Annals of Nuclear Energy 185 (2023) 109740

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Modelling and simulating of premixed layer in stratified fuel coolant configuration

Janez Kokalj [a,*], Mitja Uršič [b], Matjaž Leskovar [a], Renaud Meignen [a]

[a] Jožef Stefan Institute (JSI), Jamova cesta 39, 1000 Ljubljana, Slovenia
[b] Institut de Radioprotection et de Sûreté Nucléaire (IRSN), Cadarache Nuclear Center, BP 3 13115 Saint-Paul-lez-Durance, France

ARTICLE INFO

Keywords:
Severe accident
Fuel–coolant interaction
Vapour explosion
Stratified configuration
Premixed layer

ABSTRACT

A hypothetical severe accident in a nuclear power plant can lead to significant core damage, including melting of the core. The interaction between the molten core and the coolant water is known as a fuel–coolant interaction. One of the consequences can be a rapid transfer of a significant part of the molten corium thermal energy to the coolant in a time scale smaller than the characteristic time of the pressure relief of the created and expanding vapour. Such a phenomenon is known as a vapour explosion. Given possibly a large amount of thermal energy, initially stored in the liquid corium melt at about 3000 K, and pressure peaks of the order of 100 MPa, vapour explosion can be a credible threat to the structures, systems and components inside the reactor containment. It can also threaten the integrity of the reactor containment itself, which would lead to the release of radioactive material into the environment and threaten the general public safety. In analyses of severe accidents in nuclear power plants, a fuel–coolant interaction was mostly addressed in a geometry of a melt jet poured into a coolant pool. Based on some experimental and analytical work from the past a geometry with a continuous layer of melt under a layer of water, called stratified configuration, was believed to be incapable of producing energetic fuel–coolant interaction of sufficient magnitude to likely fail the containment. However, the results from recent experiments performed at the PULiMS and SES facilities (KTH, Sweden) with corium simulants materials contradict this hypothesis. In some of the tests, a premixing layer of ejected melt drops in water was clearly visible and was followed by strong spontaneous vapour explosions.

The purpose of our research is to improve the knowledge, understanding and modelling of the fuel–coolant interaction and vapour explosion in stratified configuration. Based on the past experimental and analytical research, mechanisms for the premixed layer formation are identified and a model for the melt-coolant premixed layer formation in stratified configuration is presented. The analyses on the PULiMS and SES experimental results demonstrate the model's capability to describe the premixed layer formation.

1. Introduction

During a hypothetical severe accident in a light water nuclear power plant, the molten reactor core may come in contact with the coolant water (Seghal, 2012). The consequence can be a rapid transfer of a significant part of the molten corium thermal energy to the coolant in a time scale smaller than the characteristic time of the pressure relief of the created and expanding vapour. Such a phenomenon is known as a steam explosion. Behind the shock wave front, the relative difference between the melt and surrounding coolant enhances further melt drops fine fragmentation, which causes a significant increase of the interface area and consequently an increase of the heat transfer between both liquids. An important condition for the possible energetic steam explosion and the self-sustained process of the shock wave propagation is the existence of a premixture of fragmented melt and coolant. Given the amount of thermal energy, initially stored in the liquid corium melt at about 3000 K, the steam explosion can be a credible threat to the systems and components inside the reactor containment. It can also threaten the integrity of the reactor containment itself, which would lead to the release of radioactive material into the environment and threaten the general public safety.

In analyses of severe accidents in nuclear power plants, a fuel–coolant interaction is mostly addressed in a configuration of a melt jet poured into a coolant pool (Berthoud, 2000). Based on some

* Corresponding author.
E-mail address: janez.kokalj@ijs.si (J. Kokalj).

https://doi.org/10.1016/j.anucene.2023.109740
Received 26 September 2022; Received in revised form 24 January 2023; Accepted 1 February 2023
Available online 8 February 2023

experimental and analytical work from the past, a geometry with a continuous layer of melt under a layer of water, called stratified configuration, was believed to be incapable of producing energetic fuel–coolant interaction of sufficient magnitude to likely fail the containment (Kudinov, 2017). However, the results from recent experiments performed at the PULiMS and SES facilities (KTH, Sweden) with corium simulants materials (Kudinov, 2017; Grishchenko, et al., 2013) and research work at AREVA (Fischer and Keim, 2020) contradict this hypothesis. In some of the tests, a premixed layer of ejected melt drops in water was clearly visible and was followed by strong spontaneous vapour explosions. It is then believed that a major task for modelling such type of interaction is to provide a description of this premixed layer, in contrast with previous models assuming flat interfaces and a vapour film separating the melt and the coolant (Corradini et al., 1988).

The purpose of this research work is to improve the knowledge, understanding and modelling of the fuel–coolant interaction and vapour explosion in stratified configuration. In the paper, a short overview of the previously performed experimental and analytical research is given first and the mechanisms for the premixed layer formation are identified and evaluated. Further, our developed model (Kokalj et al., 2021) for the melt-coolant premixed layer formation in stratified configuration, developed based on the visual observations and some available mechanisms from the literature, is presented. Finally, the model validation on available PULiMS and SES experimental results is discussed. The presented analysis demonstrates the model's capability to describe the premixed layer formation in agreement with the experimental data.

2. Past Experimental And Analytical Research

Some of the experiments providing valuable information about the vapour explosions in stratified configuration were not primarily devoted to the investigation of this phenomenon (Grishchenko, et al., 2013; Dinh et al., 2000). Therefore, one of the difficulties is a lack of measurements and visual observations, which would further enlighten the phenomenon.

