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MC3D simulations of ex-vessel steam explosions in IDPSA framework

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Abstract

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The analysis cases are studied for two different vessel failure modes and by using two fragmentation models. The basis case is a single large central hole in the reactor pressure vessel lower head, and the second melt ejection mode is a result from multiple simultaneous failures of vessel penetrations, representing instrumentation and control rod guide tube failures. Limited sensitivity analyses are performed for fragmentation model parameters and for explosion triggering time.

Results showed generally quite large pressures and impulses in comparison to e.g. results obtained in OECD's SERENA program [2], and for multiple melt jets the pressure loads were even higher than for single jet case. Throughout the analyses there were difficulties to trigger explosions and to compare different cases thus became more complicated. Although it is difficult to validate results and more detailed modelling would be necessary in order to draw more credible conclusions, this study produced useful information e.g. from IDPSA perspective and also enhanced modelling capabilities at VTT.

Key words

IDPSA, PSA, FCI, Ex-vessel steam explosions, Level 2 PRA, MC3D

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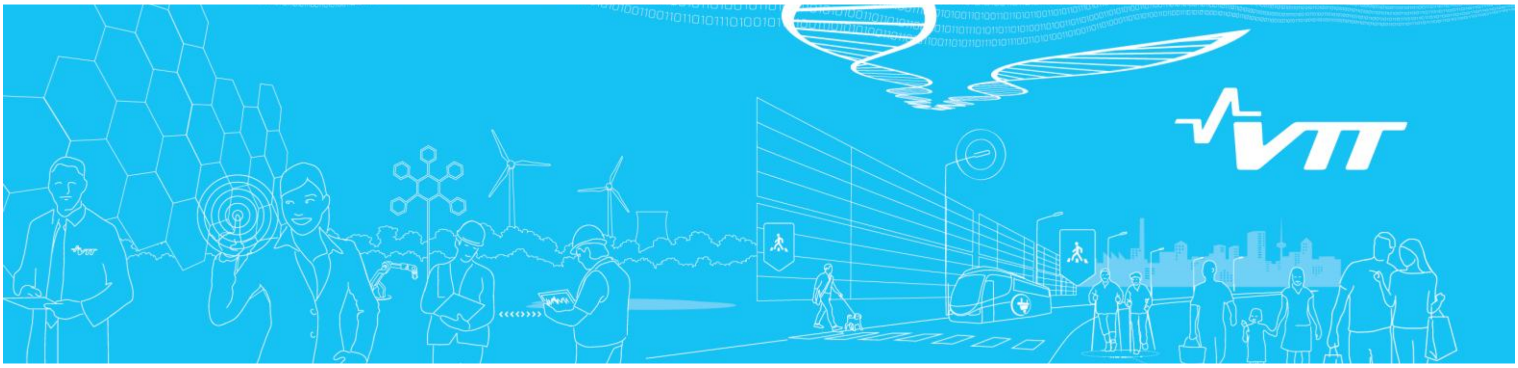

RESEARCH REPORT

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Preface

This report has been prepared under the research project PRADA, which concerns development and application of probabilistic risk assessment methods. The project is a part of SAFIR2014, which is a national nuclear energy research program. PRADA project work in 2014 is funded by the State Nuclear Waste Management Fund (VYR), Technical Research Centre of Finland (VTT), Aalto University, Nordic Nuclear Safety Research (NKS) and OECD HRP, which is gratefully acknowledged. The work was carried out at VTT.

Espoo, 14.5.2014

Author

Abbreviations

BWR	Boiling Water Reactor
CONST	CONST fragmentation model in MC3D
CRGT	Control Rod Guide Tube
FCI	Fuel Coolant Interaction
IDPSA	Integrated Deterministic and Probabilistic Safety Assessment
IGT	Instrumentation Guide Tube
KH	KELMHOLTZ fragmentation model in MC3D
LDW	Lower Drywell
NPP	Nuclear Power Plant
PRA	Probabilistic Risk Assessment
RPV	Reactor Pressure Vessel

Contents

1. Introduction

A steam explosion can take place if molten fuel resulting from a severe accident gets in contact with water and vaporizes it so rapidly that the resulting sudden pressure peak meets all the characteristics of an explosion. More generally such processes are called fuel coolant interactions (FCI). Steam explosions are considered plausible both in the reactor pressure vessel (RPV) and underneath it in the lower drywell (LDW) of a boiling water reactor (BWR) containment. Ex-vessel explosions are at issue if vessel melt-through occurs and melt is ejected into a flooded LDW. Steam explosions pose a risk also to pressurized water reactors (PWR). Although general phenomenology is common, there are some differences between BWR and PWR scenarios when it comes to steam explosions, including e.g. water pool depth, melt composition and premixing of melt and coolant, but this work concerns only ex-vessel scenarios in BWR type of reactors.

An ex-vessel steam explosion case study for Olkiluoto NPP units 1 and 2 was performed earlier in [1], and the current study aims to supplement previous work by providing more detailed analysis. The already performed case study focused on IDPSA (integrated deterministic and probabilistic safety assessment) methodologies in level 2 PRA (probabilistic risk assessment) context, and it used pressure load information from literature. In this work a more case-specific approach is pursued by conducting FCI simulations. The simulations are carried out by using MC3D code, and the analysis cases are derived from the scenarios that were analysed in [1]. This study is a preliminary one and the model lacks many features such as production of hydrogen. There is a VTT employee who is specializing in steam explosion modelling and MC3D this year, and it should be possible to obtain more detailed results for level 2 purposes regarding Olkiluoto BWR in the future. Therefore it is also unlikely that the model presented in this study would be further refined by the author (or anyone else, for that matter).

A review of steam explosion phenomenology, fundamental differences between ex- and in-vessel cases and effect of reactor parameters is given in [1], and this report does not discuss these issues. In section 3, the analysis tool MC3D and the analysis scenarios are introduced. Also the MC3D simulation phases (premixing & explosion) and progression along with results and quantities of interest are presented. Section 4 deals with simulation results from both premixing and explosion phases for two different vessel failure modes and includes also a brief sensitivity analysis. Sections 5 and 6 contain discussion and conclusions of the work carried out in this study, respectively.

2. Goal

This study aims to produce case-specific results of pressure loads on LDW wall due to ex-vessel steam explosions in a BWR plant. Outcome of the analysis can be used to enhance level 2 PRA model developed within the PRADA project for Olkiluoto NPP last year. Thus the analysis can be regarded to be an application of IDPSA methodology. An important goal is also to increase general understanding and modelling capabilities of FCI phenomena, although focus is on safety analysis and complex physics and mathematical modelling are given less attention.

3. Steam explosion simulations

MC3D is a multidimensional numerical tool devoted to study multiphase and multi-constituent flows. It is developed especially to analyze FCI phenomena but it can calculate very different situations including direct containment heating and even debris coolability. For FCI applications, MC3D is practically divided into two separate parts, the first of which calculates the premixing phase whereas the latter proceeds from premixing to calculation of explosions themselves. [3]

MC3D uses finite volume method for mass and energy balance equations and finite difference method to write momentum balance equations. Momentum balances are used to express velocities, and this expression is integrated in energy and mass balance equations. By combining all these equations one obtains a pressure system. Calculation domain can be expressed by Cartesian coordinates or by cylindrical coordinates if one intends to exploit symmetries. Scalar variables (temperature, pressure etc.) are centered in cells but velocities are specified on cell boundaries. Initial conditions for a simulation play a significant role and they must therefore be properly defined. MC3D has become one of the reference tools to evaluate FCI phenomena [4].

Simulation cases used in this study are defined so that they are representative of those scenarios analysed in [1] that resulted in vessel melt-through. Each case is studied using two different fragmentation models and two different vessel failure modes (single large jet vs. multiple smaller jets), i.e. each case is simulated four times. Only some major parameters such as water subcooling or vessel and LDW pressures are unique for each case, although some sensitivity considerations regarding fragmentation parameters and effect of triggering time are included as well.

3.1 Premixing phase

In order to accurately predict steam explosion energetics, one must first evaluate the mixing process of corium melt into water, i.e. premixing. This process has time scales of a few seconds and melt particle sizes can vary from millimetre scale to about one metre. Premixing involves heat transfer processes with large temperature and pressure differences. There can be multiple fragmentation and mixing processes simultaneously going on. The main variables in premixing application in MC3D are the volume and mass fractions, velocities, pressure and temperature. The premixing application is a complex model that allows the use of the code for other purposes besides FCI as well, such as direct containment heating. The physical models used to model premixing are introduced in detail in [4].

One of the most important processes to be modelled in premixing is the melt fragmentation because it increases interfacial area and affects heat transfer. The problem of jet fragmentation is challenging for FCI modelling and the theory is not well established. Fragmentation controls both void production and melt-drop solidification which are major limiting effects of the explosion strength. The fragmentation itself occurs primarily from the jet and secondarily from the drops themselves. [4]

In MC3D, the jet fragmentation can be activated principally with 2 types of models, although there is also a numerical non-physical fragmentation model available. The first model assumes that the fragmentation can be obtained through a correlation considering only the local physical properties of the fuel, liquid and vapor. The model is related to fine fragmentation and the fragmentation is due to the friction of the vapor film. It is strictly speaking applicable only for specific situations with large hot jets in water. The implementation of the model is such that velocities are treated globally but other properties are considered locally. The model has been observed to be quite insensitive to ambient pressures [4]. In the code this model is referred to as the CONST model.

The second model (KELMHOLTZ in the code) is based on Kelvin-Helmholtz instability model and considers local velocities. It has been made available in MC3D in order to be able to simulate various flows and it has also been used in direct containment heating calculations. The standard Kelvin-Helmholtz model is very sensitive to local conditions and also to the mesh used in analysis. Validation and further development of the KELMHOLTZ model is underway. [4]

There are many other important phenomena besides fragmentation that are modelled during premixing. For instance frictions, heat and mass transfers and oxidation have been taken into account. With respect to transition from premixing calculation to explosion phase, an interesting quantity called explosivity criterion is provided by the code. Its purpose is to give an idea of how explosive the mixture is in the course of premixing process. There are three criteria available, and the second of them is used in this study. The criterion can be expressed as

$$crit = \sum_{all\ cells} H\left(\frac{\alpha_L}{\alpha_L + \alpha_G} - 0.3\right) \alpha_D \rho_D V, \tag{1}$$

Where H is the Heaviside step function, α_L, α_G and α_D are volume fractions for (continuous) liquids, (continuous) gases and drops, respectively. ρ_D is density of melt drops and V corresponds to volume. The criterion gives the total volume of drops in cells where liquid volume fraction is larger than 0.3. This criterion is representative of mass of fragmented drops, but is quite arbitrary and should not be considered as a prediction of explosion potential, although an approximate link between the criterion and the explosivity of the mixture exists. [3]

This work concentrates on explosion loads and they are the main results from the simulations, but some results are presented from the premixing calculations as well. In addition to explosivity criterion, it is also possible to plot the actual mass of melt droplets during the simulation in order to get an idea of how the fragmentation progresses in each analysis case. Both CONST and KELMHOLTZ fragmentation models are used and the results are compared to each other.

3.2 Explosion phase

Explosion phase follows premixing calculations. In explosion phase a pressure wave propagates in the mixture composed of coolant and melt-drops, and induces fragmentation of the melt-drops. Pressurization during a steam explosion is primarily due to fine fragmentation of the melt, driven by both hydrodynamic and thermal phenomena. Melt fragments vaporise the coolant and thus contribute to the pressure wave. Time scales at issue are of the order of several milliseconds. The pressurization model employed in MC3D explosion calculations is based on a hypothesis of direct vaporization around the fuel fragments, thus ignoring micro-interaction mechanism which effectively means that heat from the fragment is transferred to a certain amount of water that either starts to boil or not. Explosion modeling in MC3D considers e.g. sizes and properties of coolant and melt particles, thermal transfers, mass transfers and interfacial frictions, and detailed discussion about the models along with reasoning behind using them is available in [5]. Especially heat and mass transfer modeling for film boiling around the fragments needs further development [5].

For each analysis case the maximum pressure in the LDW as a function of time is given. Also the pressure impulse on LDW wall is plotted at several locations. The results are compared to FCI induced structural loads used in containment event tree model in [1].

3.3 Analysis scenarios

In [1], a case study of steam explosions at Olkiluoto NPP was performed. Deterministic severe accident code MELCOR was used to evaluate accident progression within the containment. The case study aimed to find out how variations in timings of safety functions affect the initial conditions for ex-vessel steam explosions. Especially the influence of emergency core cooling system (ECCS) and RPV depressurization was focused on. No FCI code was used in the case study. A detailed description of the MELCOR scenarios can be seen in [1].

The MELCOR analysis was mostly performed in a bounding sense, i.e. for example ADS either functioned or not, and the sensitivity of results to ADS valve capacity was not investigated. Delay in ECCS actuation, i.e. in this case the recovery of external power supply, was the main parameter varied – for both high and low RPV pressure scenarios. After evaluating this kind of extreme situations, one can use expert judgment to interpolate to less drastic scenarios and avoid performing a very high number of simulations, which could prove quite an impractical approach. The information obtained from deterministic analyses was then implemented into a probabilistic containment event tree model.

Six different cases were studied with MELCOR, and they can be seen in Table 1. The table contains time points for e.g. when the fuel cladding temperature exceeds oxidation threshold for Zirconium (1100 K) and when the core melt relocation starts. Only cases 2, 5 and 6 end up with melt ejection into LDW, and are therefore interesting for steam explosion considerations. Other cases are not paid further attention here and the corresponding columns in Table 1 are faded.

Table 1: The analysis scenarios studied in [1]. Cases 2, 5 and 6 resulted in melt ejection into LDW and these cases are analysed with MC3D.

	Case #					
	1	2	3	4	5	6
ECCS availability?	Recovery at 3000s	Recovery at 4000s	Recovery at 18000s	Recovery at19000s	No	No
Depressurization through ADS [s]	1821	1821	-	-	1805	-
Core dry for the first time [s]	2510	2510	4650	4650	2510	4650
Zr oxidation starts [s]	2620	2620	3080	3080	2620	3080
Core support structures start to fail [s]	-	5678	7534	7534	5093	7534
Vessel breach (VB) [s]	-	17447	-	19021	13706	19018
Filtered venting (system 362) [s]	-	-	-	19078	-	19087
LDW water subcooling at VB [K]	-	65.53	-	95.84	73.61	95.84
LDW water partial pressure at VB [bar]	-	1.82	-	3.72	2.25	3.72
Melt ejected [ton]	-	159.7	-	-	183.3	185.5

Some further MELCOR simulations were made for cases 2, 5 and 6 in order to redefine them for MC3D analysis. For example some corium properties and gas temperatures in both RPV and LDW were looked into. Case-specific physical quantities such as pressures and temperatures are shown in Table 2. In case 6 there is quite a large pressure difference between RPV and LDW which is expected to have a huge influence on melt ejection and thus on fragmentation and premixing in general. Gas temperatures in RPV vary significantly from case to case. In case 2, ECCS is able to efficiently keep temperature low contrary to cases 5 and 6. However, gas temperatures are not expected to have massive influence on steam explosion occurrence or loads to containment walls but they are easily given as input to MC3D calculations. Water pool depth is the same in all cases.

The 2D mesh constructed for the analyses is shown in Figure 1. Water pool depth is 12.2 m and bottom of the RPV is at the height of 23.7 m. The mesh utilizes cylindrical symmetry and thus only half of the vessel and the LDW are explicitly modelled. With MC3D it would be possible to study also 3D scenarios but with the cost of significantly prolonged simulation durations. Thus 3D simulations are outside the scope of this study and even 2D modelling used here can be regarded as quite harsh. In addition, the benefits of 3D inspection are unclear because there are many uncertainties and open issues with steam explosion phenomena themselves.

Table 2: Atmospheric initial conditions and coolant properties at the time of vessel breach for each case that is analysed with MC3D.

	Case 2	Case 5	Case 6
LDW pressure [bar]	1.82	2.25	3.72
RPV pressure [bar]	1.82	2.25	70.0
Gas temperature in LDW [K]	330	340	370
Gas temperature in RPV [K]	420	1000	1250
Coolant temperature [K]	325	325	318
Water pool depth [m]	12.2	12.2	12.2
LDW radius [m]	4.6	4.6	4.6
Melt amount[1] [tons]	79.84	91.61	92.84

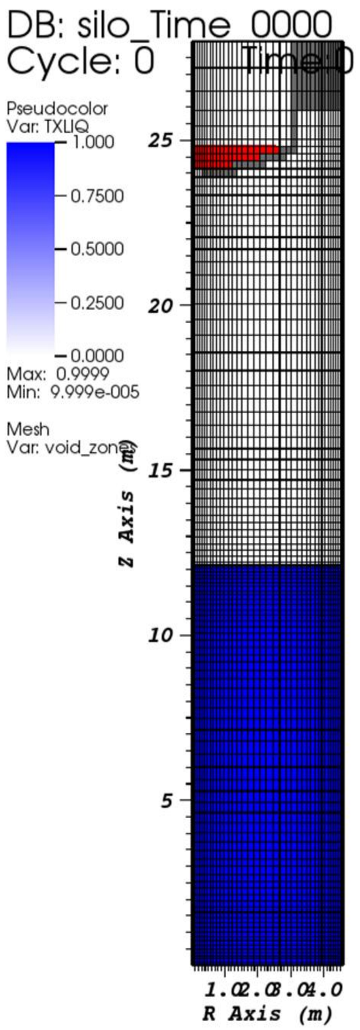

Figure 1: Mesh used in MC3D analyses.

