Analysis of WO$_3$/ZrO$_2$ vs. UO$_2$/ZrO$_2$ Fuel-Coolant Interaction in KROTOS Conditions

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ABSTRACT

A steam explosion is an energetic fuel-coolant interaction process, which may occur during a severe reactor accident when the molten core comes into contact with the coolant water. Within the nuclear reactor safety analyses steam explosions are primarily considered in melt jet-coolant pool configurations. Stratified melt-coolant configurations, i.e. molten corium layer below coolant layer, were up to now believed as being unable to generate strong explosive interactions. However, the recently performed experiments in the PULiMS and SES (KTH, Sweden) facilities with oxidic corium simulants revealed that strong steam explosions may develop spontaneously also in the stratified melt-coolant configuration. In order to validate the explosivity of the melt-coolant interaction in the stratified configuration, the explosion potential of the material that was used in the PULiMS/SES experiments, i.e. eutectic mixture of WO$_3$/ZrO$_2$, should be analysed also in the conventional melt jet-coolant pool configuration. This can be done by the evaluation of the explosivity of the WO$_3$/ZrO$_2$ melt in the conditions of KROTOS experiments, which were performed in the melt jet-coolant pool configuration with prototypic UO$_2$/ZrO$_2$ corium melt.

In the paper, the performed analysis of the explosion potential of the PULiMS/SES material WO$_3$/ZrO$_2$ is presented and discussed. Various parametric simulations were performed with the MC3D code in the KROTOS geometry for OECD SERENA project like conditions. The influence of the initial melt temperature and the explosion triggering time on the simulation results was analysed. The calculations were compared with the simulation of the SERENA KS-4 experiment with prototypic UO$_2$/ZrO$_2$ material. The results show that in the conventional melt jet-coolant pool configuration the PULiMS/SES simulant material has a significantly larger explosion potential compared to the reference prototypic corium material. The implication of the identified material influence on the stratified steam explosion energetics is addressed and suggestions for further work are given.

1 INTRODUCTION

During a hypothetical severe accident in a pressurized water reactor the molten core may be released into a flooded reactor cavity. The fuel-coolant interaction may lead to an energetic steam explosion (SE) [1]. In nuclear reactor safety analyses SE are primarily considered in the melt jet-coolant pool configuration. In such configuration sufficiently deep coolant pool conditions provide complete jet breakup and melt-coolant premixture formation, which is a necessary condition for the possible occurrence of an energetic SE. An extensive effort was put into the research of such SE, recently also within the OECD SERENA project [2]. When the water pool is shallow, the released corium melt may spread under the water creating a stratified configuration, i.e. molten corium layer below coolant layer. Stratified
melt-coolant configurations were up to now believed as being unable to generate strong explosive interactions [3]. However, the recently performed experiments in the PULiMS and SES (KTH, Sweden) facilities with oxidic corium simulants revealed that a considerable melt-coolant premixed layer may form and that strong SE may develop spontaneously also in stratified melt-coolant configurations, reaching efficiencies as high as those reported in the explosive tests carried out with the conventional melt-coolant pool configuration, prototypic corium materials and a strong external trigger. In these stratified experiments spontaneous SE occurred in 5 out of 5 tests with high melt superheat (around 200 K and above) and with water subcooling 13 – 30 K. At lower water subcooling (5 K) SE did not occur [3], [4], [5].

The objective of the presented study is to find out how the simulant material used in the PULiMS/SES stratified SE experiments would behave in typical experimental conditions of the melt jet-coolant pool configuration in comparison with a reference prototypic material. Representative experimental tests with the melt jet-coolant pool configuration were lately carried out in the KROTOS facility within the OECD SERENA project. For the purpose of this study the SERENA prototypic corium material, i.e. a mixture of 80% UO₂ / 20% ZrO₂ denoted MAT2, and the KROTOS KS-4 experimental conditions were taken as the reference [2]. Among the KROTOS tests the KS-4 experiment resulted in the strongest SE and the results were well recorded. Material MAT2 was chosen due to the near eutectic composition and its most realistic characteristics [6]. In the SES experimental tests, and in some PULiMS tests, the eutectic mixture of 84.3% WO₃ / 15.7% ZrO₂ denoted SES was used. This material was proven to be the most plausible due to a degree of similarity with the prototypic corium material (ceramic type, binary mixture of heavy metal oxides, density, etc.), due to the highest liquidus temperature among the simulants and due to other experimental advantages [4], [5].