Some of the performed experiments resulted in an explosive interaction between the hot and the cold liquid. This interaction can be spontaneous, when two liquids come in contact and energetic interaction occurs between them without additional triggering (Board and Hall, 1974; Konovalenko et al., 2012), or triggered, e.g. with external pressure pulse, tapping or in case of high impact velocity of the liquids. It seems that for an explosive interaction the temperature of the hot liquid has to be higher than the spontaneous nucleation temperature of the cold liquid (Greene and Some observations on simulated molten debris-coolant layer dynamics. , 1983) and the cold liquid has to be sufficiently subcooled. In case of the cold liquid being only slightly subcooled, no strong interaction has been observed and this may be due to a larger vapour film separating both liquids (Konovalenko et al., 2012). The explosion is not necessarily an instant event. Sometimes it took a couple of seconds to occur (Grishchenko, et al., 2013; Yamano, 1995). Prior to the explosion, some milder melt-coolant interactions, such as smaller melt eruptions (Yamano, 1995; Farmer et al., 2009), mixing (Greene and Some observations on simulated molten debris-coolant layer dynamics. , 1983), or even stronger interaction such as larger eruptions of water and melt (Yamano, 1995) could be observed. In some cases, the observed interface instabilities were marked as undesirable and suppressed (Bang and Corradini, 1989) through the installation of a plate separating the two fluids. In some cases, the increased waviness of the fluids enabled the interaction propagation to be self-sustained (Sainson et al., 1993). It seems that sometimes the first interaction (usually triggered) deformed the vapour film and the liquid interface and caused some mixing of the liquids. Therefore, in some cases, after the first explosion, more secondary explosions followed (Board and Hall, 1974; Frost et al., 1995). The propagation of the interaction was self-sustained if the inertial confinement (e.g. by the layer of the cold liquid on top) was sufficient. Increasing the confinement through the cold liquid height increased the impulse (Frost et al., 1995). The propagation velocity of the interaction was from about 5 m/s up to 250 m/s, but usually of the order of 50 m/s. With an increase in the propagation velocity, the pressure peak also increased. In some small-scale experiments, similarities of the vapour explosions in stratified configuration with experiments, where the cold liquid is injected into the hot one, were observed. This is suggesting that the phenomenon of trapping coolant in the melt takes place also in the stratified geometry. In case of supplying water through a porous concrete layer below the melt layer, only mild interaction occurred (Alsmeyer and Tromm, 1999), but the amount of water available for an energetic event was limited in that case. Sometimes, the interaction between the flowing melt and the coolant resulted in a porous layer in the debris bed. The porosity there was too large to be only due to the melt shrinkage on cooling (Dinh et al., 2000). In case of pouring melt onto the concrete basemat in the reactor cavity, the interaction between the molten core and the concrete can produce a large amount of gases and drive out bound and unbound water. Gas sparging from the molten core-concrete interaction was simulated in some experiments. Meeks et al. (Meeks, 1997) in their stratified geometry experiments uniformly injected air into the coolant pool to simulate the void in the mixture. At low air injection rates, the agitation and mixing due to the air injection increased the intensity of the interaction. At larger air injection rates, the increase in the void fraction tends to attenuate the propagating pressure wave. With a void fraction above 30 %, the explosions were suppressed (Meeks, 1997). It was also found that premixing could be suppressed by the high viscosity of the hot liquid (e.g. glycerine) (Grishchenko, et al., 2013).

Some of the experiments in a stratified-like configuration did not result in a vapour explosion. When adding the cold liquid on top of the hot one slowly (e.g. spraying), a crust was formed which prevented further energetic melt-coolant interaction (Yamano, 1995). However, some solidified tower-like structures were observed after the end of the experiments, indicating melt eruptions and freezing during the eruption (Konovalenko et al., 2012), especially during the experiments with added gas sparging (Farmer et al., 2009).

Similar experiments, studies, and observations related to the stratified vapour explosions were performed also in other research fields, such as volcanic eruptions, where lava can be in contact with water, and in case of a liquefied natural gas spillage.

In the recently performed PULiMS and SES experiments (KTH, Sweden), a superheated high melting temperature eutectic simulant of corium melt was poured as a jet into a shallow pool of subcooled water. In the PULiMS experiments, underwater melt spreading observation was the primary aim. However, unexpectedly strong spontaneous vapour explosions occurred and a premixed layer was clearly observed (Kudinov, 2017; Grishchenko, et al., 2013). At the early stage of the melt propagation, bubble growth and collapse in subcooled water were seen. When the amount of melt increased and the melt spread further away from the jet impingement, more violent interaction was observed. Splashes of melt reached up to 10 cm in height. Similar phenomena were observed also in the SES experiments (Kudinov, et al., 2015). On the contrary, the DEFOR-S and DEFOR-A experiments (KTH), using the same materials and similar temperatures as in the PULiMS experiments but a deeper water pool, which resulted in a complete jet breakup, did not result in a spontaneous vapour explosion (Konovalenko et al., 2012).

For the vapour explosion in stratified configuration, few models were developed in the past (Harlow and Ruppel, 1981; Bang and Corradini, 1991). They describe the initiation of the interaction, its propagation and mixing right in front or just behind the vapour film collapse. However, none of the models above describes the premixed layer formation as observed in some of the experiments (e.g. PULiMS and SES) or any other mixing before the initiation of the explosion.

Interestingly, it seems that the existing models, not describing any mixing before the explosion, actually affected the experimental work. For example, any possible premixed layer in the experiments was not followed or not well documented, as it was not expected. Even if any interface instabilities before the explosion were observed, they were usually marked as undesirable. Sometimes, measures were performed to minimize the instabilities (Bang and Corradini, 1989; Frost et al., 1995).

In the frame of this research, we try to fill this gap in modelling and describe the premixed layer formation. In our research, we will not assess existing models, but rather complement them. The results of our model could serve as initial conditions for any explosion model based on a pre-existing premixing in stratified configuration.

