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Numerical simulation of molten droplet deformation and disintegration under sudden accelerations

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ABSTRACT

The molten droplet fragmentation dominated by hydrodynamic mechanisms is the key process at the stage of pressure propagation in the process of the fuel–coolant interaction (FCI) which may occur during the course of a severe accident in a light water reactor (LWR). However, due to complication of the process, hydrodynamic fragmentation cannot be described by a particular mechanism, and there is no sufficient experimental studies under high pressure shock condition for this kind of fragmentation evaluation. In this paper, a multi-phase thermal hydraulic code with the Volume of Fluid Method (VOF) is developed, Continuum surface force (CSF) model is employed to compute the surface tension. The breakup process of a molten droplet under sudden accelerations is numerically analyzed to investigate the mechanism of fragmentation in vapor explosion. The results show that the breakup process experiences two stages: deformation and disintegration, which agrees with the simulation by Duan et al. (2003) using Moving Particle Semi-implicit (MPS) method. It is found that an increase in intensity of pressure pulse will accelerate the completion of breakup process and the dimensionless breakup time from the simulation is not strongly affected by Bond number (*Bo*). The simulation results suggest that the deformation imposed by the external hydrodynamic pressure distribution should be the dominant factor in breakup process for molten droplets in liquid–liquid system simulated in this paper.

1. Introduction

Fuel–Coolant Interaction (FCI) is a phenomenon that could potentially occur during a severe accident of a nuclear power plant (NPP) and may threaten the integrity of pressure vessel or containment vessel. It can take place following melting of the reactor fuel and its relocation in the bottom of the reactor vessel. Once vessel fails, molten fuel could fall into the water pool and the rapid heat transfer from the high temperature molten metal to the cold coolant with phase transition of the coolant may induce a vapor explosion which may lead to an over-pressurization.

For FCI problem, the process is generally divided into two stages: coarse mixture and pressure propagation. For the first stage, the molten melt falls into the cold liquid and then the hydrodynamic instabilities break up the molten jet and disperse it into the coolant (on the scale of 1 cm in the case of molten corium and water). After that, film boiling occurs around the molten droplets and under external pressure pulse, the vapor film can collapse, which allows the direct contact of molten metal with coolant and further causes the fragmentation of molten metal droplets. This process is defined as thermal fragmentation which leads to an increasing of the heat transfer area which evaporates the ambient liquid in a short time and generates high pressure pulse. For the stage of pressure propagation, during which the pressure peak always exceed 100 MPa (Matjaz and Mitja, 2009), it is assumed that the melt (on the scale of 0.5 mm in the case of molten corium and water) fractured during the first stage would subsequently experience a secondary breakup into even smaller droplets. This situation can be treated as impulsively acceleration-induced breakup of droplets, which corresponds to experiments where a single droplet is accelerated by a shockwave causing a step change in the velocity of the droplet relative to the ambient fluid. The fine fragmentation produces the new fuel–coolant area and then enhances the rates of heat transfer, evaporation, or chemical reaction. In this paper, the breakup behavior and mechanism during the second stage is concerned.

The sequences of pattern of deforming and fragmenting particles can be classified in groups called fragmentation modes. Experimental data of liquid–gas system were investigated by Pilch and Erdman (1987). Five types of breakup modes were demonstrated:

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Nomenclature

a	acceleration
Bo	Bond number
ζ	fractional volume
C	smoothed phase field
C_d	drag coefficient
i	diameter/deformation displacement
$\vec{n}$	unit normal vector
n	fastest growth for Rayleigh–Taylor instability
p	pressure
R	radius
t	time
t^*	dimensionless breakup time
u	velocity
U	initial velocity
We	Weber number

Greek symbols

δ	Dirac distribution
κ	curvature
ρ	density
σ	surface tension

Subscripts

0	Initial
b	breakup
cr	critical value
d	molten droplet
de	deformation
e	equator place
i	phase index
l	liquid
max	maximum
r	relative
R–T	Rayleigh–Taylor instability
s	stagnant place

Table 1
Initial parameters of calculation.

Case	d (mm)	p (MPa)	U (m/s)	We	Bo
1	5	80	53.33	14,200	6,650
2	5	100	66.67	22,200	10,400
3	5	150	100	50,000	23,400

(1) vibrational breakup regime where a parent droplet breaks up into two or more large fragments; (2) bag breakup regime where a parent droplet deforms into a more massive toroidal rim attached with a thin bag-shaped film that breaks up into finer droplets, followed by disintegration of the rim into larger droplets; (3) bag-and-stamen breakup regime where a thin bag is blown downstream while being anchored to a massive toroidal rim. A column of liquid-stamen is formed along the droplet axis parallel to the approaching flow. The bag bursts first, rim and stamen follow; (4) sheet stripping regime where a thin sheet is continuously stripped from the surface of a deforming droplet; (5) and catastrophic breakup regime where a droplet fragments due to violent surface waves. The breakup of viscous and viscoelastic droplets in the high speed airstream behind a shock wave in a shock tube was photographed with a rotating drum camera by Joseph et al. (1999), Bag and bag-and-stamen breakup were observed at very high Weber numbers, in the regime of breakup previously called catastrophic. Numerical analyses of droplet breakup were also carried out. Han and Tryggvason (2001) simulated the deformation of a liquid droplet. A small density ratio was chosen. Duan et al. (2003) studied time-dependent characteristic behavior and mechanisms of droplet breakup at around the critical Weber number using MPS method (Koshizuka and Oka, 1996) and predicted the value of the critical Weber number of 13.

It is widely known from experimental investigations (Liu and Reitz, 1997; Lee and Reitz, 2000) that Weber number has dominant effect on the behaviors of droplet breakup while the Reynolds number has little effect on breakup in all breakup regimes. The Weber number is defined as $We = \frac{\rho U^2 d}{\sigma}$, representing the ratio of pressure drag to interfacial tension force. Our study focuses on the dynamic behaviors of droplet breakup under high pressure shock wave, which is the situation for the stage of propagation process of FCI problem.

In the present study, a multi-phase thermal hydraulic code is developed and applied to simulation of the molten droplet breakup behavior under sudden accelerations for high Weber number. The VOF method based on piecewise linear interface construction (PLIC) is used to track liquid–liquid interface in the code. CSF model is employed to compute the surface tension. Surface waving, melt droplet deformation and final breakup in the fragmentation process are simulated to investigate the mechanism. The dimensionless breakup time is also examined.

2. Physical model

Liquid coolant and liquid metal droplets are considered in the calculation. For each fluid, governing equations are presented:

Mass equation:

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

Momentum equation:

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

C_i represents the fluid volume fraction of each phase which determines the fluid distribution. The transportation equation of C_i is defined as

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

The properties in the cell are determined as below

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

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

3. Numerical method

Finite volume method is used to discretize the governing equations and pressure-velocity linkage is resolved with the SIMPLE algorithm. In space discretization, the second-order central differencing scheme is used for diffusion terms and the MUSCL scheme is used for convection terms. A first order backward implicit approach is employed for the time derivative.