A numerical analysis on molten droplet hydrodynamics in sodium pool

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Abstract. The risk and consequences of vapor explosion during severe accidents are among the most critical safety problems to be considered in next-generation sodium-cooled fast reactors. The melt of the core material (corium) may be produced in the event of inadequate core cooling and/or during Loss of Coolant Accident (LOCA) leading to Core Disruptive Accident (CDA). Corium displacement can then lead to powerful fuel-coolant interactions (FCIs). One of the consequences of this molten corium-coolant interaction is that vapor formation and hence explosion may occur. Due to the problem complexity, only hydrodynamic effects of the multiphase system of a single-droplet vapor explosion phenomenon, without heat transfer, is considered. The present study focuses on simulating a molten droplet pre-conditioning (deformation before breakup) through the early stages of the molten fuel coolant interaction. In order to efficiently capture the melt-sodium interfaces and predict droplet behavior with appropriate mass conservation, calculations were conducted using the CFD code of STAR CCM+ for several melt coolant two-phase system configurations. The results demonstrate that the melt properties and velocity are the dominant factors on the melt droplet pre-conditioning behavior.

1. Introduction

The risk to the environment in a severe accident has to be estimated in the framework of safety studies for the innovative cooled sodium fast reactors. During the core melt accident, a vapor explosion might occur as a consequence of a fast and strong heat transfer following the corium-coolant interaction [1]. The molten jet collapses into smaller droplets, forming a coarse mixture. The melt droplets in this state of metastable dispersion undergo film boiling in the coolant continue until the vapor film is destabilized in a localized area, and might collapse resulting in melt-coolant direct contact. The resulting heat transferred rapidly produces a vaporization explosion of both coolant and melt fine fragmentation in a quite short time that relief of the pressure is practically impossible. The build-up of high-pressure results in shock waves that places dynamic loads on the surrounding structures.

Numerous experimental studies were conducted to help understand and describe the vapor explosion phenomenon during the interaction of melt-sodium[2],[3]. In these experiments generally, no energetic incidents were observed, where the subcooling of sodium was of the order of several hundreds of kelvin. The absence of energetic events might mainly be due to the strong impact of solidification of the melt that prevents fine fragmentation. But some studies suggested that if the melt heats the sodium in the mixing zone near the saturation temperature, a vapor explosion could occur.
those conditions the existence of the film boiling regime, which is generally agreed as a necessary initial condition for a vapor explosion, was possible. In this case, it was argued in the spontaneous nucleation model that in a fuel-water environment, but not in a large-scale fuel-sodium system, a vapor explosion might occur (Because the instantaneous temperature of contact is less than sufficient to induce sodium homogeneous nucleation). Progressive models have predicted, however, that vapor explosions can occur under favorable hydrodynamic conditions in several fluid systems (including UO2-Na) [4]. For this purpose, the current research effort has centered on defining the fundamental parameters and mechanisms involved.

It is generally accepted that a large-scale vapor explosion would require many important steps, commonly known as “(1) coarse premixing, (2) triggering, (3) escalation, and (4) propagation”[5]. “The first stage in a vapor explosion is the coarse mixing of the hot liquid throughout the cold liquid. Coarse mixing refers to a mixture of relatively large particles of molten fuel as opposed to the tiny droplets later needed for the very rapid heat transfer required for a vapor explosion”[5]. While many studies have focused on various aspects of the molten droplet deformation hydrodynamics and steam/vapor explosion[6],[7],[8], none of them deal with melt-sodium system.

This research aims to support the understanding of the FCI process in the pre-mixing phase by investigating the deformation/pre-fragmentation of the melt droplet. The emphasis is on the simulation analysis of early stage pre-fragmentation of a single droplet impinging in a sodium pool. Due to the complications involved in simulating melt droplet deformation (such as phase change, intense heat transfer, and multiphase system step changes properties), simplifications and assumptions are inevitable.