3. Mechanisms For Premixed Layer Formation

From the analysed experimental results, it can be observed, that one of the most common plausible mechanism for the premixed layer formation is the growth, expansion and collapse of vapour bubbles. The melt is usually hot enough for boiling of the coolant and if the coolant is subcooled and the coolant layer high enough, the bubbles collapse. Indeed, the mechanism of growth, expansion and collapse of the vapour bubbles was mentioned in many experiment discussions (Corradini et al., 1988; Board and Hall, 1974; Frost et al., 1995). Also in the recent PULiMS experiments, in the early stage of the melt propagation, vapour bubble formation, growth and collapse in the subcooled water were clearly observed by a high-speed camera (Kudinov, 2017; Grishchenko, et al., 2013; Konovalenko et al., 2012). A bubble collapse can be a very energetic process. At a certain frequency of the bubble collapse event, sufficient momentum flux can be transferred to the melt to sustain the premixed layer (Kudinov, et al., 2014).

Other mechanisms also seem plausible for some experiments. For the evaporation of coolant entrapped in the melt or under the melt, the most favourable geometry is the pouring of melt in a pool of coolant. This geometry was used only in a few experiments, e.g. PULiMS, SES (both KTH, Sweden) (Kudinov, 2017; De Malmazet, 2017), Board and Hall experiment (BNL, USA) (Board and Hall, 1974).

In case of pouring the coolant on the melt, e.g. Greene et al. experiment (BNL, USA) (Greene and Some observations on simulated molten debris-coolant layer dynamics. , 1983), Bang and Corradini experiment (University of Wisconsin, USA) (Bang and Corradini, 1989), Sainson et al. experiment (Gaz de France, France and Gas Research Institute, USA) (Sainson et al., 1993), some smaller amount of coolant can become entrapped in the melt. In this case, the phenomena are local, but can disturb the melt surface and cause some melt ejection.

For the mechanism of release of gases from the interaction of melt with concrete, the necessary condition is the presence of concrete, which is not the case in most of the experiments. Experiments with the concrete were e.g. S3E (KTH, Sweden) (Dinh et al., 2000), and KATS (FZK, Germany) (Dinh et al., 2000). However, in some cases, e.g. Meeks et al. experiment (University of Wisconsin, USA) (Meeks, 1997), the MCCI was simulated with a gas injection through the bottom plate. In the experiments, the bubbles of gases cause instability of the melt surface and they can push the melt to the overlying coolant. Due to the vaporization of water in the concrete and related vapour pressure, small pieces of the concrete also broke off, which resulted in a significant disturbance of the spreading melt and a small amount of melt was splashed outside. The gas injection can be considered also as the simulation of the release of non-condensable gases during melt cooling. However, it seems unlikely for cooling or any other process (e.g. oxidation) to produce enough gases to cause any substantial instabilities.

In the mechanism of jet breakup, impingement and splattering, different contributions are covered. The melt jet breakup, most known from the classical melt jet – coolant pool geometry, is greatly dependent on the coolant pool depth. In the case of a deeper coolant pool, its contribution should be more pronounced. In the case of jet geometry, e.g. PULiMS, SES (both KTH, Sweden) (Kudinov, 2017; De Malmazet, 2017), Board and Hall experiment (BNL, USA) (Board and Hall, 1974), the momentum of the melt jet falling onto the melt surface can cause instabilities. However, the jet geometry was not present in all the experiments where the premixed layer was observed (e.g. Meeks et. al experiment (Meeks, 1997), SES S1 experimental test (De Malmazet, 2017). In addition, the melt jet breakup and impingement on the melt free surface are not very sensitive to the coolant subcooling. Therefore the effect of the coolant subcooling should be minor on the premixed layer formation phenomena which is contradictory to the comparison of the SES-E3 and other tests (Kudinov, et al., 2014).

Apart from the jet of melt, the jet of coolant was also considered, e.g. Greene et al. experiment (BNL, USA) (Greene and Some observations on simulated molten debris-coolant layer dynamics. , 1983), Bang and Corradini experiment (University of Wisconsin, USA) (Bang and Corradini, 1989), Sainson et al. experiment (Gaz de France, France and Gas Research Institute, USA) (Sainson et al., 1993). In fact, this configuration was more often in the experiments but should be emphasised that the melt instabilities in this case would be localized. From the experiments, it can be noted that the jet geometry can cause instabilities but the premixed layer is formed also after the jet pouring stopped.

The formation, growth and collapse of vapour bubbles seems to be the most plausible amongst the described mechanisms (Kokalj et al., 2019). Thus, our developed models for the premixed layer formation in stratified melt-coolant configuration are based on it. However, as stressed above, besides the bubble formation, growth and collapse, other mechanisms, relevant for the individual experimental geometry (e.g. jet break-up), could serve as an additional source of the melt instabilities. Additionally, a contribution to the amount of melt-coolant mixture, which could participate in the vapour explosion, can be a consequence of mixing during the explosion itself.

4. Model For Premixed Layer Formation

It was concluded that one of the most common plausible mechanisms for the premixed layer formation is the boiling of the coolant. Due to the Rayleigh-Taylor instabilities, the bubbles arise from the vapour film. In subcooled water, bubbles condense and collapse. During the bubble collapse, water at the bubble interface accelerates towards the melt surface, creating a so-called coolant micro-jet (Caldarola and Kastenberg, 1974). The coolant micro-jet impacts on the melt surface and can produce melt surface instabilities and fragmentation of the melt.

Our model describes the premixed layer formation with three key characteristics, i.e. size of ejected melt drops, their initial velocity and the fragmentation rate of the continuous melt phase.

