On the fragmentation and phase-change heat transfer during melt-jet breakup

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Abstract

During such a severe accident of nuclear power plants, the reactor core is expected to be damaged. Even if the event is non-energetic, a considerable amount of the fuel may melt in the core region. Heat removal from the melt material must be part of the safety assessment. If cooling performance can be evaluated based on an appropriate physical model, it will greatly contribute to the safety evaluation of the nuclear reactor. The objective of this dissertation is to elucidate fragmentation mechanism and establish melt-coolability assessment methodology. Breakup of jets in liquid-liquid systems and phase-change heat transfer were experimentally and numerically studied to better understand the fundamental processes between melt jet and coolant.

First, a detailed experimental study to understand the jet fragmentation is presented. The study mainly focuses on hydrodynamic interaction of jet breakup. The experiments were carried out in an immiscible liquid-liquid system. The indices of refraction in the two liquids were matched, so that the vertical plane of jet flow was clearly visualized using laser-induced fluorescence (LIF). The jet breakup length obtained by image processing is compared with the existing correlations. Then, the breakup regimes were organized on a dimensionless operating diagram, with the derived correlations representing the criteria for regime boundaries of a liquid-liquid system based on the observation and analysis results. The experimental data were extrapolated to the expected reactor conditions.

In order to investigate parameter ranges that can not be observed by experiments, we proposed a numerical method and conducted numerical simulations. A three-dimensional color-fluid lattice Boltzmann model for immiscible two-phase flows was developed in the framework of a three-dimensional 27-velocity (D3Q27) lattice. This model was applied to liquid-jet-breakup simulations. The reproducibility of the regime map for liquid-liquid systems was confirmed.

Then, we further improved the numerical method to investigate the hydrodynamic jet flow in the reactor-equivalent condition. This successfully combined a three-dimensional nonorthogonal central-moment-based lattice Boltzmann scheme with the color-gradient lattice Boltzmann model. Hydrodynamic melt-jet breakup simulations showed that the proposed model is significantly more stable, even for flow with extremely high Reynolds numbers, up to $O(10^6)$. This enabled us to investigate the phenomena expected under actual reactor conditions.

Heat transfer from particles generated from molten jet to coolant was numerically investigated. The problem was set as forced convection boiling around the cylinder to simplify the actual situation. We used the phase-change lattice Boltzmann method with some improvements on the numerical stability. A series of pool boiling process, such as nucleation, growth, coalescence, and departure of vapor bubbles were successfully simulated. The simulation results were compared with existing film boiling heat transfer correlations.

Appropriate physical models for melt-jet breakup in coolant were identified by integrating the experimental and numerical simulation results. The correlations required for the melt-coolability assessment were determined, which are supported by the experimental or numerical evidences. The sensitivy analysis showed the coolability performance of the melt jet in coolant under various conditions.

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Chapter 1

Introduction

1.1 Background

Especially since the Industrial Revolution, power and energy have made a great contribution to the development of humankind. Among various energy sources, nuclear energy is one of the important sources invented by humankind, which has brought great benefits to humanity so far. It is undeniable fact that a large number of technological developments have been made to keep nuclear energy oparetable and safe. It goes without saying that a great deal of scientific knowledge has been accumulated in many kind of academic and industrial fields in the process. On the other hand, it is also the science's discipline that the negative side is attached to the back of the benefit. In this regard, we have experienced three severe accidents (*i.e.*, accompanied by core melting) of the nuclear power plants (NPPs) in the past: the Three Mile Island accident in 1979, the Chernobyl accident in 1986, and the Fukushima Dai-ichi accident in 2011 [1].

Most of the current nuclear reactors are nuclear reactors of the type called light water reactors (LWRs), that use light water as a coolant. Fuel burned in the nuclear reactor (spent fuel) includes uranium remaining without burning, newly formed plutonium, and radionuclides with a long half-life (minor actinide). Recovering and reusing useful substances from spent fuel is also an important issue in that the uranium itself is a depleting resource. In addition, it can be said that some solution is also required to treat with minor actinides in spent fuel.

Figure 1.1: Schematic of melt-coolability assessment model.

That is what is expected of the fast reactor. In general, nuclear reactors that cause the next reaction without decelerating neutrons born by fission while maintaining fast neutrons are called fast reactors. In the fast reactor, improvement of utilization efficiency of uranium resources by conversion of uranium 238 to plutonium 239 and reduction of radioactive waste by splitting minor actinides are expected. Sodium-cold fast reactors (SFRs), which are positioned as fourth-generation (Gen IV) nuclear reactors, is a type of fast reactor.

During such a severe accident of NPPs, the reactor core is expected to be damaged. In that case, nuclear reactors are desirable to shut down passively and non-energetically. Even if the event is non-energetic, a considerable amount of the fuel may melt in the core region. Phenomena which would be expected between the melt fuel and coolant are sometimes called fuel-coolent interactions (FCIs). This core material is required to be held in the reactor vessel for a long time after it has solidified and cooled sufficiently. In other words, heat removal from the melt material must be part of the safety assessment. If cooling performance can be evaluated based on an appropriate physical model, as in Fig. 1.1, it will greatly contribute to the safety evaluation of the nuclear reactor.

One possible scenario includes that the melt material flows into the coolant as “melt jets”. For that scenario, it is particularly important to deeply understand the behavior known as melt-jet

breakup in the coolant. To date, there have been many experimental efforts under various conditions that have been aimed at clarifying the melt-coolant interaction, including UO_2 into sodium [2,3], molten oxide into sodium [3–5], molten metal into sodium [3,4,6,7], corium into water [8–11], molten oxide into water [12–17], and molten metal into water [18–29]. The aim of all these experiments and tests was not limited to understanding phenomena in an SFR; a severe accident in a LWR was also included as a possible scenario. Iwasawa and Abe [30] provided comprehensive reviews of experimental works on the FCI phenomenon, especially, fragmentation of a melt jet during a severe accident. In addition to the experimental works, numerical efforts have also been made to deepen the understandings of FCI phenomena (*e.g.*, for LWRs [31] and for SFRs [32]).

Now let use review the experimental work conducted for SFR safety. In the context of FARO/TERMOS, Magallon et al. [2] performed two experiments that involved pouring 100 kg-scale molten UO_2 into sodium. These experiments are often referenced as T1 and T2. Part of the debris was collected to analyze the size distribution of particles that settled in the test section. The evaluated particle sizes were in the range of 10^1–10^3 μm. The penetration distance of the melt was estimated to be as much 1 m, whereas the released diameters were 50 mm (T1) and 80 mm (T2). Suzuki et al. [33] pointed out that the distance was much smaller than that predicted by the Saito correlation [34] (see Fig. 22 in Ref. [33]). Matsuba et al. carried out experiments involving molten aluminum (Al) into sodium [6] and molten alumina (Al_2O_3) into sodium [5]. Although the debris that settled onto the bottom of the test section could be collected after the experiments, it was difficult to visualize and observe the jet breakup process in detail.

During the interactions between melt jet and coolant, thermal interactions (e.g., surface freezing or coolant-vaporization) and hydrodynamic interactions (e.g., interfacial instability between two fluids, such as Kelvin–Helmholtz and/or Rayleigh–Taylor instabilities, and liquid entrainment or stripping from the interface) are considered to occur simultaneously. Hence, a number of experimental studies have focused on the hydrodynamic interactions by using various test fluids in immiscible liquid-liquid systems [23, 35]. Separate investigations of these thermal and hydrodynamic interactions would help to further understand the fundamental processes of

Figure 1.2: Expected fundamental process of melt-jet breakup process.

melt-jet breakup and its coolability. If one can appropriately separate the complex phenomena into individual phenomena, as in Fig. 1.2, and understanding the respective effects, this will eventually lead to understanding of the phenomenon in general.

1.2 Motivation and objective

Based on the current status, we can consider and classify the types of previous tests (or experiments) as in Fig. 1.3. The larger tests have good side from the viewpoint of *prototylicality*; however, it would be very difficult to investigate the phenomena directly in an reactor using actual materials. Moreover, the phenomena will result in many kind of complex interactions, including hydrodynamic and thermal ones. In those cases, it is quite difficult to identify the essence of the phenomena.

Different from such approach, this dissertation focuses on fundamental processes of the melt-jet breakup as in Fig. 1.2. A scoping study of the fundamental process is an effective approach to understanding the actual situation. The objective of this dissertation is to elucidate fragmentation mechanism and establish melt-coolability assessment methodology. After understanding the individual phenomenon in detail by experiment and numerical analysis, we integrate and generalize these findings. Then, we provide discussion on the reactor conditions. Through this

Figure 1.3: Relationship between reactor-accident phenomena and the existing tests or experiments.

dissertation, we assess the SFR condition as the reactor condition.

We briefly mention the structure of this dissertation. To this end, this dissertation is structured by seven chapters as shown in Fig. 1.4. In Chapter 2, we will deal with jet breakup of liquid-liquid two-phase system as one of the individual effects. Visualization technique combined with high-speed visualization enables us to measure the jet breakup length. Also, we generalize the flow regime transition of liquid-liquid jet breakup on the dimensionless number space, based on the visualization under wide-range parameters and phenomenological considerations.

In order to investigate parameter ranges that can not be observed by experiments, we will propose a numerical method and conduct numerical simulations in Chapter 3. Starting from the multiphase lattice Boltzmann method, we show some improvements of the stability to deal with liquid-jet breakup systems. Validity of the proposed numerical method is confirmed against the experimental data given in Chapter 2.

Then, we further improive the numerical method to investigate the hydrodynamic jet flow in the reactor-equivalent condition in in Chapter 4. Two types of melt-jet experiments are targeted: melt jets in water and in liquid sodium. Also, we assess the validity of dimensionless map generalized from the experiments.

Figure 1.4: Structure of the dissertation.

In Chapter 5, we will numerically evaluate heat transfer from particles generated from molten jet to coolant. The problem is set as forced convection boiling around the cylinder to simplify the actual situation. To solve this problem, we use the phase-change lattice Boltzmann method with some improvements on the numerical stability. The simulation results are compared with existing film boiling heat transfer correlations.

In Chapter 6, appropriate physical models for melt-jet breakup in coolant will be identified based on the above experimental and numerical simulation results. The correlations required for the melt-coolability assessment are determined, which are supported by the experimental or numerical evidences. The sensitivy analysis shows the coolability performance of the melt jet in coolant.

Chapter 2

Liquid-Liquid Jet Experiments

2.1 Literature review

Abe et al. [36] improved the crude mixed heat transfer model pmjet developed by Moriyama et al. [37]. The cooling performance of the molten fuel was evaluated. The outline of this model is shown in Fig. Several correlation equations for predicting jet breakup length corresponding to Lbrk in Fig. 1.1 have been proposed, and Saito et al. correlation [34] and Epstein–Fauske correlation [38]. It is often used as a comparison with results. Regarding SFR actual conditions, Suzuki et al. [33] compares Saito et al. correlation [34] with the jet break-up length estimated from the FARO/TERMOS experiment [2]. He said that he overestimates the breakup length. Saito's equation and Epstein's equation are also derived based on hydrodynamic instability, but experimental results according to Saito's equation [24], experiments in accordance with Epstein's equation results [26,39] and experimental results according to any correlation [28] are mixed. In order to accurately predict jet break-up length, it is necessary to clarify concrete application conditions for these correlation equations. In addition, the linear decrease in jet diameter as shown in Fig. 1.1 is just an assumption, and it is necessary to verify what kind of decrease behavior the jet diameter actually shows.