2 MODELLING AND CALCULATION CONDITIONS

The simulations were performed with the MC3D v3.8 computer code, which is being developed by IRSN, France [7], [8]. It is a multi-dimensional Eulerian code devoted to study multi-phase and multi-constituent flows in the field of nuclear safety. The SE simulation is being carried out in two steps. First the premixing phase is simulated and then the succeeding explosion phase, using the premixing simulation results as initial conditions and applying an explosion trigger. The simulations were carried out in the KROTOS geometry in the 2-D axisymmetric cylindrical coordinate system on a mesh with 20 x 120 cells and with the calculation domain size 0.356 m x 2.6 m, Figure 1. Standard calculation models and adequate modelling parameters were chosen (from detailed simulation analysis of KS-4 test [6]). The calculation time was 2 s for the premixing and 10 ms for the explosion phase. The initial calculation conditions based on the KS-4 experiment are summarized in Table 1.

<table>
<thead>
<tr>
<th>Initial melt temperature</th>
<th>2963 K</th>
<th>Melt mass</th>
<th>3.21 kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water temperature</td>
<td>333 K</td>
<td>Ambient pressure</td>
<td>0.21 MPa</td>
</tr>
<tr>
<td>Subcooling</td>
<td>60 K</td>
<td>Trigger pressure</td>
<td>15 MPa</td>
</tr>
</tbody>
</table>

The analysis of the explosion potential of the SES material (eutectic mixture of WO₃/ZrO₂) is carried out by the comparison with the KROTOS MAT2 material (nearly eutectic mixture of UO₂/ZrO₂). Table 2 compares and summarizes the material properties that are influential and have to be provided to the MC3D code. The MAT2 material properties were taken from the default and specified data used in previous calculations [6], [10]. The main SES material properties (melting temperature, specific heat, latent heat and density) were taken from the summarized data in [5] and the others from [11].
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Figure 1: KROTOS interaction tube [9] (left) and the applied MC3D calculation mesh (right).

Table 2: Comparison of material properties of MAT2 and SES material (*[11]).

<table>
<thead>
<tr>
<th>Material properties</th>
<th>Units</th>
<th>MAT2</th>
<th>SES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material composition</td>
<td></td>
<td>80% UO₂ / 20% ZrO₂</td>
<td>84.3% WO₃ / 15.7% ZrO₂</td>
</tr>
<tr>
<td>Melting temperature (solidus/liquidus)</td>
<td>K</td>
<td>2870 / 2920</td>
<td>1504</td>
</tr>
<tr>
<td>Specific heat (solidus/liquidus)</td>
<td>J/kgK</td>
<td>450 / 510</td>
<td>591</td>
</tr>
<tr>
<td>Latent heat</td>
<td>kJ/kg</td>
<td>280</td>
<td>322</td>
</tr>
<tr>
<td>Density</td>
<td>kg/m³</td>
<td>7500</td>
<td>6866</td>
</tr>
<tr>
<td>Emissivity coefficient</td>
<td></td>
<td>0.75</td>
<td>0.7 *</td>
</tr>
<tr>
<td>Surface tension</td>
<td>N/m</td>
<td>0.5</td>
<td>0.4 *</td>
</tr>
</tbody>
</table>

According to the material characteristics in Table 2 the considered two materials have comparable calorific properties (density, specific and latent heat). The major influence can be therefore expected from the significantly different material melting temperatures.

Based on the SES and MAT2 material properties various qualitative conclusions can be done. For the same initial melt temperature it is expected that the SES material droplets stay liquid for a longer time than the MAT2 droplets due to the lower melting temperature and consequently a larger melt superheat. The SES droplets are expected to stay longer liquid even for the same melt superheat due to the lower heat transfer rate at the lower SES droplets temperature. Thus more efficient explosions may be expected with the SES material because in a steam explosion only liquid melt droplets may participate efficiently. To get a quantitative insight in the explosion potential of the SES material in comparison to the MAT2 material the following simulation strategy was applied. The simulations were performed with both materials for the KS-4 experiment conditions (Table 1), i.e. with the same initial melt temperature. Additionally, two simulations with the SES material were performed, applying the same melt superheat as in the KROTOS KS-4 and SES E-1 [5] experiments. Table 3 summarizes the premixing simulation cases.

