NKS-344
ISBN 978-87-7893-426-0

Analysing Steam Explosions with MC3D

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July 2015

Abstract

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In the sensitivity analysis the effect of three input parameters, melt temperature, triggering time and ambient pressure, is varied to see how changes in these affect the results. Out of these, changing the triggering time had the largest impact on the steam explosion occurrence and strength.

The experiments chosen for simulation were performed as part of the OECD/NEA SERENA program and were run at the TROI research facility. The report also contains a brief description of the OECD/NEA SERENA program, and a more detailed description of the two test facilities used in the program, KROTOS and TROI.

An automated simulation script was developed to speed up the simulation process. The new method also reduces the possibility of human error and makes it possible to queue up simulations.

Key words

steam explosion, fuel-coolant interaction, MC3D, TROI experiments

NKS-344
ISBN 978-87-7893-426-0
Electronic report, July 2015
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Acknowledgements

NKS conveys its gratitude to all organizations and persons who by means of financial support or contributions in kind have made the work presented in this report possible.

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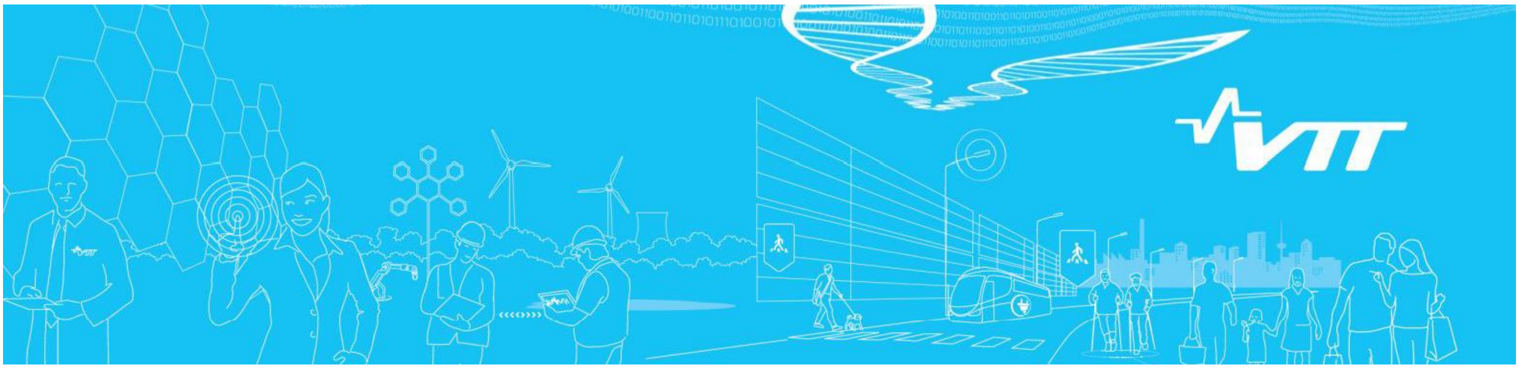
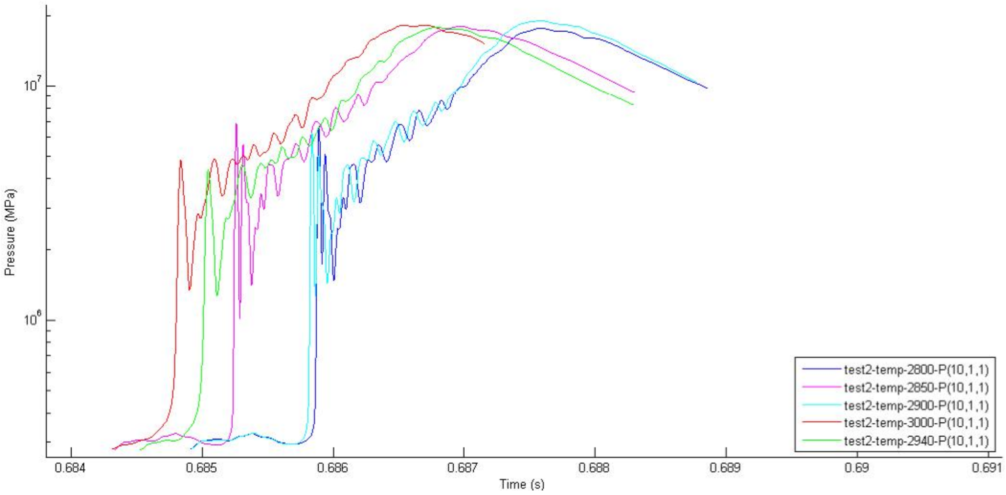


RESEARCH REPORT

VTT-R-00489-15



Analysing Steam Explosions with MC3D

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Confidentiality: Public

Report's title

Analysing Steam Explosions with MC3D

Customer, contact person, address SAFIR2014 Research Programme	**Order reference** SAFIR 26/2014
Project name Vessel failures, vapour Explosions and Spent fuel Pool Accidents	**Project number/Short name** 81659 / VESPA2014
Author(s) Magnus Strandberg	**Pages** 27
Keywords Steam Explosion, MC3D, Fuel Coolant Interaction (FCI), TROI TS-5, TROI TS-3, OCED/NEA SERENA 2	**Report identification code** VTT-R-00489-15

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Confidentiality	Public

ESPOO 25.2.2015

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Distribution (customer and VTT)

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1 Introduction

Steam explosions are energetic Fuel Coolant Interactions(FCI) that might occur when molten fuel comes into contact with the coolant. This report focuses on the experiments performed in the frame of OECD/NEA SERENA 2 program and MC3D simulations. The experiments that are simulated were performed in the TROI experimental facility in South Korea, as part of the SERENA 2 program. The report also contains a short review of different stages and progression of steam explosions.

After this in chapter 3 follows a presentation of the capabilities of the MC3D code, which is developed by IRSN and CEA in France. The MC3D is a multidimensional Eulerian code used to simulate multiphase and multi-constituent flows for nuclear safety applications.

OECD/NEA SERENA 2 program is shortly presented together with the two modern experimental facilities utilized in the program, KROTOS in France and TROI in South Korea, in chapter 4. Also the most important properties of the facilities are compared. There is also a description of two older experimental facilities that are no longer in use.

In the beginning of chapter 5 two of the performed experiments at the TROI facility are presented in more detail. Later the results of the MC3D simulations of the TROI TS-3 and TROI TS-5 experiments are compared to the available experimental data. The simulations were continued to give a slight insight into how sensitive steam explosions and simulation results might be to changes to the different initial conditions, via a so called sensitivity analysis, of which results are presented at the end of chapter 5.

2 Steam explosions in short

Steam explosions are fuel coolant interactions that could occur when molten corium fragments into water. Although molten metal fragmentation into water is a precursor to a steam explosion, it is not a certainty that a steam explosion will occur just because of it, as steam explosions are highly stochastic events. Steam explosion phenomena are usually divided into three stages: premixing, triggering and propagation. The different stages occur at different timescales and involve different physical phenomena. For example premixing can take up to a couple of seconds while both triggering and propagation takes place on a microsecond scale.

Premixing is the first stage, when the melt fragments into drops due to hydrodynamic forces. The drops are surrounded by a vapor film, since the temperature of the melt is very high. The premixing is very sensitive to the initial conditions of both the melt and the coolant as well as injection velocity, and the geometry of the structure where the mixing takes place. Table 1[Strandberg (2014)] an overview of the different initial conditions and how they effect the explosion probability and strength. The most important conditions affecting whether a steam explosion will take place or not and how strong it will be, are the amount of melt that is able to take part in the explosion and the temperature of the melt. An increase in these increase both the explosion probability and strength.

The triggering stage begins when the drop-vapor system is locally disturbed so that the coolant comes into direct contact with the melt, which leads to further fragmentation. A trigger can be either external or internal. The internal trigger is originating from inside the melt configuration itself, it could for example be water that becomes trapped when the melt impact with the bottom of a water filled dry-well. The external trigger is when the disturbance comes from outside the coolant mixture, for example a pressure

Table 1. A quick overview of the different premixing parameters and their effect on the explosion probability and strength.

Property		Explosion probablity	Explosion strength
Amount of melt	↗	↗	↗
Melt temperature	↗	↗	↗
Melt density	↘	↗	↗
Hydrogen production	↗	↗	↘
Void fraction	↗	↗	↘
Ambient pressure (<0.8MPa)	↗	↗	↗
Ambient pressure (>0.8MPa)	↗	↘	↗
Coolant temperature	↘	↘	↗

wave coming from something impacting with the vessel wall due to an external explosion. It should be noted that a triggering event does not necessarily lead to a steam explosion as the shock wave might not be able to ignite the mixture.

The last stage is known as the propagation stage. In this stage the shock wave from the trigger event propagates through the coolant-vapor-melt mixture and ignites it by collapsing the instable drop-vapor system. In the case that the triggering event is successful in igniting the mixture the shock wave will propagate at supersonic speed. If the mixture will not ignite, the progression speed will be much slower. The shock wave further fragments the drops, due to thermohydraulic forces and the differential velocity between the water and the melt.

There are three different types of steam explosions that need to be analyzed in a nuclear power plant safety perspective: in-vessel and ex-vessel steam explosions, as well as steam explosions that can occur when the debris bed is reflooded. The in- and ex-vessel cases differ a bit what comes to initial conditions but the progression is the same. For example ex-vessel cases usually contain more water that is subcooled to a greater degree than the in-vessel case. In the debris bed reflooding cases the melt is “stationary” and it is the water that is injected, instead of the melt as in the other cases.

3 MC3D

The MC3D (Multi Component 3D) code is developed by IRSN and CEA in France. The MC3D is a multidimensional Eulerian code used to simulate multiphase and multi-constituent flows for nuclear safety applications. It is usable for both research and safety usage. As the name indicates, the code can be used to simulate 3D scenarios as well as 2D. Though in this report only 2 dimensional simulations will be done, as a 3D simulation would not yield drastically improved results. This is because 3D geometries are typically approximately symmetric in respect to the rotational axis. 2D simulations will also shorten the simulation time.[Meignen and Picchi (2012)] Shorter simulation times are eligible as this report contains a sensitivity analysis where several simulations with small parameter changes are analysed.