As mentioned in Chapter 1, the hydrodynamic interaction is considered to be an important factor in melt-jet breakup. Nishimura et al. [7] suggested a hydrodynamic fragmentation model

that agreed well with their copper/sodium experiments at high ambient Weber numbers (> 200). The ambient Weber number,

$$\mathrm{We}_a = \frac{\rho_c u_{j0}^2 D_{j0}}{\sigma}, \tag{2.1}$$

is often used to characterize the jet breakup length [21,40,41] and the diameters of the resulting fragments [5,7]. Matsuo et al. [26] concluded from their melt-water experimental data that the dominant effect on jet breakup was the shear force that acted on the interface. They further concluded that, in such shear-force-dominated conditions, the Epstein–Fauske correlation [38] could be used to predict the jet breakup length. The key aspect of the Epstein–Fauske correlation is the assumption of entrainment on the basis of the Kelvin–Helmholtz instability. Epstein and Fauske [38] indicates that their correlation agreed well with the previous data on breakup length, which are considered to be in the atomized state. The conditions for the appearance of atomized breakup in liquid-liquid systems is an issue that is yet to be clarified. Identifying those conditions would enables us to use a simplified physical model to predict breakup length and fragment diameter and hence be able to evaluate melt coolability (e.g., Abe et al. [18,36]).

The breakup of a liquid jet into droplets is itself an important phenomenon in natural and industrial processes, so the instability of liquid jets has been studied extensively (see the comprehensive reviews by Eggers and Villermaux [42], Lin and Reitz [43], and McCarthy and Molloy [44]). Based on his experimental observation, Ohnesorge [45] showed that liquid jets generally falling into one of four regimes [46,47]:

(0) Slow dripping from the nozzle under gravity with no formation of a jet (dripping regime),
(I) Breakup of a cylindrical jet by axisymmetric perturbations of the surface (varicose regime),
(II) Breakup by screw-like perturbations of the jet (sinuous regime),
(III) Atomization of the jet (atomization regime).

Furthermore, he expressed the criteria for the breakup regimes I–III qualitatively on a dimensionless operating diagram (see Fig. 1 in Ohnesorge [45] or Fig. 4 in McKinley and Re-

nardy [44]). According to his article, the appropriate dimensionless groups are the Ohnesorge number Oh and the Reynolds number Re based on the dispersed phase:

$$\mathrm{Oh} = \frac{\mu_j}{\sqrt{\rho_j \sigma D_{j0}}}, \tag{2.2}$$

$$\mathrm{Re} = \frac{\rho_j u_{j0} D_{j0}}{\mu_j}. \tag{2.3}$$

The operating diagram considers the inertia, viscous, and interfacial forces of a liquid jet. The boundaries of each regime can be described in following functional form:

$$\mathrm{Oh} = a\mathrm{Re}^b \text{ or } \mathrm{Re} = a\mathrm{Oh}^b, \tag{2.4}$$

where a and b are arbitrary constants that are generally determined by fitting from experimental data. Based on Ohnesorge's experimental data, Kolev [46] later provided a quantitative expression for the functional form of the boundaries between regimes I–III [1] :

$$\mathrm{Re} = 46\ \mathrm{Oh}^{-4/5} \text{ (between I and II)}, \tag{2.5}$$

$$\mathrm{Re} = 270\ \mathrm{Oh}^{-4/5} \text{ (between II and III)}. \tag{2.6}$$

Using the aforementioned functional forms, the jet breakup regimes can be estimated approximately. Functional forms similar to Eqs. (2.5) and (2.6) have been proposed elsewhere [48–50].

Liquid-liquid jet dynamics occur in fields such as chemical engineering [51–56]) and ocean engineering [57, 58]. Experiments using a characteristic of liquid-liquid systems known as refractive index matching have also been reported to further understand jet breakup dynamics [59, 60]. Takahashi and Kitamura [55] observed jet breakup in liquid-liquid systems using various combinations of test fluids and focusing on jets in the laminar state. Riestenberg et al. [57] injected water into liquid CO_2 and classified the data into three regimes similar to those of Ohnesorge [45]. While studies on liquid-liquid systems such as those discussed above provide significant insights into the jet breakup regimes, most have been limited to dripping or laminar flows;

[1] Note that the coefficient values in Eqs. (2.5) and (2.6) are simply fitting values; it remains to identify the physical meaning of the constants (Kolev, private communication).

there have been fewer studies on the transition from dripping to atomization in liquid-liquid systems.

In this chapter, we carried out jet injection experiments using test fluids to investigate the dynamics of jet breakup and droplet formation in immiscible liquid-liquid systems as a fundamental process of melt-jet-coolant interactions.

2.2 Experimental method

2.2.1 Experimental apparatus

Figure 2.1 is a schematic diagram of the experimental apparatus, consisting of a test section, a light source and a high-speed video camera. A test fluid for the dispersed phase was injected into an acrylic reservoir (200×200×450 mm) that was filled with a second test fluid for the continuous phase. The dispersed-phase fluid was kept at a constant hydraulic head in an overflow tank, as shown in Fig. 2.1, thus forming a steady-state jet flow in the test section. The injection velocity was adjusted by changing the opening ratio of a needle valve. We employed four types of cylindrical nozzle with inner diameter D_{j0} = 3, 5, 7, and 10 mm. A high-speed video camera (FASTCAM mini UX100, Photron) was installed to record the flow images of the jet interface. The high-speed visualization was performed at 500–4,000 fps with a shutter speed of 0.000125–0.00025 s depending on the injection conditions. The image resolution of image was 512×1024 pixels. A metal halide lamp (HVS-SL, Photron) was placed at the opposite side of the test section to the high-speed camera to provide backlight illumination.

2.2.2 Test fluids and experimental conditions

We employed two pairs of immiscible liquids as the test fluids, the combinations and physical properties of which are summarized in Tables 2.1 and 2.2. The experiments were carried out at room temperature (25 °C).

Figure 2.1: Schematic diagram of experimental apparatus.

The fluids pair in Table 2.1 was used in Sec. 2.3. Silicone oil KF-96L-0.65 CS having a known refractive index of 1.375 was used as the fluid of the continuous phase. As the fluid of the jet, an aqueous glycerol solution whose refractive index can be adjusted by mass concentration was used. When the concentration of glycerin aqueous solution is 34.4 wt%, it is possible to make the refractive index of glycerin aqueous solution 1.375, which is the same refractive index as silicone oil. Adjusting the refractive index of the test fluid makes it possible to reduce the influence of refraction due to the complexly deformed interface shape by using the *laser-induced fluorescence* (LIF). The jets and continuous phase test fluids shown in Table 2.1 are not mixed with each other, and the fluorescent dye Rhodamine 6G is only dissolved in the jet.

The fluids pair in Table 2.2, The pairs were Fluorinert (FC72, 3M Co.) into water and water into silicone oil (KF-96L-0.65CS). In both combinations, the heavier fluid was injected into the lighter fluid.

Under actual SFR conditions, the dispersed and continuous phases are the mixed oxide (MOX) fuel and sodium, respectively, whose physical properties are given in Table 2.3 for reference. One of the major characteristics of the system is that sodium has a comparatively low viscosity. The physical properties in Table 2.3 will be used in Sec. 2.4.6 to estimate the reactor conditions.

Table 2.1: Physical properties of test fluids for Sec. 2.3 at 25 °C. Refractive indeces are mathed in this case (1.375).

Dispersed phase			Continuous phase			
Substance	Density [kg/m^3]	Viscosity [mPa·s]	Substance	Density [kg/m^3]	Viscosity [mPa·s]	Surface tension [mN/m]
34wt% grycerol-water mixture	1,082	2.9	Silicone oil	760	0.49	39

Table 2.2: Physical properties of test fluids for Sec. 2.4 at 25 °C.

Dispersed phase			Continuous phase			
Substance	Density [kg/m^3]	Viscosity [mPa·s]	Substance	Density [kg/m^3]	Viscosity [mPa·s]	Surface tension [mN/m]
FC-72	1,680	0.67	Water	997	0.89	52
Water	997	0.89	Silicone oil	760	0.49	40

2.3 Visualization and measurement by LIF

2.3.1 Visualization results

Figure 2.2 shows the image of the jet vertical section obtained by LIF measurement. In this study, by using the test fluid of Table 2.1, it was possible to bring the refractive index of the jet and the continuous phase close to each other, so that a clear image can be obtained as shown in Fig. 2.2, whereby the core of the jet and it became possible to discriminate and observe atomized matter. From Fig. 2.2, it can be seen that the jet interface becomes unstable at any jet speed, and atomized matter is generated at the tip and side of the jet. It is observed that the faster the jet speed, the more the proportion of fine particles stripped off at the side of the jet is increasing. In addition, as the jet speed increases, the number of fine particles to be produced increases and the diameter of fine particles tends to decrease.

Table 2.3: Physical properties of SFR conditions [61, 62].

Dispersed phase			Continuous phase			
Substance	Density [kg/m^3]	Viscosity [mPa·s]	Substance	Density [kg/m^3]	Viscosity [mPa·s]	Surface tension [mN/m]
MOX fuel (3000 °C)	8,663	4.0	Sodium	856	0.28	465

Figure 2.2: Snapshots of jet cross section by using LIF. (a) $u_{j0} = 0.96$ m/s, (b) $u_{j0} = 1.8$ m/s, and (c) $u_{j0} = 2.2$ m/s. Since the refractive indices of jet and ambient fluid are almost equal, the visualization results are net cross section of the jet.

Figure 2.3: Image processing procedure to obtain jet core length.

2.3.2 Image processing procedure

We describe the procedure of image processing to obtain the jet break length from the visualized image obtained in Sec 2.3.1. An example of an image in each process of image processing is shown in Fig. 2.3. The image obtained by LIF measurement [Fig. 2.3 (a)] is subjected to gradation inversion and binarization, thereby obtaining vertical cross-sectional information [Fig. 2.3 (b)] of the jet including the fine particles. Processing, the so-called labeling, is applied to this image. In the labeling process, different numbers are allocated to pixel areas where black portions are consecutive. As a result, the region representing the core of the jet connected from the nozzle and other regions can be identified [Fig. 2.3 (c)]. Then, by excluding the pixel area with the number assigned to the area other than the one to be connected from the nozzle, one can extract the image of only the jet core [Fig. 2.3 (d)]. Through this series of processes, by applying this process to all the measured images, the time change of the core length of the jet was obtained.

2.3.3 Behavior of jet core and calculation of jet breakup length

Figure 2.4 shows the tip position of the jet including the fine particles and the tip position of the core of the jet. The position of the nozzle exit was set to 0 m. The solid line represents the tip position of the jet including the atomized material, and the graph until the point of reaching the lower end of the visible region is displayed in the graph. From Fig. 2.4, it can be seen that, at any jet velocity, the tip of the jet including the atomized material separates from the tip of the jet core with the portion indicated by the circle in the figure as the boundary, and then the two do not coincide. Since the length at which the core of the jet disappears is considered to be the jet break up length, in this research it is judged that the jet breaks up at the point shown in the circle in Fig. 2.4, and the length of the jet core after that point is Jet breakup length was taken. The position of the tip of the jet core fluctuates over time because the fluid mass is formed at the tip of the jet and repeating the behavior of detaching from the core of the jet when it is of a certain size. Since the jet break-up length fluctuates with time, after break-up occurred, the time average was taken within the range shown in Fig. 2.4.

