CFD Simulation of Liquid-Liquid Jet Breakup: Kelvin-Helmholtz Instability

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1. Introduction

In reactor severe accidents, the contact of molten fuel and coolant in-vessel or ex-vessel may bring an energetic steam explosion. To estimate the potential magnitude of steam explosion impulse loading to the surrounding structures, many analytical codes have been developed worldwide. The code simulations showed that the corium melt jet breakup is one of the important physics that strongly influence the steam explosion intensity.

As for the jet breakup mechanism, it is generally acknowledged that the jet leading edge breaks up by the boundary layer stripping (BLS) and the jet lateral surface breaks up by the Kelvin-Helmholtz instability (KHI). The BLS mechanism has been successfully simulated by a CFD model with finer mesh size (~0.2 mm) enough to resolve the drop size [1]. Meanwhile, the KHI mechanism has been conceptually studied with the interfacial instability theory and has provided a formulation for the fastest growing wavelength of Eq. (1).

$$\lambda_D = \frac{3\pi(\rho_1 + \rho_2)\sigma}{\rho_1 \rho_2 (V_1 - V_2)^2} \tag{1}$$

When the fluids of melt, liquid and vapor are involved, it becomes more difficult to get the analytical solution for KHI [2]. In this study, computational fluid dynamics simulation of melt jet breakup by the KHI mechanism has been attempted using the ANSYS Fluent code.

2. Mathematical Model

To track the interface between the melt and coolant during the jet breakup process, the Volume of Fluid (VOF) model was selected in Fluent code. The VOF model solves only one momentum equation and the volume fraction of each phase is computed. The cell properties are calculated as volume-weighted. The governing equations are:

- Continuity equation $\frac{1}{\rho_q} \left[\frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \bullet (\alpha_q \rho_q \overrightarrow{v_q}) = S_{\alpha_q} + \sum_{p=1}^n (\dot{m}_{pq} - \dot{m}_{qp}) \right] (2)$ - Momentum equation

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \bullet (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \bullet [\mu (\nabla \vec{v} + \nabla \vec{v}^{T})]
+ \rho \vec{g} + \vec{F}$$
(3)

$$\frac{\partial}{\partial t}(\rho E) + \nabla \bullet (\vec{v}(\rho E + p)) = \nabla \bullet (k_{eff} \nabla T) + S_h$$
(4)

Details of the mathematical models can be obtained in the Fluent theory guide [3].

To correctly track the interface of melt and coolant, the computational mesh size must be small enough to resolve the growing waves. The preliminary purpose of this study is to compare the fastest growing wavelength between the instability theory and the CFD simulation, thus calculations were done for two-dimensional domain.

3. Result and Discussion

3.1 Simulation of inclined interface under gravity

To make a relative motion of two fluids, which are initial at rest, in the direction of interface, a box containing two fluids of heavier fluid in the lower layer and lighter fluid in the upper layer is suddenly tilted at 8° [4]. Two sets of fluid pair were tested: water/salt water and water/Woods metal. The density of water, salt water, and Woods metal is 998, 1075, and 9330. Fig. 1 shows two-dimensional computational domain and mesh. The mesh size was 1.0 mm in both x and y directions.

The transient behavior of water/salt water interface is shown in Fig. 2. It is observed that at about 0.3 second the wave crests already rolled over to breakup from the



Fig. 2 Water and salt water ($\Delta V = \sim 0.3 \text{ m/s}$)

interface. The relative velocity (ΔV) and the dominant wavelength of the interface were calculated at selected time and compared with estimate of Eq. (1) as shown in Table 1. It is interesting to note that the relative velocity increased as time elapsed, thus the predicted λ_D decreases. But the CFD simulation showed larger wavelength as time elapsed. This is perhaps because the wavelength observed later time was the one that originated from the earlier time when the wave began to grow. This must be checked with the results of various different conditions.

Table 1. Comparison of λ_D in water/salt water [mm]



The simulation results of water/Woods metal interface are shown in Fig. 3. In this case, the interfacial instability seemed weak compared to water/salt water case. Also, the wavelength of simulation was much longer than the theoretical fastest growing wavelength: 90 mm vs. 1.3 mm of Eq. (1).