Each case is analysed for two different vessel failure modes which both are shown in Figure 2. On the left hand side of the figure is the first failure mode which concerns a single large centrally located break. The hole has a 0.6 m diameter and this failure mode results in a single thick melt jet. The second failure mode deals with a situation where the vessel bottom is

[1] Due to exploitation of symmetry, melt amounts in the table are half of the actual amounts.

breached from several locations simultaneously. This is a feasible failure mode in BWR reactors due to the control rod and instrumentation guide tube (CRGT and IGT) penetrations through the vessel bottom. CRGT diameter is around 0.2-0.3 m and for IGT the diameter is a few centimetres. As shown by right hand side of Figure 2, there are five holes with diameters in the range of 0.1-0.25 m resulting in five melt jets that are fragmented during the premixing process. The objective is to find out how the different failure modes affect properties of the premixture (e.g. explosivity criterion of equation (1)) and the subsequent explosion.

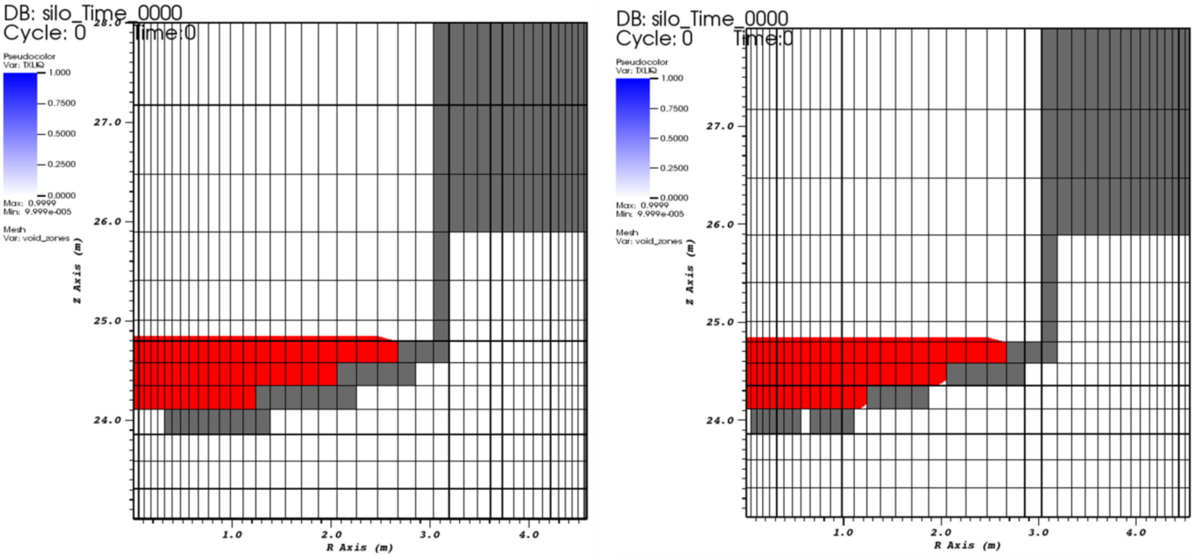

Figure 2: Vessel geometries when there is a single hole (left) in the vessel vs. multiple holes (right).

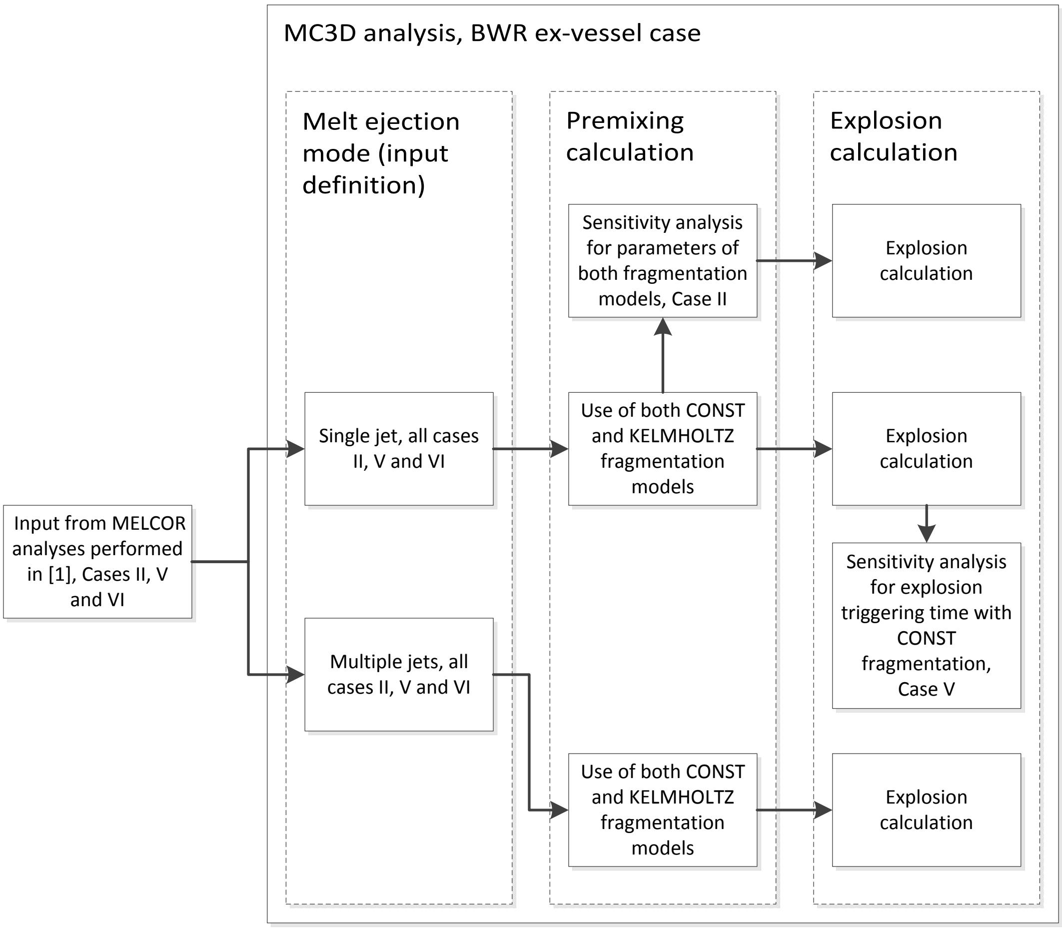

Figure 3: Summary of analyses performed with MC3D.

Figure 3 summarizes the simulations to be performed with MC3D. All cases derived from MELCOR analyses are investigated for both single jet and multiple jets melt ejection modes. Two melt fragmentation models (CONST & KELMHOLTZ) are used for premixing calculations, and premixing sensitivity analysis is conducted for case 2. All premixing simulations are followed by calculation of explosion phase, and explosion strength sensitivity to triggering time is evaluated for case 5. All sensitivity analyses concern single jet melt ejection mode.

3.3.1 Melt properties

Also some melt properties were looked into by using results from MELCOR simulations. It was observed that there are quite large differences in melt temperatures at the instant of vessel failure. In case 2, the RPV was depressurized and ECCS was recovered at 4000 s. The water injected provided also cooling to the vessel and thus delayed melt-through and the melt temperature had time to ascend to around 3100 K. In case 5, there was no cooling provided by ECCS and vessel breached earlier than in case 2, and melt temperature was around 2690 K. According to MELCOR results, melt heating is much slower in pressurized case 6. Therefore vessel also fails significantly later than in depressurized scenarios. Melt temperature at vessel breach in case 6 was just 2200 K. However, when these lower melt temperature values were used in simulations, there were problems in getting the premixture triggered, i.e. no explosion calculations could be performed. Because of that a decision was made to use the melt temperature and other melt properties from case 2 also in the rest of analysis cases.

Melt densities were observed to vary as a function of time, which is a result from altering melt compositions and conditions. A representative average value around the time of vessel failure was in the range of 7500-8000 kg/m^3. In [6], a corium density value of 7660 kg/m^3 for

Nordic BWRs was used, and the same value is adopted in this study. MELCOR results were not used to obtain other melt properties such as heat capacities or conductivities. Instead values representative of UO2/ZrO2 80/20 corium composition was used [7]. Melt properties used in the analyses are collected in Table 3.

Table 3: Melt properties used in MC3D simulations (UO2/ZrO2 80/20 [7]). The same values were used in all analysis cases.

Solidus melt temperature [K]	3050
Liquidus melt temperature [K]	3100
Liquid heat capacity [J/kg/K]	510
Solid heat capacity [J/kg/K]	450
Surface tension [N/m]	0.45
Fusion latent hear [J/kg]	2.8E5
Origin temperature for internal energy and enthalpy calculation [K]	3100
Solid density [kg/m^3]	7660
Liquid density [kg/m^3]	7660
Heat conductivity [W/m/K]	2.3
Dynamic viscosity [Pa.s]	4.0E-3
Radiative emissivity (dimensionless)	0.7

3.3.2 Fragmentation

Each case (cases 2, 5 and 6) is analysed for two different vessel failure modes (see Figure 2) and for two different fragmentation models (CONST and KELMHOLTZ) discussed in section 3.1. Thus each case is calculated 4 times and total number of different analysis scenarios rises up to 12. In addition, sensitivity analysis for some fragmentation parameters is performed and discussion can be seen in sections 4.3.1. The default values for parameters regarding both fragmentation models can be seen in Table 4. Sauter diameter, in fluid dynamics, means the average particle size. It is defined as the diameter of a sphere that has the same volume or surface area as the particle of interest. The fragmentation models have also many other parameters that the user can modify, but in this work they are not taken into account in sensitivity considerations.

Table 4: Fragmentation models and default values of their parameters.

CONST model		KELMHOLTZ model	
Parameter	Default value used	Parameter	Default value used
Jet fragmentation rate in gas [m3/s/m2]	0.01	Coefficient for the fragmentation rate	0.15
Jet fragmentation rate in water [m3/s/m2]	0.075	Ratio of new born fragment diameter to wave length	6
Corium drop Sauter diameter [m]	2.5E-3	Characteristic radius of the jet	0.3 for single jet, 0.075 for IGT/CRGT failure mode
Velocity of melt drops that diverge from the melt jet [m/s]	0.5		

4. Results

In the following sections, the results from the analysis cases are presented. First, results from simulations that concerned single jet vessel failure mode are shown. Premixing and explosion phases are dealt with separately. Results from premixing phase concern mainly the explosivity criterion of equation (1) as a function of time. Also the actual mass of melt fragments is plotted. Explosion phase results show the maximum pressure in both the whole domain and along the LDW wall. Also pressure impulses along the LDW wall are given.

Simulation progression can be visualized by using VisIT, and it can be applied both to premixing and explosion phases. As an example, in Figure 4 is a series of figures from premixing calculations for case 2 using CONST premixing and single jet release mode. Red regions in the figure represent continuous melt fields, i.e. melt jet or melt pool. Orange particles or dots that emerge from the melt jet represent fragmented melt. Note that in the figure the fragments are magnified for visualization purposes and they do not represent a realistic physical situation in that sense. Melt jet reaches the water at around 1.66 s and starts to fragment at a higher rate than in air. A little before 2.71 s the melt front gets in contact with the bottom of the LDW, which is a typical candidate for a triggering event. All premixing calculations are set to terminate at the time 3.5 s.

In Figure 5 is a series of figures that show how the explosion starts and progresses from the premixing calculations of Figure 4. Colours indicate pressures in different regions, but note that the pressure scale changes from picture to picture and e.g. red colour may stand for ~1E8 Pa in one picture and ~1E7 Pa in another. Triggering time was selected on the basis of explosivity criterion which is assumed to indicate the worst possible time for explosion trigger in terms of threat posed to containment integrity. A conventional candidate for triggering time is the moment when melt gets in contact with the LDW floor. Each explosion calculation was predetermined to last for 100 ms, which is quite a long time when it comes to explosion dynamics, but this way there should be enough time for high pressures to fade away so that the full extent of the loads imposed to the walls could be evaluated.

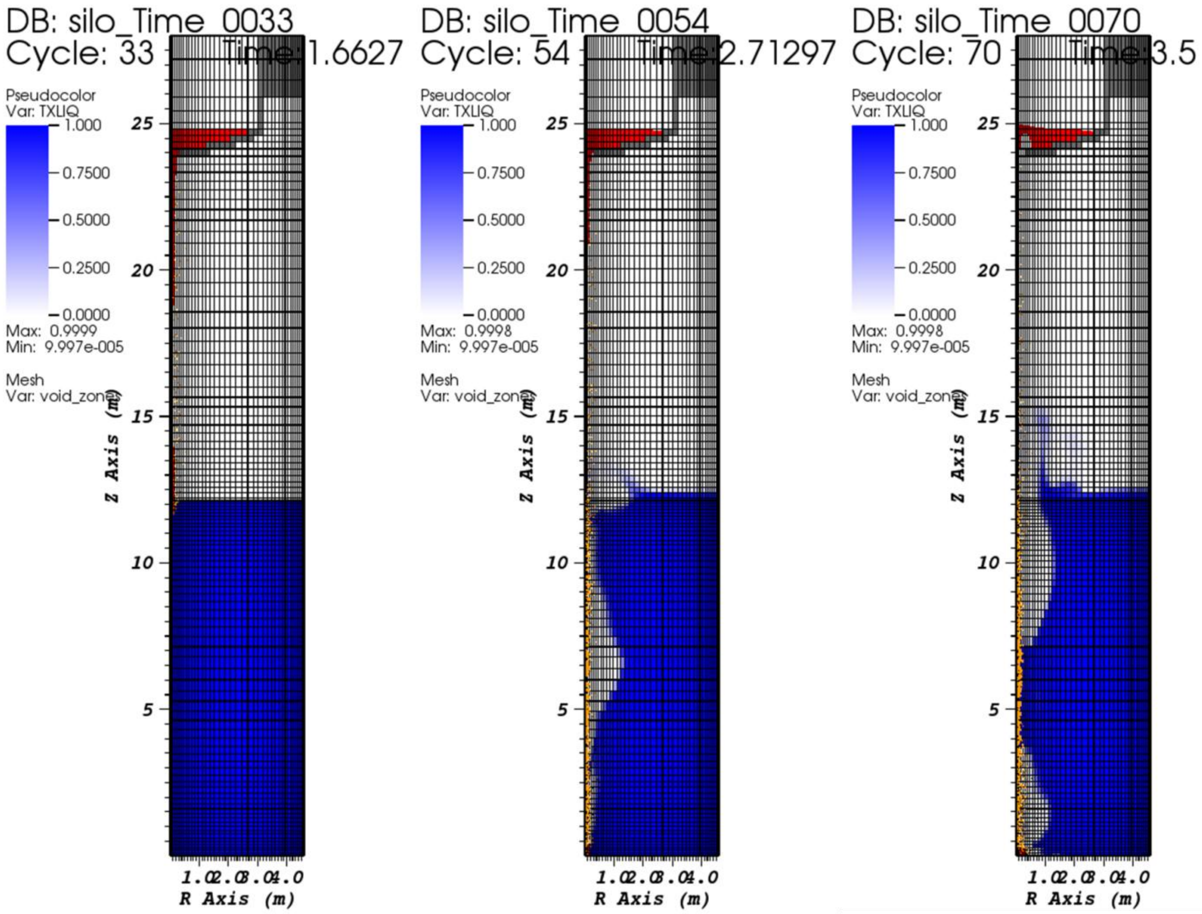

Figure 4: Penetration of melt jet into the water in case 2 during premixing calculations using CONST model and single jet melt ejection mode.

The first picture in the upper left corner of Figure 5 takes place a little after the explosion was triggered (2.4000 s). The highest pressures (~265 MPa) were obtained at this early stage of the explosion. In the next picture right to the first one it is clearly seen how the pressure wave propagates in water and in the third picture the pressure wave is reflected back from the LDW wall and floor. Right after this reflection, the maximum pressure (28.3 MPa at 0.0048 s since trigger) along the LDW wall is reached. The bottom left picture shows how the high pressure zone fills more or less the whole liquid space in the LDW, with a pressure concentration at right bottom corner. After that a new trigger seems to take place at the time 0.0172 since the trigger, this time at a somewhat higher location, but this latter explosion does not lead to as high pressure loads as the earlier one and the high pressures fade away. After ~30 ms there are no more extreme pressures present in the LDW and the rest of the simulation can actually be regarded as gratuitous.