The modelling values depend on the scale of the instabilities, given by the value of the most dangerous wavelength on the surface, i.e. for which the instability growth rate is the highest – in our case this is the distance between the formed bubbles (Berenson, 1961):

$$\Lambda = 2\pi\sqrt{\frac{3\sigma_L}{g(\rho_L - \rho_G)}}, \tag{1}$$

where σ_L is the liquid coolant surface tension at saturation temperature, g the gravity acceleration and ρ_L and ρ_G the density of the liquid and gaseous phase of the coolant, respectively.

The melt surface instabilities can result in fragmentation of the melt. The size of the ejected melt drops in our model is related to the instability wavelength. The hypothesis by Leclerc and Berthoud (Leclerc and Berthoud, 2003) for the thermal fragmentation of a single melt drop is adopted, where the melt drop diameter is defined as one quarter of the instability wavelength. Based on the performed analysis (Kokalj et al., 2021), the melt drop diameter in our model is multiplied by the factor C_d, being 1.25. The melt drop diameter most affects the fine fragmentation rate and the consequent explosion duration, and based on the comparison with the experimental results, the best-case factor C_d was determined.

$$d = C_d \cdot 0.25 \cdot \Lambda. \tag{2}$$

The fragmentation rate of the melt layer can be established from the size of the ejected melt drops and the frequency of their ejections per melt area. The size of the melt drop is defined in Eq. (2). The single melt drop ejects from the surface area that is defined with the wavelength as given in Eq. (1). It should be emphasized that in this area we have node and antinode, therefore the effective surface area is $\frac{1}{2}\Lambda^2$. Based on the performed analysis (Kokalj et al., 2021), the fragmentation rate in our model is multiplied with the factor C_f, being 0.5. Varying this factor shows a tendency towards stronger explosions with higher fragmentation rates but only until a certain plateau. More pronounced is the influence of higher melt fragmentation rates producing a shorter peak of the force signal with higher maximal force. Based on the analysis and comparison with the experimental results, the best-case factor C_f was determined.

$$\Gamma = C_f \cdot \frac{\pi d^3 F}{3\Lambda^2}. \tag{3}$$

The frequency of the melt ejections F is proportional to the frequency of the bubble formations and collapses. It can be derived from the relation by Berenson (Berenson, 1961) for the bubble detachments for a horizontal surface film-boiling heat transfer, considering the Rayleigh-Taylor instabilities. With some simplifications due to the large differences in the liquid and vapour density, the following equation is obtained:

$$F = \frac{1}{2\pi}\sqrt{\frac{\rho_G v_{vf}^2 n}{\rho_L a} + gn - \frac{\sigma_L n^3}{\rho_L}}, \tag{4}$$

where n is wavenumber and v_{vf} and a vapour velocity and vapour film thickness:

$$v_{vf} = 0.45\frac{\lambda_{vf}\Delta T}{\rho_{vf}\Delta H a^2 n}, \tag{5}$$

$$a = 2.35 \cdot \frac{\sigma_L^{\frac{1}{8}}}{(g\rho_L)^{\frac{3}{8}}} \cdot \left(\frac{\mu_{vf}\lambda_{vf}\Delta T}{\Delta H \rho_{vf}}\right)^{\frac{1}{4}}, \tag{6}$$

where index vf stands for the vapour film, ΔT is the temperature difference between the melt and the coolant and ΔH is the average enthalpy difference between vapour and liquid coolant. The constant factors of Berenson (Berenson, 1961) are used in correlations.

The initial velocity of the ejected melt drops is calculated from the available energy. As shown in experiments by Caldarola and Kastenberg (Caldarola and Kastenberg, 1974), the available energy (and consequently velocity) lies between the transmitted (energy due to the shock wave from a hemispherical source to the surrounding medium) and the acoustic (energy of the elastic wave travelling in the fuel) energy limits. Thus, the velocity as calculated from the acoustic energy (lower limit) is in our model multiplied by a free factor C_v. Based on the performed analysis (Kokalj et al., 2021), C_v was assessed to 6. This value most agrees with the visual observation of the premixed layer while it does not significantly affect the explosion strength.

$$v = C_v\sqrt{C_{v1} \cdot C_{v2} \cdot \frac{(p_{max} - p_0)^2 \Delta T_{sub}^2}{\Lambda^{0.8}\sqrt{\Delta p}}}, \tag{7}$$

where p_0 is the ambient pressure, p_{max} is the pressure of coolant micro jets acting on the melt, ΔT_{sub} is the water subcooling, Δp is the pressure difference between inside and outside of the bubble, C_{v1} is a constant, related to the dimension of the formed coolant micro-jet generated after the bubble collapse and its value is around 0.01. C_{v2} is related to the material properties:

$$C_{v2} = \frac{(\rho_M - \rho_L)\rho_L^{1.9}}{(\rho_M + \rho_L)\rho_M^2 \rho_G^2} \cdot \frac{\lambda_L^{\frac{4}{3}} c_p^{\frac{2}{3}}}{c g^{0.2} L^2 \sigma_L^{0.2} \mu_L^{\frac{8}{15}}}, \tag{8}$$

where index M stands for melt, λ is thermal conductivity, c_p is specific heat, c is sound velocity, L is latent heat and μ is dynamic viscosity.

Our model, reduced to the three equations for the melt drops diameter (Eq. (2)), fragmentation rate (Eq. (3)) and ejected melt drop initial velocity (Eq. (7)), can be implemented into the fuel–coolant interaction codes to mathematically describe the phenomenon of the premixed layer formation in stratified configuration.