To begin with, the current study is limited to melted droplet hydrodynamics in a sodium tank, without taking into account heat transfer or phase shifts throughout the interaction. Another assumption in this simulation is that melt and sodium are considered to be immiscible fluids. Since vapor formation and the subsequent explosion is considered (in the scope of this study) to be a result of an intense and fast increasing of droplet deformation/pre-fragmentation, and hence more surface is exposed to cooling. Therefore, the purpose of this study is to analyze the impact of different effective factors that determines the vapor explosion’s accompanied intensity and energetics during the premixing phase.

The study started with an investigation of the VOF method’s capabilities to simulate two immiscible fluids (water and diesel) hydrodynamics with rapid grade changes of physical properties across the liquids confluences. The objective is to ensure that, with sufficient mass conservation, the system can observe the boundaries and their development. Further calculations are performed following the basic qualification of the code to analyze the effect of several variables (such as droplet Weber number and physical properties of the material) on the molten droplet preconditioning before the vapor explosion.

2. Numerical Method

Various methods are used for interface tracking, such as the level set method, volume of fluid (VOF) method [9], and the simplified line interface calculation (SLIC) [10]. Other calculation methods for fluid interfaces are found in[11]. According to Rudman [12] volume tracking method is more accurate than the interface tracking scheme by Unverdi and Tryggvason [13] that is using the Lagrangian interface to represent density field on Eulerian mesh. Using the level set method [14], large liquid droplet behavior is simulated [15] in the water tank. However, it does not guarantee the conservation of mass in substantially distorted flows, as discussed in[12].

The VOF method is selected in the present study as it quite simple, precise, and accessible in the STAR CCM+ code. The VOF method is a numerical formula used to track non-immiscible fluid-fluid interfaces. The summation of volume fractions for all phases in each control volume is equal to unity. Particularly the volume of fraction unit value resembles a cell filled with fluid whereas the cell contained no fluid is designated by zero value. At least one interface has to be comprised in any cell with a volume fraction between zero and one. The continuity equation is solved for one or more
phases in order to monitor interfaces between phases. The STAR CCM+ code provides VOF method under multiphase flow; more details can be found in its user-guide (STAR CCM+13.04).

With sufficient meshing performed within STARCCM+, a rectangular field of 20 mm (x-axes) x 50 mm (y-axes) is considered. Atmospheric pressure at the upper and lower side is applied to the boundary. Field function is used to initialize the top of the boundary melt droplet (5 mm and 0 mm away). Field functions are used in STAR CCM+ code to visualize the computed fields, to specify boundary, and region values, or to define initial conditions. Based on assuming circular shaped droplet in 2D analysis, 0.003 m, 0.004 m, and 0.006 m are considered to be the droplet diameter. The Courant number (Co), \( (\Delta t*V_{fluid})/\Delta x \) is used to control time step calculation, where \( \Delta t \) denotes the time step, \( V_{fluid} \) stands for fluid velocity, and \( \Delta x \) is grid element size. For all the two-phase equations discussed in the paper, Co = 0.15 is used. In the continuity and momentum equation, the convergence parameters are held at 0.001.

As the interface instability defines the vapor explosion occurrence, a simple Rayleigh–Taylor instability phenomenon is examined first to determine the efficiency of the VOF methodology for interface monitoring. The interface behavior between two immiscible water and diesel liquids is modeled using a starting structure that positions the water (heavier) on top of the diesel (lighter).