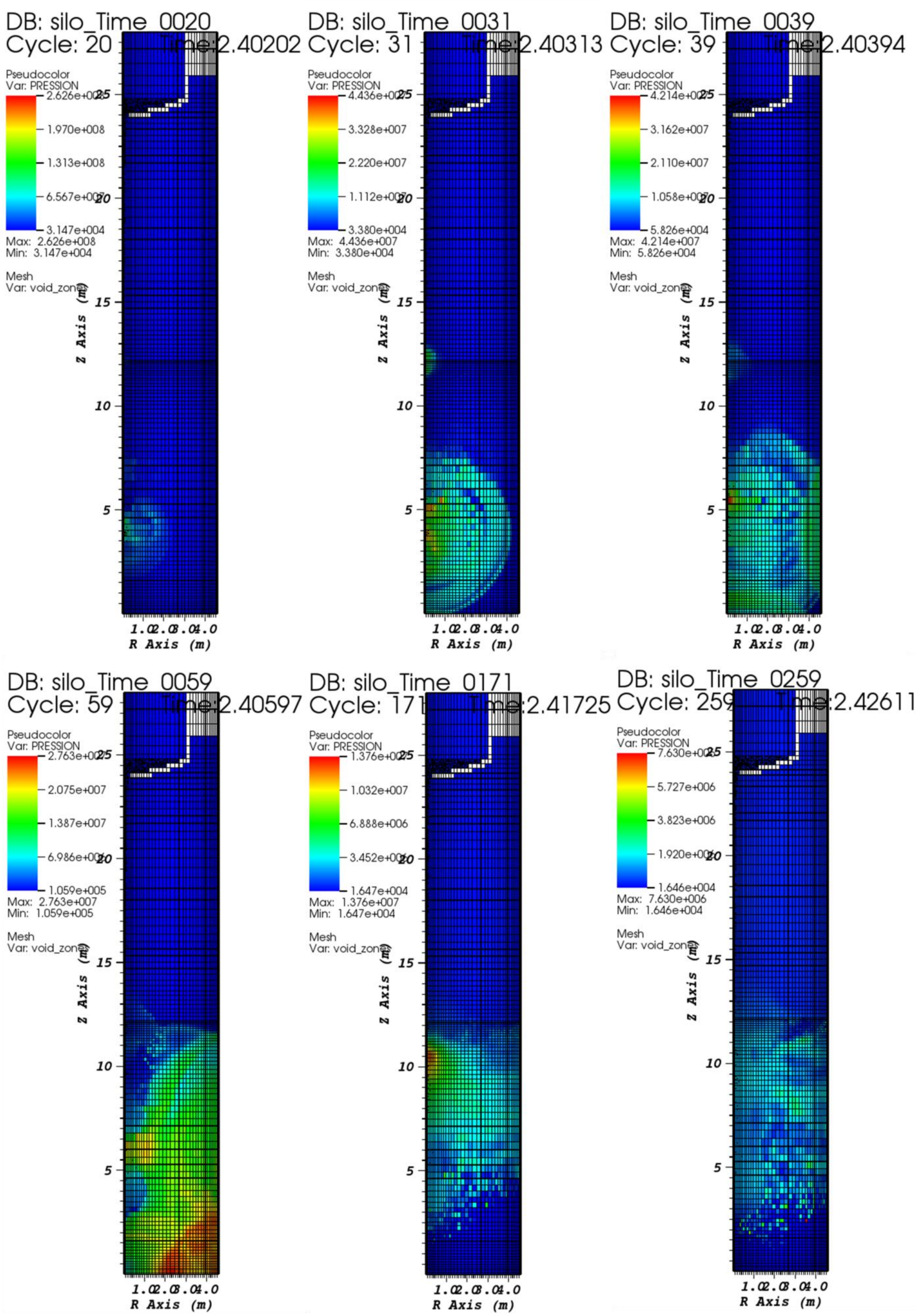

Figure 5: Progression of the explosion pulse in case 2 and single melt jet mode. Initial state was calculated with CONST premixing model. Explosion is assumed to trigger already before contact with the LDW bottom.

4.1 Single jet

Results from calculations with single break in the centre of the RPV lower head can be regarded as the core of this study, partly because these results are seen as more reliable than results with multiple failures in the vessel (due to relative simplicity of situation with only one melt jet). As already discussed, premixing for each case is calculated with two different fragmentation models and each premixing simulation is followed by calculation of the explosion phase. However, there were difficulties with triggering of explosions, and therefore e.g. a little different triggering times had to be chosen for different cases which hinders the comparability of results. Also all the sensitivity considerations in section 4.3 concern scenarios with single melt jet.

4.1.1 Premixing phase

In Table 5 is a summary of basic results from premixing calculations with single melt jet. Explosivity criterion values for cases 2 and 5 are of the same order of magnitude for both premixing models, but maximum seems to be achieved somewhat later for case 5. For case 6 the explosivity value is significantly higher because of pressurized melt ejection, and CONST premixing model yields even higher figures than KH model. Contrary to explosivity criterion, KH model yields generally higher total mass of melt drops than the CONST model. Also this time results for cases 2 and 5 are quite near to each other while case 6 produces values multiple times higher than the other two cases.

Premixing model does not have any significant effect on propagation of the melt jet, i.e. for a particular case the melt jet front progresses quite similarly regardless of premixing model employed. There are also no vast differences between cases 2 and 5 regarding the time the melt jet reaches surface of the water pool or the bottom of the LDW. In case 6 the pressurized melt ejection means that the melt jet and drops have high speed and penetrate water very early. The fragmentation in case 6 is so intense that from result with KH model it is difficult to say when or if the jet reaches the bottom of LDW because the jet seems to practically fragment away.

Table 5: Results from premixing calculations with single jet melt ejection mode.

	Explosivity criterion maximum and the corresponding time	Mass of melt droplets at the end of premixing calculations [kg]	Melt jet reaches water [s]	Melt jet reaches LDW bottom [s]
Case 2 CONST	939.5 at 2.445 s	7136.1	1.61	2.71
Case 5 CONST	923.2 at 2.722 s	7942.4	1.62	2.72
Case 6 CONST	4156.3 at 1.139 s	49686.4	0.29	0.71
Case 2 KH	126.9 at 2.855 s	10951.1	1.61	2.65
Case 5 KH	208.4 at 3.496 s	11773.3	1.62	2.64
Case 6 KH	1382.2 at 2.418 s	68791.2	0.23	(no melt in jet form to reach bottom)

Figure 6 contains explosivity criterion values as a function of time for CONST model and Figure 7 shows similar information for KELMHOLTZ premixing model. Case 6 stands out clearly with multiple times higher values than other cases produce. Fragmentation also begins almost immediately in case 6 while in cases 2 and 5 fragmentation begins later. Start of fragmentation corresponds roughly the time the melt jet gets in contact with water. The reason behind oscillating behavior in case 6 for KELMHOLTZ model is unclear. In Figure 8 is the development of mass of melt drops in time for each case. Yet again, case 6 yields highest values. Values for KELMHOLTZ model are systematically higher than those of CONST cases.

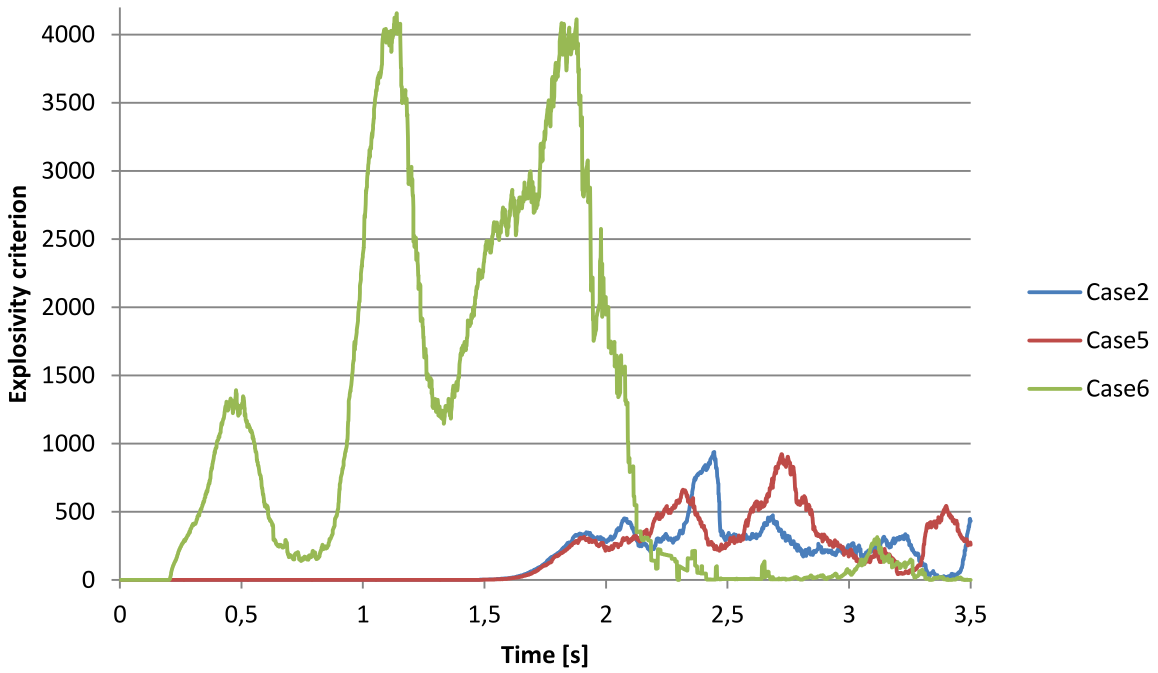

Figure 6: Explosivity criterion as a function of time with CONST premixing model and single jet melt ejection mode.

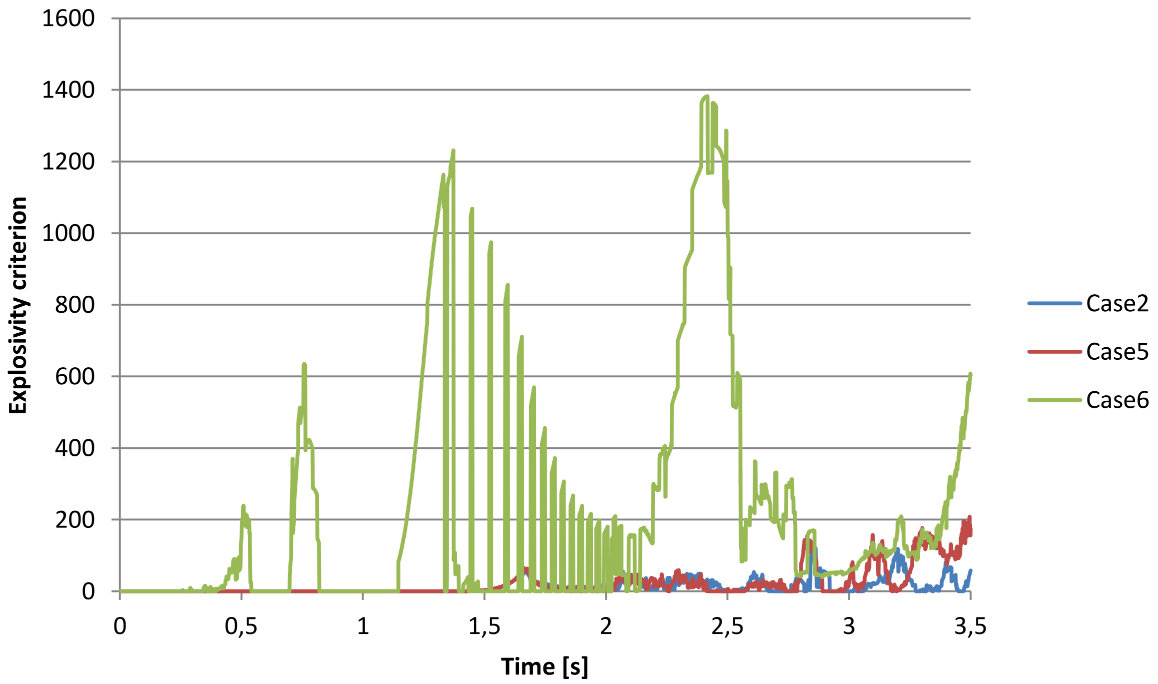

Figure 7: Explosivity criterion as a function of time with KELMHOLTZ premixing model and single jet melt ejection mode.

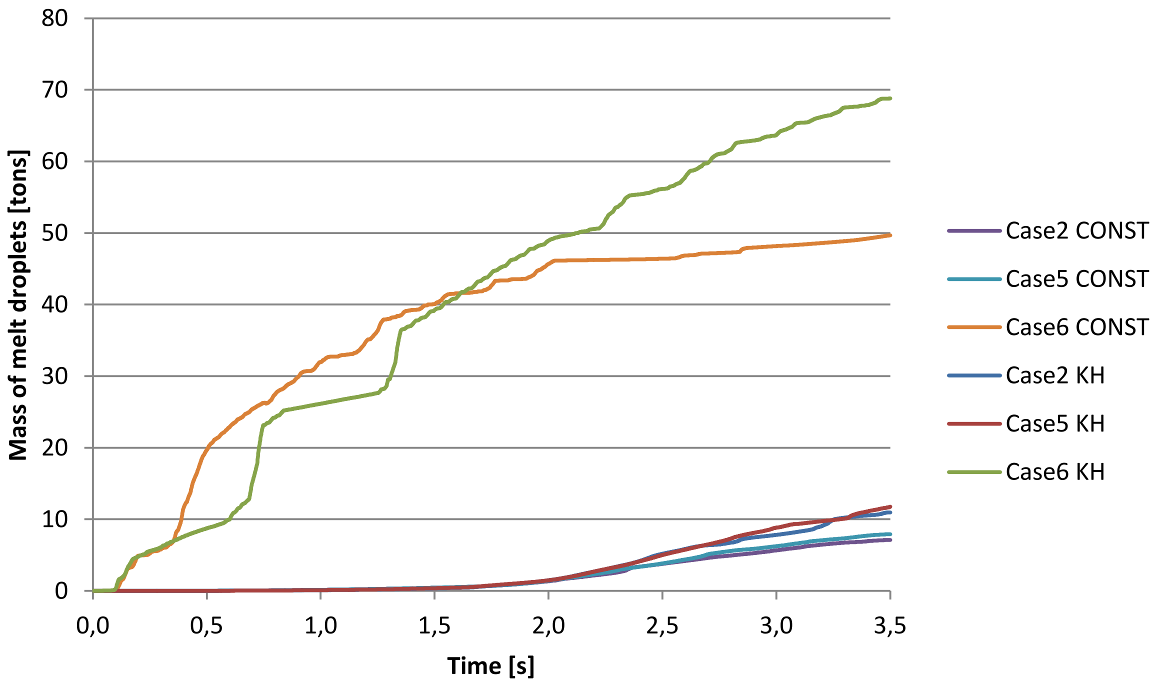

Figure 8: Melt drop mass as a function of time for both premixing models and single jet melt ejection mode.

4.1.2 Explosion phase

Table 6 contains main results from explosion calculations that were performed using premixing results discussed in section 4.1.1 as input. Trigger time was decided to be as near as possible to the explosivity criterion maximum, but in almost every case there were difficulties to initiate the trigger and therefore compromises regarding triggering time had to be made. Now all triggers occur already well before the melt reaches LDW bottom, and for KELMHOLTZ cases the triggering time had to be chosen so early that the melt jet had penetrated only a few meters in the water pool which is 12.2 m deep in total. For case 6 it was impossible to trigger the explosion at any time irrespective of fragmentation model used.

Table 6: Results from explosion calculations with single jet melt ejection mode. In two cases the trigger could not be initiated at all.

	Trigger time [s]	Explosivity criterion value (eq. (1)) at trigger	Melt jet height at triggering time [m]	Maximum pressure in whole domain [MPa]	Maximum pressure along LDW wall [MPa]	Impulse on the LDW wall [MPa.s]
Case 2 CONST	2.4000	817.304	3.71	264.8 (at 0.0019 s)	27.7 (at 0.0048 s)	0.168
Case 5 CONST	2.2957	585.988	4.85	330.1 (at 0.0017 s)	27.6 (at 0.0090 s)	0.158
Case 6 CONST	-	-	-	-	-	-
Case 2 KH	1.8939	16.957	9.04	207.3 (at 0.0011 s)	13.6 (at 0.0097 s)	0.053
Case 5 KH	1.9621	18.122	8.32	158.1 (at 0.0011 s)	12.8 (at 0.0094 s)	0.055
Case 6 KH	-	-	-	-	-	-

Table 6 includes also maximum pressures both in the whole simulation domain and along the LDW wall. Courtesy of higher explosivity criterion values, maximum pressures for CONST cases are higher than for KELMHOLTZ calculations, and the highest pressure, around 330 MPa, is obtained in case 5. Differences in pressures along the LDW wall are smaller for cases that are calculated with the same fragmentation model, and for CONST cases the pressure values are around twice as high as for KELMHOLTZ cases.

Impulses on the LDW wall were measured at four different locations along the LDW wall with varying heights from the LDW bottom (0.1 m, 2.9 m, 9.1 m and 12.1 m). In Figure 9 are pressure impulses for case 2 with CONST premixing. It can clearly be seen that the highest impulses are obtained near the LDW bottom. This is actually true for all cases analysed in this study, also for those cases where explosion is triggered near the surface of water. Figure 10 shows time development of pressure impulse maxima for each case where explosion could be triggered and the end values are present in Table 6 as well.

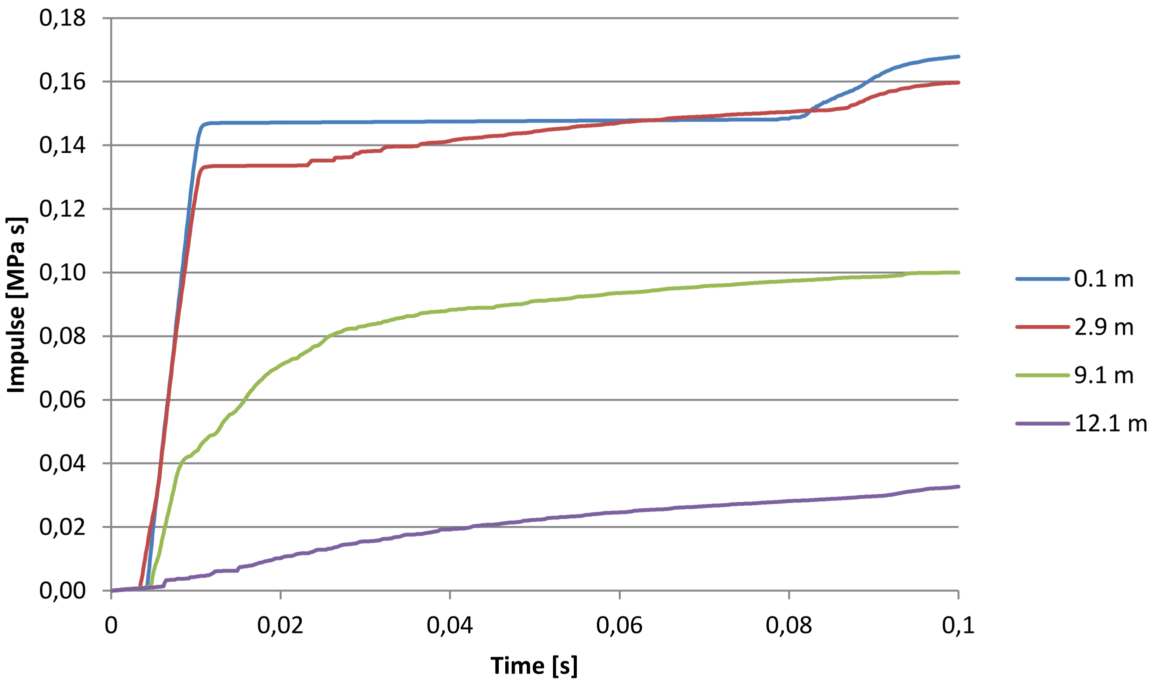

Figure 9: Pressure impulses at different heights along the LDW wall. Case 2 with CONST premixing and single jet melt ejection mode.