5. Modelling With MC3D

The developed model for premixed layer formation was implemented as a patch in the computational multi-fluid dynamic code MC3D V3.9.0.p1, which is being developed at IRSN (France) with fuel–coolant interactions in mind. MC3D is one of the leading codes in the field of fuel–coolant interactions and it is suitable for the planned purpose because it covers both the premixing phase and the explosion phase of the fuel–coolant interaction. The premixing phase module (Meignen, 2014) deals with the initial mixing of the melt and the coolant and this module was upgraded with the premixed layer formation model, developed in the frame of our research work. To compute the explosion phase, the results from the premixing phase module serve as an input for the explosion phase module (Meignen, 2014). The explosion phase module concerns the fine fragmentation of the melt during the explosion and the heat transfer between the created fine fragments and the coolant. It is not modified in our modelling.

MC3D is an Eulerian code in which for each phase (melt drops, continuous melt, liquid coolant, vapour coolant, non-condensable gases) a set of continuity equations for the mass, momentum and energy are solved. Numerically, the phases are represented by three types of fields: volumes, velocities, and temperatures. Primary fragmentation is represented by a mass transfer from the continuous melt field to the (discrete) melt drops fields (Fig. 1). It is not possible to represent with a single Eulerian field the trajectories of the melt drops, which are typically ejected upwards and are falling back downwards, thus having a different velocity sign. However, the melt drops can be represented with a multi-drop model where different melt drop volume fields are characterized by a specific diameter (MUSIG method). As many fields can be used as necessary, but they must be grouped in one or two (at maximum) velocity fields. In the standard model of MC3D, the mass transfer can occur between the drop fields according to the secondary fragmentation model (large drops being fragmented into smaller ones). Premixing and explosion modelling follows the same rules, but in the explosion model, the continuous melt field is not used, whereas an additional field is used to represent the small fragments coming from the fine fragmentation resulting from the explosion.

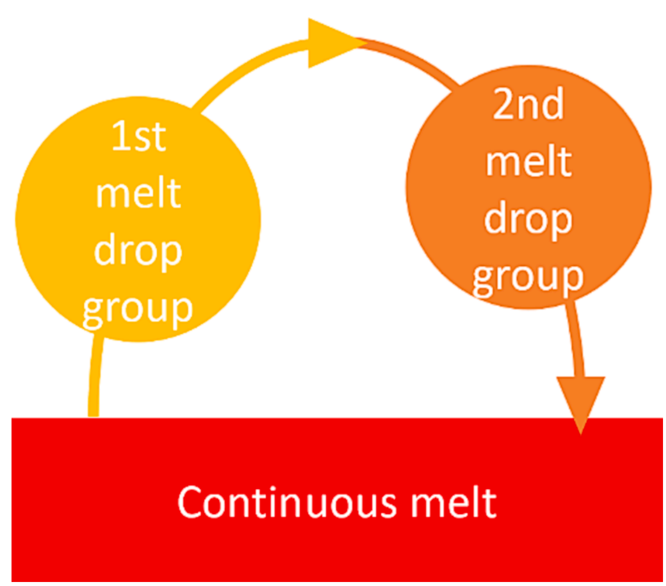

Fig. 1. Chematic overview of the two-melt-drop-group approach.

For the melt drop description of the premixed layer, a two-melt-drop-group approach is used (Fig. 1) with two volume fields, each with its own velocity, and its own temperature field. The model is modified in a way that one group is reserved for the drops moving upward (positive velocity) and one group for the drops falling downwards. The group for the drops moving upward is fed by the continuous melt fragmentation at the fragmentation rate and with the drop size and the initial drop velocities as defined in Section 4. The second group is fed through a modification of the mass transfer law, which occurs in the cells corresponding to the highest position of the (1st group) drops.

The explosion modeling has not been modified.

For the premixing phase of the simulations, the material properties of the melt, the initial conditions (melt, water and gas temperature) and the initial geometry are the input parameters. Among the available melt fragmentation models in the code, only our newly incorporated model for the melt fragmentation in stratified configuration is considered. For the explosion phase of the simulations, the results of the premixing phase serve as the input. The explosion is triggered by the defined trigger (location, composition, pressure).

6. Application To Experiments

The complex phenomena of premixed layer formation as described by our model was assessed on the experimental results by simulating the SES S1 and PULiMS E6 experimental tests. On these tests, some previous simulation analyses were performed, but without modelling the premixed layer formation (Leskovar, 2019).

6.1. SES S1 experimental test

The SES experiments were performed at KTH (Sweden). The test section consisted of a square tank of the size of 1 m^2, filled with water to the height of 25 cm. The melt was released in the water through the funnel, which ended in the water, 25 mm above the melt spreading surface. The initial melt temperature was 1303 K, which corresponds to 160 K of superheating. The melt material properties (Table 1) are determined from the literature (Grishchenko, et al., 2013; Konovalenko et al., 2012; Plinius, 2010; Moriyama and Furuya, 2020; Kudinov, et al., 2012; Konovalenko and Kudinov, 2012; Centrih and Leskovar, 2014), except the velocity of sound in the melt is arbitrarily set to 1800 m/s.

The water was at 348 K. During the release of the melt under water, a spontaneous vapour explosion occurred after 0.6 s. A more detailed description is given in (De Malmazet, 2017).

The 3D calculation domain contains half of the experimental tank applying symmetry boundary conditions at the symmetry plane. The melt pouring and spreading is not modelled. Therefore, initially, all the continuous melt is described as a 5 mm high melt pool with a diameter of around 25 cm. The analyses are based on the best-case (Kokalj et al., 2021), with parameters C_v, C_d and C_f being 6, 1.25 and 0.5.

Firstly, the premixed layer formation phase was simulated. After the initial transient of the first melt drops being ejected, quasi-stationary conditions are developed. The melt drops are constantly being ejected from the continuous melt and coalescing back. In Fig. 2, the formed premixed layer is shown. The largest melt volume fraction is at the bottom, as a shallow pool of continuous melt remains there. The ejected melt drop volume fraction increases towards the top of the premixed layer because numerically the velocity of the melt drops decreases and all the melt drops reach approximately the same height. The phenomenon of the premixed layer formation is not completely homogeneous, which indicates the complexity of the feedback loops. Namely, heating of the coolant water, vaporization and flow currents of the vapour, water and melt affect the height of the premixed layer and the melt fraction distribution. Nevertheless, the simulation results where the maximum reached height of melt drops is around 10 cm seem to be close to the experimental observation.