The analysis was further implemented to droplet in sodium pool (two phase system). In this study vapor formation and hence explosion is considered to be a result of an intense and fast increase of droplet deformation/pre-fragmentation, and as a result more surface is exposed to cooling. The research therefore seeks to analyze the influencing factors during the pre-mixing stage which determine the intensity and energy of the vapor explosion. To achieve this analysis is carried by changing the initial Weber number, droplet size, and selecting various material properties for the droplet (density and surface tension); as shown in Table 1.

| Thermophysical and Physical Property | Stainless steel | Uranium | Na |
|-------------------------------------|-----------------|---------|----|
| Density (kg/m³)                     | 8920            | 7954    | 17797 | 17300 | 892 |
| Kinematic viscosity (mm²/s)         | ---             | 0.775   | ---   | 0.309 | 0.456 |
| Surface tension (mN/m)              | ---             | 1830    | ---   | 1550  | 182  |

3. Results and Discussions

3.1. Code validation approach

It is recognized that the Successful simulation of Rayleigh-Taylor instability is a standard for validating interface capturing codes. The instability between two immiscible fluids water and diesel in this analysis is simulated. Starting from induced sinusoidal interface disruption the water suspended above begins to penetrate down through the diesel driven by gravitational force. The volume fraction contour plots at various time intervals demonstrating the instability growth over time illustrated in Figure 1.
Due to gravitational force, the heavier would go down from the side. Hirts and Nichols [9] has found that the instability grows linearly in the initial phase and then later the effects of non-linear becomes more pronounced. The current outcomes that show non-linear development of the interfaces are in line with the literature on the behavior of global interfaces [18],[12] where the initial growth creates a spike that goes down near the sidewall and starts to roll up, gradually becoming more deformed. In this regard, there were several related studies performed to model Rayleigh-Taylor instability using the Boltzmann method[19],[20]. According to the above mentioned, the present approach can provide a realistic simulation of the interface pattern between two immiscible liquids.

3.2. droplet behavior in sodium pool

The two-phase arrangement of droplet and sodium was assumed in the analysis. In the simulation, the vapor resulting from film boiling is neglected as the analysis focuses on the key factors that trigger vapor explosion during the early phase of premixing. In the calculation, the droplet is initialized at a distance of 0.0035 m on top of the pool surface and subsequently falls. For simplicity, round shape droplet is considered. Fig.4. indicates the distortion in the stagnant sodium pool of a molten stainless steel droplet of diameter equal to 0.003 m with 2.5 m/s starting speed ($We = 9.139$). Launched at the very beginning as a circular form, the droplet develops a nearly ellipsoidal form and then transforms into a half-circle. The sustained distortion subsequently results in a sickle shape. Ma et al.[15], observed comparable pattern of deformation here, where it starts to release segments from its horizontal edges that imitate the sheet strip-ping breakup.
3.3. Effect of weber number
Steel droplets with various preliminary Weber numbers were selected in conjunction with the case of droplets falling in a sodium pool, as defined in Section 3.2 to measure the Weber number's impact on droplet distortion. The droplet to coolant density ratio, $\rho_d/\rho_c$ is 8.9. The Weber number ($We$) is a measure of a fluid's inertia relative to its surface tension, and can be formulated as follows:

$$We = \frac{\rho_d V^2 D_0}{\sigma_0}$$

(1)

Weber number is important for studying droplets and bubbles formation. Calculations are performed for various initial Weber numbers: 87, 244, 405, and 566. The comparison of the droplet aspect ratio against time is shown in Fig.3. The ratio of the droplet surface area to its original value is known as aspect ratio $A_s/A_{s,\text{init}}$ which is a factor that describes accurately deformation of the droplet and is determined using the STAR-CCM+ ‘isosurface’ function. It could be shown that, with the increase in Weber number, the aspect ratio, as well as the distortion, increases dramatically in a given time frame. This demonstrates that hydrodynamic distortion is more noticeable at higher droplet velocity as well as lower surface tension.