In Figure 11 are the pressure maxima in the whole simulation domain for each case. Pressure peaks are achieved in the early stages of the calculations, before 5 milliseconds since the trigger. After roughly 15 milliseconds there are no more pressures above 50 MPa in any of the simulation cases. Figure 12 illustrates maximum pressures along the LDW wall, and as already stated above, pressure values are lower for KELMHOLTZ premixing cases. For case 2 with CONST premixing there is a second pressure rise along the LDW wall after approximately 80 milliseconds from the trigger which indicates a second, milder explosion to have occurred.

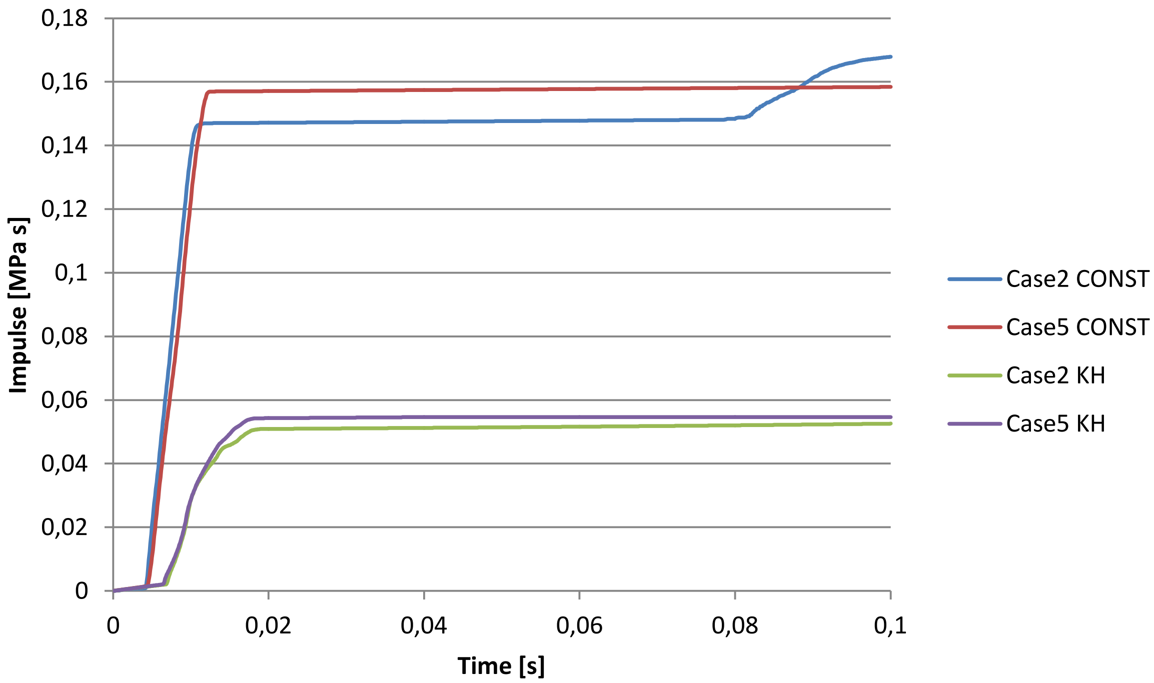

Figure 10: Pressure impulses at 0.1 m height from the LDW bottom for cases 2 and 5 with both premixing models and single jet melt ejection mode.

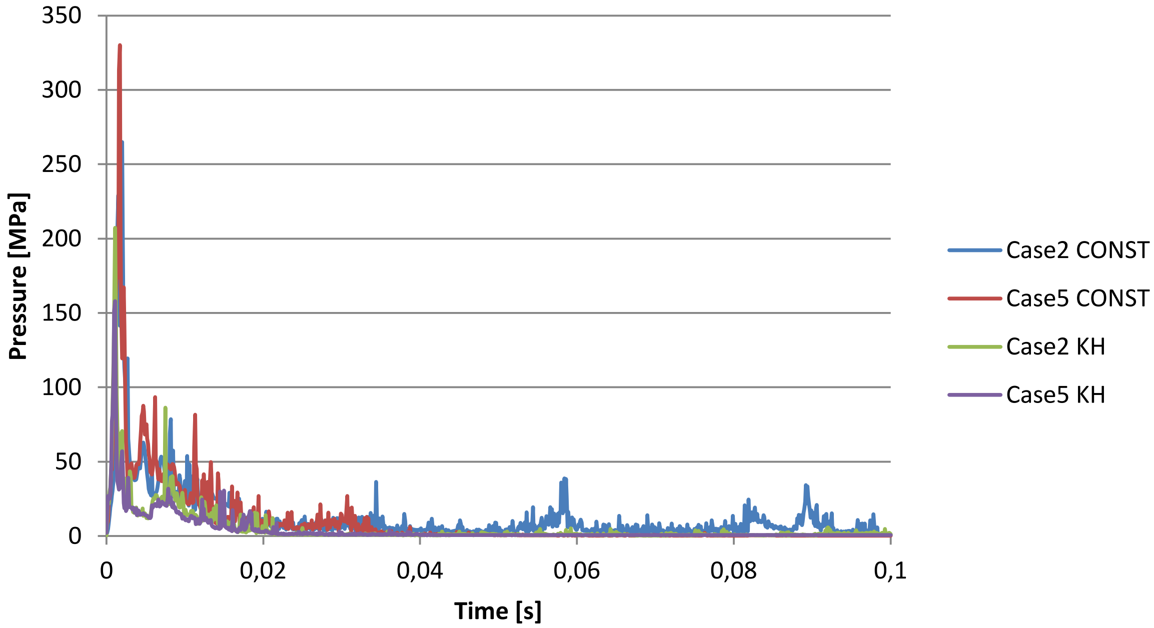

Figure 11: Maximum pressures in the whole domain during explosion calculations with both premixing models and single jet melt ejection mode.

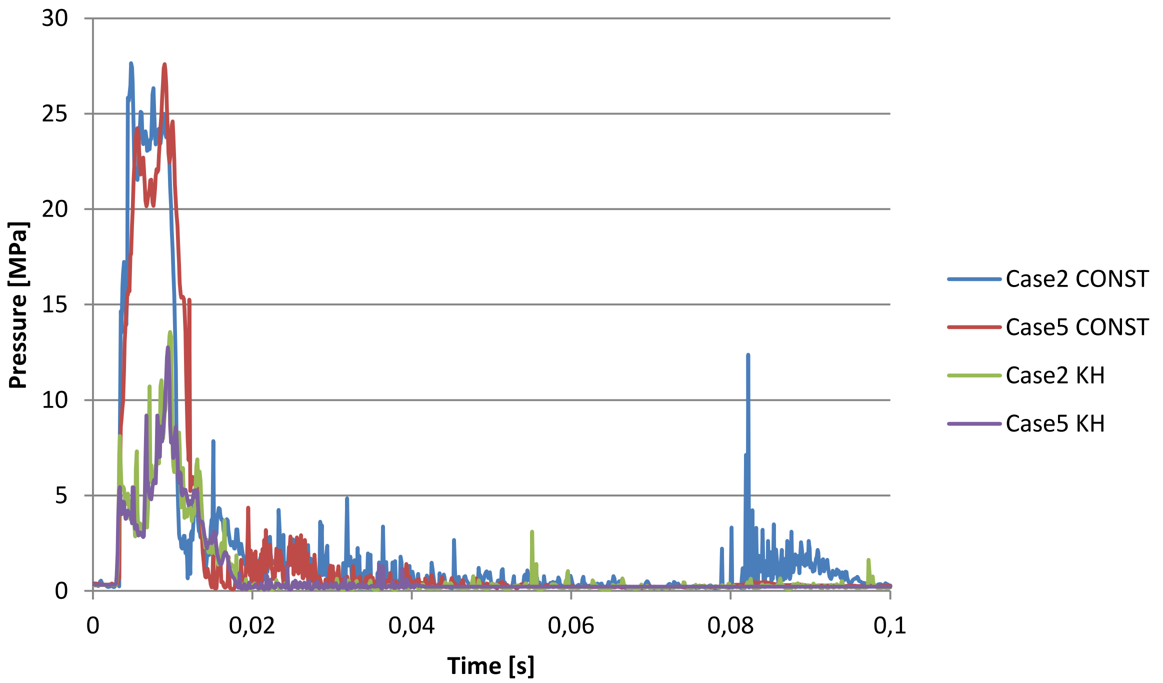

Figure 12: Maximum pressures along the LDW wall during explosion calculations with both premixing models and single jet melt ejection mode.

4.2 Multiple jets

The same three cases were analysed for a little different vessel geometry as well. Now there are multiple holes in the LDW lower head which represent a situation where some of the bottom penetrations (CRGT and IGT) have failed simultaneously. The mesh used in simulations can be seen in Figure 2. The analyses proceed in similar fashion to those performed for single jet vessel failure mode, i.e. premixing is calculated with two fragmentation models for each case and each premixing calculation is followed by simulation of the subsequent explosion phase. Also the results are presented with similar tables and figures as results from single jet scenarios.

4.2.1 Premixing phase

In Table 7 are explosivity criterion maxima, total mass of melt drops and time when melt jet reaches water for each simulation. Because there are now multiple melt jets which also enables higher total fragmentation rate, it is difficult to say from the results if melt reaches the LDW bottom in jet form and when. Therefore no data on that is displayed in Table 7. However, the time melt jet reaches water can be interpreted from results, and for cases 2 and 5 there are no huge differences compared to single jet scenario, but for case 6 it takes now a little longer time for the melt to reach water. Both explosivity criterion and mass of melt drops are generally multiple times higher than for single break melt ejection mode. KELMHOLTZ fragmentation model yields now higher values in terms of explosivity criterion than CONST model but for melt drop mass it is not easy to see a clear dependence on fragmentation model used.

Figure 13 and Figure 14 show how the explosivity criterion behaves as a function of time for both fragmentation models. For case 6 fragmentation starts about one second earlier than in cases 2 and 5. Characteristic of case 6 is that the highest explosivity values are reached quite early and thereafter the values drop to levels lower than those of cases 2 and 5. Figure 15 illustrates the development of melt drops, and case 6 is distinguishable from all other cases which are easiest grouped according to the fragmentation model used.

Table 7: Results from premixing calculations with multiple melt jets vessel failure mode. There is no melt in clear jet form to reach LDW bottom.

	Explosivity criterion maximum and the corresponding time	Mass of melt droplets at the end of premixing calculations [kg]	Melt jet reaches water [s]	Melt jet reaches LDW bottom [s]
Case 2 CONST	5173.1 at 1.914 s	62402.7	1.57	-
Case 5 CONST	3906.1 at 1.911 s	54411.3	1.58	-
Case 6 CONST	9855.4 at 1.228 s	84395.1	0.49	-
Case 2 KH	8825.6 at 2.418 s	54840.2	1.64	-
Case 5 KH	6441.0 at 2.025 s	69634.5	1.68	-
Case 6 KH	10048.5 at 1.074 s	85060.0	0.41	-

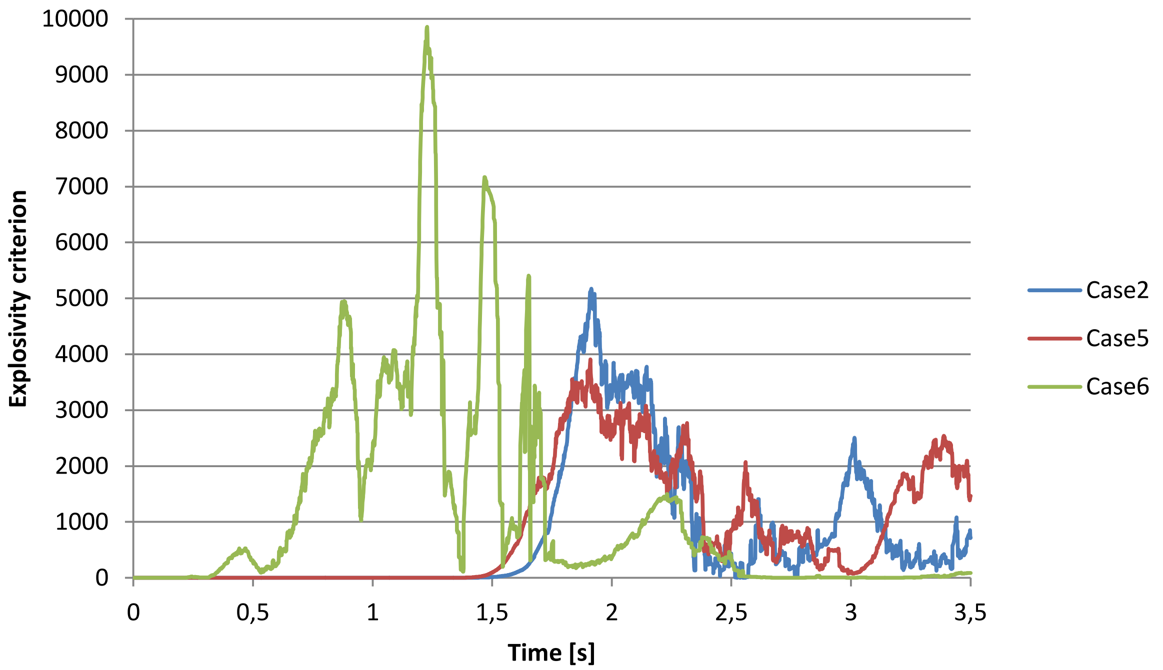

Figure 13: Explosivity criterion as a function of time with CONST premixing model and multiple jets melt ejection mode.

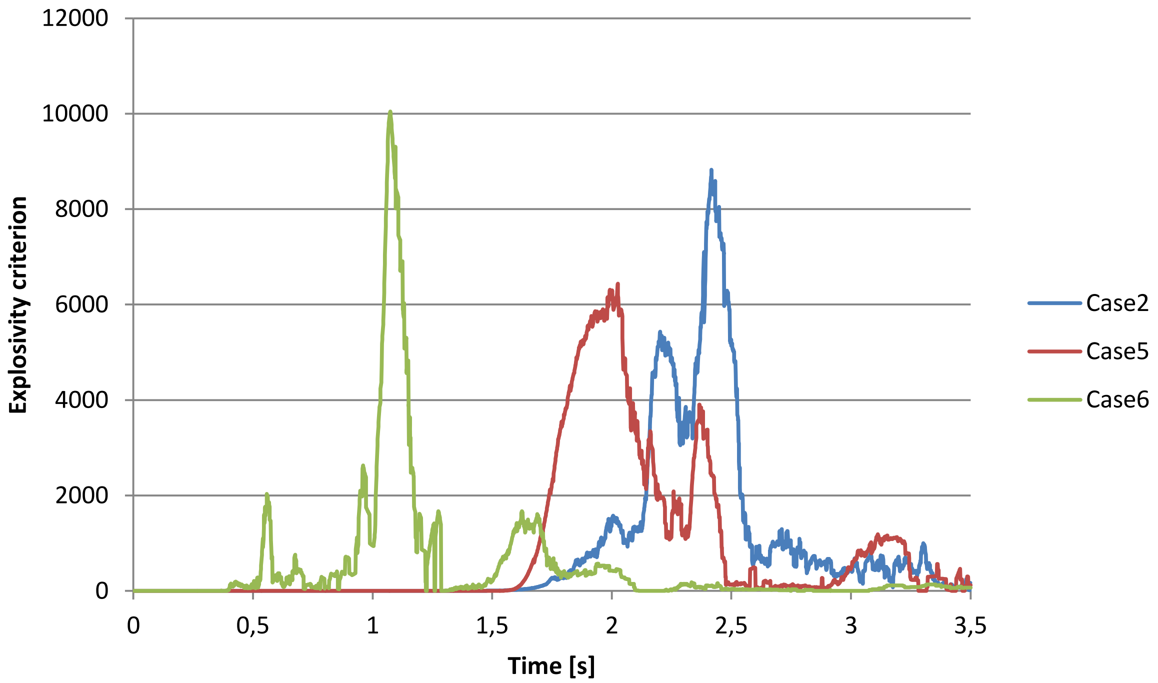

Figure 14: Explosivity criterion as a function of time with KELMHOLTZ premixing model and multiple jets melt ejection mode.