2.3.4 Arrangement of calculated jet break-up length by dimensionless number

We will organize the obtained jet breakup length by an important dimensionless number and compare it with existing correlation formula. There are Saito et al. correlation [34] and Epstein–Fauske correlation [38] as representative correlation equations relating to jet break-up length. assuming that the inertial force of the jet is balanced with the buoyancy received from the surrounding fluid and the resistance due to the vapor flow, Saito et al. [34] obtained the following equation,

$$\frac{L_{\mathrm{brk}}}{D_{j0}} = 2.1\mathrm{Fr}^{\frac{1}{2}} \left(\frac{\rho_j}{\rho_c}\right)^{\frac{1}{2}}, \tag{2.7}$$

where $\mathrm{Fr} = u_{j0}^2/gD_{j0}$ is the Froude number.

Figure 2.4: Time series of jet leading-edge including fragments (solid line), and jet core length (dashed line).

On the other hand, Epstein and Fauske [38] obtained the following equation on the assumption that the velocity of the jet and the speed of entrainment due to atomization are proportional.

$$\frac{L_{\mathrm{brk}}}{D_{j0}} = \frac{1}{2E_0}\left(\frac{\rho_j}{\rho_c}\right)^{\frac{1}{2}}. \tag{2.8}$$

E_0 in Eq. 2.8 is called the entrainment coefficient, and in the literature [38] it states that the value of 0.05 to 0.1 is in good agreement with the experimental result. Also, when $E_0 = 0.1$, it is shown that it agrees with the formula derived by Taylor (1963) in the range of 6%. As shown in Fig. 2.5 (a), Saito et al. correlation depends on Froude number, whereas Epstein–Fauske correlation depends only on E_0.

Figure 2.5 (a) shows the jet breakup length against the Froude number. The Froude number is a dimensionless number representing the ratio of inertial force and gravity, and the larger the value, the more the influence of inertial force excels as compared with gravity. The figure also shows the results of existing experiments in the case where the molten metal is injected into water under the liquid-liquid contact condition [26] and the case where the molten metal is injected at the interface solidification condition [39] ing. Matsuo et al., Jet break-up length obtained by the experiment of Iwasawa et al. Is a value estimated from time change of jet tip position. From Fig. 2.5 (a), no dependence of Froude number was observed in any of the experimental results, and a tendency to follow Epstein's equation was obtained. On the other hand, according to the experimental result of Saito et al. [34] used in the derivation of Saito et al. correlation it is seen that the jet is covered with a vapor film from the visualized image. In addition, in the experimental results [24] according to the Saito formula reported in the existing research, a relatively high temperature melt is injected into the water, and a stable vapor film is formed between the jet and the coolant It is thought that it was generating. The Epstein equation in Fig. 2.5 (a) and the difference between this experimental result and Saito et al. correlation may be affected by presence or absence of a vapor film between the jet and the surrounding fluid.

Figure 2.5 (b) shows the jet breakup length againt the Weber number ($= \rho_c u_{j0}^2 D_{j0}/\sigma$). The Weber number is a dimensionless number representing the ratio of the inertial force and the interfacial tension, which means that the influence of the inertial force is superior to the interfacial tension as the value is larger. If the Weber number is sufficiently large and the influence of the inertial force is superior to the interfacial tension, it is considered that the influence of atomization becomes remarkable in jet breakup. For this reason, it is conceivable that results based on Epstein–Fauske correlation on the premise of entrainment due to atomization were obtained. In addition, from Fig. 2.5 (b), it can be considered that Epstein–Fauske correlation can be applied as a predicted correlation equation of jet breakup length when the Weber number is about 10 to 1000. In the case where the Weber number is smaller than the order of 10, it is presumed that the entrainment at the jet interface presumed by Epstein–Fauske correlation is suppressed, so a separate examination is necessary. In addition, although a separate study

Figure 2.5: Comparison of the jet breakup length with (a) Froude number and (b) Weber number.

is required for the case where the Weber number is larger than the order of 1000, looking at the trend in Fig. 2.2, regarding the case where the jet speed further increases and the Weber number becomes larger. It is inferred that it is difficult to think that the core of the jet reaches even deeper because the influence of atomization is dominant.

Based on our results shown in Fig. 2.5, we calculated the jet breakup length by performing a series of new image processing including labeling after using LIF as a visualization method, and the Weber number was 10–1000, the tendency that the jet breakup length follows the formula of Epstein was obtained. This result is similar to the results of existing experiments using different evaluation methods [26, 39]. Since the Epstein–Fauske correlation is derived on the premise of entrainment at the interface [38], if the jet is covered with a vapor film by film boiling, the entrainment is inhibited and the model advocated by Epstein matches It is inferred that it will disappear. High temperature melting bodies are also used in existing experiments [26, 39], including the effect of nucleate boiling or transition boiling. As shown in Fig. 2.5, the condition of boiling and the result of this experiment carried out by liquid-liquid adiabatic system also follow Epstein–Fauske correlation also implies that the effect of nucleate boiling or transition boiling on jet break length is considered to be small.

Here, consider the SFR condition. It is expected that the phenomena under the SFR consition is sufficiently lower than the minimum film boiling temperature, and the influence of vapor film is sufficiently small [24,33]. Assuming the physical property values in Table 2.3, the jet velocity u_{j0} =1–5 m/s, and the jet diameter D_{j0} = 55 mm, the Weber number can be calculated from 101 to 2531, and under the actual machine condition, it is within the range of the horizontal axis and a slightly larger Weber number than that. In the case where the Weber number becomes as large as 2000 as mentioned above, a separate examination is necessary, but for a region where the Weber number is about 10 to 1000 under actual machine conditions, the jet break length is predicted by Epstein's equation It is thought that.

2.3.5 Averaged shape of jet core

In the existing research, cooling performance evaluation of molten fuel by coarse mixed heat transfer model has been performed, but assumption that the shape of melt jet in the model linearly decreases from the coolant liquid level is placed [36, 37]. Such an assumption seems to be due to the fact that the core of the jet actually decreases, there is no experimentally observed example. In this section, we investigate the average decreasing behavior of the jet diameter from the measurement result of the jet cross section.

Figure 2.6 shows the procedure for calculating the average of the diameters of the jets. The image to be used is an image where fragments are eliminated as shown in Fig. 2.3 (d). First, as shown in Fig. 2.6 (a), a black area in the horizontal direction is counted with respect to the image of the core of the jet at a certain time, and this is taken as the jet diameter. By applying this processing to each image at each time, as shown in Fig. 2.6 (b), a time change of the jet diameter at each height position is obtained. Finally, the average diameter of the jet diameter obtained in Fig. 2.6 (b) is taken to obtain the average jet diameter as shown in Fig. 2.6 (c). The time to start taking the average and the time to take the average are the same as when calculating the jet break up length in Sec 2.3.3.

Figure 2.7 shows the result of time average with respect to the diameter of the jet. The figure aligned on the right side of the graph is visualized on the assumption that the horizontal cross

Figure 2.6: Estimation procedure of mean jet core diameter.

section is circular based on the calculated jet diameter. 1 is assigned to the internal area of the average jet diameter, 0 is assigned to the external area, and an isosurface where the value is 0.5 is displayed. From Fig. 2.7, it can be seen that at any jet speed, the jet diameter slightly increases immediately after flowing, after which the jet gradually becomes thinner and finally the diameter becomes zero. The results shown in Fig. 2.7 show that the radial dimension of the continuous jet core decreases in the flow direction. In this method, an image excluding micronized particles detached from the core of the jet is used, and as a result, it is considered that the behavior of the jet core becoming thinner due to atomization is reflected. Regarding the slight increase in jet diameter, due to friction between the jet immediately after flowing out of the nozzle and the surrounding fluid, force is exerted in the direction in which the interface is kept in place, and fluctuation of the unstable interface is considered. Although the decrease in jet diameter is not linear, a model [36, 37] that the core portion of the jet shown in Fig. **??** gradually becomes thin due to atomization is a jet break with atomization It is considered appropriate for up behavior.

Figure 2.7: Averaged jet-core diameter at each jet velocity. The jet-core diameter does not reduce linearly.

2.4 Flow regime transition criteria

2.4.1 Typical breakup regimes and breakup-length curve

Firstly, we conducted qualitative observations of the jet breakup regimes in the present experiments, typical snapshots of which are shown in Fig. 2.8. The test fluid pair was water (dispersed phase) and silicone oil (continuous phase); the nozzle diameter D_{j0} was 7 mm. Thus, the variable parameter was the injection velocity u_{j0}. From left to right, we can see that the droplet size decreased and the number of droplets increased with increase of jet velocity. Also, the scale of the waves on the interface became smaller with the velocity was increased.

Next, we measured the jet breakup length. The term breakup length refers to the length of the continuous liquid column from the nozzle [43, 44]. Jet breakup length is one of the indices that characterize the jet breakup behavior. The measured jet breakup length L scaled on the nozzle diameter D_{j0} is plotted in Fig. 2.9 against the ambient Weber number $\mathrm{We_a}$ [Eq. (2.1)]. The conditions were the same as those mentioned in the previous paragraph. The jet breakup length was defined as the mean continuous jet length over 1.0 s. The corresponding visual

images are also included in the figure. The curve of jet breakup length in Fig. 2.9 shows certain characteristic behavior. With increase of $\mathrm{We_a}$, the breakup length increases at first to a local maximum, decreases to a local minimum, then increases again. For $\mathrm{We_a} > 100$, it was difficult to identify the breakup length from the backlight visual images. Thus, results from index-matched laser-induced fluorescence (LIF) measurements are additionally plotted in Fig. 2.9 with the corresponding snapshots [63]. Note that the latter measurement results were processed based on vertical-plane images of the jet flow, and suggest that the Weber number dependence of the breakup length is no longer significant.

The variation in breakup length shown in Fig. 2.9 is similar to that reported for liquid-gas systems [21, 40]. It is also similar to results from numerical simulations of Wood's metal into water [41]. We found the quantitative tendency of the breakup-length curve for our liquid-liquid system to be similar to that for a liquid-gas system.

Figure 2.8: Snapshots of typical breakup regimes observed in the experiments. The jet velocity increases from left to right: (a) 0.041 m/s, (b) 0.076 m/s, (c) 0.21 m/s, (d) 0.83 m/s, (e) 2.1 m/s. The scale bar in each image represents 5 mm.

Figure 2.9: Jet breakup length versus ambient Weber number. Open circles (○) represent data obtained via planar LIF (laser-induced fluorescence) using the index-matching technique (Saito et al. [63]). The three images on the right are of the vertical plane of the jet illuminated by a laser sheet.

2.4.2 Droplet formation process and droplet size distribution

Droplet analysis procedure

Image processing was used to analyze the droplet size. Because the droplets were not necessarily circular in outline, an elliptical approximation was used instead to evaluate the droplet diameter.

