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Numerical analysis on molten droplet hydrodynamic deformation and surface waves under high pressure pulse

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ABSTRACT

A multi-phase hydrodynamic code using volume of fluid method (VOF) is used to simulate the molten droplet deformation, and the surface waves at the stages of pressure propagation and expansion in steam explosion (SE). Both melt-liquid system and melt-gas system are simulated using the code. A benchmark case of Joseph et al.'s experimental data (1999) is performed to validate the code. In this paper, effects of vapor film and surface tension on the droplet behavior under high pressure pulse are investigated. In addition, effects of material density and pressure pulse magnitude on the droplet deformation, and the growth of surface waves are also analyzed. Results of simulation analysis suggested that vapor film can be neglected and the effect of surface tension is not significant for hydrodynamic process under high pressure pulse. Results of simulation also demonstrate that material density and pressure pulse play a significant role in the process of droplet deformation and surface wave growth. The research shows that the effect of hydrodynamic deformation is significant for droplet fragmentation, and droplet penetration can more likely be achieved by surface wave instability at the stages of propagation and expansion in steam explosion.

1. Introduction

In a postulated severe accident in nuclear power plant (NPP), high temperature molten fuel may fall into the containment cavity after the reactor vessel failure. During the process of fuel–coolant interaction (FCI), steam explosion, which may be triggered due to rapid heat transfer between high temperature molten metal and cold coolant, induces high pressure wave and causes potential system damage.

FCI process is commonly divided into four stages: coarse mixture, trigging, propagation and expansion. At the first stage, the continuous molten fuel falls into the cavity water and disperses into droplets, which is covered by vapor films as a result of liquid evaporation. Once the film collapses due to the instability or the external pressure pulse during triggering stage, the coolant water could be directly in contact with the molten droplets, which will result in sudden evaporation of water and cause droplet fragmentation. This progress is defined as thermal fragmentation (Ciccarelli and Frost, 1994; Kim and Corradini, 1998) which involves an increase in heat and mass transfer and further pressure wave propagation. At the propagation stage, more liquid fuel droplets will further fragment and cause more heat and mass transfer, and pressure pulsation. The process can be treated as hydrodynamic fragmentation which involves acceleration-induced droplets breakup. The last stage, the expansion stage, destructive pressure peaks could exceed 100 MPa (Leskovar and Uršič, 2009) and post a severe challenge to containment integrity.

According to experimental investigations (Liu and Reitz, 1997; Lee and Reitz, 2000), the hydrodynamic force and surface tension force are critical factors in the process of droplet breakup. Weber number $We = \frac{\rho U^2 d}{\sigma}$, is widely used to characterize effect of hydrodynamic force and surface tension force. Based on initial Weber number, the patterns of deforming and fragmenting particles can be classified in groups called fragmentation modes. Pilch and Erdman (1987) summarized five modes using experimental data of droplet breakup in liquid–gas system: (1) vibrational breakup regime; (2) bag breakup regime; (3) bag-and-stamen breakup regime; (4) sheet stripping regime where a thin sheet is continuously stripped from the surface of a deforming droplet; (5) and catastrophic breakup regime. Using a rotating drum camera, Joseph et al. (1999) conducted a photographic experiment on viscous droplets breakup under the high speed airstream in a shock tube. In Joseph's study, mode 2 and 3 were observed at the very high Weber numbers which should belong to mode 5 region. Hansson et al. (2009) studied micro-interactions of a single droplet during

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Nomenclature

a	acceleration (m/s^2)
Bo	Bond number
C	fractional volume
d	diameter/deformation displacement (m)
L	wave amplitude (m)
$\vec{n}$	unit normal vector
n	fastest growth for Rayleigh–Taylor instability
p	pressure (MPa)
R	radius (m)
t, T	time (s)
u, v, V	velocity (m/s)
We	Weber number

Greek symbols

δ	Dirac distribution
κ	curvature
ρ	density (kg/m^3)
σ	surface tension (N/m)
λ	wave length (m)
μ	dynamic viscosity (Pa s)

Subscripts

0	initial
d	molten droplet
c	coolant
i	phase index

triggering phase in steam explosion and found that the molten droplet experiences interfacial instabilities and deformation before fragmentation. Hansson reports that the molten droplet's initial deformation/pre-fragmentation helps coolant to penetrate liquid film. This phenomena is named "preconditioning" mechanism.