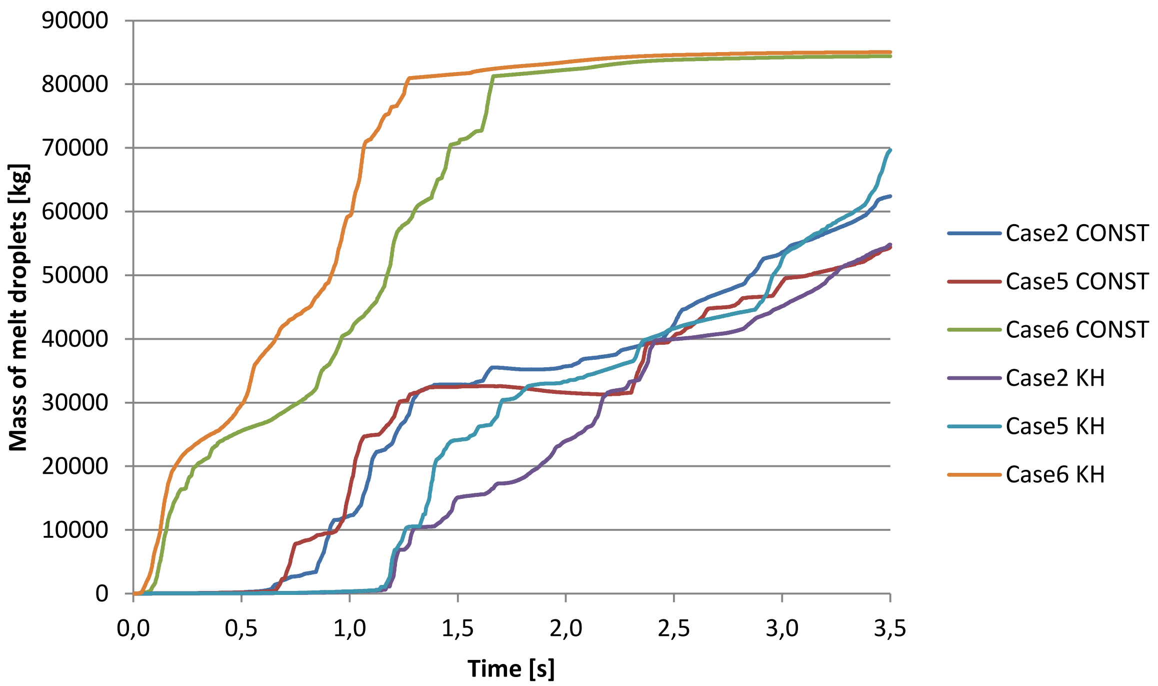

Figure 15: Melt drop mass as a function of time in all cases and both premixing models for multiple jets melt ejection mode.

4.2.2 Explosion phase

Calculation of explosion phase induced several kinds of difficulties. Even though explosivity criterion values were systematically high for all simulations, there were problems getting the explosion triggered. Calculation of explosion phase for case 6 turned out impossible regardless of fragmentation model used. The same holds true also for case 5 with KELMHOLTZ model. Explosion simulation of cases 2 and 5 with CONST premixing could be initiated but the calculations were terminated prematurely. However, the most important early phases of explosions were calculated and e.g. pressure peak maximum along the LDW wall was most likely achieved. Impulses along the wall would have probably increased further but an idea of their magnitude was obtained. In any case, the pressure maxima and impulses for CONST premixing are now significantly higher than for single jet cases. Pressure impulse maxima are about twice as high, which suggests that the amount of melt involved in premixing plays an important role. The only KELMHOLTZ case for which the explosion could be calculated was case 2, and the explosion had to be triggered very early at the time 1.6 seconds with only a little melt involved and a modest explosivity criterion value of 3.0. Therefore the explosion was also relatively mild. Results from multiple melt jets explosion calculations are shown in Table 8

Table 8: Results from explosion calculations with multiple jets melt ejection mode. In all but two cases the trigger could not be initiated.

	Trigger time [s]	Explosivity criterion value (eq. (1)) at trigger	Maximum pressure in whole domain [MPa]	Maximum pressure along LDW wall [MPa]	Max impulse on the LDW wall [MPa.s]
Case 2 CONST	3.0001	2167.6	376.6	33.8	0.340
Case 5 CONST	2.6073	1367.8	397.4	35.6	0.293
Case 6 CONST	-	-	-	-	-
Case 2 KH	1.6000	3.0	38.4	2.8	0.057
Case 5 KH	-	-	-	-	-
Case 6 KH	-	-	-	-	-

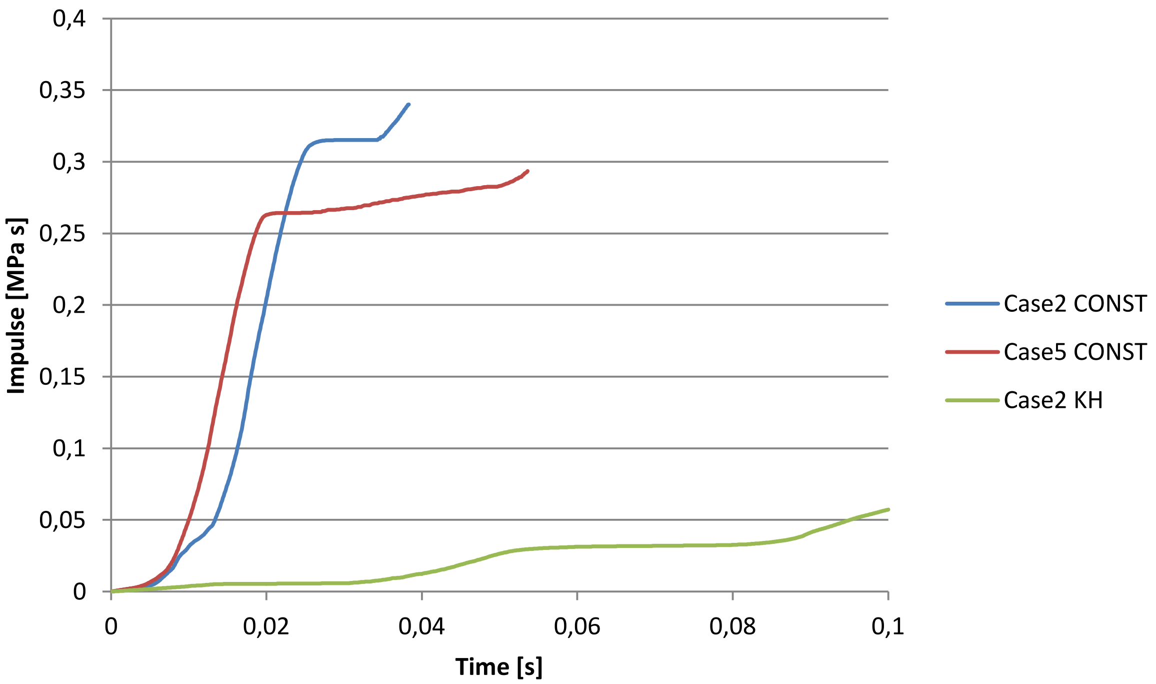

Figure 16: Pressure impulses maxima for all cases where explosion could be triggered with multiple jets melt ejection mode. For CONST cases calculations terminated prematurely.

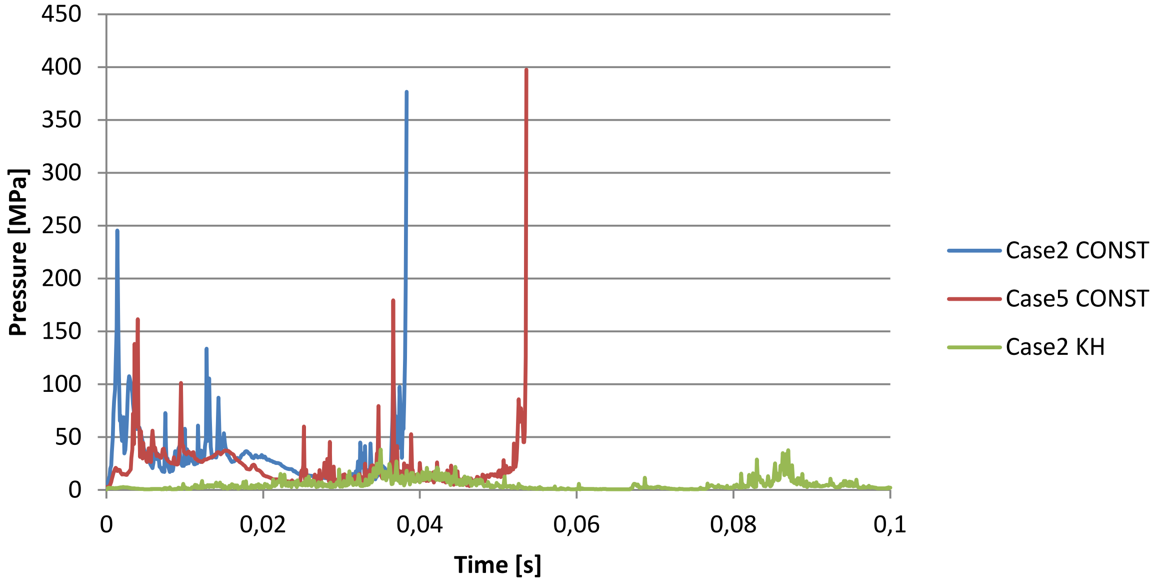

Figure 17: Maximum pressures in the whole domain for all cases where explosion could be triggered with multiple jets melt ejection mode. Extreme pressure peaks most likely induced premature termination of CONST calculations.

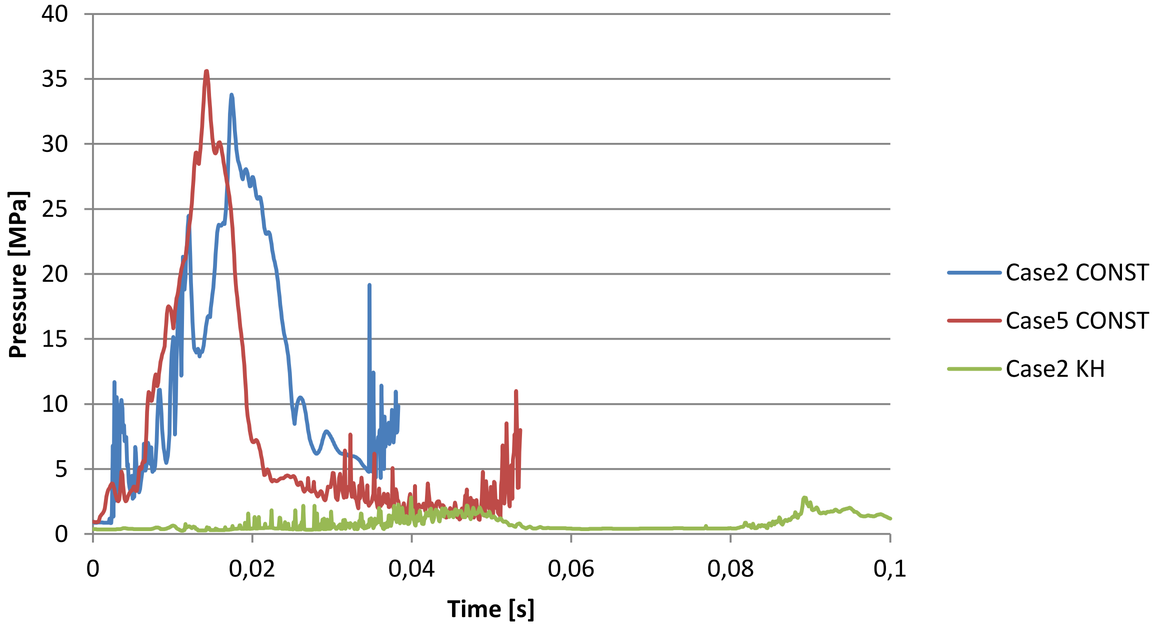

Figure 18: Maximum pressures along the LDW wall for all cases where explosion could be triggered with multiple jets melt ejection mode. For CONST cases calculations terminated prematurely.

A noteworthy observation from pressure impulse results is that now the impulse values are close to maximum value even at the height of around 9 meters from the LDW bottom. Even at water surface level the impulse value is near to that of single jet case. Figure 16 illustrates pressure impulse maxima along the LDW wall for all cases that could be triggered and shows how the very early trigger in KELMHOLTZ case leads to low impulse values. Figure 17 shows maximum pressures in whole of the domain and gives a slight hint what could have led to premature termination of CONST calculations. Results show that extreme pressures near 400 MPa occurred and possibly somehow caused simulations to end. These perhaps nonphysical pressure peaks should probably be ignored, and use the second largest values, which are 245.4 MPa and 179.5 MPa for cases 2 and 5, respectively. Figure 18 illustrates the pressures along the LDW wall, and it can be seen that the highest values are distributed around the time of 20 milliseconds after the trigger occurred. In both Figure 16 and Figure 17 the pressures for KELMHOLTZ case are very low in comparison to CONST cases, due to reasons discussed above.

4.3 Sensitivity analyses

Sensitivity analyses were performed for both fragmentation models by varying some of their parameters. Analyses did not limit to premixing calculations but proceeded to explosion phase as well. The effect of triggering time was investigated for a single input from premixing calculations. Single jet melt ejection mode was used for all sensitivity analyses and case 2 was used for fragmentation and case 5 for triggering time analyses.

4.3.1 Fragmentation parameters

A brief sensitivity analysis was performed for fragmentation parameters in order to see how they affect the premixing process and the subsequent explosion strength. The investigation was limited to fragmentation rate and the melt drop sizes (or related parameters). An increased fragmentation rate and smaller melt particles both are assumed to result in higher explosion potential because of higher melt surface area available for heat transfer. The analysis was conducted by using case 2 and the single jet vessel failure mode as a basis.

Table 9: Fragmentation parameter values used in sensitivity analysis. Case 2 serves as a basis for the sensitivity inspection. Also default values are shown.

CONST model				KELMHOLTZ model			
Parameter	Default	Case 2Ca	Case 2Cb	Parameter	Default	Case 2Ka	Case 2Kb
Jet fragmentation rate in gas [m3/s/m2]	0.01	0.01	0.02	Coefficient for the fragmentation rate	0.15	1.0	0.15
Jet fragmentation rate in water [m3/s/m2]	0.075	0.075	0.1	Ratio of new born fragment diameter to wave length	6.0	6.0	1.0
Corium drop Sauter diameter [m]	2.5E-3	1.0E-3	2.5E-3	Characteristic radius of the jet	0.3	0.3	0.3
Velocity of melt drops that diverge from the melt jet [m/s]	0.5	0.5	0.5				

Once again, there were difficulties to induce trigger, i.e. the explosion phase could not always be calculated. For KELMHOLTZ cases the explosivity criterion values and the melt drop masses were systematically smaller than for CONST cases. However, explosion phase could not be calculated for every CONST case either. In order not to diminish potential for explosion, sensitivity analysis cases were calculated only with higher fragmentation coefficient values and smaller particles in comparison to default values, independent of the fragmentation model used. Combined effect of parameter variations was not investigated. Due to computational burden, only two extra calculations were performed for each fragmentation model, i.e. the analysis cannot be regarded as a proper sensitivity analysis. However, an impression of the order of magnitude of the influence the above mentioned fragmentation parameter variations can have, was obtained.

Table 9 contains the basic initial information for sensitivity analysis cases. Also default parameter values are included for comparison’s sake. When it comes to CONST modelling, case 2Ca has default fragmentation rates but melt drops are of smaller diameter. Case 2Cb, on the other hand, has higher fragmentation rates but melt fragments are of default size. Melt drop velocities are not varied at all. For KELMHOLTZ model, the fragmentation coefficient is increased for case 2Ka and ratio of new born fragment diameter to wave length is decreased in case 2Kb (to represent smaller diameters).

Table 10: Premixing calculation results for fragmentation sensitivity analysis.

	Explosivity criterion maximum and the corresponding time	Mass of melt droplets at the end of premixing calculations [kg]	Melt jet reaches water [s]	Melt jet reaches LDW bottom [s]
Case 2 CONST default	939.5 at 2.445 s	7136.1	1.61	2.71
Case 2Ca	213.2 at 2.616 s	7250.7	1.61	2.70
Case 2Cb	873.8 at 2.995 s	10140.8	1.61	2.78
Case 2 KH default	126.9 at 2.855 s	10951.1	1.61	2.65
Case 2Ka	1297.5 at 3.444 s	13850.5	1.62	(no melt in jet form to reach bottom)
Case 2Kb	117.2 at 3.122 s	9613.2	1.61	2.64

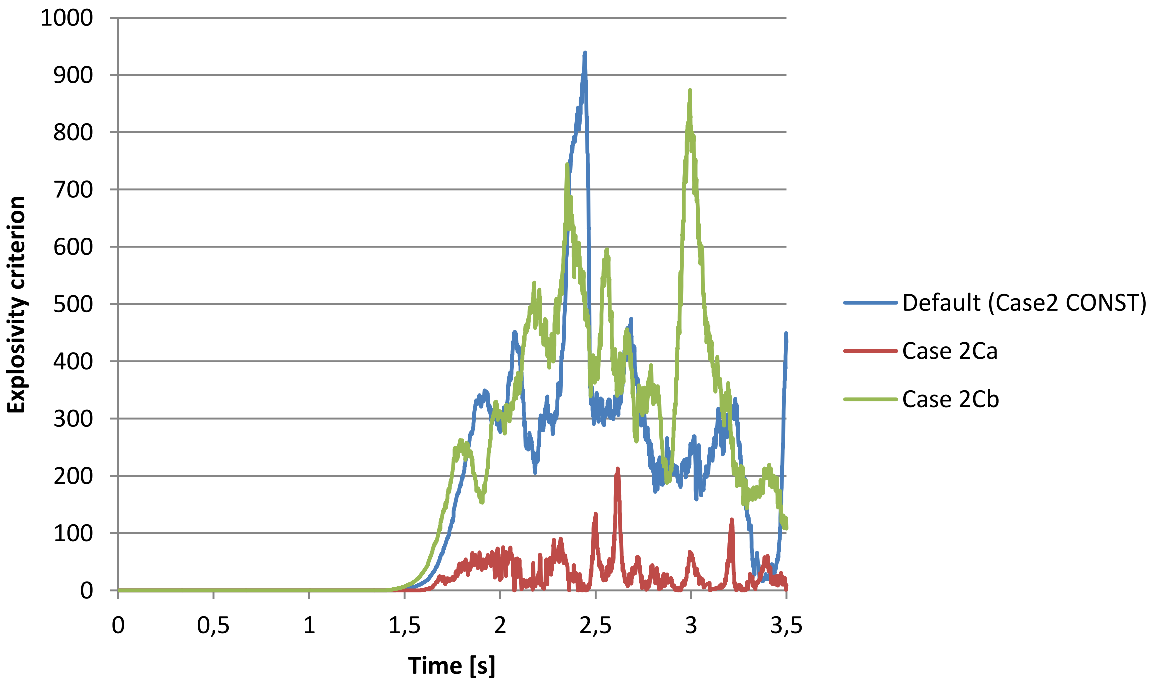

Figure 19: Explosivity criterion for sensitivity analysis cases as a function of time with CONST premixing model and single jet melt ejection mode.

