. The initial conditions are set for premixing time 0.25 s. The fraction of melt droplets mass was 80%.

4 CONCLUSION

The purpose of the work was to gain steam explosion model parameters for pre-calculations of planned experiments in the TROI facility. For that reason the TROI-13 FCI experiment was analysed with the computer code MC3D. Although the recommended and default MC3D values were used as far as possible, information from [6] was used to

determine some premixing simulation parameters, which could have an influence on the mechanisms of the jet break-up process, coalescence process, melt droplets coarse break-up and solidifications effects of the melt droplets. All those processes influence the amount and characteristics (like size and temperature profile) of the melt droplets at steam explosion triggering. The droplets are important because they drive the heat transfer and represent the source for fine fragmentation during explosion.

Comparison of premixing results with experimental measurements revealed that premixing simulations underestimate SDM if damping functions are suppressed and overestimate coalescence if the damping factors are used or not. There were no experimental data to evaluate the jet fragmentation model. Nevertheless, premixing simulations were used for help to define the initial conditions for the steam explosion simulations. The results of steam explosion simulations presented on Figure 4, were comparable with experimental measurements. The results of steam explosion simulations indicate that the mass of droplets involved in the steam explosion has an important influence on the pressure impulse. The results also indicate that, due to solidification effects, not all of the melt droplets can participate in the steam explosion. Around 60 – 80% of the injected jet mass presented as melt droplets was participating in the steam explosion. The premixing simulation predicted that at triggering time about 77% of the melt mass in water was in form of droplets. The steam explosion was triggered at or near the bottom of the test vessel.

The results indicate a need for improving the FCI code to be able to take into account the proper mass of active droplets and its characteristics when the steam explosion occurs. One of the ways is to increase the significance of melt droplet solidification in MC3D code. The improvement would help to decrease the coalescence effect and would improve the prediction of the melt droplet mass participating in the steam explosion.

ACKNOWLEDGMENTS

The authors acknowledge the support of the Ministry of Higher Education, Science and Technology of the Republic of Slovenia within the research project J2-6565 and the cooperative CEA-JSI research project (contract number 3211-06-000459). The Jožef Stefan Institute is a member of the Severe Accident Research Network of Excellence (SARNET) within the 6th EU framework programme.

REFERENCES

[1] M. Leskovar, B. Mavko, “Pre-calculations of KROTOS/PLINUS Steam Explosion Experiment with MC3D”, Proc. Int. Conf. Nuclear Energy for New Europe, 2006, Portorož, Slovenia, September 18-21, Nuclear Society of Slovenia, 2006, pp. 809.1-809.14.

[2] D. Magallon, “Steam explosion in light water reactors”, Severe Accident Phenomenology Short Course, 2006, Cadarache, France, January 9-13, SARNET.

[3] M.L. Corradini, B.J. Kim, M.D. Oh, “Vapor Explosions in Light Water Reactors: A Review of Theory and Modeling”, Progress in Nuclear Energy, **22**, 1988, pp. 1-117.

[4] D. Magallon, J.H. Song, R. Meignen, N.D. Suh, “SERENA: Proposal for a Phase 2 programme”, OECD Research programme on fuel-coolant interaction, Revision 2, 31 May 2006.

[5] I.K. Park, Y.J. Chang, Y.S. Shin, C.H. Kim, B.T. Min, S.W. Hong, J.H. Song, H.D. Kim, “Steam Explosion Experiments in the “Test for Real corium Interaction with water (TROI)” Program”, Transactions, SmiRT 16, Washington DC, August 2001, paper 1925.

[6] J.H. Song, I.K. Park, Y.S. Shin, J.H. Kim, S.W. Hong, B.T. Min, H.D. Kim, “Fuel coolant interaction experiments in TROI using a UO_2/ZrO_2 mixture”, Nuclear Engineering and Design, **222**, 2003, pp. 1-15.

[7] R. Meignen, “MC3D Version 3.5: Support guide to the use of MC3D”, IRSN Report, 2006.

[8] M. Leskovar, B. Mavko, “Material Properties Influence on Steam Explosion Efficiency: Prototypic versus Simulant Melts, Eutectic versus Non-Eutectic Melts”, Proc. Int. Conf. Nuclear Energy for New Europe, 2006, Portorož, Slovenia, September 18-21, Nuclear Society of Slovenia, 2006, pp. 811.1-809.15.

[9] D. Magallon, K.H. Bang, S. Basu, G. Berthoud, M. Burger, M.L. Corradini, H. Jacobs, R. Meignen, O. Melikhov, K. Moriyama, M. Naitoh, J.H. Song, N. Suh, T.H. Theofanous, “Results of Phase 1 of OECD Programme SERENA on Fuel-Coolant Interaction”, ERMSAR-2005, Aix-en-Provence, France, 14-16 November 2005, pp. 1-12.