Figure 2.10 shows the original image to be processed [Fig. 2.10(a)] and the post-processed analyzed image [Fig. 2.10(b)]. The procedure of the present analysis can be summarized briefly as follows:

1. The five coordinate values were extracted from the visual image of droplets.

2. The elliptical approximation was applied to the five coordinate values.

3. An area-equivalent diameter was calculated from the ellipse equation.

The Cartesian coordinate system used for droplet analysis is shown schematically in Fig. 2.11. In general, the shape of an ellipse with angle θ is given by

$$\left[\frac{(x-x_0)\cos\theta+(y-y_0)\sin\theta}{a}\right]^2+\left[\frac{-(x-x_0)\sin\theta+(y-y_0)\cos\theta}{b}\right]^2=1, \tag{2.9}$$

where a and b are the major and minor half widths of the ellipse, respectively, and (x_0, y_0) is the central point of the ellipse. Equation (2.9) can be expanded as follows:

$$x^2+Axy+By^2+Cx+Dy+E=0, \tag{2.10}$$

where A, B, C, D, and E are constants. In the droplet analysis, the five coordinate values are substituted to Eq. (2.10), and then the area-equivalent diameter of the droplet de was calculated by

$$d_e=2\sqrt{ab}. \tag{2.11}$$

Hereinafter, we will evaluate the area-equivalent diameter d_e as the droplet diameter d using the aforementioned procedure.

Figure 2.10: Example of droplet size analysis: (a) pre-processed original image, (b) analyzed image.

Figure 2.11: Coordinate system for image processing of a droplet.

Table 2.4: Summary of breakup regimes.

Regime	Characteristics
0	Dripping from nozzle (no jet formation)
I	Varicose breakup
IIa	Sinuous breakup *without* entrainment
IIb	Sinuous breakup *with* entrainment
III	Atomization

Characteristics of breakup regimes

We now classify the breakup regimes obtained from the experiments. In the present study, we extend the classical Ohnesorge classification [45, 47] to liquid-liquid systems based on the observation results. The five types of breakup regimes as shown in Fig. 2.8 are subjected to Ohnesorge's classification. A brief summary of the classified breakup regimes and their characteristics is given in Table 2.4. The Roman numerals for each regime correspond to those mentioned in Chapter 1, except for Regime II. Since different droplet-formation processes were observed experimentally, Regime II is divided into two sub-regimes: Regime IIa and Regime IIb. Details of the characteristics of each sub-regime are given later in this section.

Next, we investigate the droplet size and its distribution. The droplet size itself and its distribution are also considered to be characteristics of the jet breakup behavior in conjunction with the breakup length. The number of measured droplets n was 100–500 depending on the conditions, although that of Regime 0 was only approximately 20. Since the injection velocity was

very small in Regime 0, fewer droplet images were available compared with the other regimes.

Figure 2.12 shows typical snapshots of the whole jet flow (left panel), the vicinity of droplet formation (upper-right panel) and the evaluated droplet-size distribution (lower-right panel) in each breakup regime. The histograms show the probability density of the measured droplet diameter. The vertical axis, pdf (probability density function), is normalized by number of droplets n, thus the area is to be 1 when it is integrated over the entire range. The pdfs here are based not on droplet volume but on droplet number. The droplet formation process and characteristics of droplet size distribution in each regime are described below.

Regime 0 (Dripping) – The results for Regime 0 are shown in Fig. 2.13(a). A droplet formed very near the nozzle by expansion of the neck part; no obvious liquid column formed. The so-called pinch-off phenomenon was dominant during this breakup regime. The resulting droplet was marginally wider than the nozzle. This tendency is similar to that predicted by classical Rayleigh theory [64] for a liquid column in a vacuum:

$$d = \sqrt[3]{\frac{3\pi}{1.4}} D_{j0}, \tag{2.12}$$

Equation (2.12) leads to $d \sim 1.89 D_{j0}$, which appears to overestimate the present experimental results slightly. According to Kolev [46], breakup in this regime is influenced by density ratio and gravity. The difference in density ratio between liquid-gas and liquid-liquid systems is considered to be partly responsible for such an overestimation.

Regime I (Varicose breakup) – The results for Regime I are shown in Fig. 2.13(b). Clearly, a continuous liquid column now formed from the nozzle, unlike in Regime 0. The liquid column was nearly axisymmetric (varicose), and droplets formed at its top. Two types of breakup pattern were observed in this regime: droplet pinch-off and the formation of satellite droplets just after the pinch-off. This explains the obvious double-peaked histogram of droplet size. Since the satellite droplets were much smaller than the nozzle diameter, the two distributions can be easily identified. The larger one corresponds to pinch-off droplets whose sizes ranged around the nozzle diameter, which is a little different from classical theory [64, 65]. As pointed

out by Kitamura et al. [52], the theoretical prediction may be valid only when the velocity difference across the interface is sufficiently small.

Regime IIa (Sinuous breakup without entrainment) – The results for Regime IIa are shown in Fig. 2.13(c). The liquid column transitioned to being asymmetric (sinuous) in this regime. However, droplets continued to form at the column tip, as in Regime I. The droplet size distribution seems to possess two peaks, but this tendency is no longer as clear as it is in Regime I. The observed process of droplet formation was again pinch-off and satellite formation. One of the reasons why the liquid column became sinuous in this regime is considered to be that the settling velocity exceeded the jet velocity at the inlet. The settling velocity of a particle is given by

$$u_s = \sqrt{\frac{4}{3c_f}}\sqrt{\frac{\rho_p - \rho_a}{\rho_a} d_p g}, \tag{2.13}$$

where c_f is the drag coefficient, d_p is the particle diameter, ρ_p is the particle density, and ρ_a is the density of the ambient fluid. By replacing ρ_p and ρ_a with ρ_j and ρ_c, respectively, and assuming that (i) the particle diameter dp for a pinch-off droplet is equal to the nozzle diameter D_{j0}, and (ii) the drag coefficient acting on the particle is $c_f \approx 0.44$ (Newtonian regime), the settling velocity is evaluated as $u_s \approx 0.25$ m/s for the conditions in Fig 2.8. The jet velocity in this regime [Fig. 2.8(c)] was 0.21 m/s, which is clearly comparable with the predicted settling velocity.

Regime IIb (Sinuous breakup with entrainment) – The results for Regime IIb are shown in Fig. 2.13(d). The sinuous shape of the liquid column was similar to that in Regime IIa. Regarding the droplet formation process, droplet entrainment at the side of the liquid column began in this regime, with pinch-off and satellite formation at the tip of the liquid column. As can be seen in the relevant histogram, the diameters of the entrainment and satellite droplets were less than the nozzle diameter. It was difficult to identify from the visual images whether such small droplets were due to satellite formation or entrainment. In this regime, droplets comparatively larger than the nozzle diameter could be observed, although they were few in number.

Regime III (Atomization) – The results for Regime III are shown in Fig. 2.13(e). The liquid

column was now covered with a proliferation of entrainment droplets that were much smaller than the nozzle diameter. Note that in this regime, pinch-off and satellite formation may still have been occurring at the tip of the liquid column, but the overwhelming number of entrainment droplets prevented us from identifying such behavior.

The observed droplet-formation process can be finally classified to three types: pinch-off, satellite formation, and entrainment. It is known that the processes of breaking up into droplets can be divided into the so-called primary breakup [66,67] and secondary breakup [68,69] during liquid jet breakup [70]. Primary breakup forms droplets directly from the liquid column, after which secondary breakup occurs depending on the flow conditions. Pinch-off and entrainment are elements of primary breakup; satellite drop formation is part of secondary breakup. Hereinafter, the droplets formed by primary breakup (pinch-off and satellite) and secondary breakup (satellite formation) will be considered separately for droplet size evaluation.

The distribution of droplet diameter and the typical droplet-formation process in each breakup regime are summarized in Fig. 2.13. We can see that the dominant process transitioned from pinch-off to entrainment with increase of jet velocity. Qualitatively, the characteristic droplet size decreases as we progress through the series of breakup transition regimes.

2.4.3 Breakup regimes on dimensionless map

The experimental results classified into the regimes defined in Table 2.4 are shown in Fig. 2.14 with available experimental data [55,71]. A schematic illustration describing the characteristics of each regime is also shown within the figure. For reference, the boundaries of the liquid-gas systems of Ohnesorge [45] (Eqs. (2.5) and (2.6), obtained by Kolev [46]) are drawn as the dashed lines. We can see that the correlations for liquid-gas systems cannot be applied to liquid-liquid systems on the diagram. The increase of ambient density is considered to be responsible for the difference between liquid-liquid and liquid-gas systems. In general, the density ratio (dispersed phase to continuous phase) γ is of the order of 1 for liquid-liquid systems and 1,000 for liquid-gas systems. Modification or reformulation of the boundaries into those for liquid-liquid systems is required in order to predict the breakup regime in liquid-liquid systems.

(a) Regime 0: Dripping from nozzle (no jet formation).

(b) Regime I: Varicose breakup

(c) Regime IIa: Sinuous breakup without entrainment

Figure 2.12: Droplet formation process and evaluated droplet-diameter distribution in each breakup regime.

(d) Regime IIb: Sinuous breakup with entrainment

(e) Regime III: Atomization

Figure 2.12: (*cotinued*)

Figure 2.13: Summary of transitions in droplet diameter distribution (left) with typical snapshots of the droplet formation process (right).

2.4.4 Evaluation of median diameter

Droplet size in each regime

Next, we calculate the median diameter to evaluate the droplet size. Here we use the mass-median diameter (MMD) as the index of droplet size. The MMD has been employed by several authors to evaluate the fragment size during melt-coolant interactions (e.g., Refs. [5, 7, 26]). Therefore, we can compare our results with the available data on the same basis. The discussion including available experiments will be given later.

The results plotted in Fig. 2.15 show the velocity dependence of MMD for $D_{j0} = 7$ mm for

Figure 2.14: Operating diagram of jet breakup regimes observed in the present experiments and in previous studies [55, 71]. Dashed lines are the boundaries for liquid-gas systems obtained by Kolev [46] based on Ohnesorge's experimental data [45]. The correlations for liquid-gas systems are not applicable to liquid-liquid systems.

water and silicone oil. It should be noted that we defined two MMDs for the same jet velocity condition when two peaks were observed in the droplet size distribution [e.g., Figs. 2.12(b) and (c)]. Such a double-peaked distribution was observed whenever satellite drops formed. Satellite droplets were smaller than pinch-off ones, but the numbers of each were comparable. This indicates that the total mass of the satellite droplets can be neglected, and that treating them separately would not yield a significant effect on the MMD. Singly distributed droplets and the larger ones in the double-distributions were mainly due to pinch-off or entrainment. Also, the vertical error bars in Fig. 2.15 indicate the 95% confidence interval for MMD, which we use to express the width of the droplet size distributions even though the distributions were not necessarily Gaussian ones. Unless otherwise stated, the procedure mentioned in this paragraph will be adopted in the rest of this article.

From Fig. 2.15, we find that when the jet velocity is small (Regimes 0, I, and IIa), the droplets are either the same size as the nozzle diameter or a little larger. In contrast, at high velocity (Regime III), the droplet diameter seems to depend on the jet velocity.

Figure 2.15: Velocity dependence of droplet size, with histograms of droplet diameter distribution. The vertical and horizontal axes in the histograms denote the probability density and droplet diameter (d/D_{j0}), respectively.

Comparison with classical hydrodynamic instabilities

According to previous work, the fragment size is affected by classical instabilities [18, 19, 26, 36, 72]. The relationship between the evaluated droplet size and the critical wavelength of each instability is compared here.