Numerical analyses of droplet breakup were also carried out by numerous researchers. Han and Tryggvason (2001) performed numerical studies on deformation of small density liquid droplet, and found absence of backward-facing bag mode is absent. Han and Tryggvason also reported that Reynolds number affects the value of critical Weber number at transition of different breakup modes, and droplet deformation rate decreases with the increase of droplet viscosity. Duan et al. (2003) studied time-dependent characteristic behavior and mechanisms of droplet breakup near critical Weber number using moving-particle semi-implicit (MPS) method (Koshizuka and Oka, 1996). The critical Weber number was proposed to be 13 for uranium dioxide droplets in water. Thakre et al. (2013) reported a triggering pressure less than 5 MPa in a numerical study of molten droplet deformation using CFD code FLUENT. Results of separate-effect study quantitatively demonstrated the importance of droplet velocity and melt properties on the melt droplet preconditioning. However, in Thakre's study, the surface wave was not discussed, and the triggering pressure pulse is not as high as what have been observed in experiments reported by other literatures. Zhong et al. (2014) analyzed the droplet deformation and disintegration under sudden accelerations. Their study, with main focus on the droplet breakup process and breakup time, illustrates a triggering pressure pulse of approximately 100 MPa, which satisfies the condition of pressure propagation or expansion stages. Their findings also indicate that an increase of pressure pulse intensity will accelerate the completion of breakup process and the dimensionless breakup time is nearly independent of Bond number (Bo).

It is widely accepted that hydrodynamic fragmentation of molten droplets under high pressure pulse is an important phenomenon in steam explosion. However, due to various difficulties in steam explosion experiments with high pressure shock wave, availability of a detailed observation with accurate surface wave tracing is truly limited. In this study, a multi-phase hydrodynamic code is used to simulate the behavior of molten droplet deformation and surface waving under high pressure pulse (100 MPa, 150 MPa). The volume of fluid (VOF) method based on piecewise linear interface construction (PLIC) is utilized to track melt-liquid/gas interface. Molten droplet evolutions in both melt-liquid and melt-gas system are modeled in the simulation. In addition, effects of vapor film and surface tension on the droplet behavior are investigated. And, in the end, effects of material density and pressure pulse magnitude on droplet deformation and wave development are reported.

2. Physical model and numerical methods

During the process of hydrodynamic fragmentation of molten droplets under high pressure pulse, the effect of hydrodynamics is predominant. Therefore, this study mainly focuses on the hydrodynamic behavior of the molten droplet, and heat transfer and the phase change are not modeled in simulation. Duan et al. (2003), Thakre et al. (2013) and Nomura et al. (2001) suggest that use of isothermal condition is valid in the simulation of hydrodynamic fragmentation of molten droplets because of very short time scale of the process. Yuan et al. (2008) developed a multi-phase hydrodynamic code to simulate the behavior of molten droplet during FCI, and it is also used in this paper. Physical model and numerical methods used in this code is discussed in detail in Yuan et al. (2008). Thus, only a brief introduction of governing equations is presented in the following.

Mass and momentum equations used in this study are presented:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\rho \vec{u}\vec{u}) = \nabla \cdot \mu(\nabla \vec{u}) - \nabla p + \rho g + \sigma \kappa \delta_s \vec{n} \tag{2}$$

The surface tension term $\sigma\kappa\delta_s\vec{n}$ in momentum equation is calculated in by continuum surface force (CSF) model (Brackbill et al., 1992), which was also used in the simulation Thakre et al. (2013) and Zhong (2014). The transport equation of volume fraction C_i of each phase is expressed as

$$\frac{\partial C_i}{\partial t} + \nabla(C_i \vec{u}) = 0 \tag{3}$$

The properties in the cell are obtained by:

$$\rho = \sum C_i \rho_i \tag{4}$$

$$\mu = \sum C_i \mu_i \tag{5}$$

Finite volume method is used to discretize the governing equations and pressure–velocity linkage is resolved with the SIMPLE algorithm. In order to obtain the distribution of fluid volume fraction C, Eq. (3) is solved by VOF method. In this study, the Youngs VOF