In Table 10 are results from premixing calculations for all fragmentation sensitivity analysis cases. For CONST cases the default parameters yield highest explosivity criterion value but case 2Cb with increased fragmentation rates is not far behind. According to results, case 2Ca with smaller drop Sauter diameter has significantly decreased potential for explosion. For case 2Ka the fragmentation coefficient was increased remarkably and this can also be seen in explosivity criterion values. Decrease in ratio of new born fragment diameter to wave length did not induce significant changes in comparison to default parameter values. Explosivity criterion values as a function of time for each sensitivity analysis case are shown by Figure 19 and Figure 20.

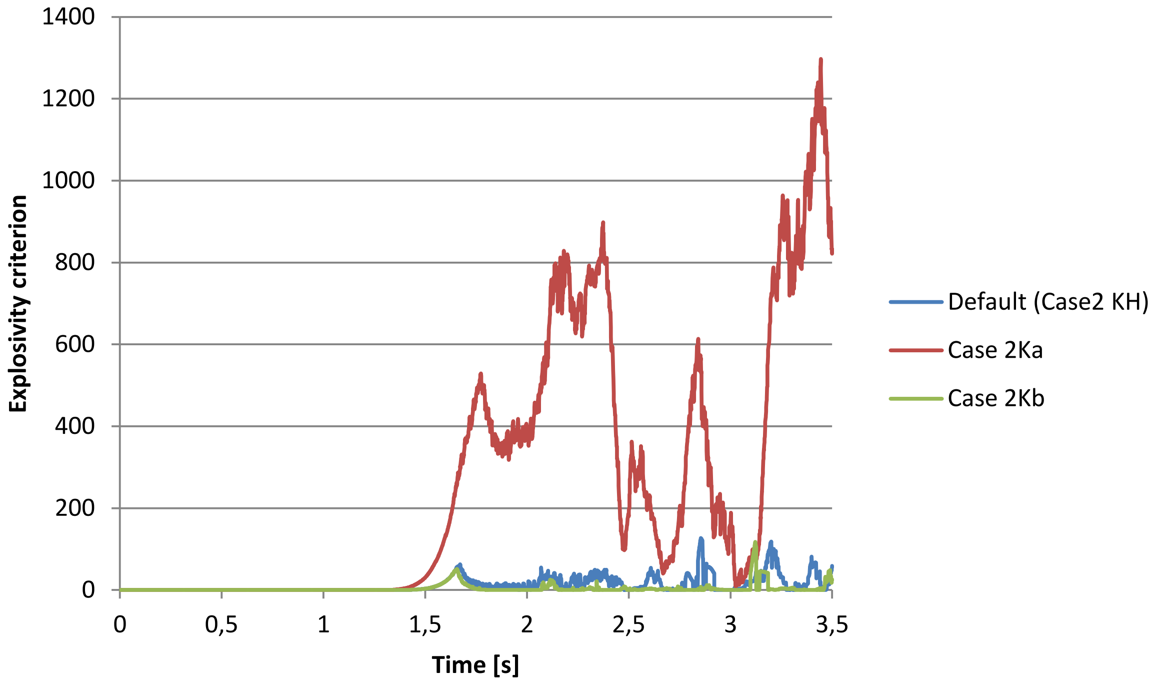

Figure 20: Explosivity criterion for sensitivity analysis cases as a function of time with KELMHOLTZ premixing model and single jet melt ejection mode.

Melt drop masses varied between 7 and 14 tons depending on the case, as shown by Figure 21. KELMHOLTZ fragmentation yielded highest values, especially for case 2Ka with high fragmentation rate. Decreased ratio of fragment diameter to wave length resulted in somewhat smaller mass of melt drops. Of CONST cases, 2Cb with increased fragmentation rate produces more melt drops than the other two cases which are quite even.

Table 11 contains information on explosion simulations that were performed for the fragmentation sensitivity analysis cases. For two cases explosion could not be triggered, and for those cases that could be triggered the triggering times were quite different from each other, which makes it difficult to compare results. For case 2Ca (decreased melt drop Sauter diameter) the explosion is a lot milder than for the default CONST case. Case 2Kb produces also a lot lower pressure values than the default KELMHOLTZ case but max impulses are practically the same.

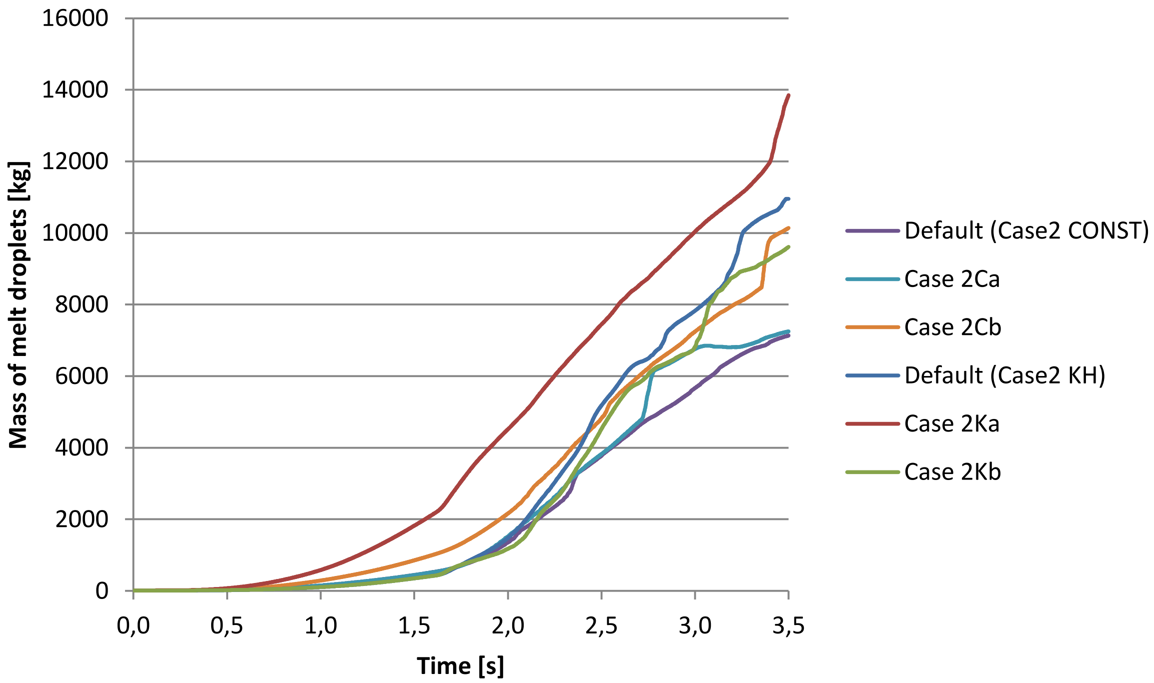

Figure 21: Melt drop mass as a function of time in all sensitivity analysis cases for single jet vessel failure mode.

Figure 22 shows pressure impulses near the LDW bottom for all fragmentation sensitivity analysis cases. Default case impulses reach their maximum after 0.1-0.2 ms whereas for other cases the impulse rises more gradually. Figure 23 and Figure 24 illustrate maximum pressures during simulations in the whole simulation domain and along the LDW wall, respectively. CONST default case is easily distinguishable from both figures while others display more moderate pressure behaviour.

Table 11: Explosion calculation results for fragmentation sensitivity analysis.

	Trigger time [s]	Explosivity criterion value (eq. (1)) at trigger	Melt jet height at triggering time [m]	Maximum pressure in whole domain [MPa]	Maximum pressure along LDW wall [MPa]	Impulse on the LDW wall [MPa.s]
Case 2 CONST default	2.4000	817.304	3.71	264.8 (at 0.0019 s)	27.7 (at 0.0048 s)	0.168
Case 2Ca	3.2133	125.207	0.00	97.5 (at 0.0012 s)	16.1 (at 0.0114 s)	0.111
Case 2Cb	-	-	-	-	-	-
Case 2 KH default	1.8939	16.957	9.04	207.3 (at 0.0011 s)	13.6 (at 0.0097 s)	0.053
Case 2Ka	-	-	-	-	-	-
Case 2Kb	2.5040	3.925	1.31	72.0 (at 0.0009 s)	5.5 (at 0.0041 s)	0.058

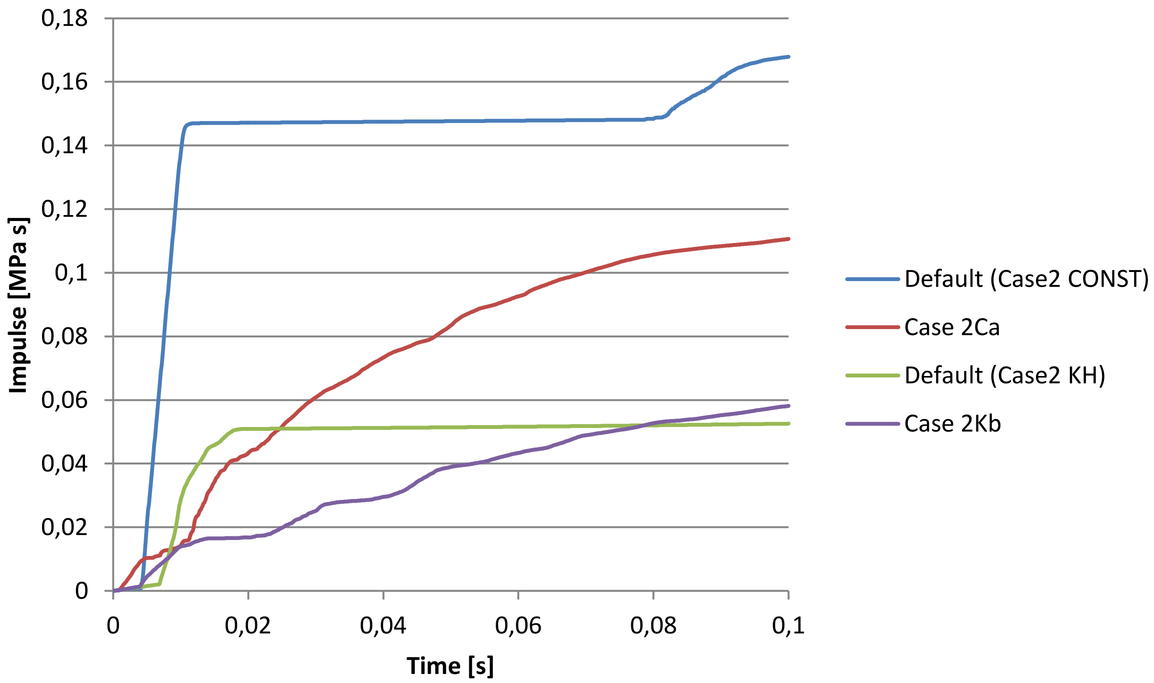

Figure 22: Pressure impulse maxima for fragmentation parameter sensitivity analysis. All impulse maxima take place at 0.1 m height from the LDW bottom.

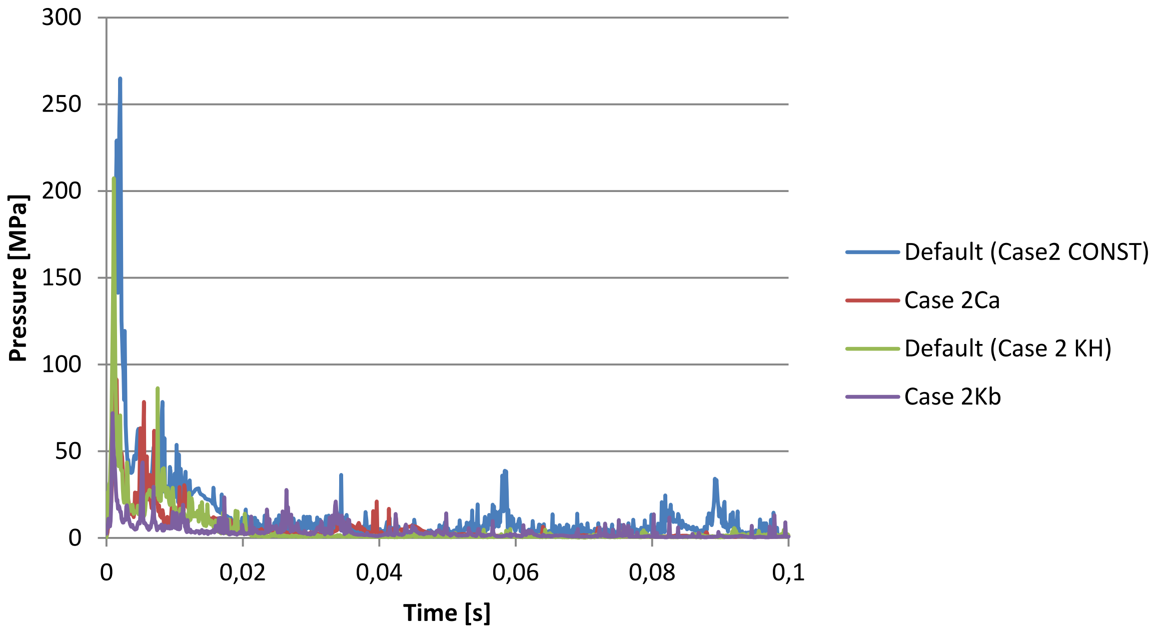

Figure 23: Maximum pressures in the whole domain during explosion calculations for fragmentation parameter sensitivity analysis.

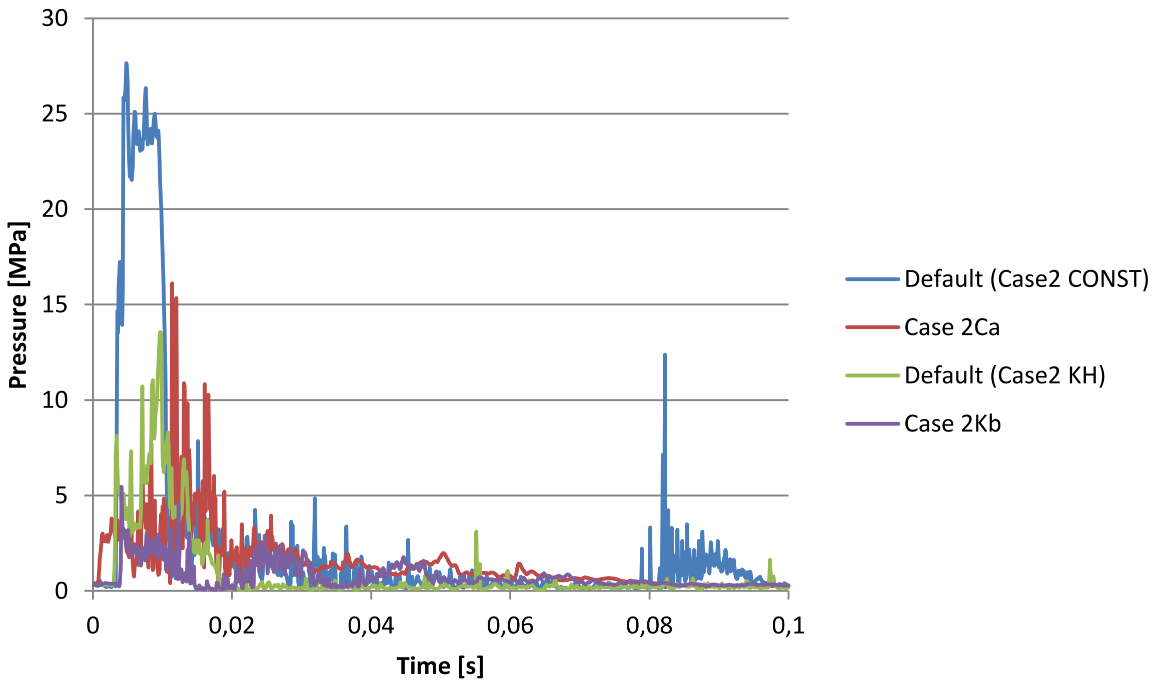

Figure 24: Maximum pressures along the LDW wall during explosion calculations for fragmentation parameter sensitivity analysis.

4.3.2 Triggering time

Explosion phase of case 5 with CONST premixing model and default fragmentation parameters was calculated with different triggering times in order to see how big an impact it can have on explosion strength. Table 12 contains the different triggering times and includes also results for case 5 from initial analyses discussed in section 4.1.2 (triggering time t2 = 2.2957 s). For the first two triggering times the melt jet has not got in contact with LDW bottom yet, contrary to the latter two cases.

Table 12: Effect of triggering time variation on explosion calculation results. Case 5 with CONST premixing and default fragmentation parameters was used.

Trigger time [s]	Explosivity criterion value (eq. (1)) at trigger	Melt jet height at triggering time [m]	Maximum pressure in whole domain [MPa]	Maximum pressure along LDW wall [MPa]	Max impulse on the LDW wall [MPa.s]
t1=2.2001	443.452	5.82	192.7 (at 0.0017 s)	27.7 (at 0.0090 s)	0.151
t2=2.2957	585.988	4.85	330.1 (at 0.0017 s)	27.6 (at 0.0090 s)	0.158
t3=2.9008	327.292	0.0	249.5 (at 0.0012 s)	8.2 (at 0.009 s)	0.175
t4=3.4016	545.489	0.0	210.3 (at 0.0013 s)	15.0 (at 0.0084 s)	0.236

Default case (t2) yields the highest pressures both in the whole domain and along the LDW wall, but in the cases analysed, it appears that the later the trigger occurs the bigger the pressure impulse. Also, as can be seen from Figure 25, for early triggers (t1 and t2) the impulse maxima are reached at 10 ms but for late triggers the impulses rise more steadily during the simulation. A possible explanation is that if trigger takes place late, there is more melt involved in premixing and it can be distributed more widely, which can lead to such behaviour as seen in the results. Figure 27 also demonstrates that for triggers t1 and t2 there are high pressures along the wall only for a limited time, and thereafter pressures drop to near zero. On the other hand, for triggering times t3 and t4 the peak pressures are more moderate but last longer thus resulting in higher total impulses. Figure 26 contains maximum pressure curves in the whole domain. After early peaks all pressures drop quite soon to a little elevated values near to initial pressure.