3.1 MC3D general description

MC3D utilises two different Fuel Coolant Interaction (FCI) codes that have a common numeric solver. One of the codes is for the premixing stage and the other for the explosion stage. The triggering stage is

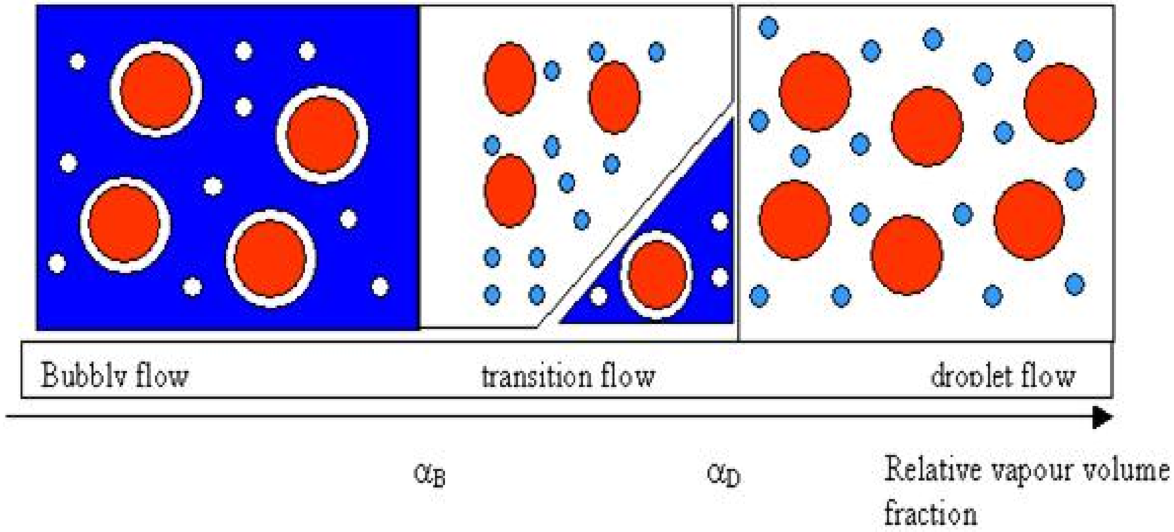

Figure 1. Different flow regions in MC3D Premixing[Meignen and Picchi (2014)]

incorporated into the code used for the explosion stage. This splits the simulation into two parts. In the first part the fragmentation of the melt jet, the vapour build-up and the heat transfer is simulated. The second part, that can be started at a time chosen by user, handles the rapid fragmentation of the melt drops and the heat transfer from the molten drops to the coolant. [Meignen and Picchi (2012)]

3.2 Premixing stage description

In the premixing stage the fuel can be present in three different stages: as continuous fuel, as drops or as fragments. The fragments stage is optional and the continues stage contains several forms of continuous fuel, for example molten fuel jet or a molten pool. The stages are connected via mass transfer equations that move fuel from one stage to another. The three different stages are handled by different sets of equations.

The mass transfer of the continuous fuel field is calculated utilizing a Volume of Fluid-Piecewise Linear Interface Construction(VOF-PLIC). VOF-PLIC is a commonly used method for computational fluid dynamics (CFD). VOF handles multiphase fluids by calculating cell fractions and constructing an interface in cells where the fraction is not 1 or 0. PLIC is then used as a method to construct the interface as a line or plane in the cell depending on the fraction[Karch et al. (2013)]. The fragmentation of the continuous fuel into drops is handled either with a global correlation model that uses a specific user specified fragmentation parameter for that type of fuel jet in water, or with a local fragmentation model that utilises the Kelvin-Helmholtz extension model to calculate the drop diameter. The Kelvin-Helmholtz model originates from the difference in velocity between the melt jet and the coolant. The coalescence of drops is handled via a geometrical model.

Regions containing moving drops and the medium they are suspended in is called the flow. In figure.1, the different flow types, i.e. bubbly flow, transition flow and droplet flow are illustrated. The vapour volume fraction in the cell determines the flow type and the limit between the different regions can be specified by the user. In the premixing stage of the simulation the fragments are in equilibrium with the water. [Meignen et al. (2005)]

3.3 Explosion stage description

In MC3D the triggering time is a user specified parameter. In addition to the moment it occurs triggering is defined also by specifying a cell or a zone of cells of which pressure is artificially increased to achieve an external trigger.

MC3D uses a direct vaporization approach, meaning that there is vapor production around the fragments, leading to pressurization. This is achieved via the Epstein-Hauser model for heat transfer correlation.

For the fine fragmentation there are two available models. A standard model where the fine fragment size is constant and user specified, as well as the with fragmentation rate. Also a new model has been implemented that calculates the fragment size variation using Weber criterion of drop stability (1). The new model is still under development.[Meignen et al. (2005)]

$$D_f = We_c \frac{\sigma}{\sigma_a V_{ad}^2} \tag{1}$$

4 OECD/NEA SERENA 2 Program

This chapter gives a description of the OECD/NEA SERENA 2 program, first shortly about the program in general and then a more detailed description of the two experimental facilities used in the program. The goal of the OECD/NEA SERENA 2 program was to establish the status of current FCI codes and their capabilities as well as to analyse the loads induced by a steam explosion in reactor accident scenarios. This was done by setting up and performing a number of tests, and analysing a large amount of parameters in regards to melt composition and interaction. Also analytical work was performed to test the codes capabilities to work with reactor case codes. The main finding of the program was that an in-vessel steam explosion would not challenge the integrity of the nuclear reactor containment. However, the ex-vessel steam explosions still needs further study.

The OECD/NEA SERENA and SERENA 2 projects were not the first experimental research programs in the field of steam explosions, as research has been done since the 60's. Since then several facilities have been used to analyse phenomena related to steam explosions. Some of the most notable experimental facilities that are not in use anymore are listed in table 2[Strandberg (2014)]. In parallel to this the methods to predict, approximate and simulate steam explosions have also been developed, both to the advancement of computer code, and also the increase in computational power.

Table 2. Experimental facilities that are no longer in use that were used for steam explosion research

Name	Year	Comments
FARO	1993	Prototypic, i.e. closer to reactor scale steam explosion. Used to determine the boiling feedback in a closed vessel under high pressure and the possible thermal attack on the lower vessel head
MAGICO	1992	Steel balls of mm-size dumped into saturated water, to better understand premixing.
MIXA		Prefragmented melt in even streams, with posibility to observe jet fragmentation under fall.

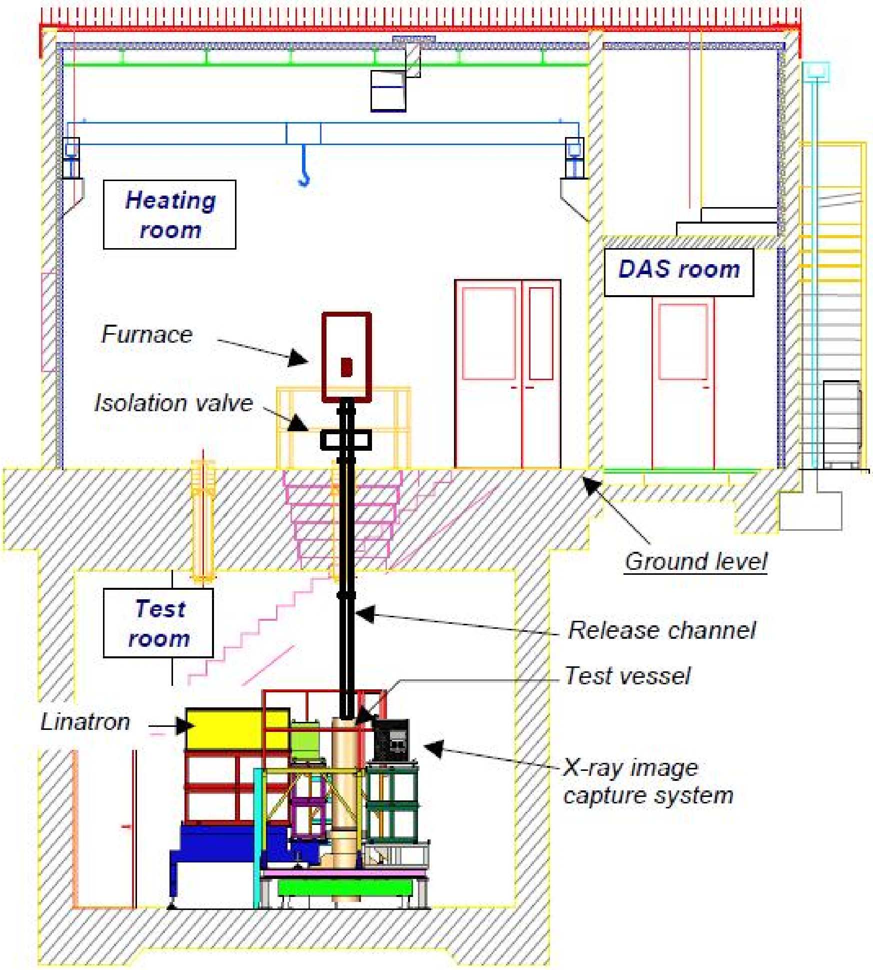

Figure 2. Schematic figure of the KROTOS test facility used in the OECD/NEA SERENA 2 experiments[HONG et al. (2009a)].

4.1 KROTOS

The KROTOS facility in Cadarache, France, is operated by the Commissariat A'l'Energie Atomique(CEA). It was one of the test facilities used in the OECD/NEA SERENA and SERENA 2 program.[Cassiaut-Louis and P. Piluso (2011)]

The geometry of the interaction vessel makes it more suitable for 1D and 2D axisymetric tests than 3D tests. The most important feature of the KROTOS facility is its X-ray radioscopy equipment that allows detailed studies of the fragmentation of the melt jet as it enters into water. It is also equipped with an external trigger device.