Table 1
Melt material properties used in calculations.

Property	Value
Melting point	1143 K
Density	7811 kg/m^3
Specific heat	473 J/(kg·K)
Latent heat	170 kJ/kg
Thermal conductivity	5.3 W/(m·K)
Surface tension	0.2 N/m
Dynamic viscosity	0.016 Pa·s
Emissivity	0.7
Sound velocity	1800 m/s

Because of the lack of more detailed experimental data regarding the premixed layer, further analyses and comparison of our model with the experiments are made regarding the explosion phase, as seen in Fig. 3. The force signal on the bottom of the test section and the total gained impulse are compared. The total gained impulse is in the simulation around 20 % lower, compared to the experimental one. Initially, the simulation's impulse is almost identical to the experimental one. The difference is made in the second half of the explosion when the explosion in the simulation decays earlier.

For the simulation case, the force signal is more fluctuating compared to the experimental one, although in the experimental results two force peaks can be also observed. In the simulation, the pressure shock waves are reflected and when meeting, a local increase in fine fragmentation increases pressure and a maximum in the force signal can be observed. The force signal in the simulation decreases more gradually compared to the experiment.

Considering the uncertainty in simulating the vapour explosions, the simulation results for the SES S1 experimental test seem to be in relatively good agreement with the experimental findings. The height of the developed premixed layer seems to be similar to the experimental one and the total impulse of the simulation is around 80 % of the experimental one. The difference in the impulse builds up towards the end of the explosion. This might indicate an additional contribution to the strength of the explosion from the coarse mixing between melt and coolant during the explosion. The so-produced melt drops would also undergo fine fragmentation and contribute to the explosion strength.

6.2. PULiMS E6 experimental test

The PULiMS experiment was simulated in addition. The PULiMS experiment was performed at KTH (Sweden). The main experimental conditions and results are summarized here, while a more detailed description is given in (Kudinov, 2017; Konovalenko et al., 2012). The test section consisted of a rectangular tank of the size of 2 m × 1 m, filled with water to the height of 20 cm. The melt was released through the funnel, which ended 20 cm above the water surface. The initial melt temperature was 1322 K, which corresponds to 179 K of superheating. Water was at 348 K. During the release of the melt, a spontaneous vapour explosion occurred after around 7 s.

The 3D calculation domain contains half of the experimental tank applying symmetry boundary conditions at the symmetry plane. The continuous melt is described as a 25 mm high melt pool with a diameter of around 40 cm. The analyses are based on the best-case (Kokalj et al., 2021) with the same parameters as in the SES case - C_v; C_d and C_f being 6, 1.25 and 0.5.

For the PULiMS E6 case, the simulated premixed layer also seems to be close to the experimental observations. However, the explosion for the PULiMS E6 case is underpredicted to around one third of the experimental impulse in the simulation analysis (Fig. 4). Although the impulse of the explosion is underpredicted in the simulations, the force signal is initially almost identical to the experimental one, indicating similar initial development of the explosion.

Overall, it seems that the simulation does not describe the explosion phenomena as well as the SES S1 case. Similar to the SES S1 case, an

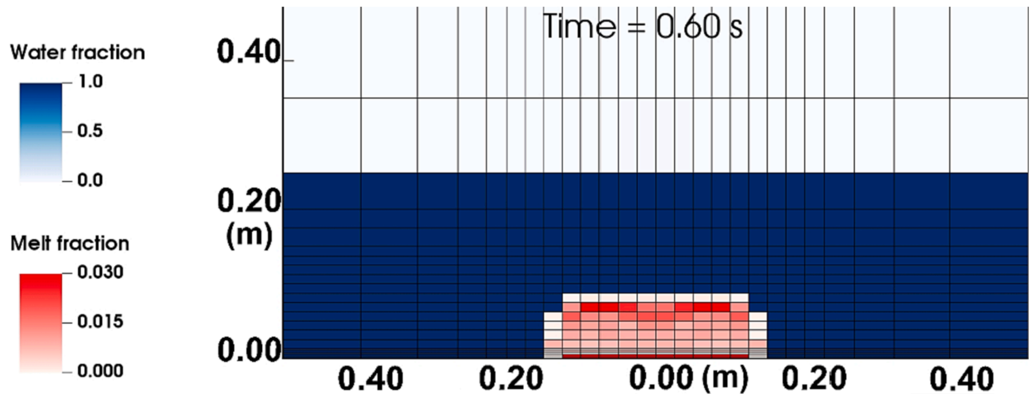

Fig. 2. Imulated premixed layer for the ses s1 experimental test after 0.6 s. Melt fraction (melt drops and melt pool in the two bottommost cells) is shown where its volume fraction exceeds 0.001.

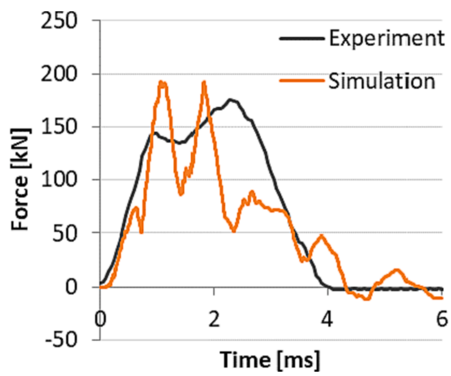

Fig. 3. Comparison of the force and total gained impulse on the bottom plate for SES S1 simulation and experiment.