The critical wavelengths of the classical Rayleigh–Taylor and Kelvin–Helmholtz instabilities in two-dimensions are given by [73]

$$\lambda_{\mathrm{cr,RT}} = 2\pi \left[\frac{\sigma}{(\rho_j - \rho_c)g} \right]^{\frac{1}{2}}, \tag{2.14}$$

$$\lambda_{\mathrm{cr,KH}} = 2\pi \frac{\rho_j + \rho_c}{\rho_j \rho_c} \frac{\sigma}{u_{j0}^2}, \tag{2.15}$$

respectively, where σ is the interfacial tension and g is the gravitational acceleration. The jet

velocity is used as the scaling velocity under the assumption that the ambient fluid is stationary in Eq. (2.15). One can draw the critical wavelength curve for the data using the same physical quantities.

Figure 2.16 shows the variation in MMD when jet velocity for various nozzle diameters, and the critical wavelength curves described by Eqs. (2.14) and (2.15). The test fluid pair was again water/silicone oil. The wavelength of the Rayleigh–Taylor instability is constant (26.4 mm for the present liquid-liquid system) with velocity, whereas that of the Kelvin–Helmholtz instability depends on the jet velocity. All the nozzle diameters used in the present study were smaller than the critical wavelength of the Rayleigh–Taylor instability. From Fig. 2.16, the size of the droplets formed at lower velocities are of the same order as the nozzle diameter and smaller than the wavelength of the Rayleigh–Taylor instability. The velocity dependence on droplet diameter seems to appear at higher velocity regardless of nozzle diameter. The slope of this variation is similar to that of the Kelvin–Helmholtz instability, although there is some discrepancy between droplet size and instability wavelength. In Fig. 2.16, the dominant mechanism of droplet formation transitioned from pinch-off to entrainment among 0.3–0.7 m/s. The observation through the present experiments showed that the size of the pinch-off droplets depended on the nozzle diameter. In contrast, the size of the entrainment droplets clearly depended on velocity regardless of nozzle diameter.

It is noticeable that that the velocity dependence seems to appear beyond the intersection point of the Rayleigh–Taylor and Kelvin–Helmholtz instabilities. This would imply that the intersection point is related to the transition between breakup regimes, namely whether or not entrainment dominates.

Summary of droplet size and comparison with melt-coolant experiments

Next, we plot all the present experimental results against the ambient Weber number [Eq. (2.1)] to summarize the data obtained in different systems and to quantitatively compare the available experimental data from melt-coolant systems.

Figure 2.16: Comparison of measured droplet diameter for variable nozzle diameters and two-dimensional hydrodynamic interfacial instability theories: Rayleigh–Taylor (dotted) and Kelvin–Helmholtz (broken) instabilities.

Figure 2.17 shows the droplet MMD obtained from the present experiments and the fragment MMD obtained from the previous works: U-alloy78/water system [26], copper/sodium system [7], and aluminum-oxide/sodium system [5]. The vertical axes in Fig. 2.17(a)(b) differ as to whether or not they are normalized by nozzle (inlet) diameter. The normalized MMD at lower Weber number is around 1 ($d = D_{j0}$) except for the satellite droplets [see Fig. 2.17(b)]. The normalized MMD obtained by Matsuba et al. [5] was evaluated as being much smaller than in the present liquid-liquid experiments. Two reasons for this can be considered. Firstly, the nozzle diameters used in their experiments were 40–63 mm, which is larger than those in other experiments (3–10 mm (present), 7–20 mm [26], 7.6–18 mm [7]). Based on such diameters, the normalized MMD of Matsuba et al. [5] results in much smaller values compared with the others. Secondly, Matsuba et al. used melt oxide as the jet material. As pointed out by Schins and Gunnerson [3], the thermal stress characteristics of molten oxide lead to fracturing-type fragmentation. At higher Weber numbers, the non-normalized MMD of the present experiment and the previous data are well correlated [see Fig. 2.17(a)]. This seems to suggest that droplet formation at higher Weber numbers is dominated by the mechanisms that are independent of

nozzle size; the Kelvin–Helmholtz instability correlates with droplet formation at higher Weber numbers. This fact is reasonable because the Kelvin–Helmholtz instability itself is independent of nozzle (inlet) diameter.

The threshold value at which the tendency of droplet or fragment size changes is found to be $\mathrm{We_a} \approx 20$. This value is the same order of magnitude as the critical Weber numbers for droplets: 12 [67] or 18 [26].

2.4.5 Breakup regime map for liquid-liquid systems

Formulation of breakup-regime boundaries

As discussed in Sec. 2.4.3, the regime boundaries in liquid-gas systems are not suitable for liquid-liquid systems on the dimensionless operating diagram. We consider the physical meanings of the boundaries for liquid-liquid systems and modify the boundaries. In the framework of linear theory, the following dimensionless parameters are considered to describe the breakup of a viscous jet in a viscous fluid [43]:

$$(\gamma,\ \eta,\ \mathrm{Re},\ \mathrm{We},\ \mathrm{Fr})\,, \tag{2.16}$$

where γ is the density ratio and η is the viscosity ratio. The Ohnesorge number can be written as $\mathrm{Oh} = \mathrm{We}^{1/2}/\mathrm{Re}$. By using the above dimensionless groups, we obtain the functional form on the Ohnesorge's operating diagram. We follow here the functional form expressed by Eq. (2.4).

As mentioned in Sec. 2.4.2, the transition from varicose to sinuous breakup (Regime IIa) may be explained from the viewpoint of the settling velocity of a formed pinch-off drop by Eq. (2.13). We assume that the transition from varicose breakup (Regime I) to sinuous breakup (Regime IIa) occurs at the point at which the jet velocity at the inlet corresponds to the settlement velocity:

$$u_{j0} = u_s,\ \text{or},\ u_{j0} = \sqrt{\frac{4}{3c_f}}\sqrt{\frac{\rho_j - \rho_c}{\rho_c} D_{j0} g}. \tag{2.17}$$

Figure 2.17: Experimental results compared with available experimental data, including U-alloy 78/water [26], copper/sodium [7] and aluminum-oxide/sodium [5]: (a) normalized by nozzle diameter, (b) dimensional expression.

By transforming Eq. (2.17) to the form of Eq. (2.4) using the dimensionless groups [Eq. (2.16)], one can obtain the following relation:

$$\mathrm{Oh} = \left[\frac{4}{3c_f}(\gamma - 1) \cdot \mathrm{We} \cdot \mathrm{Fr}^{-1}\right]^{\frac{1}{2}} \mathrm{Re}^{-1}, \tag{2.18}$$

where $\gamma = \rho_j/\rho_c$, $\mathrm{We} = \rho_j u_{j0}^2 D_{j0}/\sigma$, and $\mathrm{Fr} = u_{j0}^2/gD_{j0}$.

As mentioned in Sec. 2.4.4, the intersection point of the Rayleigh–Taylor and Kelvin–Helmholtz instabilities can be viewed as the transitional point. Beyond this point, the droplet size showed a clear dependence on the jet velocity, which suggests that entrainment now dominates the breakup behavior. Here, we assume the following relationship:

$$2\pi\left[\frac{\sigma}{(\rho_j - \rho_c)g}\right]^{\frac{1}{2}} = 2\pi\frac{\rho_j + \rho_c}{\rho_j\rho_c}\frac{\sigma}{u_{j0}^2}. \tag{2.19}$$

With the dimensionless groups, Eq. (2.19) can be rewritten as

$$\mathrm{Oh} = \left[(1+\gamma)\sqrt{1 - \frac{1}{\gamma}} \cdot \mathrm{Fr}^{-\frac{1}{2}}\right] \mathrm{Re}^{-1}. \tag{2.20}$$

We find that the value of the exponent part [or b in Eq. (2.4)] is -1 in both Eqs. (2.18) and (2.20) based on these simple assumptions. The coefficient [or a in Eq. (2.4)] is, however, in a complicated form in both Eqs. (2.18) and (2.20), so we determined the value instead by least-squares fitting the experimental data by using the breakup-regime data as shown in Fig. 2.18. Finally, the following correlations describing the boundaries of each breakup regime in liquid-liquid systems can be obtained from the present study and previous work [55, 71]:

$$\mathrm{Oh} = 2.8\ \mathrm{Re}^{-1}\ \text{(between I and IIa)}, \tag{2.21}$$

$$\mathrm{Oh} = 22\ \mathrm{Re}^{-1}\ \text{(between IIb and III)}. \tag{2.22}$$

The ambient viscosities considered in Eqs. (2.21) and (2.22) were 0.36–0.89 mPa·s; the related dimensionless parameters [appeared in Eqs. (2.18) and (2.20)] were $\gamma = 1.3$–1.8, $\mathrm{We} = 8.2 \times 10^{-3}$–$1.3 \times 10^3$, and $\mathrm{Fr} = 2.9 \times 10^{-3}$–$1.1 \times 10^2$.

Figure 2.18: Fitting to determine the coefficient between: (a) Regime I and Regime IIa, (b) Regime IIb and III.

2.4.6 Summary of experimental data and extrapolation to SFR accident conditions

Figure 2.19 summarizes again the experimental results with the obtained boundaries for liquid-liquid breakup regimes [Eqs. (2.21) and (2.22)]. On the diagram, the boundaries for liquid-liquid systems result in being located in the left-hand side compared with those for liquid-gas systems. As discussed in Sec. 2.4.3, the difference of density ratio in each system is considered to be responsible for such a shift in the diagram.

The boundaries of the jet breakup regimes were extrapolated to the region in which no experimental data is available. The FARO/TERMOS experiments (UO_2/sodium system) carried out by Magallon et al. [2] are also plotted in Fig. 2.19 with the symbol '×', where the release channel diameter and the velocity upon impact with the sodium (see Table 1 in Ref. [2]) were taken as the characteristic length and velocity, respectively. We find that Magallon et al.'s experimental data are in the atomization regime. One of the characteristics of jet atomization is that the droplets are much smaller than the jet diameter [43]. From a hydrodynamic viewpoint, this might explain the fact reported by Magallon et al. [2] that the debris was observed to be fine

fragments whose size was of the order of 10^1–10^3 μm.

The expected SFR conditions are also shown in Fig. 2.19 as the closed (grey) region with dashed line. The reactor conditions were estimated using the physical properties of the dispersed phase in Table 2.3 and the following conditions:

- jet diameter D_{j0} = 10–500 mm,
- jet velocity u_{j0} = 0.5–50 m/s.

By using the above assumptions, the UO_2/sodium data of Magallon et al. [2] can be included in the reactor conditions. We can see that most of the expected reactor conditions are located in Regime III. It is only the case of low jet velocity and small diameter (u_{j0} = 0.5 m/s and D_{j0} = 10 mm) that is in Regime II. The reactor conditions do not extend to Regimes 0 or I under the aforementioned assumptions. Of course, thermal interactions could be involved in promoting jet breakup in actual situations, such as the local vaporization of sodium [5] or surface freezing [74]. However, the hydrodynamic interactions considered in this article imply that the jet breakup regimes under SFR conditions appear to be in the atomization regime. Thus, the fragments would be much smaller than the jet diameter in an actual reactor.

2.5 Summary

The dynamics of jet breakup and droplet formation in immiscible liquid-liquid systems were studied experimentally in order to better understand the fundamental interactions between a melt jet and the surrounding coolant. We performed experiments using two-types of test-fluid pairs under isothermal conditions.