Due to the radioscopy equipment the facility is constructed in two levels, with the lower level located underground. The levels are separated by a thick concrete slab to protect against upward scattered X-ray radiation. Figure 2 is a schematic overview of the facility. The figure also shows where is also presented the main parts of the setup; the furnace, the release channel and the test vessel.Table 3 lists the KROTOS experiments performed during the OECD/NEA SERENA 2 program.

Table 3. KROTOS experiments performed as part of the SERENA 2 project.

Properties	KF-C	KF-1	KF-2	KF-3	KF-4	KF-5	KF-6
Melt Mass(kg)	2.681	2.419	4.121	0.786	3.211	2.331	1.293
Melt Temperature(K)	29362	2969	3049	2850	2958	2864	2853
Initial pressure (MPA)	0.390	0.440	0.200	-	0.210	0.210	0.210
Jet Diameter (mm)	20	15	10/spray	30	30	30	30
Triggering time (ms)	440	931	922	-	851	1127	1542
Void at triggering (Vol.%)	12	6.7	27	1	6	16	12
Max pressure (MPa)	32.3	34.7	23.3	-	44.7	-	9.4
Impulse(N*s)	342	584	743	-	898	-	-
Conversion ratio (%)	0.10	0.10	0.08	-	0.18	-	-

4.2 TROI

The TROI (Test for Real cOrium Interaction with water) research facility in South Korea is maintained by the Korean Atomic Energy Research Institute, KAERI. The facility is located in Daejon in the Republic of Korea. It has been used in the OECD/NEA SERENA Phase 1&2 projects. The construction begun in 1999 and the first preliminary tests started in July 2000. In April 2001 the the first test with a UO_2 & ZrO_2 mix was conducted.

The test facility consist of a furnance vessel, a pressure vessel, a quick-opening valve with an intermediate melt catcher and an interaction vessel. Figure 3 shows a schematic figure of the facility, and a close-up of the of the melt catcher valve can be seen in figure 4. The molten material is melted inside the furnace vessel by using of an electromagnetic furnace, supplied via an 150kW R.F generator. The furnace vessel contains an equipment for measuring the melt temperature(a Pyrometer), as well as ambient pressure. It also incorporates argon(Ar) gas injection for aerosol removal. Also a sample of the contents of the ambient gas can be collected. When the melt has reached desired temperature it is released down to the interaction vessel via the intermediate melt catcher. The interaction vessel contains the measurement equipment needed for the experiments including multiple temperature and pressure sensors. The trigger equipment is placed at the bottom of the interaction vessel and it is automatically governed by sensors in the melt release channel with a timed backup.

Due to the geometry of the interaction vessel the TROI facility is well suited for studying the 3D-effects of steam explosions. It can also be used to test relatively large samples: close to 18 kg of melt material was used in the OECD/NEA SERENA 2 program.

The KROTOS and TROI experiments are both built to examine phenomena related to the steam explosions, but their construction and test focus differ. Due to the larger melt masses of the TROI experiments and better design of the facility for 3D analyses the TROI experiments can better be used as a starting point for plant application simulations cases,Therefore the TROI experiments have been chosen for further study in this report. Table 4 lists the TROI experiments performed in the OECD/NEA SERENA 2 project.

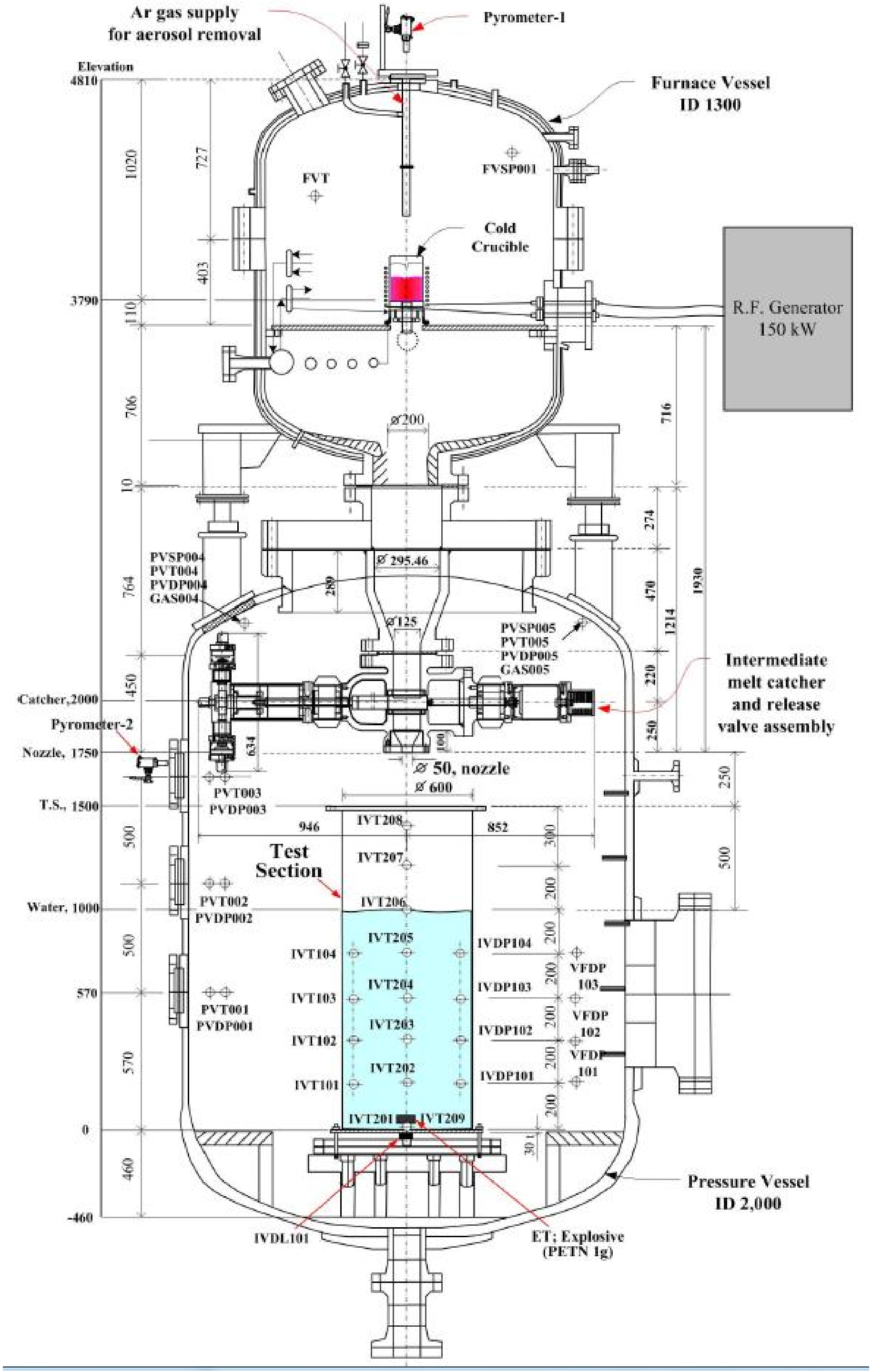

Figure 3. Schematic figure of the TROI test facility used in the OECD/NEA SERENA 2 experiments. [HONG et al. (2009a)].

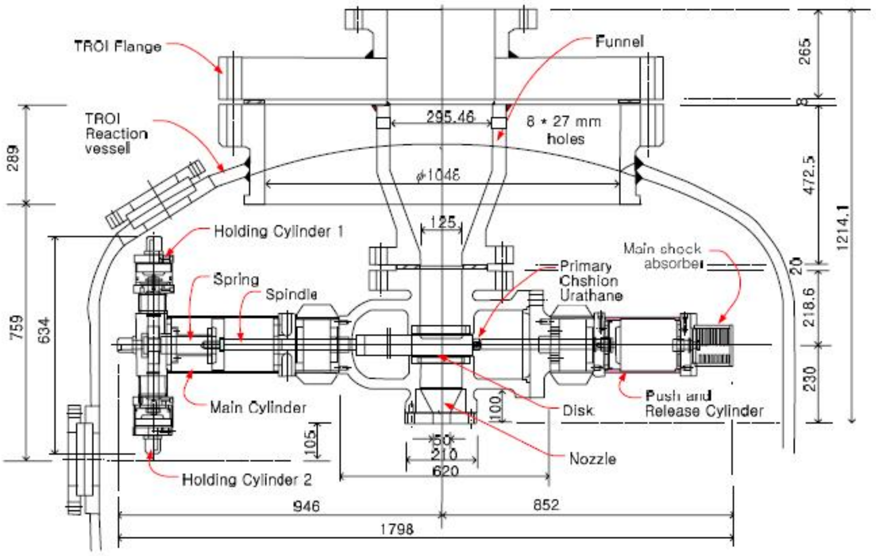

Fig. 2.1.4 Intermediate melt catcher on the quick-opening valve assembly (unit : mm)

Figure 4. Schematic figure of the intermediate melt catcher of the TROI test facility used in the OECD/NEA SERENA 2 experiments. [HONG et al. (2009a)].

Table 4. TROI experiments prefrormed as part of the SERENA 2 project.

Properties	TS-1	TS-2	TS-3	TS-VISU	TS-4	TS-5	TS-6
Delivered Melt Mass (kg)	15.385	12.479	15.877	19.179	14.319	17.882	9.262
Delivered Melt Temperature (K)	3000	30632	31072	30242	30112	29402	29102
Melt composition (wt%)							
UO_2	73.4	68	71	75	81	76	73.32
ZrO_2	26.6	32	29	25	19	18.3	18.45
Zr						5	
U						0.7	
Fe_3O_3							4.89
$FissionProducts$							3.34
Initial Pressure (MPa)	0.402	0.22	0.223	0.226	0.231	0.211	0.213
Jet Diameter (mm)	50	50	50	50	50	50	50
Triggering Time(ms)	939	875	875	No	1 040	1 046	1 050
Void at Triggering(Vol.%)	4	3	2	10	14-24	12-34	4-10
Max. Pressure (MPa)	17	10	12		20	7	25
Impulse(N*s)	6640	>8000	9000		»9000	4680	»9000
Conversion Ratio (%)	0.12	0.28	0.22		0.35	0.06	0.66

5 MC3D Simulations

The focus of this report is in simulating the TROI experiments that contain U and Zr as oxides or metals, and that were conducted as part of the OECD/NEA SERENA 2 program. In the next sub-chapters the selected experiments and the results of the simulations presented.