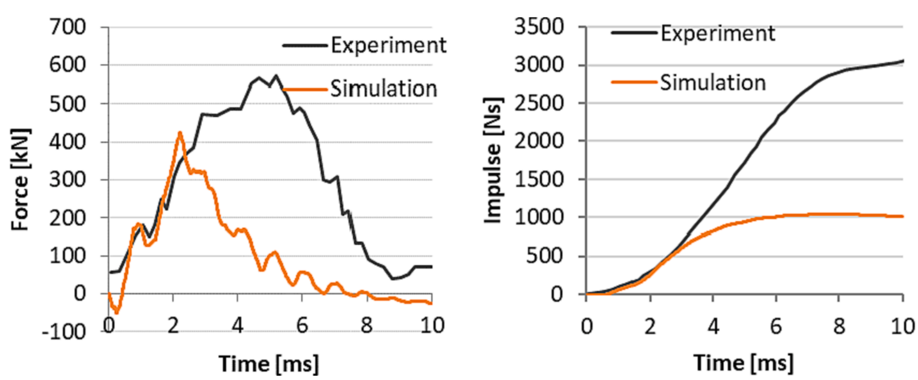

Fig. 4. Comparison of the force and total gained impulse on the bottom plate for PULiMS E6 simulation and experiment.

additional contribution to the amount of melt, participating in the explosion, can be a consequence of mixing during the explosion itself. However, additional observed underestimation of the explosion strength in simulation might indicate possible additional contributions from the other mechanisms related to the melt-coolant mixing, premixed layer formation and vapour explosion. In the PULiMS E6 experimental test, contrary to the SES S1 experimental test, the melt jet falls through 20 cm of water. This geometry presents the potential for some amount of mixing between the melt and the coolant as a consequence of the melt jet breakup.

7. Conclusions

The recent experimental results from the PULiMS and SES (KTH, Sweden) experimental facilities with spontaneous vapour explosions again raised interest in vapour explosions in the stratified configuration. During the experiments, an extensive premixed layer was observed prior to the explosion. From the perspective of nuclear safety studies, it is important to be able to simulate potential energetic fuel–coolant interactions in stratified configurations with the preceded premixed layer of ejected melt drops in the coolant layer.

A short overview of the experimental and analytical research is given. Based on the experiments, possible mechanisms for the premixed layer formation are given and assessed. The developed model for the premixed layer formation, based on the bubble formation and collapse mechanism is presented in the paper. The model was implemented into the Eulerian fuel–coolant interaction code MC3D (IRSN, France) and validated against the SES S1 and the PULiMS E6 experimental results.

The simulation results are in agreement with the experimental results regarding the expected premixed layer. For the explosion phase, it seems that the simulations accurately describe the initial phase of the vapour explosion in both aspects – force and impulse, but underestimate the explosion strength of the second part.

The observed underestimation of the explosion strength in simulations might indicate possible additional contributions from the other mechanisms related to the melt-coolant mixing, premixed layer formation and vapour explosion. Some amount of mixing between the melt and the coolant could be a consequence of the melt jet breakup, especially in the PULiMS case, where in the experiment the melt jet falls through 20 cm of water. For a melt jet diameter of 20 mm, the typical melt jet breakup length can be estimated to be in the order of 30 cm (Manickam et al., 2017). A very rough estimation of 20 cm of water pool depth breaking up around two thirds of the melt jet and creating a corresponding amount of premixture seems in high correlation with the observed one third of vapour explosions strength coming from the premixed layer only. However, this is only a speculative estimation and should be further investigated, e.g. as an analysis of vapour explosion in combined melt jet and stratified configuration. An additional contribution to the amount of melt, participating in the explosion in both cases, can be a consequence of mixing during the explosion itself.

In line with this assessment, the simulation results with our model, considering only the bubble formation, growth and collapse mechanism, underestimate the experimental results. This indicates some other plausible contributions, for research of which the future experimental and analytical work would be of great help. With improved experimental observations, a more detailed comparison of the premixed layer characteristic would also be possible.

Also, the uncertainties of material thermophysical properties would affect the results. Simplified, their integral effect on the model can be analysed as the model constants uncertainty. Therefore, further sensitivity and uncertainty analysis of simulated premixed layer and vapour explosion in stratified configuration are perspectives for future work.

Overall, the proposed premixed layer formation model enables a more reliable assessment of the stratified vapour explosion risk in nuclear power plants and other industries.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors do not have permission to share data.

Acknowledgments

The authors acknowledge the financial support of the Slovenian Research Agency, grants P2-0026, Z2-4437 and L2-1828.

References

Alsmeyer, H. and W. Tromm, *The COMET concept for cooling core melts: Evaluation of the experimental studies and use in the EPR*. 1999, Institut für Kern und Energietechnik, Forschungszentrum Karlsruhe, Germany. p. 94.

Bang, K.H., Corradini, M.L., 1989. Stratified vapor explosion experiments. Chemical Engineering Communications 86 (1), 31–42.

Bang, K.H., Corradini, M.L., 1991. Vapor explosions in a stratified geometry. Nuclear Science and Engineering 108 (1), 88–108.

Berenson, P.J., 1961. Film-boiling heat transfer from a horizontal surface. Journal of Heat Transfer 83 (3), 351–356.

Berthoud, G., 2000. Vapor explosions. Annual Review of Fluid Mechanics 32 (1), 573–611.

Board, S.J., Hall, R.W., 1974. Propagation in thermal explosions. In *2nd Specialist MeetIng On Sodium Interaction In Fast Reactors*. Ispra, Italy.

Caldarola, L., Kastenberg, W.E., 1974. Mechanism of fragmentation during molten fuel/coolant thermal interactions. In: Fast reactor safety meeting. Beverly Hills, California, USA, pp. 937–954.