Visualization measurement of jet breakup behavior by LIF was performed using a fluid immiscible as a test fluid and having the same refractive index. From the visualization result of the jet vertical section by LIF, the jet break length was measured as the length of the jet core. In the condition that the Weber number is about 10 to 1000, the correlation formula of Epstein is

Figure 2.19: Flow transition criteria of jets in liquid-liquid systems with experimental data and expected accident conditions.

suitable as a correlation formula of jet break up length. Also, the generated fine particles were excluded and the time average of the diameters of the jets of the jet was calculated. It turned out that the jet accompanying atomization gradually became thinner and break up after the diameter slightly increased with respect to the flow direction.

The jet breakup behavior was observed by changing the jet velocity. The variation of measured breakup length with ambient Weber number obtained in the present liquid-liquid system was similar to that in a liquid-gas system. The breakup regimes were classified based on Ohnesorge's idea. However, it was found that the empirical correlations representing the boundaries of the breakup regimes in liquid-gas systems could not be applied to liquid-liquid systems. The droplet size distribution in each breakup regime was analyzed using image processing. Observations showed that pinch-off, entrainment, and satellite formation appeared as the droplet formation process. The characteristics of the droplet diameter distribution changed demonstrably with the breakup-regime transitions. The velocity-dependence of droplet size was confirmed when entrainment was dominant. Comparison with hydrodynamic instabilities suggested that the velocity-dependence was correlated with the Kelvin–Helmholtz instability. The variation of

droplet size with ambient Weber number was compared between the present study and available melt-jet experiments. The droplet diameter normalized by the inlet diameter was well correlated with Weber number at lower Weber numbers; at higher Weber numbers, the droplet size in dimensional (non-normalized) form was well correlated with Weber number.

Based on the observation and analysis results, the breakup regimes were organized on a dimensionless operating diagram. By using simple assumptions, the correlations representing the criteria for the regime boundaries of liquid-liquid systems were derived as follows:

$$\mathrm{Oh} = 2.8\ \mathrm{Re}^{-1}\ \text{(between I and IIa)},$$

$$\mathrm{Oh} = 22\ \mathrm{Re}^{-1}\ \text{(between IIb and III)}.$$

Finally, extrapolation of the experimental data to the expected conditions of an SFR was considered. The extrapolation results implied that most of the hydrodynamic conditions during an accident would be covered by Regime III, the atomization regime. It should be noted that the present results were performed under isothermal liquid-liquid systems, thus they did not simulate a high-temperature conditions with phase changes from the views of prototypicality. It is necessary to separately evaluate the thermal interactions; such studies have also been carried out by many researchers (e.g., surface solidification [39, 75] and coolant subcooling [15]). As far as the SFR conditions are considered, thermal interactions would promote jet fragmentation [33]. A careful consideration on the thermal interactions in the reactor conditions should be taken into account to assess the reactor conditions. In this regard, very recently, Iwasawa and Abe [76] provided a scaling analysis and discussed the effect of sollidification based on their experimental data.

Chapter 3

Liquid-Liquid Jet Simulations

3.1 Literature review

Multiphase and multicomponent flows appear in many natural and industrial processes. A liquid jet injected into another fluid is an interesting example of such a flow. Significant efforts have been put into understanding the breakup of a liquid jet for more than a century. Since the pioneering works of Plateau [77] and Rayleigh [64], extensive studies on this subject have been performed theoretically, experimentally, and numerically [42–44, 78].

Drops form directly from the nozzle at low injection velocities, and a liquid jet issues from the nozzle and then breaks into droplets in various patterns at higher injection velocities. The occurrence of such a regime is of interest in the study of liquid-jet breakup. [45] classified his results into four types of breakup regimes: (0) dripping, (I) varicose, (II) sinuous, and (III) atomization [46, 47]. He also provided a regime map of liquid jets in a gas using the Ohnesorge and Reynolds numbers. After Ohnesorge's work, much research on this subject has been performed (e.g., [48–50]). The majority of investigations have focused upon liquid-gas systems (liquid jet into gaseous atmosphere). Breakup of jets in liquid-liquid systems (liquid jets into another liquid) has not been investigated as extensively. Our focus in this paper is therefore on the breakup of liquid jets in immiscible liquid-liquid systems.

The liquid-liquid-jet systems can also be found in several fields, e.g., chemical processing [51,53, 55] and CO_2 storage in oceans [57,79]. In the field of nuclear engineering, interactions between melt and coolant must be well understood for safety design of nuclear reactors and have therefore been extensively investigated in the literature [18,23,24]. In experiments, a high-temperature melt is often used to simulate the core melt materials. [18] discussed the relationships between the fragment size and the Rayleigh–Taylor and Kelvin–Helmholtz interfacial instabilities [73].

Numerical simulations of liquid-liquid jets involve the solution of the Navier–Stokes equations for two fluids with specified boundary and interface conditions. Several approaches to solving these types of free-surface problems are available in the literature. As a first attempt, [80] investigated the axisymmetric steady-state laminar jet based on the volume-of-fluid (VOF) method [81]. [41] also used the VOF method provided by a commercial code, FLUENT, to simulate a melt jet into water. They successfully reproduced a variation in the breakup length [21]; later, a similar variation was confirmed by experiments [63,82]. [83] numerically investigated liquid-liquid-jet breakup using a front-tracking method [84,85]. They mapped different breakup modes on a plot of Weber number vs. viscosity ratio. The drawback of their front-tracking simulations was that they neglected the coalescence of generated drops. The aforementioned numerical simulations [41,80,83] were limited to two-dimensional cases.

A completely different approach is the use of a lattice Boltzmann method. Several authors have investigated liquid-liquid-jet flows using multiphase lattice Boltzmann models [86–88]. In recent years, this method has been recognized as a powerful tool for analysis of complex fluid dynamics, including multicomponent and multiphase flows [89]. Compared with other macroscopic CFD methods based on the Navier–Stokes equations, the lattice Boltzmann method, which is constructed using mesoscopic kinetic equations, has several advantages. For instance, it is easy to incorporate mesoscale physics such as interfacial breakup or coalescence. Moreover, the computational cost for simulating realistic fluid flows is reasonable compared with particle-based methods (e.g., molecular dynamics). The relations of the scale properties in fluid flows are schematically illustrated in Fig. 3.1.

Two-phase or multiphase lattice Boltzmann models can be classified into four categories:

Figure 3.1: Relationship between multiscale properties of a fluid flow and a simulation method.

- Color-fluid model [90, 91],
- Pseudo-potential model [92, 93],
- Free-energy model [94, 95],
- Mean-field model [96].

This classification may not be exhaustive, for instance, the latter two models are sometimes identified as phase-field models [97] since the Cahn–Hilliard or similar interface tracking equations can be derived from them. For details about the multiphase lattice Boltzmann models, interested readers can refer to the comprehensive review papers [89, 97–101] and references therein. In this paper, we focus upon the color-fluid model. This model possesses many strengths in simulations of multiphase/multicomponent flows, including strict mass conservation for each fluid and flexibility in adjusting the interfacial tension [102]. A static drop test is no longer needed to determine the interfacial tension; it can be directly obtained without any analysis or assumptions. Moreover, the color-fluid model shows a very small dissolution property for tiny droplets or bubbles [101].

Color-fluid models, which are often referred to as R-K or color-gradient models, were first developed by [90], who extended the two-component lattice gas automata model of [103]. Later, [91] enabled the introduction of density and viscosity ratios by modifying the forms of the distribution functions. [104] replaced Gunstensen's maximization-recoloring step with a formulaic

segregation algorithm. Instead of widening the interface width, Latva-Kokko–Rothman's recoloring algorithm solves some issues with the previous color-fluid-type model, namely, the lattice-pinning problem and the spurious velocities. [105] extended the model to common a two-dimensional nine-velocity (D2Q9) lattice. They modified the perturbation operator to recover the Navier–Stokes equations correctly.

[106] demonstrated that integrating Latva-Kokko–Rothman's recoloring operator [104] into Reis–Phillips' perturbation operator [105] greatly improves the numerical stability and accuracy of solutions over a wide range of parameters. Using an isotropic gradient operator also enhanced numerical stability and accuracy [107]. [108] derived a generalized perturbation operator using the phase-field (or order parameter) instead of a color-gradient and formulated the color-fluid model in three dimensions. Very recently, [109] generalized the color-fluid-type lattice Boltzmann model in two and three dimensions.

Galilean invariance is one of the issues to be improved in the color-fluid family. Following [110], a source term to improve the Galilean invariance was derived by [111] and incorporated into an equilibrium distribution function. The enhanced equilibrium distribution function showed an improvement of the momentum-discontinuity problem through numerical tests on a layered Couette flow. Recently, [102] have modified an equilibrium distribution function based on the third-order Hermite expansion of the Maxwellian distribution. They also showed that discontinuous velocities were improved by this modification.

It is known that the LB method suffers from numerical instability in low-viscosity conditions. Modification of the collision operator is one method for overcoming this issue [112]. A multiple-relaxation-time (MRT) collision operator or generalized lattice Boltzmann equation [113–115] has been widely used, even for multiphase flows, to enhance numerical stability and accuracy and to reduce spurious current near the interface.

We return to the issue of lattice Boltzmann simulations of liquid-jet breakup. [116] successfully introduced an MRT operator to the multiphase lattice Boltzmann model and performed liquid-jet breakup simulations [86]. They assumed that the flow was axisymmetric in two dimensions. They investigated the influence of interfacial tension, injection velocity, and liquid viscosity

under a density ratio of 5. However, three-dimensional simulations are required to further understand breakup characteristics, since liquid-jet breakup is an essentially three-dimensional flow, as shown in Fig. **??**.

In this chapter, we present the three-dimensional two-phase lattice Boltzmann model for immiscible two-phase flows and its application to liquid-jet breakup. We formulate the three-dimensional two-phase lattice Boltzmann model for immiscible two-phase flows in the framework of a three-dimensional 27-velocity (D3Q27) lattice. The collision operator consists of D3Q27 versions of three sub-operators: an MRT-collision operator, a generalized-perturbation operator [108], and a formulatic-recoloring operator [104]. A D3Q27 version of the enhanced equilibrium distribution functions [111] is also incorporated into this model to improve its Galilean invariance.

3.2 Methodology

The present model is formulated on a D3Q27 lattice. The key to the formulation is the combination of previous work and their extension to the D3Q27 framework. The main points of this process can be briefly summarized as follows:

- Introducing a D3Q27 MRT collision operator [117] and relaxation parameters [118]
- Extending an enhanced equilibrium distribution function [111] to the D3Q27 lattice
- Extending a generalized perturbation operator [108] to the D3Q27 lattice

For the present three-dimensional lattice Boltzmann model, distribution functions move on a

Figure 3.2: Three-dimensional 27-velocity (D3Q27) lattice.

D3Q27 lattice with the lattice velocity $\mathbf{c}_i$ defined as follows:

$$\mathbf{c}_i = (c_{ix}, c_{iy}, c_{iz}) = \begin{cases} (0,0,0)c, & i = 1, \\ (\pm1,0,0)c,\ (0,\pm1,0)c,\ (0,0,\pm1)c, & i = 2,3,\ldots,7, \\ (\pm1,\pm1,0)c,\ (0,\pm1,\pm1)c,\ (\pm1,0,\pm1)c, & i = 8,9,\ldots,19, \\ (\pm1,\pm1,\pm1)c, & i = 20,21,\ldots,27, \end{cases} \tag{3.1}$$

where $c = \delta_x/\delta_t$, δ_x is the lattice spacing and δ_t is the time step. The schematic structure of the D3Q27 lattice is shown in Fig. 3.2. The D3Q27 model is a straightforward extension of the D2Q9 model [119].