First an experiment that contains no metal, i.e. the TROI TS-3 experiment. This purely oxidic experiment is used as a starting point to test the mesh, and also used in developing the new simulation process script, which is presented in Appendix A. Next more complicated experiment TROI TS-5, in which the melt included also metals, is presented and simulation results are analysed. Last in this chapter the results of a simple sensitivity analysis are presented, in order to study the effect of some parameters to the simulation results.

5.1 Non-metallic experiment

5.1.1 Presentation of the TROI TS-3 experiment

TROI TS-3 was chosen as starting point for the sensitivity analysis. The TS-3 test was performed with a melt mixture consisting of 71% of UO_2 and 29% of ZrO_2.Other important parameters of the experiment are presented in table 5, where are listed for example the melt mass and temperature as well as the initial pressure of the reaction vessel.

Figure 5 shows two snapshots of the melt injection into the test chamber. It is visible from the figures that the jet is continuous.

The melt jet front progression is shown in figure 6. This is important for defining how much melt can take part in the explosion. This has a great impact on the explosion strength. In addition it is a factor that can be easily compared between the experiment and the simulation.

Figure 7 shows the dynamic pressure measured in the TS-3 experiment at various levels. The blue line represents the progression of the external trigger in the mixture followed by the steam explosion front that is illustrated by the red line. As can be seen the pressure of the steam explosion front peak reaches over 8 MPa in the explosion.

5.1.2 Simulation results

The goal of simulating the TROI TS-3 experiment was to approximate the starting parameters for the TS-5 simulation, presented in 5.2.2. Another reason for the more simple, and therefore faster to simulate, simulation was that it was used to develop and test the automatic simulation script presented in appendix A.

In table 5 the actual parameters from the test are presented together with the parameters used in the simulation. The final parameters where chosen so that the results match the experiment. In the iteration process the experiment parameters were used as a starting point. The simulation was done as a 2D

Table 5. List of the initial parameters for the TROI TS-3 test [HONG et al. (2009a)]. The right column shows the selected parameters for the MC3D simulations presented in section 5.1.2.

	Experimental value	Simulation value
Melt Properties		
Delivered Melt Mass [kg]	15.877	
Delivered Melt Temperature [K]	2861	3150
Liquidus Temperature[K]		3000
Overheating[K]		150
Melt Composition [wt%]		
UO_2	71	
ZrO_2	29	
Test section		
Depth [m]	1	1
Temperature Water [K]	331	
Initial Sub-cooling [K]	42.15	
Initial Pressure [MPa]	0.223	0.223
Saturation Temperature[K]		
Fall Distance [m]	1	1
Vessel Inner Diameter [cm]	60	60

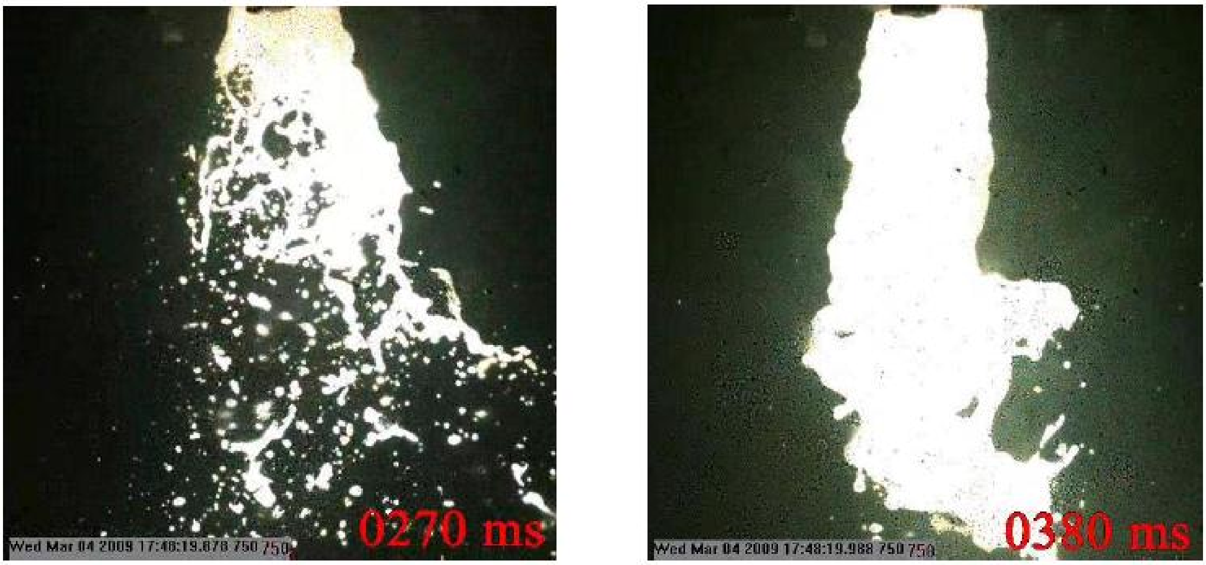

Figure 5. The melt jet injection in the TS-3 experiments at two different times.[HONG et al. (2009b)]

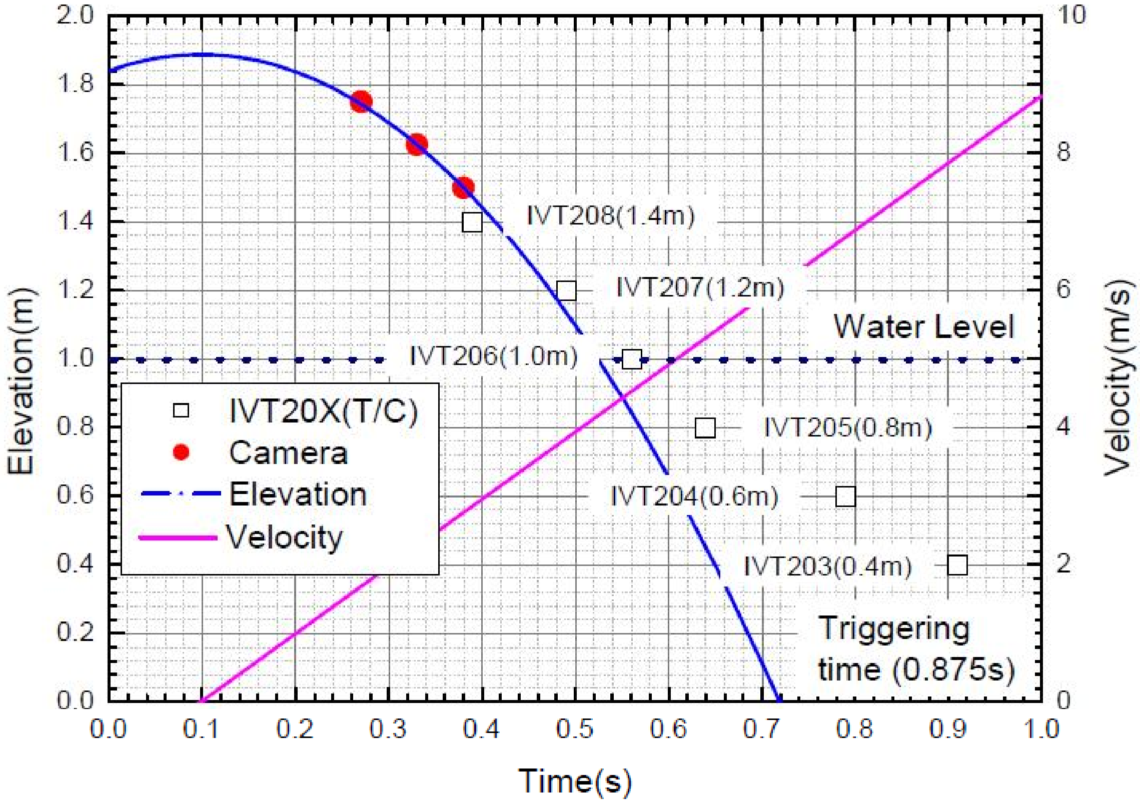

Figure 6. Melt progression in the TS-3 experiment, showing both the melt velocity and position as well as the indication devices used for data extraction.[HONG et al. (2009b)]

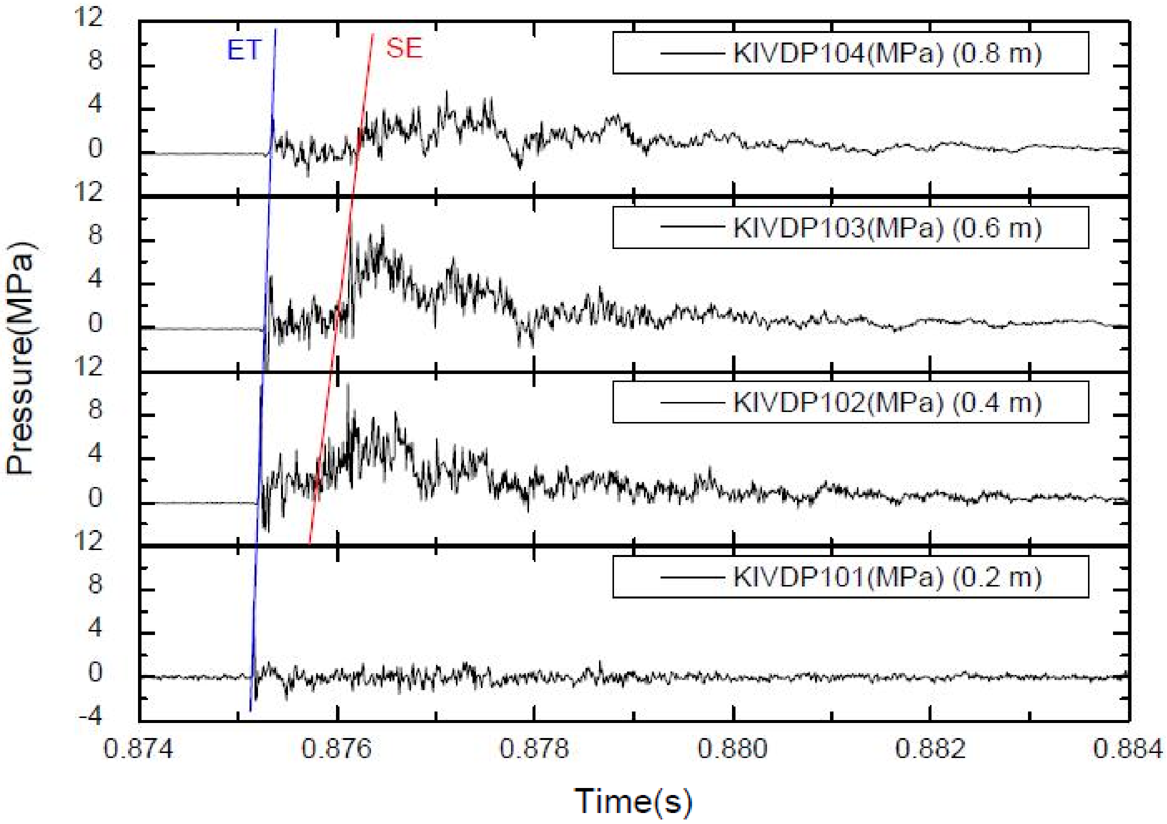

Figure 7. Pressure measurments from the TROI TS-3 experiment. Blu line indicates the progression of the trigger and the red line that of the steam explosion. [HONG et al. (2009b)].