![Figure 3. Illustration of the droplet's aspect ratio versus time at different Weber numbers.](image)

3.4. Effect of droplet density
Two droplets with different densities were selected and analyzed to investigate the material density effect on droplet deformation: stainless steel ($\rho_d = 7954$ kg/m³) and uranium ($\rho_d = 17300$ kg/m³). Choosing two materials with a significant difference in density (the density of uranium is more than twice that of steel) helps to clearly illustrate the density effect over the required preconditioning time. In both cases, an equivalent value of initial $We = 40$ is considered. It can be observed that the rate of deformation is higher in the droplet of higher density and especially that the distortion is 9% higher at the end of 6 ms, even though it showed earlier that the less dense droplet underwent slightly higher deformation rate. It could therefore be established that the denser droplet is subjected to greater deformation and the coolant is therefore exposed to a comparably larger surface.
3.5. Size effect on droplet behavior

Because of the reliance of aerodynamic forces on their size, it has been recognized that smaller droplets gains and loses speed faster than bigger droplets[21]. It is important to consider the droplet size impact in the coolant at which density ratio of droplet to coolant may be about 8 to 20 (the density ratio of uranium to sodium is around 20). Another important quantity necessary to be determined in this analysis is the terminal velocity of droplets falling in the field of gravity, which for gaseous or liquid mediums given as:

$$V_t = \left( \frac{4gD}{3C_d} \right) \left( \frac{\rho_d - \rho_c}{\rho_c} \right)^{\frac{1}{2}}$$  

Where $g$ denotes gravitational acceleration, $D$ stands for the diameter of the droplet, $C_d$ Implies the drag coefficient, $\rho_d$ indicates the droplet density and $\rho_c$ represents the coolant density. The drag coefficient for a solid sphere is about 0.4 in a turbulent regime.

With their terminal velocity, two separate droplets of different sizes, 0.004 m and 0.006 m, were Introduced $V_f(0.004 \text{ m}) = 0.938 \text{ m/s}$ and $V_f(0.006 \text{ m}) = 1.149 \text{ m/s}$, calculated by implying the same coefficient of drag as the solid sphere ($C_d = 0.47$). The relative velocity ($V_r$) that works on the droplet may be expressed as,

$$V_r = V_f - V_t$$

It is assumed in Eq.2. that both droplets were forced to fall at same velocity ($V_f$) that is higher than terminal velocity ($V_t$). Therefore, the 0.004 m relative velocity is,

$$V_r = V_f - 0.938$$

For 0.006 m droplet, it will be,

$$V_r = V_f - 1.149$$

Equations (3) and (4) shows that, regarding the 0.004 m droplets, the relative velocity between droplet-coolants is greater. To explain the above statement, calculations are performed where both droplet sizes were given initial velocity of 4 m/s. The deformation pattern of both droplets is shown in Figure 4. Aspect ratio versus time for different droplet densities.

![Figure 4. Aspect ratio versus time for different droplet densities.](image-url)
Fig. 5, suggesting that the deformation rate is higher in 0.004 m droplet comparing to 0.006 m droplet and a more visible effect observed after 4 ms. If droplets of different sizes are subjected to an equivalent force, droplets of small sizes are observed to deform at a higher rate.

Figure 5. Comparison of distortion rate versus time; for different size droplets falling at 4 m/s.

4. **Summary and Conclusions**

The paper describes the findings of an attempt to model the preconditioning (deformation before breakup) of a molten droplet in a sodium pool before vapor explosion using the VOF method in the STAR CCM+ code.

The ability of the VOF approach to predict a two-phase flow problem was verified by obtaining results consistent with previous research literature through the successful simulation of the Rayleigh-Taylor instability interface behavior between immiscible fluids.

It is found that with the increase in Weber number, the aspect ratio, as well as the distortion, increased dramatically. Thus the hydrodynamic deformation is more pronounced in the droplet of higher velocity and lower surface tension.

The effects of melt density on the rate of deformation have been examined as well showing that the denser droplet is subjected to greater deformation and larger surface therefore comparably exposed to coolant.

The analysis of droplet size demonstrates that when droplets of different sizes were subjected to an equivalent force, droplets of small sizes underwent larger deformation.

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