Numerical modelling of melt droplet interaction with water

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Abstract. A collapse of the vapour film separating a hot melt droplet from the surrounding water due to sudden ambient pressure rise is considered. The pressure peak causes a direct contact between water and melt, leading to significant disturbances of the melt droplet surface. Results of numerical simulations performed by the VOF method are presented. Parametric analysis of the interaction process is performed for a molten tin droplet with initial temperature of 950 K, immersed in subcooled water having the temperature of 353 K. The interaction is initiated by sudden rise of the ambient pressure to as much as 8 MPa, imitating the arrival of a thermal detonation wave, with its gradual decrease towards the initial pressure of 0.1 MPa. Simulations reveal the collapse of the vapour film, impingement of water on the droplet surface, and subsequent expansion of vapour due to rapid water evaporation. Significant disturbances of the melt droplet surface are obtained, and implications for the steam explosion problem are discussed.

1. Introduction

The phenomenon of steam explosion embraces rapid phase transitions occurring when a cold volatile fluid (water) is brought in contact with a hot fluid (melt) having its temperature above the boiling point of the cold fluid. In the cases when the vapor film separating the two fluids and limiting the heat transfer between them becomes unstable, the interaction can proceed explosively [1]. The problem of steam explosion is of particular interest in relation to industrial safety problems, especially in severe accidents at nuclear power reactors where explosive interaction can occur between the molten materials of the degraded reactor core (corium) and reactor coolant (usually, water) [2]. The coupled transient processes during such an interaction are quite complex, and many uncertainties still remain despite the significant experimental, theoretical, and numerical efforts undertaken [3].

Experimental studies on steam explosions may be broadly classified into small-scale studies of single melt droplet interaction with coolant with the mass of melt about of 1 g [4]–[6], and larger-scale integral experiments where the mass of melt is from few to dozens of kilograms [7]–[8]. The former approach is handy for revealing the fine details of the interaction, including the development of vapor film instability, as well as the shape of both the melt droplet and the surrounding steam bubble. The latter approach, on the contrary, provides the first-hand data on the overpressures and shock impact caused by the thermal detonation; however, the interaction details often remain obscured due to intense boiling and formation of fine debris making water opaque.
Several mechanisms were considered to explain the explosive interaction of a single melt drop with the surrounding coolant. These are related to the development of vapor film instability and impact of water micro-jets on the melt surface, capture of water by the melt with subsequent explosive evaporation of water in the bulk of the melt droplet, cooling and freezing of the molten surface with subsequent growth of thermal stresses in the thin crust causing its cracking, propagation and interaction of pressure waves in the liquid melt droplet caused by local water impingement and leading to cavitation in the bulk of the droplet material. It may be stated that no single mechanism available so far is capable of explaining all available experimental data on the dependence of droplet fragmentation in water on the droplet material and superheat, water subcooling, presence of non-condensable gases, etc. Therefore, the problem of melt droplet interaction with water still remains in the focus of research attention worldwide.

In the current work, an attempt is undertaken to perform three-dimensional simulations of melt droplet interaction with surrounding coolant, aimed at revealing the fluid-dynamical aspects of the problem; the known Volume Of Fluid (VOF) model is used to describe the phases separated by sharp interfaces. A similar approach was taken in the recent paper [9] presenting two-dimensional results of VOF simulations. We consider a single molten tin droplet surrounded by a thin vapor film separating it from the ambient subcooled water. The interaction is initiated by sudden increase in the ambient pressure with its gradual decrease to the ambient level, imitating the arrival of a triggering pressure wave. The main attention is paid to the evolution of vapor film and melt droplet surface in the course of the interaction process. This research extends our previous activity in the simulation of three-phase melt-water-vapor interactions [10].