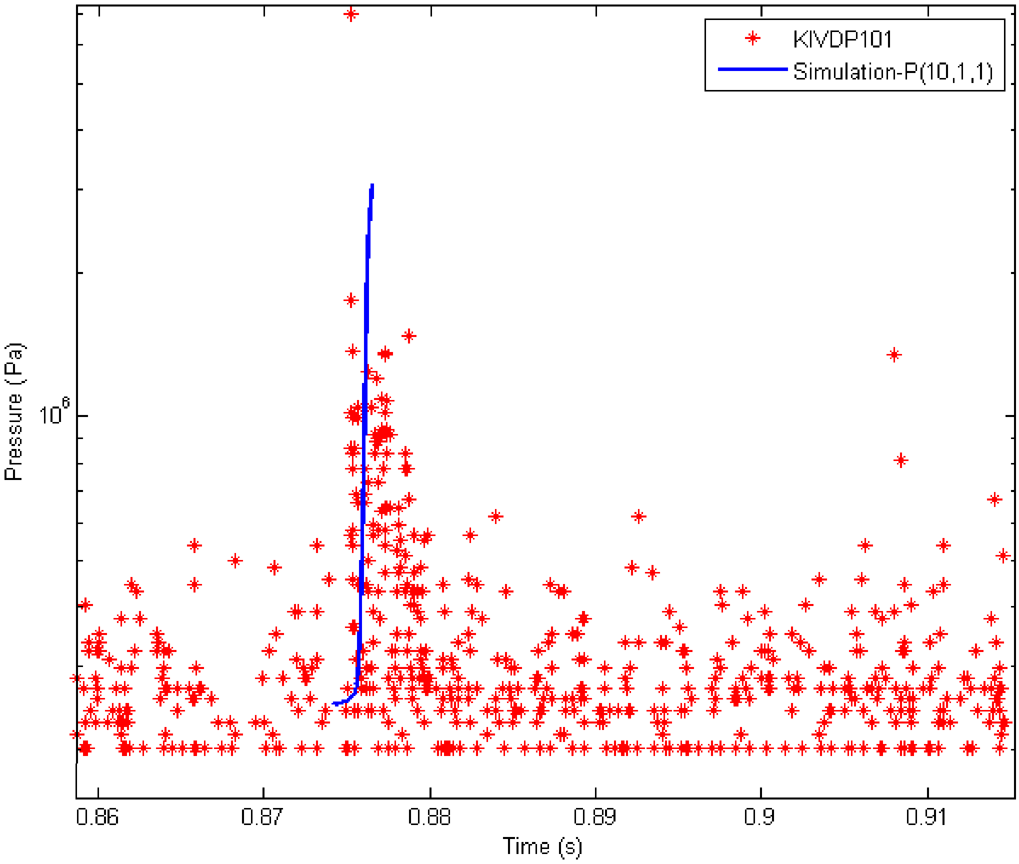

Figure 8. The simulated pressure peak plotted against the experimental data. Red markers are the experimental data and blue is the simulated results.

simulation as the setup is symmetrical and 3D simulations would result in significantly longer simulation times. The simulation is relatively simple because the effects of hydrogen production do not have to be taken into account in this experiment.

The simulation was done using a custom user defined melt, instead of one of the predefined, and the initial values for solidus and liquidus temperatures were defined with the help of ASTEC as 2 973 K and 3 136 K, respectively. Some modifications for the values were needed to achive similar results with experiment.

The simulated dynamic pressure can be seen in figure 8. The blue line represents the simulated pressure and the red markers are the raw experimental data. As can be seen from table 5 the initial parameters were changed quite a lot. The melt temperature was increased from 2861K to 3150K.

5.2 Metallic experiment

5.2.1 Presentation of the TROI TS-5 experiment

In this subsection a more complex experiment case with more reactorlike properties is presented. In this case the hydrogen production is taken into account.

The experiment chosen for the metallic experiment is the TROI TS-5, composed of 76% of UO_2, 18.3% of ZrO_2, 5% of Zr and 0.7% of U. The idea is that adding metal into the mixture will result in more realistic melt, as in a reactor accident scenario the melt would probably not be fully oxidized, which would have effects on the steam explosion progression as the hydrogen production would increase the void build up. In table 6 the different experiment parameters are presented[HONG et al. (2011)], together with parameters used in the simulation.

According to SONG et al. (2007), the steam explosion will be weaker if the hydrogen production is ample, although it is hard to determine if the hydrogen production will occur in huge quantities due to the fragmentation. In one such experiment there were no signs of a large amount of hydrogen being produced and the resulting steam explosion was very energetic.

In figure 9 the melt progression is shown. From the figure it is possible to see that this experiment had marginally higher velocity when contacting the water surface and that it contacted the bottom of the vessel slightly faster than the TS-3 experiment that was presented in the previous subsection.[HONG et al. (2011)]

Figure 10 shows the dynamic pressure measured with the KISTLER sensors during the melt coolant interaction. From the graph it can be read that the pressure was as high as 6MPa. In [HONG et al. (2011)] the maximum impulse was calculated to be about three kilo newton seconds(kNs). The calculated efficiency of interaction was $0,06\%$ compared to the calculated thermal energy in the delivered melt.

In the TS-5 experiment a so called steam spike occurred before the actual triggering. A steam spike is a significant increase in the void fraction and steam, without major increase in pressure. Figure 11 shows another graph of the pressure showing the recorded pressure in the top of the interaction vessel and in the melting vessel. From the graph it can be seen that the pressure seems to be rising at a semiconstant speed and that the trigger is not efficient to really trigger a steam explosion, and also that it is not possible to distinguish between the steam spike and the trigger.[Meignen (2015)]

During the TS-5 experiment a sample of the ambient gas was collected twice, once 5 minutes before the opening the quick-opening valve and also 10 minutes after the opening of the valve. Two samples were collected at both instances. One of the samples collected after the explosion showed a measurable increase in hydrogen content. Compared to the other TROI TS experiments it had a higher hydrogen content than all the rest except for the TS-4. It has been speculated that the Zr metal in the melt was oxidized during the experiment.[HONG et al. (2011)]

5.2.2 Simulation results

For the metallic experiment the TROI TS-5 was chosen for a simulation exercise, composed of 76% of UO_2, 18.3% of ZrO_2, 5% of Zr and 0.7% of U[HONG et al. (2011)]. In table 6 the actual parameters

Table 6. List of the initial parameters for the TROI TS-5 test [HONG et al. (2011)]. In the right column are the selected parameters for the MC3D simulations presented in section 5.2.2.

	Experimental value	Simulation value
Melt Properties		
Delivered Melt Mass [kg]	17.882	17.8
Delivered Melt Temperature [K]	2940	2940
Liquidus Temperature[K]	2800	-
Overheating[K]	140	-
Melt Composition [weight %]		
UO_2	75.97	
ZrO_2	18.32	
U	0.73	
Zr	4.99	
Test section		
Depth [m]	1	1
Temperature [K]	337	
Initial Sub-cooling [K]	36.15	
Initial Pressure [MPa]	0.205	
Saturation Temperature[K]	394.67	
Fall Distance [m]	1	1
Vessel Inner Diameter [cm]	60	60