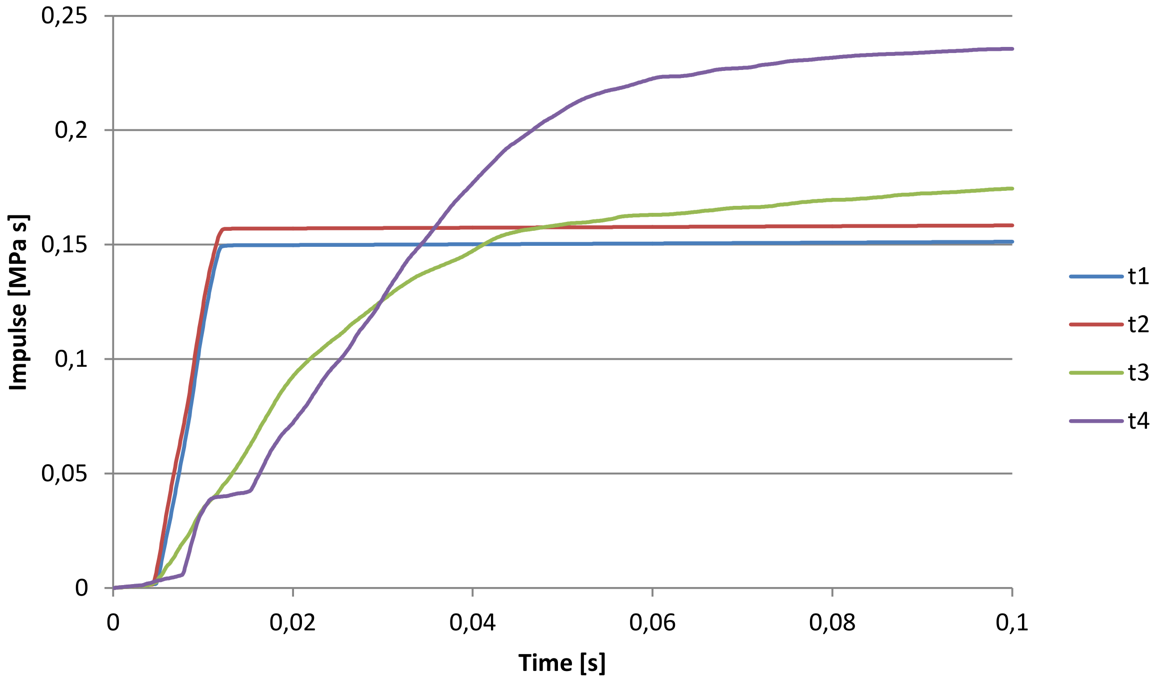

Figure 25: Pressure impulse at the height of 0.1 m from the LDW bottom for triggering time sensitivity analysis.

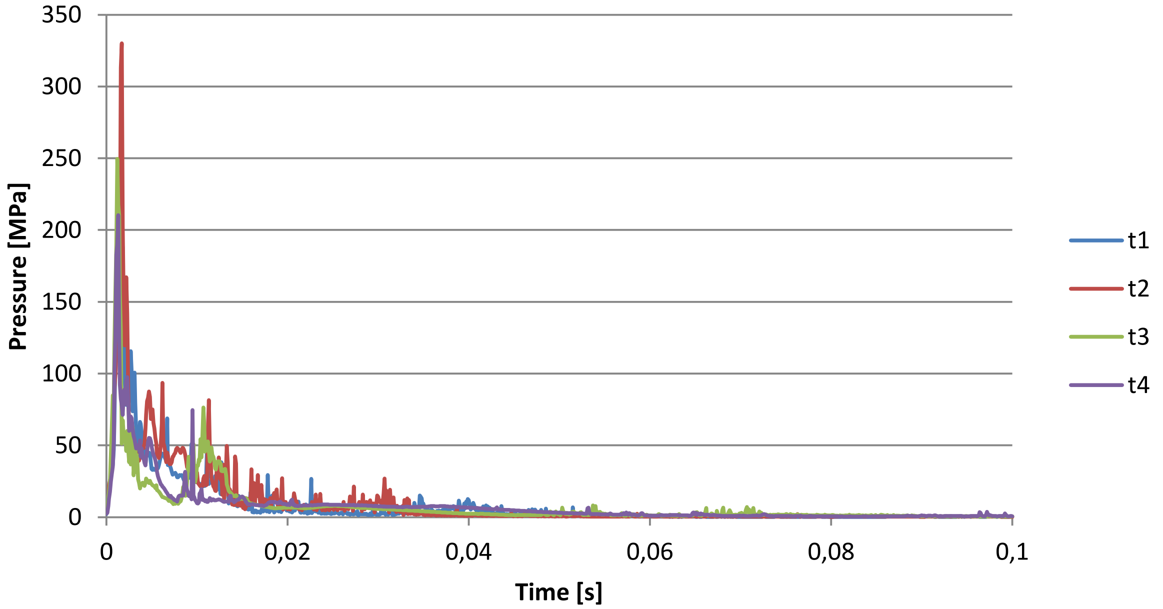

Figure 26: Maximum pressures in the whole domain for triggering time sensitivity analysis.

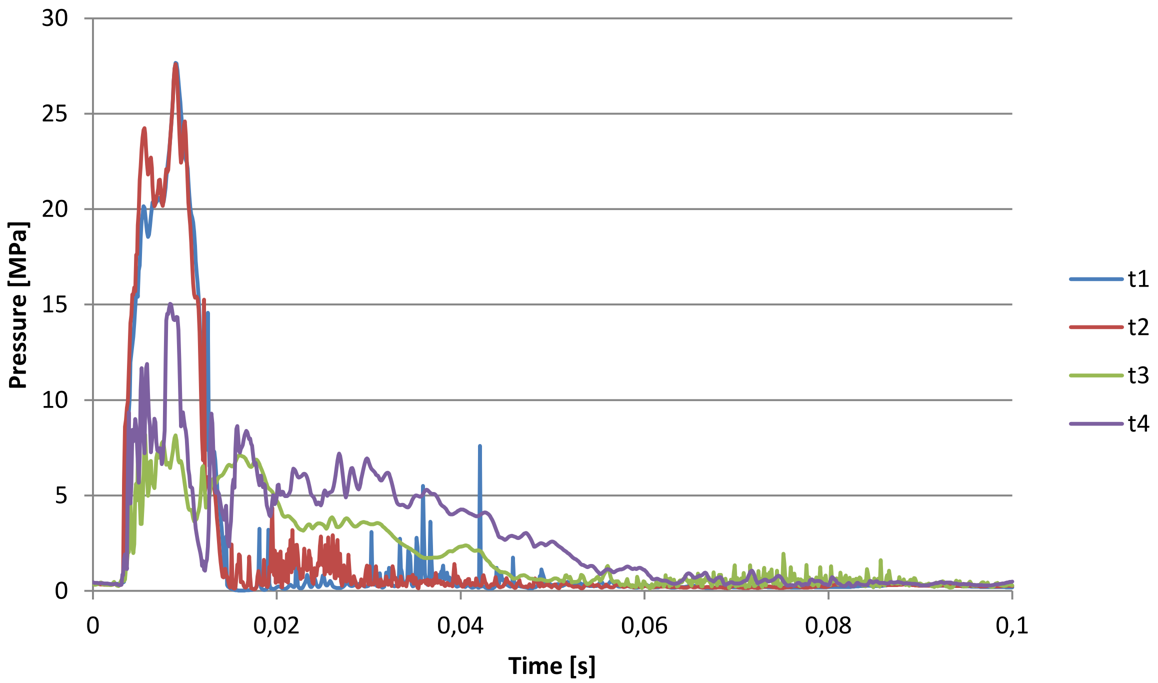

Figure 27: Maximum pressures along the LDW wall for triggering time sensitivity analysis.

5. Discussion and implications for level 2 PRA

Generally speaking, results obtained from simulations in this study showed quite high loads posed to containment. OECD's SERENA program (reference [2]) discusses results obtained from ex-vessel steam explosion simulations for reactor cases representing "a plausible LWR situation", and thus offers a good point of reference. Several FCI codes were used in SERENA program, including MC3D. Analyses considered only gravity-driven melt pours and they were performed, depending on analysis tool used, in 1, 2 or 3 dimensions. Trigger was applied when the melt reached cavity (or LDW) bottom.

Pressure peaks at the bottom of the cavity reported in [2] were mainly in the range of 60-80 MPa with the highest value at about 110 MPa. Maximum pressure in the whole domain in this work exceeded 300 MPa i.e. the difference is big. However, pressure values at the LDW bottom were not investigated in this study and these values are therefore not adequately comparable. Results at the side wall in [2] vary between 10 and 40 MPa and are consistent with results shown in this report which were mainly between 10 and 30 MPa and a little over 30 MPa for multiple jets cases. Pressure impulses in [2] ranged from a few kPa.s to 130 kPa.s, although one case yielded much higher values. Most cases analyzed in this study had impulses well above 100 kPa.s, with the highest value as large as 340 kPa.s for one of the multiple melt jets cases. However, also values around 50 kPa.s were obtained, which are well consistent with impulses discussed in [2]. It can be concluded that pressure loads simulated in this study were somewhat larger than expected and presented in literature.

Reference [8] investigated ex-vessel steam explosions for a PWR plant, also by using MC3D. Melt release location, cavity water temperature, primary system over-pressure at vessel failure and the triggering time were all varied in the analyses. Similar to results obtained in this study, also in [8] the pressure loads are very large in comparison to those of SERENA program. Maximum pressures are close to 300 MPa and impulses at the cavity bottom as much as over 500 kPa.s, although impulses on cavity wall were smaller (<300 kPa.s) and thus closer to impulses obtained in this work. One possible explanation for very high pressures suggested in [8] is that MC3D over-predicts the amount of melt droplets.

A problem that caused troubles throughout this work was the triggering of explosions. Typically it was not possible to choose any given triggering time and one had to be content if explosion could be initiated at all. As a consequence, different analysis cases were difficult to compare with each other as for one case the trigger occurred right after the melt penetrated into water and for another case only after contact with LDW bottom. It is unclear if these problems emerged from physical reasons, i.e. from the fact that such melt-water configuration is unlikely to produce a steam explosion. Another explanation is related to MC3D code and its numerics which necessarily do not have anything to do with actual physical conditions that govern the explosion potential of the premixture.

Cases 2 and 5 do not differ drastically from each other. Regarding initial conditions, case 5 has a little higher ambient pressure and gas temperature. There is also more melt involved. It is practically impossible to draw any conclusions between cases 2 and 5 regarding premixing calculations with this few simulations. Sometimes case 2 yields higher explosivity criterion values and sometimes case 5. The same holds true for explosion results as well, i.e. cases 2 and 5 cannot really be distinguished from each other with any certainty. Case 6 is a whole different story due to pressure difference between RPV and LDW atmosphere which results in pressurized melt ejection. Therefore premixing calculations yield much higher explosion criterion values and mass of melt drops for case 6 than for other cases, although for multiple jets melt ejection mode the difference is less clear than for single jet. Unfortunately, none of premixing calculations for case 6 could be brought to explosion phase due to problems with initiation of the trigger.

Initial intention was to use a little different, more case-specific melt properties for each case 2, 5 and 6, as discussed in section 3.3.1. For the main part the scenarios would have differed with respect to melt temperature and other properties easily obtained from MELCOR simulations (unlike e.g. viscosity). Some simulations were run with case-specific melt properties, but because unsurmountable difficulties emerged regarding, once again, explosion trigger, it was decided to use the same melt properties for all cases. Of course it would be tempting to conclude that cases for which explosion cannot be triggered are safe and infeasible for explosion, but this implication is discarded here. On the contrary, the assumption is that each case taken into analysis can also be triggered.

Multiple melt jets enable bigger melt amounts to be involved in premixing, and thus, in theory, also have potential for bigger explosions. Indeed, at least according to explosivity criterion and mass of melt drops, multiple melt jets cases result in situations more prone to strong explosions. Explosion phase simulation results confirm this hypothesis with pressure impulse values nearly twice as high as for single jet analysis cases. Multiple breaks in the lower head of the vessel make it possible for the melt to distribute more evenly and also to fragment more efficiently. High pressure loads also appear not to be equally focused near the LDW bottom as for single jet cases and impulses are as high as 150 kPa.s near the surface of water as well.

In the course of analyses it soon became evident how sensitive premixing and subsequent explosion is both to fragmentation model and corresponding parameter values used. Two fragmentation models, namely CONST and KELMHOLTZ, were used and the default parameter values utilized were those recommended in [7]. With default fragmentation parameters, CONST model resulted in systematically higher explosion potential for single jet cases, but for multiple jets vessel failure mode the situation turns the other way around. However, all explosions that followed CONST premixing were stronger than KELMHOLTZ cases, but this probably resulted mainly from very early triggering times that had to be used for KELMHOLTZ cases. In [7] it was mentioned that CONST fragmentation model is currently better suited for safety analysis, whereas KELMHOLTZ is physically more accurate but may need to be developed further in order to be applicable in reactor scale situations.

Increase in fragmentation rate (CONST) or coefficient (KELMHOLTZ) did yield higher mass of melt drops but unlike for KELMHOLTZ, there was no significant effect on explosivity criterion values for CONST fragmentation. Unfortunately, for neither model with increased fragmentation rate the explosion phase could be calculated. Smaller melt fragments, on the other hand, seem to produce smaller explosivity criterion values and also smaller (or equal for CONST fragmentation) mass of melt drops. Respectively, explosion loads appear to be smaller as well. However, in the course of analyses it was observed that explosivity criterion value at trigger does not correlate very well with the strength of the subsequent explosion, and mass of melt droplets might be a more accurate indicator of explosion potential. The effect of decrease in size of melt fragments was a little surprising as it was expected that with constant fragmentation rate but smaller particles the increased melt drop surface area would lead to higher heat transfer capacity and thus also bigger explosions.

Problems with explosion trigger compelled to use very different triggering times throughout analyses which impeded comparison between different cases. Therefore it was important to investigate the effect of trigger timing using a certain premixing calculation as input (case 5 with single jet and CONST premixing). Results indicate that for early triggers that occur before melt gets in contact with LDW floor the explosion dynamics are a little different from explosions that take place later. For early explosions the pressure impulses last only ~10 ms whereas for late triggers there are clearly elevated pressures along the LDW wall as late as 50-60 ms since the trigger. Maximum pressures, however, are notably higher for early explosions. According to results it seems that the later the trigger, the higher the total impulses on the LDW wall. A plausible explanation for higher impulses is that the amount of melt involved in premixture increases if trigger occurs late, but the mechanism behind altered explosion dynamics is unclear.

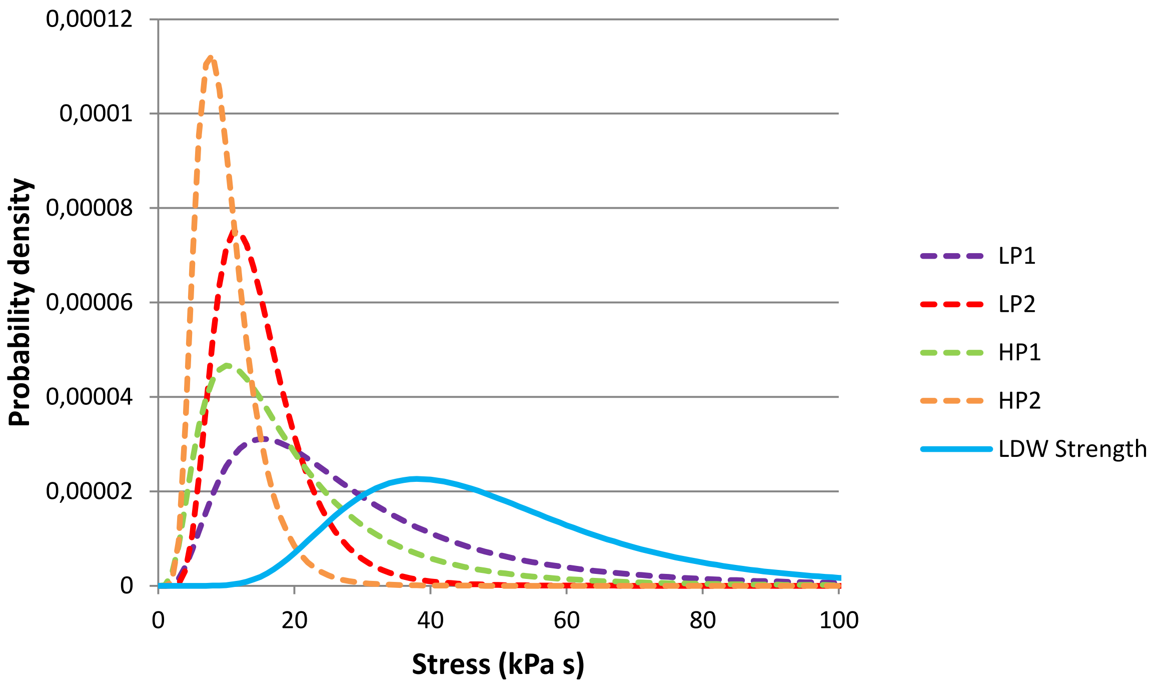

Figure 28: Distributions used in [1] to determine the probability of LDW failure due to pressure impulse caused by ex-vessel steam explosion. LP1 = low pressure, much melt; HP2 = high pressure, little melt etc. Impulses obtained in this study are much higher.