In this model, two immiscible fluids are represented as pseudo red and blue fluids, respectively. The distribution function, f_i^k, is introduced to represent the fluid k, where $k = r$ and b denote the colors "red" and "blue," respectively, and i is the lattice-velocity direction. The total distribution function is defined as $f_i = f_i^r + f_i^b$. The evolution of the distribution function is expressed by the following lattice Boltzmann equation:

$$f_i^k(\mathbf{x} + \mathbf{c}_i\delta_t, t + \delta_t) - f_i^k(\mathbf{x}, t) = \Omega_i^k(\mathbf{x}, t), \tag{3.2}$$

where $\mathbf{x}$ and t are the position and time, respectively. The collision operator Ω_i^k is made up of

three sub-operators [120]:

$$\Omega_i^k = \left(\Omega_i^k\right)^{(3)} \left[\left(\Omega_i^k\right)^{(1)} + \left(\Omega_i^k\right)^{(2)}\right], \tag{3.3}$$

where $(\Omega_i^k)^{(1)}$ is the single-phase collision operator, $(\Omega_i^k)^{(2)}$ is the perturbation operator, and $(\Omega_i^k)^{(3)}$ is the recoloring operator. Using the MRT operator, the single-phase collision operator can be written as

$$\left(\left|\Omega^k\right\rangle\right)^{(1)} = -\mathbf{M}^{-1}\mathbf{K}\mathbf{M}\left(\left|f^k\right\rangle - \left|f^{k(e)}\right\rangle\right) + \left|F\right\rangle. \tag{3.4}$$

The density of the fluid k is given by

$$\rho_k = \sum_i f_i^k. \tag{3.5}$$

The total fluid density is given by $\rho = \sum_k \rho_k$, and the total momentum is defined as

$$\rho\mathbf{u} = \sum_i \sum_k f_i^k \mathbf{c}_i + \frac{1}{2}\mathbf{F}\delta_t, \tag{3.6}$$

where $\mathbf{F}$ is the body force. Note that Eq. (3.6) indicates that the local velocity is modified to incorporate the spatially varying body force [121]. In Eq. (3.2), $\mathbf{M}$ and $\mathbf{K}$ are, respectively, the 27×27 transformation and relaxation matrices. In this paper, Dirac's bra-ket notation is employed. Here, the "bra" operator $\langle f|$ denotes a row vector along each lattice-velocity direction, i.e., $(f_1, f_2, \ldots, f_{27})$, and the "ket" operator $|f\rangle$ denotes a column vector, i.e., $(f_1, f_2, \ldots, f_{27})^{\mathrm{T}}$, where the superscript "T" is the transpose operator.

The MRT collision operator in three dimensions is usually implemented with the D3Q15 or D3Q19 lattices. As an early attempt for the D3Q27 MRT collision operator, Dubois and Lallemand [122] and Premnath and Banerjee [123] presented the formulation independently in 2011. Dubois and Lallemand [122] arranged the D3Q27 orthogonal basis vectors for the moments according to their character (scalars, vectors, and tensors, etc.) and then used *raw moments* to formulate an MRT lattice Boltzmann model. On the other hand, Premnath and Banerjee [123] arranged the D3Q27 orthogonal basis vectors based on the increasing order of moments and used *central moments* to formulate an MRT lattice Boltzmann model. Later,

Geier et al. [117] provided the following orthogonal moment set for the D3Q27 lattice:

$$
\mathbf{M} = \begin{bmatrix}
\langle 1| \\
\langle c_{ix}| \\
\langle c_{iy}| \\
\langle c_{iz}| \\
-2\langle 1| + \langle |\mathbf{c}_i|^2| \\
2\langle c_{ix}^2| - \langle c_{iy}^2 + c_{iz}^2| \\
\langle c_{iy}^2 - c_{iz}^2| \\
\langle c_{ix}c_{iy}| \\
\langle c_{iy}c_{iz}| \\
\langle c_{iz}c_{ix}| \\
-4\langle c_{ix}| + 3\langle c_{ix}c_{iy}^2 + c_{iz}^2c_{ix}| \\
-4\langle c_{iy}| + 3\langle c_{iy}c_{iz}^2 + c_{ix}^2c_{iy}| \\
-4\langle c_{iz}| + 3\langle c_{iz}c_{ix}^2 + c_{iy}^2c_{iz}| \\
4\langle c_{ix}| - 6\langle c_{ix}c_{iy}^2 + c_{iz}^2c_{ix}| + 9\langle c_{ix}c_{iy}^2c_{iz}^2| \\
4\langle c_{iy}| - 6\langle c_{iy}c_{iz}^2 + c_{ix}^2c_{iy}| + 9\langle c_{ix}^2c_{iy}c_{iz}^2| \\
4\langle c_{iz}| - 6\langle c_{iz}c_{ix}^2 + c_{iy}^2c_{iz}| + 9\langle c_{ix}^2c_{iy}^2c_{iz}| \\
4\langle 1 - |\mathbf{c}_i|^2| + 3\langle c_{ix}^2c_{iy}^2 + c_{iy}^2c_{iz}^2 + c_{iz}^2c_{ix}^2| \\
-8\langle 1| + 12\langle |\mathbf{c}_i|^2| - 18\langle c_{ix}^2c_{iy}^2 + c_{iy}^2c_{iz}^2 + c_{iz}^2c_{ix}^2| + 27\langle c_{ix}^2c_{iy}^2c_{iz}^2| \\
2\langle c_{iz}^2 + c_{iy}^2| + 3\langle c_{ix}^2c_{iy}^2 + c_{iz}^2c_{ix}^2| - 4\langle c_{ix}^2| - 6\langle c_{iy}^2c_{iz}^2| \\
2\langle c_{iz}^2 - c_{iy}^2| + 3\langle c_{ix}^2c_{iy}^2 - c_{iz}^2c_{ix}^2| \\
-2\langle c_{ix}c_{iy}| + 3\langle c_{ix}c_{iy}c_{iz}^2| \\
-2\langle c_{iy}c_{iz}| + 3\langle c_{ix}^2c_{iy}c_{iz}| \\
-2\langle c_{iz}c_{ix}| + 3\langle c_{ix}c_{iy}^2c_{iz}| \\
\langle c_{ix}c_{iy}^2 - c_{iz}^2c_{ix}| \\
\langle c_{iy}c_{iz}^2 - c_{ix}^2c_{iy}| \\
\langle c_{iz}c_{ix}^2 - c_{iy}^2c_{iz}| \\
\langle c_{ix}c_{iy}c_{iz}|
\end{bmatrix}, \tag{3.7}
$$

where $|\mathbf{c}_i| = \sqrt{c_{ix}^2 + c_{iy}^2 + c_{iz}^2}$. The transformation matrix transfers the distribution functions from velocity space to moment space. Using the MRT collision operator instead of a traditional single-relaxation-time (or BGK) collision operator contributes to enhancement of numerical stability and accuracy, even with additional computational costs. The practical forms of the transformation matrix and its inverse are given in Ref. [124]. The relaxation matrix $\mathbf{K}$ is the diagonal matrix given by [118]

$$\begin{aligned}\mathbf{K} &= \mathrm{diag}\left[s_1, s_2, \ldots, s_{27}\right] \\ &= \mathrm{diag}[s_1, s_1, s_1, s_1, s_5, s_6, s_6, s_8, s_8, s_8, \\ &s_{11}, s_{11}, s_{11}, s_{14}, s_{14}, s_{14}, s_{17}, s_{18}, s_{19}, s_{19}, s_{21}, s_{21}, s_{21}, s_{24}, s_{24}, s_{24}, s_{27}],\end{aligned} \tag{3.8}$$

where the elements $0 < s_i < 2$ represent both the hydrodynamic and non-hydrodynamic relaxation parameters. The hydrodynamic parameters satisfy the following relations:

$$\nu = \frac{1}{3}\left(\frac{1}{s_6} - \frac{1}{2}\right) = \frac{1}{3}\left(\frac{1}{s_8} - \frac{1}{2}\right), \tag{3.9}$$

$$\zeta = \frac{1}{3}\left(\frac{1}{s_5} - \frac{1}{2}\right), \tag{3.10}$$

where ν and ζ are the kinematic viscosity and the bulk viscosity, respectively. In this paper, we use the optimized parameters proposed by Suga et al. [118]: $s_1 = 0$, $s_5 = 1.5$, $s_{11} = 1.5$, $s_{14} = 1.83$, $s_{17} = 1.4$, $s_{18} = 1.61$, $s_{19} = s_{21} = 1.98$, and $s_{24} = s_{27} = 1.74$. We confirmed that these parameters significantly enhanced the numerical stability even at extremely low kinematic viscosity with the order of $O(10^{-4})$.

For the single-phase collision operator, an enhanced equilibrium distribution function proposed by [111] is used in this paper:

$$f_i^{k(e)}(\rho_k, \mathbf{u}, \alpha_k) = \rho_k \left(\varphi_i^k + w_i \left[\frac{3}{c^2}(\mathbf{c}_i \cdot \mathbf{u}) + \frac{9}{2c^4}(\mathbf{c}_i \cdot \mathbf{u})^2 - \frac{3}{2c^2}\mathbf{u}^2\right]\right) + \Phi_i^k. \tag{3.11}$$

In the case of $\Phi_i^k = 0$, Eq. (4.11) recovers the common form of an equilibrium distribution function. Using the form of Eq. (4.11), the Galilean invariance is improved for variable density and viscosity ratios under the hypothesis of a small pressure gradient [111, 125, 126]. However,

it should be noted that this can only partly restore Galilean invariance, as still the third order diagonal equilibrium moments are not independently supported, and are related to the corresponding first moments. Consequently, there will be cubic velocity errors in Galilean invariance even for the D3Q27 lattice, which could become perceptible for flows under high shear. This issue can be solved by making some additional corrections to the collision operator, as suggested recently by [127].