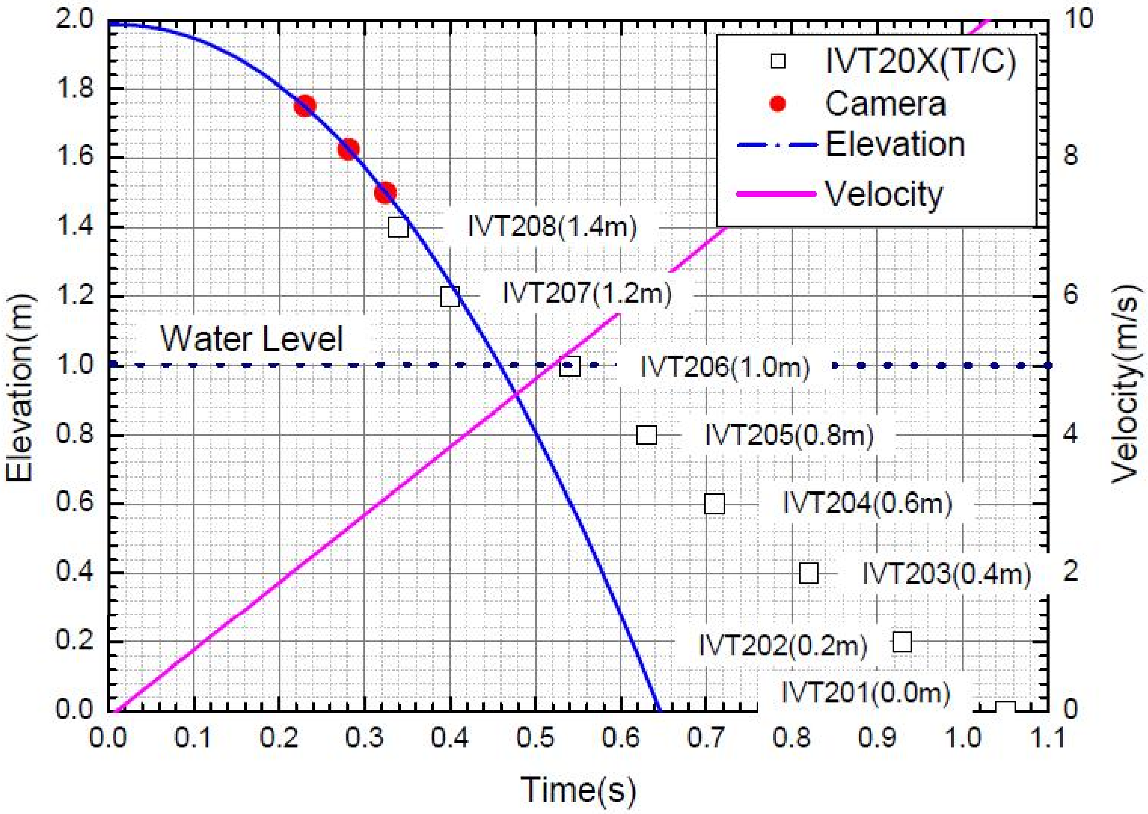

Figure 9. The melt progression in the TS-5 experiment, showing both the melt velocity and position as well as the indication devices used for data extraction.[HONG et al. (2011)]

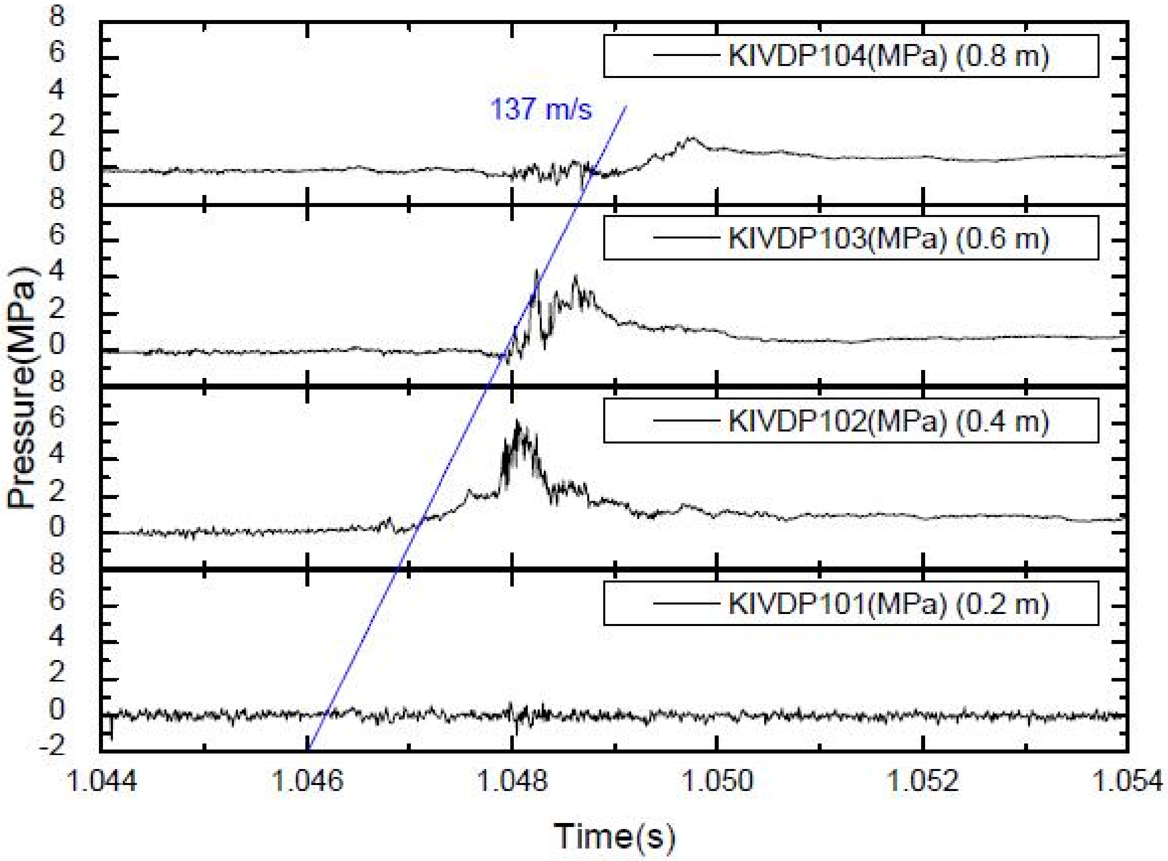

Figure 10. Pressure measurements from the TROI TS-5 experiment. No steam explosion was detected in this experiment.[HONG et al. (2011)].

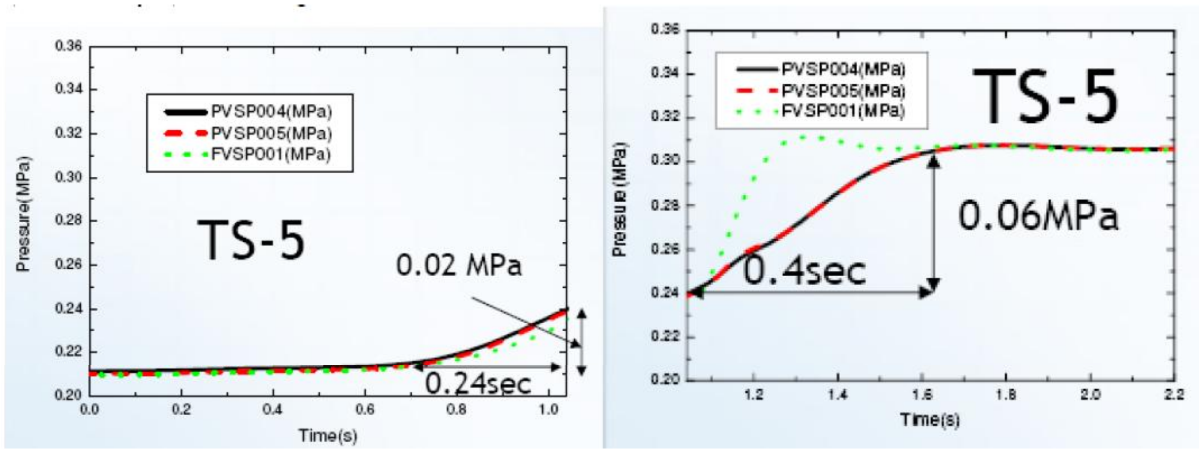

Figure 11. The pressure rise recorded from three different points in the TS 5 experiment, showing the appearance of a so called steam spike. PVSP are from the top of the interaction vessel, FVSP is from the melting vessel. The rise in the FVSP line at 1.15 does not to be seem related to an event occurring in the reaction vessel.[Meignen (2015)]

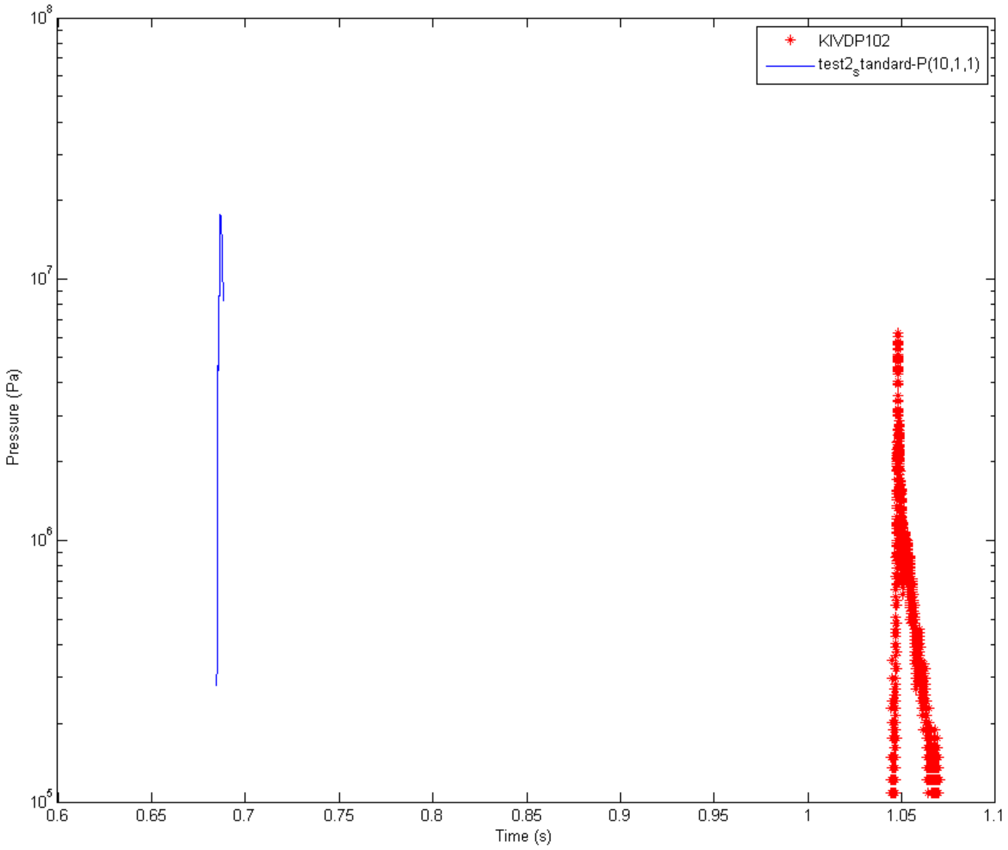

Figure 12. The simulated pressure peak plotted against the experimental data. Red markers are the experimental data and blue is the simulated results.

from the test are presented alongside with the parameters that where used to produce the graph in figure 12. In the simulation a default mixture for the melt was used, as a custom user defined melt added unnecessary complexity, due to the way MC3D handles hydrogen production. From figure 12 can be seen the simulated pressure peak produced by a simulated steam explosion with a trigger at 0.68 seconds compared to the values recorded in the experiment. In the simulation the fragmentation process also produced hydrogen. The hydrogen production rate, in the premixing stage, can be seen in figure 13.