2. Mathematical model

A three-phase system is considered which includes the melt (subscript m), liquid water (w), and water vapor (v) separated by sharp interfaces; phase change can occur on the boundary between water and vapor. The Volume Of Fluid (VOF) method, e.g., in [11] is applied by introducing an effective fluid with the properties depending on the volume fractions \( \alpha \) and respective properties of each fluid:

\[
\rho = \sum_k \alpha_k \rho_k, \quad \rho h = \sum_k \alpha_k \rho_k h_k, \quad \eta = \sum_k \alpha_k \eta_k, \quad \lambda = \sum_k \alpha_k \lambda_k
\]

Here, \( \rho \) is the density, \( h \) is the specific sensible enthalpy, \( \eta \) is the dynamic viscosity, and \( \lambda \) is the thermal conductivity (the phase properties are denoted by subscript \( k = m, w, v \)). The phase volume fractions \( \alpha_k \) satisfy the compatibility condition \( \alpha_m + \alpha_w + \alpha_v = 1 \). The governing equations for the flow take the form:

\[
\frac{\partial \rho_k \alpha_k}{\partial t} + \nabla (\rho_k \alpha_k \mathbf{U}) = \Gamma_k
\]

\[
\rho \frac{D \mathbf{U}}{Dt} = -\nabla P + \nabla \tau + \mathbf{F}_s
\]

\[
\rho \frac{D h}{Dt} = \frac{DP}{Dt} + \nabla \lambda \nabla T - \Gamma \Delta h_{ev}
\]

Here, \( t \) is the time, \( P \) and \( T \) are the pressure and temperature, \( \mathbf{U} \) is the velocity vector, \( \Gamma_k \) is the phase source term due to phase transitions; in the current problem \( \Gamma_m = 0, -\Gamma_w = \Gamma_v = \Gamma \), where \( \Gamma \) is the water evaporation rate per unit volume, and \( \Delta h_{ev} \) is the latent heat of evaporation. The stress tensor is expressed via the dynamic viscosity and velocity gradients as \( \tau = \eta (\nabla \mathbf{U} + \nabla \mathbf{U}^T - \frac{2}{3} \mathbf{I} (\nabla \cdot \mathbf{U})) \). The surface tension force \( \mathbf{F}_{s,k} \) acting on \( k \)-th liquid phase \( (k = m, w) \) is described by the continuous surface force (CSF) model [11]:
\[ F_{s,k} = \sigma_k \kappa_k \nabla \alpha_k \]  

(5)

where \( \sigma_k \) is the surface tension of \( k \)-th liquid on the interface with vapor, and \( \kappa_k = -\nabla \left( \frac{\nabla \alpha_k}{1 \mid \nabla \alpha_k} \right) \) is the surface curvature of \( k \)-th liquid. The total surface tension force in (3) is defined by \( F_s = \sum_k F_{s,k} \).

The continuity equation for the effective fluid is obtained by the summation of the continuity equations for the phases (2); after some transformations it is reduced to the velocity constraint

\[
\nabla U = -\sum_{k=1}^{K} \frac{\alpha_k}{\rho_k} \frac{D \rho_k}{Dt} + \Gamma \left( \frac{1}{\rho_v} - \frac{1}{\rho_w} \right)
\]

(6)

with the right-hand side containing two terms describing the phase compressibility effects and dilatation due to evaporation, respectively. Equations (2) are transformed to make them suitable for effective numerical solution for the phase volume fractions \( \alpha_k \):

\[
\frac{\partial \alpha_k}{\partial t} + (U \cdot \nabla) \alpha_k + \alpha_k (\nabla U) = -\frac{\alpha_k}{\rho_k} \frac{D \rho_k}{Dt} + \frac{\Gamma_k}{\rho_k}
\]

(7)

The liquid phases \((k=m,w)\) are considered as weakly compressible fluids, and for the vapor the ideal-gas law is applied.

In the previous work [10], the phase change rate \( \Gamma = \Gamma^+ - \Gamma^- \) was described by a simple model by Lee [12] widely used in simulations with phase change. However, its major drawback is an unknown constant which varies significantly between different authors. In this work, the evaporation rate is formulated in line with the ideas of work [13]; the evaporation rate \( \Gamma^+ \) is

\[
\Gamma^+ = \frac{3 \sqrt{2} \lambda_c}{5 \Delta x} \left\| \nabla \alpha_v \right\| \max(T - T_{sat}, 0)
\]

(8)

where \( \Delta x \) is the cell size, \( T_{sat} (P) \) is the saturation temperature at the local pressure (the condensation rate \( \Gamma^- \) is written in a similar way, with the rightmost factor changed for \( \max(T_{sat} - T, 0) \)).