For each premixing case two explosion simulations were performed, varying the explosion triggering time to evaluate its influence. In the experiments the explosion is typically triggered at the melt bottom contact (MBC). Therefore the following triggering
times were chosen: the MBC time in the KS-4 experiment, which is 1.18 s, and the average MBC time in the simulated premixing cases, which is approximately 0.9 s.

Table 3: Simulation strategy – premixing cases.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Material</th>
<th>Initial melt temperature</th>
<th>Superheat</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAT2</td>
<td>MAT2</td>
<td>2963 K</td>
<td>43 K</td>
<td>reference simulation</td>
</tr>
<tr>
<td>SES-A</td>
<td>SES</td>
<td>2963 K</td>
<td>1459 K</td>
<td>same init. temperature as MAT2</td>
</tr>
<tr>
<td>SES-B</td>
<td>SES</td>
<td>1675 K</td>
<td>171 K</td>
<td>middle init. temp. (as SES E-1 [5])</td>
</tr>
<tr>
<td>SES-C</td>
<td>SES</td>
<td>1547 K</td>
<td>43 K</td>
<td>same superheat as MAT2</td>
</tr>
</tbody>
</table>

3 SIMULATION RESULTS AND ANALYSIS

Four simulations denoted MAT2, SES-A, SES-B and SES-C were performed for the premixing phase (Table 3). After that the explosion simulations were carried out for two triggering times.

3.1 Premixing

The melt front propagation and pressure comparison are shown in Figure 2 and the global void fraction (VF) development is shown in Figure 3. In each graph the two triggering times are marked with vertical dashed lines. The green lines depict the MAT2 simulation and the orange lines with different intensities depict the SES simulations.

It may be observed in Figure 2 that all simulations predict a similar melt front penetration. Two simulations with the high initial temperature (MAT2, SES-A) reach the melt bottom contact (MBC) at 0.9 s, while the other two express a slightly shorter MBC time. A similarity may be perceived between the pressure build-up (right graph in Figure 2) and the void fraction development (Figure 3). The VF and pressure increases for MAT2 even after MBC since many droplets have been already solidified and do not coalesce at the bottom, providing enough surface area for further heat transfer to the water. For SES-A the void and pressure build up stop after MBC since many droplets are still liquid and coalesce at the bottom and thus significantly reduce the area for further heat transfer. The heat transfer is significantly lower for SES-B and SES-C due to the low initial temperatures. The void production and the consequent pressure build-up are therefore significantly reduced.

Figure 4 summarizes the total (liquid+solid), liquid and active droplet mass evolution. Liquid droplets are defined as droplets that are liquid enough to be able to undergo fine fragmentation during the explosion. Active droplets, i.e. droplets that may efficiently contribute to the explosion, were defined as liquid droplets in regions with less than 60% of void fraction (red line in diagrams), since in too voided regions the ability for the heat transfer from the melt droplets to the water is reduced. The liquid (blue) and active droplet lines in the diagrams diverge significantly more for MAT2 and SES-A due to the much larger VF (Figure 3). The comparison shows that noticeably more liquid mass is available in the SES simulations especially at the crucial moments of triggering (dashed vertical lines). The liquid droplet mass in the SES simulations is slightly reduced for the low initial melt temperatures compared to SES-A. However there is a bit more active droplet mass available for the simulations with the low initial melt temperature (SES-B and SES-C) due to the significantly lower VF. It may also be observed that the MAT2 droplets start to solidify quite early (total and liquid lines separate at approx. 0.6 s) and the total droplet mass preserves its maximum value because the solidified droplets cannot coalesce at the bottom. In the SES simulations all droplets stay liquid (total and liquid lines overlap) almost till the end of the simulation.
Figure 2: Melt propagation (left) and pressure build-up (right).

Figure 3: Global void fraction (VF) development.