Figure 28 shows distributions for pressure impulse loads used in [1]. A distribution for LDW capacity/strength is also given. LP stands for low pressure (i.e. gravity driven) melt ejection and HP means a case where RPV remains pressurized. Number code 1 means that a lot of melt is released whereas number 2 indicates that less melt is involved. According to results obtained in this study, the impulse loads are significantly higher than those of Figure 28, and even the smallest impulse value was above 50 kPa.s which exceeds LDW strength mean value of 40 kPa.s. Because explosion phase of pressurized cases could not be simulated, it is impossible to say whether the assumption of milder explosions related to pressurized melt ejections is correct or not. Also no simulations were performed with remarkably smaller melt amounts. Some conclusions can be made regarding vessel failure mode as the simulations suggest that multiple breaks in the vessel result in higher loads. Another question is the feasibility and relative probability of the different vessel failure modes, but this issue is not considered here. Under the circumstances, however, it seems plausible that the impulse load curves of Figure 28 could be shifted to the right.

Even though similar or even higher pressure load values were simulated also in [8], it is not certain by any means that these results strictly represent a plausible reactor situation, i.e. it is extremely difficult to validate such results. There seems to be a consensus in the scientific community that pressure loads presented in SERENA program are nearer to realistic values, but of course results of this study and those of [8] cannot be completely neglected. Cases calculated in this study were quite simple and there is space for more detailed approach which could have an influence on overall results and conclusions. For instance melt properties could and should be defined more specifically for each analysis case, although accurate definition of melt composition would have been more critical if there had been an attempt to model hydrogen production.

The objective of this study was to approach ex-vessel steam explosion from safety analysis perspective using a reactor scale model, thus leaving more theoretical dimensions of the problem with less attention. In fact, physics involved in FCI phenomena is far from being well understood and a lot of work is still needed in order to achieve a good level of confidence in modeling of reactor situations where large extrapolation with respect to experimental conditions is necessary. Thus FCI phenomenology itself is a major contributor to uncertainties present in the analyses of this study, along with incomplete modelling.

6. Conclusions

This study continued the work done in [1] with an aim to produce case-specific results of pressure loads due to ex-vessel steam explosions in a BWR plant by using MC3D code. Three basic analysis cases were derived from scenarios investigated in [1] resulting in RPV failure and subsequent melt ejection. Explicit differences in FCI sense between the cases remained vague because explosion phase of case 6 with pressurized melt ejection could not be simulated and the other two cases produced quite similar and even a little inconsistent results. Same melt properties were used for all cases.

Throughout the analyses there were difficulties to trigger explosions. For a particular premixing calculation there may have been only one or two if any possible points in time for initiation of the explosion. Time of trigger can affect explosion strength significantly and thus it is difficult and even dubious to compare cases that have very different triggering times. Because of inconsistent triggering times the analysis results were quite scattered, but otherwise the results were characterized by unexpectedly high pressure loads. The maximum pressure in the whole simulation domain was as much as ~300 MPa, pressures along the LDW side wall exceeded 30 MPa and the impulse maxima reached values over 300 kPa.s. However, most simulations produced remarkably weaker explosions.

Each case was analyzed for two RPV failure modes (see Figure 2). First failure mode was characterized by a single large central break in the RPV, and another one had multiple breaks of different sizes representing failures of RPV bottom penetrations (IGT and/or CRGT failure). It turned out that multiple breaks yielded the biggest explosions, probably simply because there was more melt involved in premixing.

Small-scale sensitivity inspection with respect to fragmentation model parameters did not reveal anything that could be considered especially important for safety analyses. It merely highlighted how important it is to keep in mind the significant impact fragmentation parameter values can have when interpreting any results. Triggering time sensitivity analysis implied that the later the trigger occurs the stronger is the explosion, which can be accounted for bigger melt amounts involved, although the issue is not necessarily that straightforward.

The high loads obtained in this study call into question e.g. the impulsion load distributions used in [1] or in any other level 2 PRA study, although a lot of room has been left for improvement regarding level of detail of modeling. At least results regarding the relative severity of multiple melt jets vs. single jet seem plausible. At the same time it must be taken into account that methods used to model FCI phenomena are not yet at a completely mature stage which introduces epistemic uncertainty into play.

The problems that were encountered in performing the simulations unfortunately degrade the applicability of results in the event tree developed in previous work [1] or in any other L2PRA model. The goal was to obtain case-specific results to be used in refining the model constructed earlier, and therefore concentrate more on utilizing the deterministic side of IDPSA methodological framework. Due to the aforementioned problems it was regarded unworthy to introduce results from MC3D simulations into the event tree model in [1]. However, general knowledge of steam explosion phenomenon and modeling capabilities was obtained.

Appendix: MC3D data set example

The following code sample is an example of data set used to run MC3D simulations. There are separate files for premixing and explosion calculations, and the example below corresponds to case 2 with single jet melt ejection mode and CONST fragmentation model.

Premixing

```
TITRE 'BWR premixing const';

*Pool depth
WATERLEV = 12.2;
*LDW radius
WATERRAD = 4.6;
*Water temperature
T_WATER=325.;
*Mesh dimensions
NFX = 41;
NFY =2;
NFZ = 106;
*LDW pressure
P_LDW=1.82D5;
*Vessel pressure
P_VES=1.82D5;
*Melt temperature
T_MELT=3100.;
*Gas temperature in LDW
T_LDW=330.;
*Gas temperature in vessel
T_VES=420.;

PASDT  DTMIN  1.0D-12   DTMAX  1.D-2  DTINIT 1.0D-5
      TMAX   3.5   NPTMAX  999999
      DTVAR  ITER 7   FREIN 0.5   ACCEL 1.25  FACSEC 0.1 ;

DOM = DOMAINE  NFX  NFY  NFZ;

*Melt properties
MATCOR
* UO2ZRO2 80/20 calculated from GEMINI MEPHISTA databas
TSOLIDUS 3050.
TLIQUIDU 3100.
CPLIQUID 510.
CPSOLIDE 450.
EFUSION 2.8D5
TENSURF 0.45
TPORIGIN  3100.
ROSOLIDE 7660.
ROLIQUID 7660.
EMISSIV 0.7
CONDUCT 2.3
VISCODYN 4.D-3
;

CALCUL = APPLI DOM  PREMEL REFRI  EAU
                     FONDU  MATUSER
```

```
                 INCOND AIR
;

*****************************************************************
*** MESH
*****************************************************************
MAILLA = MAILLAGE CALCUL CYLIND

R    MULTI PROG 20  0.00   2.25  1.07  PROG 20 2.25 WATERRAD 0.93
TETA REGU   0.000 6.283
Z    MULTI  PROG 30 0. 6. 1.05
               PROG   30 6. WATERLEV 0.95
                PROG 20 WATERLEV 18. 1.05
                PROG 20 18. 25. 0.95
                PROG  5 25. 28. 1.2
;

*****************************************************************
*** INITIALIALISATION
*****************************************************************
INIT  CALCUL  DIAGOU 1.0D-2
TEMPLIQ T_WATER
TXMEL 1.  TEMPMEL T_LDW
     UGOU 0.D0 VGOU 0. WGOU 0.D0 TXGOU 0.  TEMPGOU T_MELT
     UJET 0.D0 VJET 0. WJET 0.D0 TXJET 0.  TEMPJET T_MELT
     PGISP 1 0.5
   PRESSION  P_LDW
  XLIMGOU  1.D-6
;

*****************************************************************
*** GEOMETRY
*****************************************************************
* Debris configuration at the bottom
BED = ZONINT 1 NFX 1 2 1 5;
NEWZONE DEBRIS BED;

* Water pool (pit)
WATER = ZONINT 1  NFX 1 2 1 60;
AFFECT WATER TXLIQ 1.  TXMEL 0.;
NEWZONE PUITS WATER;

*Vessel geometry
V1=ZONINT  6 16 1 2 96 97;
ZONEVIDE V1;
V2=ZONINT  15 21 1 2 97 98;
ZONEVIDE V2;
V3=ZONINT 20 24 1 2 98 99;
ZONEVIDE V3;
V4=ZONINT 23 26 1 2 99 100;
ZONEVIDE V4;
V5=ZONINT  25 26 1 2 100 NFZ;
ZONEVIDE V5;
V6=ZONINT 26 NFX 1 2 103 NFZ;
ZONEVIDE V6;
```

```
*Vessel internals
VES=ZONINT 1 25 1 2 101 NFZ;
AFFECT VES PRESSION P_VES TEMPMEL T_VES
TXLIQ 0. TXMEL 1. TXJET 0. TXGOU 0.;
NEWZONE CUVE VES;

*Cavity wall
WALL=ZONINT 40 NFX 1 2 1 NFZ;
ZONEVIDE WALL;

*Melt zones
MELTCOM1 = COMPO  TXJET 1. TXMEL 0. TXLIQ 0. TXGOU 0.;
MELTCOM2 = COMPO  TXJET 0.24 TXMEL 0.76 TXLIQ 0. TXGOU 0.;

MELT1=ZONINT 1 15 1 2 97 98;
AFFECT MELT1 MELTCOM1
PRESSION  P_VES
;
MELT2=ZONINT 1 20 1 2 98 99;
AFFECT MELT2 MELTCOM1
PRESSION  P_VES
;
MELT3=ZONINT 1 23 1 2 99 100;
AFFECT MELT3 MELTCOM1
PRESSION  P_VES
;
MELT4=ZONINT 1 25 1 2 100 101;
AFFECT MELT4 MELTCOM2
PRESSION  P_VES
;

*Turbulent diffusion term
TQDMB DISTUB 1. 1.;

PHYTRPM
* No fragmentation of the drops
CPILCH 0.;

*Solid temperature for premixing =~( tsol + tliq) /2
 PRSOLIDE TSOLID  3075;

* Fragmentation
INTERFAC CORFRAG  CONST
*Jet fragmentation rate in gas
FRGVAP 0.01
*Jet fragmentation rate in water
FRGFLM  0.075
*Corium drop Sauter diameter
DIACRE 2.5D-3
* velocity of drops that exit the jet
VEJDR  0.5
;

******************************************************************
*** OUTPUTS
******************************************************************
```

```
IMPRIMER DOM NCRITEXP  2
IMPINI PERIODE 0.2D0 PLANXZ
     ;

POST XMGR SILO
TYP1 1.D-6
  4DIM
  3DIM
  1DIM
*masses of the drops and the jet
 'AMM(3)''AMM(4)'
*thermal energy of the drops and the jet
 'AME(3)''AME(4)'
*kinetic energy of the drops and the jet
 'AMC(3)''AMC(4)'
  SIMP
*Timestep duration, height reached by corium jet front, mean fuel diameter
  'DT()' 'FRONJET()'' DSAUTER()'
TYP2 0.5D-1
*component velocities and volume fractions
      UVWJET  UVWGOU UVWLIQ  UVWMEL
     PRESSION
     TXJET TXGOU TXLIQ TXMEL
* partial pressures
       PGI1 PVAP  PGI1SP  PRESSION
*Component temperatures
      TEMPMEL TEMPLIQ TEMPGOU  ;

SAUVEGAR TSFREQ 0.1 CRITEXP;

MC3D;

FIN;
```

Explosion

```
TITRE 'BWR explosion (const premixing)';

*Pool depth
WATERLEV = 12.2;
*LDW radius
WATERRAD = 4.6;
*Water temperature
T_WATER=325.;
*Mesh dimensions
NFX = 41;
NFY =2;
NFZ = 106;
*LDW pressure
P_LDW=1.82D5;
*Vessel pressure
P_VES=1.82D5;
*Melt temperature
T_MELT=3100.;
*Gas temperature in LDW
T_LDW=330.;
*Gas temperature in vessel
T_VES=420.;

PASDT  DTMIN  1.0D-12   DTMAX  1.D-5  DTINIT 1.0D-5
      TMAX  2.5    NPTMAX  999999
      DTVAR  ITER 7   FREIN 0.5   ACCEL 1.25  FACSEC 0.1 ;

DOM = DOMAINE  NFX  NFY  NFZ;

*Melt properties
MATCOR
* UO2ZRO2 80/20 calculated from GEMINI MEPHISTA databas
TSOLIDUS 3050.
TLIQUIDU 3100.
CPLIQUID 510.
CPSOLIDE 450.
EFUSION 2.8D5
* ?? for the rest
TENSURF 0.45
TPORIGIN  3100.
ROSOLIDE 7660.
ROLIQUID 7660.
EMISSIV 0.7
* not used
CONDUCT 2.3
VISCODYN 4.D-3
;

CALCUL = APPLI DOM EXPLO REFRI  WATER
                    FONDU  MATUSER
                    INCOND AIR
;
```

```
*******************************************************************
*** MESH
*******************************************************************
MAILLA = MAILLAGE CALCUL CYLIND

R    MULTI PROG 20  0.00   2.25  1.07  PROG 20 2.25 WATERRAD 0.93
TETA REGU   0.000 6.283
Z    MULTI  PROG 30 0. 6. 1.05
                PROG   30 6. WATERLEV 0.95
                 PROG 20 WATERLEV 18. 1.05
                 PROG 20 18. 25. 0.95
                 PROG  5 25. 28. 1.2
;

*******************************************************************
*** INITIALIALISATION
*******************************************************************
INIT  CALCUL  DIAGOU 1.0D-2  DIALIQ 1.D-3 DIAMEL 1.D-3 DIAFRA 7.5D-5
  TEMPFRA T_MELT
  PRESSION  P_LDW
  XLIMGOU  1.D-6
;

*******************************************************************
*** GEOMETRY
*******************************************************************
* Water pool (pit)
WATER = ZONINT 1  NFX 1 2 1 60;
*AFFECT WATER TXLIQ 1.  TXMEL 0.;
NEWZONE PUITS WATER;
*Vessel geometry
V1=ZONINT  6 16 1 2 96 97;
ZONEVIDE V1;
V2=ZONINT  15 21 1 2 97 98;
ZONEVIDE V2;
V3=ZONINT 20 24 1 2 98 99;
ZONEVIDE V3;
V4=ZONINT 23 26 1 2 99 100;
ZONEVIDE V4;
V5=ZONINT  25 26 1 2 100 NFZ;
ZONEVIDE V5;
V6=ZONINT 26 NFX 1 2 103 NFZ;
ZONEVIDE V6;

*Cavity wall
WALL=ZONINT 40 NFX 1 2 1 NFZ;
ZONEVIDE WALL;

* Options for maximum pressures and impulses
OPTION
IMPOPT 7 1;

*zones for max pressure and pressure impulses
WALL1=ZONINT 39 40 1 2 2 3;
WALL2=ZONINT 39 40 1 2 20 21;
WALL3=ZONINT 39 40 1 2  40 41;
```

```
WALL4=ZONINT 39 40 1 2  59 60;
NEWZONE PAROIPUI WALL1 WALL2 WALL3 WALL4;

*Solid temperature for premixing =~( tsol + tliq) /2
 PRSOLIDE TSOLID  3075;

ZTRIG = ZONINT 1 NFX 1 2 1 NFZ;

TREXPLO TEMPS 2.39
   APPREP PREMEL ZONEXPLO
*  METHOD MODALL
  TRIGGER ZTRIG TXFRA 1.D-2
   PRESSION 20.D5
  DIAFRA 7.5D-5
;
*********************************************************************
*** OUTPUTS
*********************************************************************
IMPRIMER DOM
IMPINI PERIODE 5.D-3 PLANXZ
 ;
POST XMGR SILO
TYP1 1.D-10
  4DIM
  3DIM
  1DIM
*masses of the drops and the jet
 'AMM(3)''AMM(4)'
*thermal energy of the drops and the jet
 'AME(3)''AME(4)'
*kinetic energy of the drops and the jet
 'AMC(3)''AMC(4)'
  SIMP
*Timestep duration, height reached by corium jet front, mean fuel diameter
  'DT()' 'FRONJET()'' DSAUTER()'
TYP2 1.D-4
*component velocities and volume fractions
      UVWJET  UVWGOU UVWLIQ  UVWMEL
     PRESSION
     TXJET TXGOU TXLIQ TXMEL
* partial pressures
       PGI1 PVAP  PGI1SP  PRESSION
*Component temperatures
      TEMPMEL TEMPLIQ TEMPGOU  ;

MC3D;
FIN;
```

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Abstract
max. 2000 characters

This study aims to supplement previous work performed in [1] by providing more detailed analysis on ex-vessel steam explosion loads posed to containment structure of a BWR reactor. The analyses are conducted with MC3D code, which is a multidimensional numerical tool devoted to analysis of FCI phenomena. Results can be reflected to steam explosion modelling implemented in a level 2 PRA model developed last year, and the analysis can thus be regarded to be an application of IDPSA methodology. Focus of this study is on safety considerations and complex physics and mathematical modelling are given less (if any) attention.

The analysis cases are studied for two different vessel failure modes and by using two fragmentation models. The basis case is a single large central hole in the reactor pressure vessel lower head, and the second melt ejection mode is a result from multiple simultaneous failures of vessel penetrations, representing instrumentation and control rod guide tube failures. Limited sensitivity analyses are performed for fragmentation model parameters and for explosion triggering time.

Results showed generally quite large pressures and impulses in comparison to e.g. results obtained in OECD's SERENA program [2], and for multiple melt jets the pressure loads were even higher than for single jet case. Throughout the analyses there were difficulties to trigger explosions and to compare different cases thus became more complicated. Although it is difficult to validate results and more detailed modelling would be necessary in order to draw more credible conclusions, this study produced useful information e.g. from IDPSA perspective and also enhanced modelling capabilities at VTT.

Key words: IDPSA, PSA, FCI, Ex-vessel steam explosions, Level 2 PRA, MC3D.

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