Centrih, V., Leskovar, M., 2014. Simulation of stratified steam explosion in PULiMS facility. Jožef Stefan Institute, p. 54.

Corradini, M.L., Kim, B.J., Oh, M.D., 1988. Vapor explosions in light water reactors: a review of theory and modeling. Progress in Nuclear Energy 22 (1), 1–117.

De Malmazet, E., et al. Stratified Steam Explosion Phenomena: SAFEST SES-S1 test results and preliminary analysis. in The 8th European Review Meeting on Severe Accident Research, ERMSAR-2017, Warsaw, Poland. 2017.

Dinh, T.N., Konovalikhin, M.J., Sehgal, B.R., 2000. Core melt spreading on a reactor containment floor. Progress in Nuclear Energy 36 (4), 405–468.

Farmer, M.T., Kilsdonk, D.J., Aeschlimann, R.W., 2009. Corium coolability under ex-vessel accident conditions for LWRs. Nuclear Engineering and Technology 41 (5), 575–602.

Fischer, M., Keim, T., 2020. Retrofitting of ex-vessel core catchers into operating nuclear power plants at the example of a Mark-I BWR. Annals of Nuclear Energy 146, 107646.

Frost, D.L., Bruckert, B., Ciccarelli, G., 1995. Effect of boundary conditions on the propagation of a vapor explosion in stratified molten tin/water systems. Nuclear Engineering and Design 155 (1), 311–333.

Greene, G.A., et al., *Some observations on simulated molten debris-coolant layer dynamics*. 1983, Brookhaven National Laboratory, Upton, New York, USA. p. 15.

Grishchenko, D., et al. *Insight into steam explosion in stratified melt-coolant configuration*. in *15th International Topical Meeting on Nuclear Reactor Thermal Hydraulics*. 2013. Pisa, Italy.

Harlow, F.H. and H.M. Ruppel, *Propagation of a liquid-liquid explosion*. 1981, Los Alamos National Lab., USA. p. 13.

Kokalj, J., M. Leskovar, and M. Uršič. *Premixed layer formation modelling in stratified melt-coolant geometry*. in *18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics*. 2019. Portland, USA: ANS.

Kokalj, J., Uršič, M., Leskovar, M., 2021. Modelling of premixed layer formation in stratified fuel–coolant configuration. Nuclear Engineering and Design 378, 111261–111277.

Konovalenko, A. and P. Kudinov. *Development of scaling approach for prediction of terminal spread thickness of melt poured into a pool of water*. in *The 9th International Topical Meeting on Nuclear Thermal-Hydraulics, Operation and Safety*. 2012. Kaohsiung, Taiwan.

Konovalenko, A., A. Karbojian, and P. Kudinov. *Experimental results on pouring and underwater liquid melt spreading and energetic melt-coolant interaction*. in *The 9th International Topical Meeting on Nuclear Thermal-Hydraulics, Operation and Safety*. 2012. Kaohsiung, Taiwan: American Nuclear Society.

Kudinov, P., et al., 2017. Premixing and steam explosion phenomena in the tests with stratified melt-coolant configuration and binary oxidic melt simulant materials. Nuclear Engineering and Design 314, 182–197.

Kudinov, P., et al. *Validation of the FCI codes against DEFOR-A data on the mass fraction of agglomerated debris*. in *5th European Review Meeting on Severe Accident Research, ERMSAR-2012*. 2012.

Kudinov, P., et al., *Investigation of steam explosion in stratified melt-coolant configuration*, in *The 10th International Topical Meeting on Nuclear Thermal-Hydraulics, Operation and Safety*. 2014: Okinawa, Japan. p. 16.

Kudinov, P., et al., *Investigation of steam explosion in stratified melt-coolant configuration*, in *2nd NUGENIA Review Meeting TA2.2*. 2015: Jandía, Spain. p. 37.

Leclerc, E., Berthoud, G.J., 2003. Modeling of Melt Droplet Fragmentation Following Vapor Film Destabilization by a Trigger Pulse. Nuclear Technology 144 (2), 158–174.

Leskovar, M., et al., 2019. Investigation of steam explosion duration in stratified configuration. Nuclear Engineering and Design 353, 110233.

Manickam, L., Bechta, S., Ma, W., 2017. On the fragmentation characteristics of melt jets quenched in water. International Journal of Multiphase Flow 91, 262–275.

Meeks, M.K., et al., 1997. Suppression of stratified explosive interactions. In: OECD/CSNI Specialist Meeting on Fuel-Coolant Interactions. Tokai, Japan, pp. 624–638.

Meignen, R., et al., 2014. The challenge of modeling fuel–coolant interaction: Part I – Premixing. Nuclear Engineering and Design 280, 511–527.

Meignen, R., et al., 2014. The challenge of modeling fuel–coolant interaction: Part II – Steam explosion. Nuclear Engineering and Design 280, 528–541.

Moriyama, K., Furuya, M., 2020. Kinetic energy evaluation for the steam explosion in a shallow pool with a spreading melt layer at the bottom. Nuclear Engineering and Design 360, 110521.

Plinius, 2010. Transnational Access to the Prototypic Corium Platform PLINIUS, Research report EURATOM 6th Framework Programme, Project coordinator: C. Journeau.

Sainson, J., M. Gabillard, and T. Williams. Propagation of vapor explosion in a stratified geometry experiments with liquid nitrogen and water. in CSNI Specialists Meeting on Fuel-Coolant Interactions. 1993. Santa Barbara, California, USA.

Seghal, B.R., *Nuclear Safety in Light Water Reactors: Severe Accident Phenomenology*. 2012: Elsevier Inc.

Yamano, N., et al., 1995. Phenomenological studies on melt-coolant interactions in the ALPHA program. Nuclear Engineering and Design 155 (1), 369–389.