Numerical simulations are carried in the framework of the open source CFD toolbox OpenFOAM-v1912 [14]. A new VOF solver taking into account both the phase compressibility and phase changes (unavailable in the standard distribution) is developed and implemented.

3. Geometry and parameters

We consider collapse of vapor film separating the hot melt and water, caused by the sudden surge of water pressure. Initially, the melt drop radius was \( R_m = 3.36 \) mm, the vapor film outer radius was \( R_v = 0.5 \) mm; and the rest of the space was filled with water. The computational domain was a cube with the side of length \( H = 7.32 \) mm, it covered 1/8 of the whole space, and the numerical grid contained \( 125 \times 125 \times 125 \) cells.

The left, front, and bottom boundaries were considered as symmetry planes. All other boundaries were open, with the boundary pressure varying in time as \( P_{bnd} = P_a + (P_0 - P_a) \exp(-t/t_0) \). Initially, the pressure in the melt drop and in the vapor film was set to \( P_a = 1 \) bar, whereas the pressure in water was set to a prescribed high value \( P_0 = 40 \) or 80 bars. This initial condition, together with the above-mentioned pressure boundary conditions, imitate arrival of a shock wave propagating in water, with the characteristic overpressure decay time \( t_0 \) which was varied in the simulations. The initial temperatures of the melt, water and vapor were \( T_m = 950 \) K, \( T_w = 323 \) K and \( T_v = 373 \) K (saturated vapor).
respectively. The water-vapor interface was perturbed by creating several spherical water bulges facing towards the melt droplet.

The droplet material was molten tin, a metal with a relatively low melting point, often used in experiments on fuel-coolant interaction (see e.g., [4, 5]). The present work is focused on the fluid dynamics of interaction; possible freezing of droplet and material-dependent phenomena were not considered. The properties of tin were taken from [15]: the melt density \( \rho_m = 6689 \text{ kg/m}^3 \), specific heat capacity \( c_m = 263 \text{ J/(kg K)} \), dynamic viscosity \( \eta_m = 0.9 \cdot 10^{-3} \text{ Pa s} \), conductivity \( \lambda_m = 38.4 \text{ W/m K} \), surface tension \( \sigma_m = 0.52 \text{ N/m} \), the corresponding water properties \( \rho_w = 1027 \text{ kg/m}^3 \), \( c_w = 4181 \text{ J/(kg K)} \), \( \eta_w = 0.3 \cdot 10^{-3} \text{ Pa s} \), \( \lambda_w = 0.65 \text{ W/m K} \), \( \sigma_w = 0.06 \text{ N/m} \), vapor properties \( c_{p,v} = 1800 \text{ J/(kg K)} \), \( \eta_v = 3.5 \cdot 10^{-5} \text{ Pa s} \), \( \lambda_v = 0.09 \text{ W/m K} \); the heat of evaporation \( \Delta h_v = 2.26 \text{ MJ/kg} \).

4. Results

To demonstrate the evolution of vapor film and melt droplet, simulations were carried out for the cases listed in table 1. The first four cases correspond to different intensity and pressure decay rate in the arriving shock; the fifth case was calculated at a constant high ambient pressure to see the effect of vapor expansion.

| Case | Initial pressure \( P_0 \), MPa | Time constant \( t_0 \), \( \mu s \) | Maximum pressure \( P_{\text{max}} \), MPa |
|------|------------------|------------------|------------------|
| C1   | 8                | 100              | 80.6             |
| C2   | 8                | 30               | 70.1             |
| C3   | 4                | 100              | 41.4             |
| C4   | 4                | 30               | 28.4             |
| C5   | 8                | \( \infty \)     | 163.1            |