As the TS-5 experiment produced a “steam spike” the fitting of the simulation data to the experimental data is not a viable option. When the explosion was simulated to trigger at a time that matched the experiment triggering time no explosion occurred. Because of this the trigger time was changed to 0.68 seconds which is the value at which MC3D expects the strongest explosion to occur. The input parameters were modified compared to previous analyses, in such a way that at the time of triggering not only the pressure is artificially increased in the cell that is the location for the trigger, but also extra melt drops are added to the cell to help with the triggering.

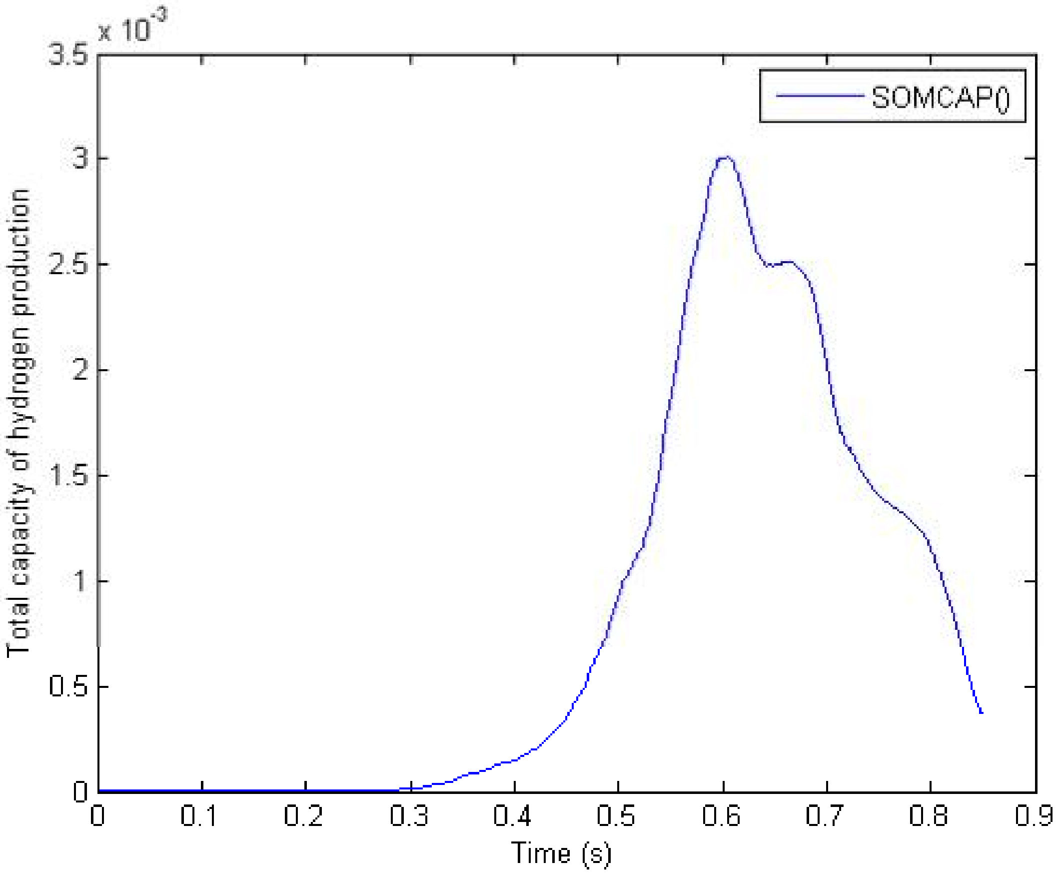

Figure 13. The simulated hydrogen production in the premixing stage of the TS-5 simulations

5.3 Sensitivity analysis

A sensitivity analysis was done for some important input parameters,using TS-5 test as a base, to evaluate their effect to steam explosion according to MC3D. Starting from the TS-5 experiment means that also in the sensitivity analysis the effects of hydrogen production is taken into account. The sensitivity analysis was done so that one parameter at a time was changed and its effect analysed.

During the fitting of the simulations to the experimental values in subsection 5.1.2 it became apparent that melt temperature has one of the greatest impacts on the explosion strength. Therefore one of the parameters selected for the sensitivity analysis was the melt temperature. Also explosion time and ambient pressure were simulated in this way. In table 1 are listed a few other conditions that impact on the occurrence and strength of steam explosions, which were not chosen to be part of the sensitivity analysis. The three parameters, melt temperature, explosion time and ambient pressure, were deemed more important at this stage, because they are assumed to have a greater impact. Changing the melt mass values to far from the experimental values, would have resulted in unrealistic ratios between the melt and the coolant masses.

In figure 14 the same input parameters are used as in the simulation of which results are presented in figure 12 but with a different melt temperature, ranging from 2800K to 3000K. A simulation with 2700K was also done but it resulted in such an unfavorable condition after the premixing that it caused the explosion stage simulation to crash. The reason for that most probably was that melt temperature of 2700K was too low to result in conditions required for a steam explosion. For the temperatures that were able to trigger a steam explosion the resulting differences in the pressures were not that huge. A reason for this could be that at the moment when the steam explosion is triggered the melt temperature is not the limiting factor of the steam explosion strength, if there is one.

Different trigger times were also simulated in a similar fashion. In figure 15 the effect on the pressure peaks can be seen. In addition to the to the cases visible in the graph, triggering at 0.5 seconds was also simulated but no steam explosion occurred. As can be seen the simulated explosion is strongest at 0.68, and a bit weaker at 0.64 seconds. The short line at 0.7 seconds is most probably a simulation glitch as the simulation stopped abruptly. The fact that triggering at 0.9 seconds also yields a steam explosion confirms this assumption.

The effect of ambient pressure was also analysed, but the results indicate that it had no notable effect on the pressure peaks. This can be explained by the fact that ambient pressure has the largest effect on the probability of the steam explosion to occur and not the strength of the steam explosion. In the simulations explosion occurred with every tested ambient pressure level.

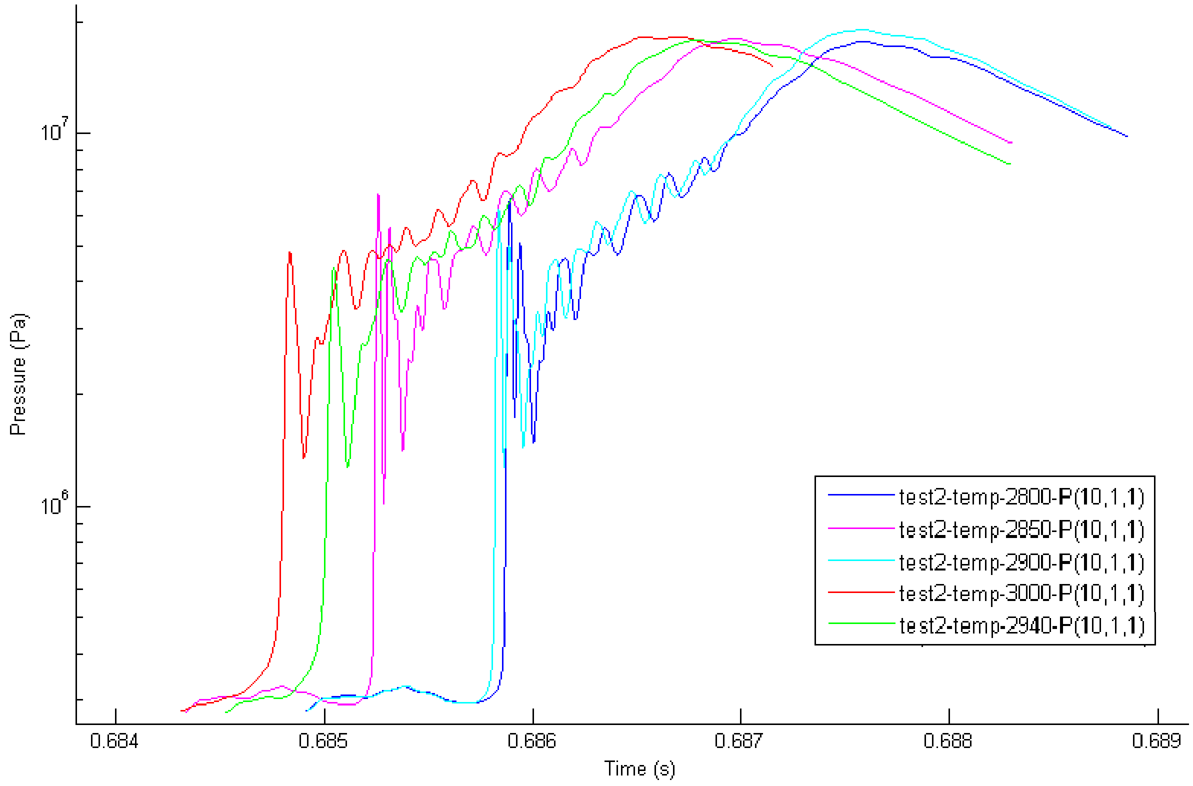

Figure 14. Impact of different melt temperatures on the simulations

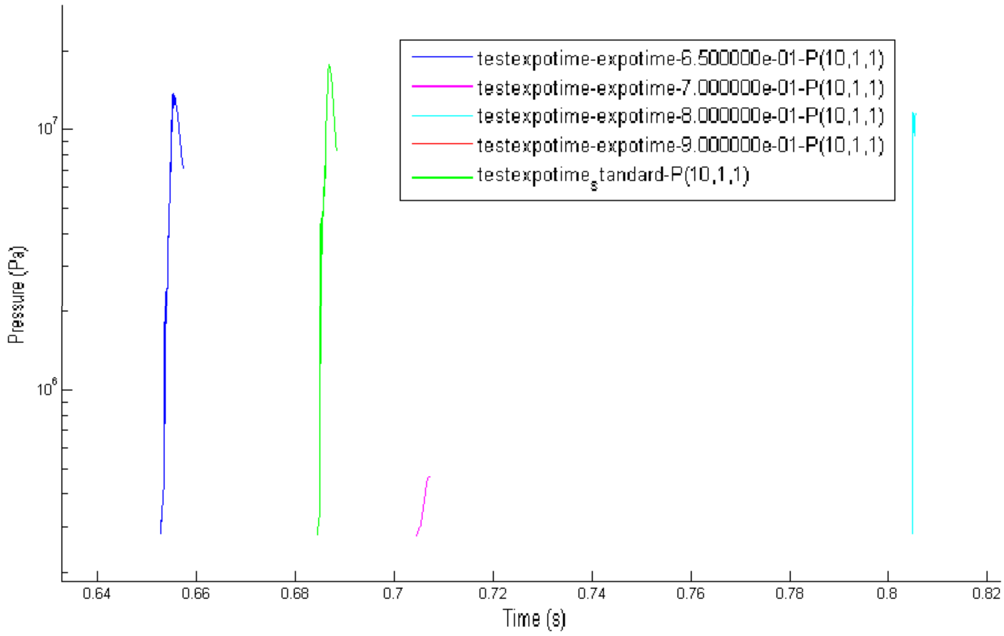

Figure 15. Impact of different trigger time on the simulations. Trigger time at 0.9 sec is scaled out of the graph as it was an invisible dot as no explosion occurred.