3.2 Simulation of vertical jet

The KHI on the surface of falling vertical jet of Woods metal in water was simulated in 2D domain as shown in Fig. 4. The initial velocity was set at 2.0 m/s for Woods metal layer and 1.0 m/s for water layer and the velocity at the inlet boundary was set at the same value as the initial velocity so that the relative velocity was maintained at 1.0 m/s from the beginning. The transient interface behavior is shown in Fig. 4. The wavelength measured in the simulation result was 53 mm, but the predicted λ_D by Eq. (1) was 5.2 mm, which is ten times smaller than that of CFD simulation.

The big difference between the theoretical wavelength and CFD result called for an investigation of mesh size effect. The mesh size was reduced from 1.0 mm to 0.1 mm, 0.25 mm, and 0.50 mm. When the mesh size was smaller, the wave became visible at earlier time at which



Fig. 4. Computational domain and vertical 2D jet of Woods metal in water ($\Delta V=1 \text{ m/s}$)

no wave was visible in case the mesh size was 1.0 mm.

To systematically analyze the dominant wavelengths at earlier time when the wave height was too small to identify, the volume fraction variation in the proximity of the interface was transformed into wave numbers per unit length using the Fast Fourier Transform technique. Fig. 5 shows the variations of Woods metal volume fraction near the interface at 0.01 s in case of 0.1 mm mesh size and the FFT result is shown in fig. 6. Since the data for FFT in this case is volume fraction versus distance along the interface, the resulting frequency from FFT corresponds to the number of waves per unit length. Thus wavelength is the reciprocal of frequency.



Fig. 5. Woods metal volume fraction at 0.01 s ($\Delta x=0.1$ mm)



Fig. 6. FFT result of data in Fig. (5)

As seen in Fig. 6, the FFT result does not show a unique frequency, but at least the dominant frequency of peak magnitude can be identified. The peak frequency in Fig. 6 is ~220, thus the corresponding wavelength is $1/220 \sim 4.5$ mm. This value seems close to the theoretical estimate of 5.2 mm by Eq. (1).

The dominant wavelength and wave height at different times and different mesh sizes are shown in Fig. 7. As the mesh size becomes smaller, smaller wave is identified at earlier time. The wave growth looks similar between the mesh size of 0.1 and 0.25 mm, and both show the steepest wave growth at 0.075 s. At this time, the wavelength is 10 to 13 mm and it is about 2 to 2.5 times bigger than the theoretical value of λ_D . It is found that for this case the mesh size must be smaller than 0.25 mm, which is about one twentieth of the theoretical λ_D .



Fig. 7. Wavelength and wave height growth

For the relative velocity of 4 m/s where the initial velocity was set at 5.0 m/s for Woods metal layer and 1.0 m/s for water layer, the interface at t=0.09 s is shown in Fig. 8. In this case, the wavelength measured in the simulation result was 55 mm, but the predicted λ_D was 0.33 mm, two order of difference. The mesh size of this calculation was 1.0 mm, but because the theoretical wavelength is 0.33 mm in this case, calculation must be done with much smaller mesh, for example, 0.01 mm. This requires much bigger computing capability, thus it will be done in the future.



Fig. 8. Woods metal and water for $\Delta V=4$ m/s

The computational results of KHI show that the theoretical fastest growing wavelength can be seen at very early time of wave growth, and then the wave becomes bigger gradually. This implies that the relation of breakup size in KHI to the theoretical fastest growing wavelength is not supported by this observation. It is to say that the small waves at the beginning become larger as they grow.

4. Conclusion

Computational fluid dynamics simulation of melt jet breakup using ANSYS Fluent code has been performed. The Kelvin-Helmholtz instability at the jet lateral surface has been simulated with the VOF multiphase model. While the CFD modeling of interface with relative velocity shows interface distortion as well as unstable growth of interface, the relation of breakup size in KHI to the theoretical fastest growing wavelength may not be supported by the present observation. The small waves at the beginning become larger as they grow. The effect of mesh size on the resolution of KHI will be further studied in the future.

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