Figure 4: Total, liquid and active droplet mass evolution comparison.
3.2 Explosion

The integral premixing conditions at the moments of the explosion triggering may be perceived from the locations marked with vertical dashed lines in Figure 4. Figure 5 shows the comparison of the explosion pressure and pressure impulse at the K1 pressure transducer, which is placed in the lower part of the test tube at 0.2 m above the bottom (Figure 1). At this height the explosion pressure impulses reached the highest values, whereas the highest pressure peaks can be reached also in the upper part of the test tube. All 4 simulations are compared for triggering at 0.9 s (left diagrams) and at 1.18 s (right diagrams). The fragmented mass development during the explosion is compared in Figure 6. It may be observed that the MAT2 simulations (green lines) give in general the weakest explosion strength. At both triggering times SES-A gives the strongest explosion according to the pressure impulses (bottom diagrams in Figure 5) and the produced mass of fragments (Figure 6). However, for each triggering time the SES simulations give quite comparable explosion strength despite the large initial melt temperature difference in premixing (Table 3). The reason is that in the high melt temperature case SES-A the premixture is highly voided and thus the heat transfer and vaporization during the explosion is less efficient, which compensates the higher available initial melt energy. The explosion strength of all SES simulations is in a noticeably higher range than the explosion strength of MAT2.

![Figure 5: Explosion pressure (upper diagrams) and impulse (bottom diagrams) comparison at K1 transducer for earlier (0.9 s – left diagrams) and later (1.18 s – right diagrams) triggering.](image)

The explosion strength at triggering time 1.18 s (right diagrams in Figure 5 and Figure 6) is reduced for all simulations compared to the early triggering at 0.9 s (left diagrams) as expected according to the available liquid and active droplet mass (Figure 4). For the later triggering time practically no explosion occurs for the MAT2 simulation due to the lack of available liquid droplet mass. Comparing the SES simulations at 1.18 s, it may be observed that for the simulations with the low initial melt temperature (SES-B, SES-C) the pressure peaks are higher and narrower, which is contributed to the fact that there is an insignificant
amount of void present compared to the SES-A simulation (Figure 3). Correspondingly the active droplet mass in SES-A is lower (Figure 4), however it seems that in SES-A the explosion ‘burns’ also the rest of the liquid droplets until the end of the simulation.

Figure 6: Fragmented mass comparison for earlier (left) and later (right) triggering.

All relevant premixing and explosion simulation results are summarized in Figure 7. The explosion strength of all SES simulations (bottom diagrams) is in a noticeably higher range than the explosion strength of the MAT2 simulation. The MAT2 explosion simulation is more sensitive to the triggering time because a significant amount of MAT2 droplets is already solidified at later times (Figure 4). The SES material droplets solidify significantly slower, providing enough ‘explosion fuel’ for a quite longer period of time. In the SES simulations the produced fragmented mass more or less corresponds to the available liquid droplet mass. It may be even slightly larger because during the explosion also the melt in the non-fragmented melt jet may undergo fine fragmentation.

Figure 7: Summary of results for earlier (0.9 s – left diagrams) and later (1.18 s – right diagrams) triggering time. Upper diagrams: total, liquid and active droplet mass together with fragmented mass. Bottom diagrams: explosion maximum pressure and impulse.
4 CONCLUSIONS

According to the performed study it can be concluded that in the jet-pool configuration of the KROTOS geometry the PULiMS/SES simulant material (eutectic mixture of WO$_3$/ZrO$_2$) has a significantly larger explosion potential than the reference SERENA prototypic material (near eutectic mixture of UO$_2$/ZrO$_2$), irrespective of the initial melt temperature of the simulant material. The PULiMS/SES simulant material is also less sensitive to the triggering time because the melt droplets solidify slower, providing enough ‘explosion fuel’ for a quite longer period of time. It is estimated that the most decisive factor for the higher explosivity of the simulant material is its significantly lower liquidus temperature. The melt is prone to remain liquid for a longer time, which is a promoting factor for the development of a strong steam explosion also in a stratified configuration despite the qualitatively different premixture formation mechanisms.

To be able to evaluate the explosion potential of prototypic corium melt in stratified configurations, which is the main purpose of the research, beside further analytical work and well instrumented experiments with simulant material also experiments with prototypic corium melt in stratified configurations would be needed. It should be explored if such experiments could be performed in the modified KROTOS facility and which facility modifications would be necessary to enable the investigation of steam explosions with prototypic corium melt in stratified configurations.

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