6 Conclusion

The objective of the work presented in this report was to broaden the expertise in MC3D use and also to evaluate the sensitivity of the simulation results to selected input parameters. During the simulations a script to automate the simulation process was developed.

The MC3D code consists of two parts, one handling the premixing and one the explosion(propagation) stage. The premixing part splits the fuel into three different modes: continuous, drops and fragments. For each mode different methods and models are applied to handle the transfer of material and heat to and from the different modes. The explosion is triggered artificially by introducing high pressure into a cell that is specified by the user. In the latest version of MC3D it is also possible to allow the program to calculate the fragment size instead of using a user specified parameter for this.

In the frame of the OECD/NEA SERENA 2 project, experiments were performed both in the KROTOS and TROI facilities. The special feature of the KROTOS facility is the X-ray spectrometry measuring equipment, which allows detailed studies of the void fraction in the interaction vessel. On the other hand, the TROI facility has a larger interaction vessel that allows bigger melt masses making the experiments more prototypic compared KROTOS. Because of this, two experiments performed at the TROI facilities were chosen to be simulated.

The first of the experiments the TROI TS-3, was used mainly to achieve a starting point for the simulation parameters of the TROI TS-5 test. However, as it is was relatively fast to simulate, it was suited to be used in the development of the simulation script.

The TROI TS-5 experiment was chosen for its partly metallic melt to demonstrate and analyse the effect of hydrogen production. In the TS-5 experiment occurred what is known as a "steam spike" which is believed to be the reason for the mixture not triggering properly. This unfortunately makes matching of the experiment to the simulation quite impossible.

In the last part of the report a simple sensitivity analysis for three different input parameters is presented, the parameters being melt temperature, trigger time and ambient pressure. The simulation results were not so sensitive to changes in melt temperature, which probably is because the melt temperature in this case is not the limiting factor for the strength of the explosion. Changing trigger time had a more visible effect as triggering too soon or too late did not result in a steam explosion. Ambient pressure had no effect on steam explosion strength in this scenario, which was to be expected as it mostly affects the probability of a steam explosion to occur.

Simulating steam explosions with MC3D can be quite a time consuming process as the program, as stated previously, should not be used as a "black box" tool. However, it is possible to achieve satisfying results in the end if the user is skilled enough. The automated script added value to the work, even though the development process took quite a lot of time. Now the future usage of MC3D will be much faster and streamlined.

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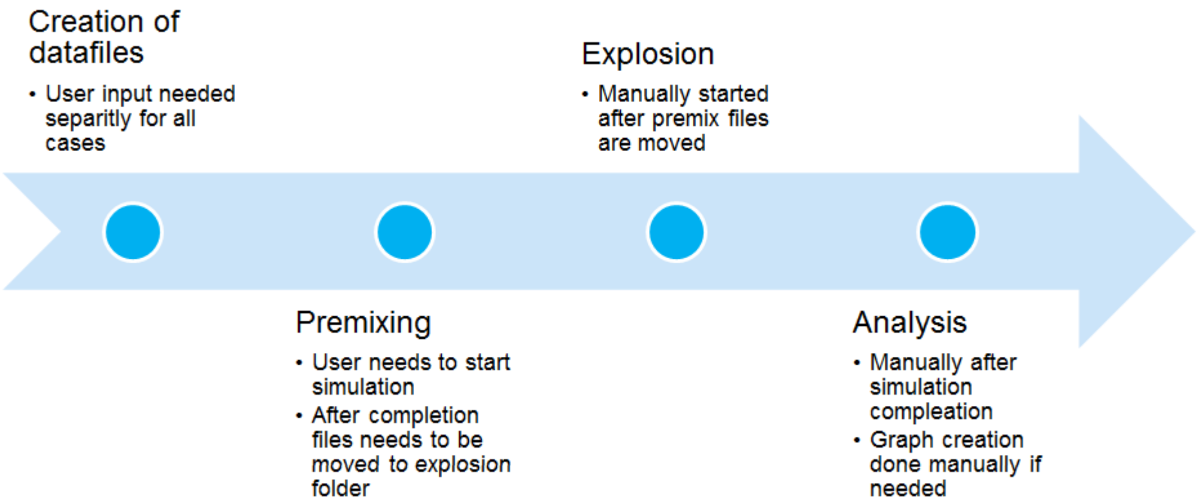

Figure 16. The old simulation process.

A Simulation procedures

For the simulations presented in this report the MC3D software was used but to make the handling and analysis of all the data more efficient and less prone to errors a Matlab script was created. The script handles the creation of simulation data directories and configuration files. The script is also able to automatically collect and plot the data to graphs. This way is considerably faster, and simpler analysis of the data is achieved.

If a simulation needs to be run manually it involves many different steps: the creation of the datafile, running of the premixing, transferring files from premix to explosion simulation, running the explosion simulation and then collecting the data into graphs. Because of this it is quite clear that the person doing the simulation has to focus only on it while the simulation is running, as there are so many manual steps. Another factor is also that the time steps in between the different manual steps vary a lot and are hard to predict.

Running the simulation through the script automates all the middle steps, and only the the data input needs to be done manually. The script can run more than one simulation in series from one data input. This makes it possible to automatically run multiple simulations easily and quickly. The script also directly prints pressure graphs that help with the first rough analysis to see if the simulation was successful or not.

Figures 16 and 17 illustrate how the manual input differs from using the script. The use of the script does not change the fact that MC3D can not be used as a black-box tool as the user still has to make the underlaying data file that is inserted into the Matlab files as a template. The user is also needed to througly analyse whether the results are realistic or not.

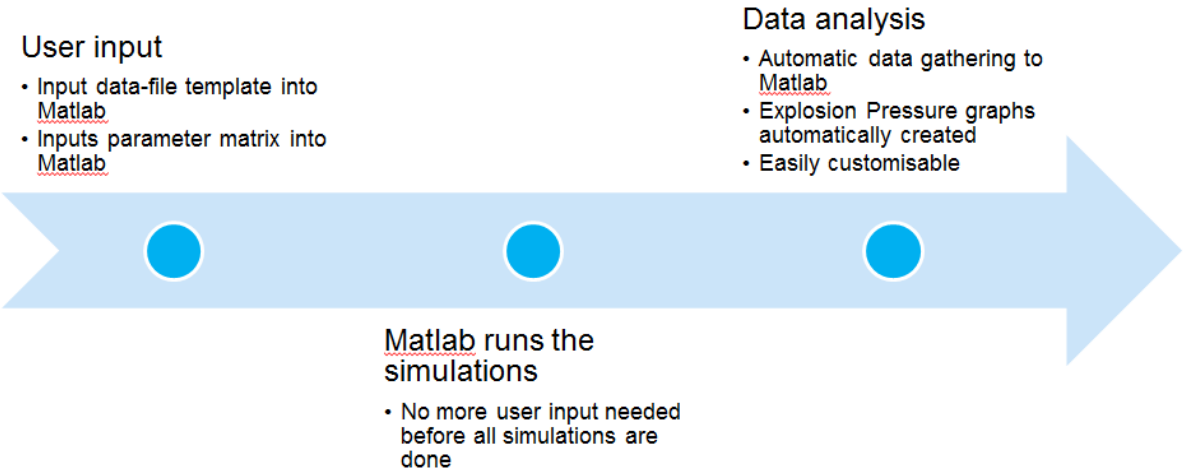

Figure 17. The simulation proiccess while running in the matlab environment.

Title	Analysing Steam Explosions with MC3D
Author(s)	Magnus Strandberg
Affiliation(s)	VTT Technical Research Centre of Finland Ltd.
ISBN	978-87-7893-426-0
Date	July 2015
Project	NKS-DECOSE
No. of pages	27
No. of tables	6
No. of illustrations	17
No. of references	11

Abstract
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MC3D is a simulation software developed to analyse steam explosions. In this report the software is presented in outline. MC3D is then used to simulate two steam explosion experiments, and the results are presented. The first of the simulations is a simple fitting test, to establish a starting point for more complex cases. The second simulation is performed also as a fitting test and in addition as a base for a sensitivity analysis.

In the sensitivity analysis the effect of three input parameters, melt temperature, triggering time and ambient pressure, is varied to see how changes in these affect the results. Out of these, changing the triggering time had the largest impact on the steam explosion occurrence and strength.

The experiments chosen for simulation were performed as part of the OECD/NEA SERENA program and were run at the TROI research facility. The report also contains a brief description of the OECD/NEA SERENA program, and a more detailed description of the two test facilities used in the program, KROTOS and TROI.

An automated simulation script was developed to speed up the simulation process. The new method also reduces the possibility of human error and makes it possible to queue up simulations.

Key words steam explosion, fuel-coolant interaction, MC3D, TROI experiments

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