In figure 1, the interaction of melt droplet with water is shown for the case C1, corresponding to the initial water pressure of 8 MPa and the pressure decay time of 100 \( \mu s \). The distributions of volume fractions are shown in the vertical plane of symmetry \( \gamma = 0 \) at five consecutive instants \( t = 10, 20, 50, 100, \) and 400 \( \mu s \), with white color denoting melt, red color corresponding to vapor, and blue color denoting water. Due to the high initial pressure drop, water is accelerated towards the melt droplet surface, causing rapid collapse of the vapor film by the time of 20 \( \mu s \); the first direct contact of melt and water naturally occurs at the points where the perturbed vapor film is the thinnest. In the contact zone, pressure surge caused by the water impact along with rapid evaporation is obtained; vapor expansion is clearly visible on the frames at times of 50–400 \( \mu s \). The growth of the vapor bubble is non-monotonic; it is featured by three oscillations of which the first one is a complete collapse, whereas the latter two are contraction and expansion of the vapor film.

The melt surface becomes significantly perturbed in the course of interaction. This is demonstrated in figure 2 where the shapes of melt surface (defined as the iso-surface of melt volume fraction \( \alpha_m = 0.2 \) ) are presented. The simulation shows the development of melt splashes, as well as fine fragmentation of melt with the formation of small dispersed fragments. The analysis shows that the positions of melt splashes correspond to the points of the first contact of water with melt; therefore, the splashes are similar to the known cumulative jets caused by the impact of water on the melt surface (see the recent experimental results [16]).

In figures 3 and 4, respective results are shown for the case C2 where faster pressure decay occurs (the time constant in the exponential decay law is 30 \( \mu s \)), promoting expansion of the vapor bubble. Qualitatively similar results were also obtained in the cases C3 and C4 for lower intensity of the triggering shock (4 vs 8 MPa). In the case C5 where the ambient pressure remained high, vapor bubble expansion was restricted, and the perturbations on the melt droplet surface were weaker.
Figure 1. Melt droplet interaction with water at times of 10, 20, 50, 100, and 400 µs (left to right), case C1.

Figure 2. Melt droplet surface at times 100 and 400 µs (left to right), case C1.

Figure 3. Melt droplet interaction with water at times of 10, 20, 50, 100, and 400 µs (left to right), case C2.

Figure 4. Melt droplet surface at times of 100 and 400 µs (left to right), case C2.

Figure 5. Maximum (solid lines) and minimum (dashed lines) pressures, vapour volume in cases C1–C4.
To compare the features of melt-water interactions, in figure 5a,b the maximum and minimum pressures obtained for cases C1–C4 are shown by the solid and dashed lines, respectively. The peak pressures obtained numerically are presented in the rightmost column in table 1. The calculated volumes of vapor are also plotted in figure 5c. It can be seen that for the slower pressure decay (cases C1, C3), the bubble oscillates 2–3 times in the course of interaction, while the faster pressure decay (cases C2 and C4) are featured by monotonous expansion of the vapor bubble after a single collapse.

Conclusions
The numerical simulations of single melt droplet interaction with water by VOF method indicate that the melt surface is disturbed significantly by water impact caused by the sudden ambient pressure rise. Melt splashing and fine fragmentation are observed in the numerical simulations. Collapse of the vapor film separating the two liquids causes direct impact of water on the melt surface, resulting in short-duration pressure pulse. The vapor bubble exhibits several oscillations during the interaction, provided that the ambient pressure decay rate is not too high; otherwise, the vapor expansion caused by the pressure drop overcomes the evaporation/condensation, resulting in monotonous growth of the vapor volume. Further research will address in more details the effect of pressure wave parameters (triggering), as well as propagation of pressure waves in the melt and possibility of cavitation as a mechanism for droplet explosion following the melt-water interaction.

The results obtained in this work are qualitatively consistent with the experimental observations [4–6] where it was shown by the superimposed optical and X-ray images that the vapor bubble around the melt droplet oscillates to or three times before droplet fragmentation occurs. Quantitative validation of VOF simulations will be performed in the future; it requires calculations in proper geometry and conditions corresponding to the experiments. Such studies will also allow the requirements to numerical grid resolution to be established.

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