The weights, w_i, are those of a standard D3Q27 lattice [119]:

$$w_i = \begin{cases} 8/27, & i = 1, \\ 2/27, & i = 2, 3, \ldots, 7, \\ 1/54, & i = 8, 9, \ldots, 19, \\ 1/216, & i = 20, 21, \ldots, 27. \end{cases} \tag{3.12}$$

Moreover, in the D3Q27 lattice, one can derive

$$\varphi_i^k = \begin{cases} \alpha_k, & i = 1, \\ 2(1-\alpha_k)/19, & i = 2, 3, \ldots, 7, \\ (1-\alpha_k)/38, & i = 8, 9, \ldots, 19, \\ (1-\alpha_k)/152, & i = 20, 21, \ldots, 27, \end{cases} \tag{3.13}$$

and

$$\Phi_i^k = \begin{cases} -3\bar{\nu}(\mathbf{u} \cdot \nabla \rho_k)/c, & i = 1, \\ +16\bar{\nu}(\mathbf{G}_k : \mathbf{c}_i \otimes \mathbf{c}_i)/c^3, & i = 2, 3, \ldots, 7, \\ +4\bar{\nu}(\mathbf{G}_k : \mathbf{c}_i \otimes \mathbf{c}_i)/c^3, & i = 8, 9, \ldots, 19, \\ +1\bar{\nu}(\mathbf{G}_k : \mathbf{c}_i \otimes \mathbf{c}_i)/c^3, & i = 20, 21, \ldots, 27, \end{cases} \tag{3.14}$$

where $\otimes$ is the tensor product and the symbol ":" indicates tensor contraction; $\bar{\nu}$ is the kinematic

viscosity interpolated by [108, 120]

$$\bar{\nu} = \frac{1+\phi}{2}\nu_r + \frac{1-\phi}{2}\nu_b. \tag{3.15}$$

Here, ϕ is the order parameter to distinguish the two components in a multicomponent flow, defined as [108]

$$\phi(\mathbf{x}, t) = \frac{\rho_r(\mathbf{x}, t) - \rho_b(\mathbf{x}, t)}{\rho_r(\mathbf{x}, t) + \rho_b(\mathbf{x}, t)}. \tag{3.16}$$

The values of the order parameter $\phi = 1, -1$, and 0 correspond to a purely red fluid, a purely blue fluid, and the interface, respectively [120]. In the framework of D3Q27 lattice, the tensor $\mathbf{G}_k$ in Eq. (3.14) is defined as

$$\mathbf{G}_k = \frac{1}{48}\left[\mathbf{u} \otimes \nabla\rho_k + (\mathbf{u} \otimes \nabla\rho_k)^{\mathrm{T}}\right]. \tag{3.17}$$

As established in [91], the density ratio between the fluids, γ, must be taken into account as follows to obtain a stable interface:

$$\gamma = \frac{\rho_r^0}{\rho_b^0} = \frac{1-\alpha_b}{1-\alpha_r}, \tag{3.18}$$

where the superscript "0" indicates the initial value of the density at the beginning of the simulation [111]. In each homogeneous phase region, the pressure of the fluid k is given by

$$p_k = \rho_k \left(c_s^k\right)^2 = \rho_k \frac{9(1-\alpha_k)}{19} c^2, \tag{3.19}$$

for the D3Q27 lattice. This corresponds to an isothermal equation of state. In this paper, we choose $\alpha_b = 8/27$, in which $c_s^b = 1/\sqrt{3}$ [88, 125].

The term $|F\rangle$ in Eq. (3.4) represents the discrete forcing term accounting for the body force $\mathbf{F}$. In the MRT framework, the forcing term reads as [128]

$$|F\rangle = \mathbf{M}^{-1}\left(\mathbf{I} - \frac{1}{2}\mathbf{K}\right)\mathbf{M}\,|F'\rangle\,, \tag{3.20}$$

where $\mathbf{I}$ is a unit matrix, $|F\rangle = (F_1, F_2, \ldots, F_{27})^{\mathrm{T}}$, and $|F'\rangle = (F'_1, F'_2, \ldots, F'_{27})^{\mathrm{T}}$ is given by

$$|F'\rangle = w_i \left[3\frac{\mathbf{c}_i - \mathbf{u}}{c^2} + 9\frac{(\mathbf{c}_i \cdot \mathbf{u})\mathbf{c}_i}{c^4} \right] \cdot \mathbf{F}\delta_t. \tag{3.21}$$

Eqs. (3.20) and (3.21) reduce to Guo *et al.*'s original forcing scheme [121] when using a single-relaxation time [128]

To model the interfacial tension, [108] derived a generalized perturbation operator based on the CSF [129] concept, and the work of [105] is employed to obtain the interfacial tension:

$$\left(\Omega_i^k\right)^{(2)} = \frac{A_k}{2}|\nabla\phi| \left[w_i \frac{(\mathbf{c}_i \cdot \nabla\phi)}{|\nabla\phi|^2} - B_i \right]. \tag{3.22}$$

Eq. (3.22) satisfies the correct form of the interfacial-tension force in the Navier–Stokes equations when the lattice-specific variables B_i are chosen correctly. We derived the values of B_i in the framework of the D3Q27 lattice as follows:

$$B_i = \begin{cases} -(10/27)c^2, & i = 1, \\ +(2/27)c^2, & i = 2, 3, \ldots, 7, \\ +(1/54)c^2, & i = 8, 9, \ldots, 19, \\ +(1/216)c^2, & i = 20, 21, \ldots, 27. \end{cases} \tag{3.23}$$

In this model, the interfacial tension can be directly given by

$$\sigma = \frac{4}{9} A\tau c^4 \delta_t, \tag{3.24}$$

where we assumed that $A = A_r = A_b$, τ is the relaxation time. Parameter A controls the strength of interfacial tension, σ.

Although the perturbation operator, $(\Omega_i^k)^{(2)}$, generates interfacial tension, it does not guarantee the immiscibility of both fluids. To promote phase segregation and maintain the interface, the

following recoloring operator is applied [104, 106, 130]

$$(\Omega_i^r)^{(3)} = \frac{\rho_r}{\rho} f_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\theta_i) f_i^{(e)}(\rho, \mathbf{0}, \bar{\alpha}), \tag{3.25}$$

$$(\Omega_i^b)^{(3)} = \frac{\rho_b}{\rho} f_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\theta_i) f_i^{(e)}(\rho, \mathbf{0}, \bar{\alpha}), \tag{3.26}$$

where

$$\cos(\theta_i) = \frac{\mathbf{c}_i \cdot \nabla \phi}{|\mathbf{c}_i||\nabla \phi|}, \tag{3.27}$$

and $f_i^{(e)}$ is evaluated using Eq. (4.11), a zero velocity, and

$$\bar{\alpha} = \frac{1}{2}(1+\phi)\alpha_r + \frac{1}{2}(1-\phi)\alpha_b. \tag{3.28}$$

For the computation of the gradient operator for an arbitrary function χ, the following second-order isotropic central scheme [108, 131–133]

$$\nabla \chi(\mathbf{x}, t) = \frac{3}{c^2} \sum_i \frac{w_i \chi(\mathbf{x} + \mathbf{c}_i \delta_t, t) \mathbf{c}_i}{\delta_t}, \tag{3.29}$$

is adopted.

3.3 Numerical tests

3.3.1 Static droplet

Static-droplet tests are performed to test the validity of interfacial tension predicted by Eq. (3.24). The computational domain is discretized into an $85 \times 85 \times 85$ lattice. A steady red droplet with radius R is immersed in a blue fluid. The density field of each phase is initialized as follows:

$$\rho_r(x, y, z) = \frac{\rho_r^0}{2} \left[1 - \tanh\left(\frac{2(r-R)}{W} \right) \right], \tag{3.30}$$

$$\rho_b(x, y, z) = \frac{\rho_b^0}{2} \left[1 + \tanh\left(\frac{2(r-R)}{W} \right) \right], \tag{3.31}$$

where $W = 4$ and $r = \sqrt{(x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2}$ with the central position of the computational domain (x_c, y_c, z_c). We set the density and kinematic-viscosity ratios as 1.5 and 1, respectively. The kinematic viscosity for each phase is set to be 1.0×10^{-3}, and gravity is neglected throughout the simulations. The parameters are A in Eq. (3.24) and initial droplet radius R (see Table 3.1). Periodic boundary conditions are imposed on all sides of the computational domain.

The Laplace equation in three dimensions is given by

$$\Delta p = \frac{2\sigma}{R}, \tag{3.32}$$

where Δp is the pressure difference across the droplet interface. The pressure for each phase is evaluated by Eq. (3.19) and is measured after 80,000 iterations using the same procedure as [106]. Figure 3.3 shows the measured pressure differences. For both the higher [Fig. 3.3(a)] and lower [Fig. 3.3(b)] interfacial tensions, the results are in proportion to the droplet curvature $1/R$, with which the Laplace law was satisfied. The theoretical prediction by Eq. (3.24), shown in Fig. 3.3 as a solid line, also agrees well with the measured pressure differences. Table 3.1 summarizes the simulation parameters and the evaluated error. The error E is calculated as [108]

$$E = \frac{|\sigma_{th} - \sigma_{Lap}|}{\sigma_{th}}, \tag{3.33}$$

where σ_{th} and σ_{Lap} are the interfaceial tension predicted by Eq. (3.24) and that measured by the Laplace equation Eq. (3.32), respectively. We confirm that the lattice Boltzmann model developed in Sec. 3.2 can predict the interfacial tension for a static case within a maximum error of 1.6%.

We should mention the influence of lattice isotropy on the so-called spurious velocity. Fig. 3.4 compares the droplet shape and velocity field at the equilibrium state for D3Q19 [Fig. 3.4(a)] and D3Q27 lattices [Fig. 3.4(b)]. The numerical test using D3Q19 is based on [88]. The maximum spurious velocities $|\mathbf{u}|_{max}$ are 1.2×10^{-2} for D3Q19 and 5.8×10^{-3} for D3Q27, respectively. Although the conditions are same except for the employed lattice geometry, the

Figure 3.3: Laplace's law for a static droplet: (a) $A = 1.0 \times 10^{-2}$ and (b) $A = 4.0 \times 10^{-4}$.

Table 3.1: Parameters and evaluated errors of static droplet tests.

R	A	$E\%$
30	1.0×10^{-2}	0.77
25	1.0×10^{-2}	0.92
20	1.0×10^{-2}	1.6
30	4.0×10^{-4}	0.63
25	4.0×10^{-4}	0.77
20	4.0×10^{-4}	1.1

simulation using the D3Q27 lattice shows better result. Enhancing the lattice isotropy (from D3Q19 to D3Q27) contributes to reducing the spurious velocity.

3.3.2 Oscillating droplet

Oscillatory-droplet tests are performed to test the model validity in an unsteady case. The simulation setup and parameters for the present numerical tests follow [134], except for the interfacial-tension coefficient. A droplet with a prolate-spheroid shape is placed at the center of a computational domain discretized by a $41 \times 41 \times 41$ lattice. The droplet's minimum and maximum radii are 11 and 15, respectively. We set a density ratio of 4. The kinematic viscosity ratio is set to be unity ($\nu = \nu_r = \nu_b$), and gravity is neglected throughout the simulations. The parameters are ν and A (see Table 3.2). Parameter A is the same as the ones provided in

Figure 3.4: Influence of lattice isotropy on the spurious velocities: (a) D3Q19 [88] and (b) D3Q27.

Sec. 3.3.1.

The analytical solution of [135] is used for comparison with the computed time periods. The frequency of the n-th mode is given by

$$\omega_n = \omega_n^* - \frac{1}{2}\chi\omega_n^{*\frac{1}{2}} + \frac{1}{4}\chi^2, \tag{3.34}$$

where ω_n is Lamb's natural resonance frequency [136]

$$(\omega_n^*)^2 = \frac{n(n+1)(n-1)(n+2)}{R_e^3[n\rho_2 + (n+1)\rho_1]}\sigma. \tag{3.35}$$

Note that R_e in Eq. (3.35) is the equivalent radius of a droplet. Subscripts 1 and 2 refer to the dispersed and continuous phases, respectively, so they can be replaced by r and b in this paper. Parameter χ is given by

$$\chi = \frac{(2n+1)^2(\mu_1\mu_2\rho_1\rho_2)^{\frac{1}{2}}}{2^{\frac{1}{2}}R_e[n\rho_2 + (n+1)\rho_1][(\mu_1\rho_1)^{1/2} + (\mu_2\rho_2)^{1/2}]}. \tag{3.36}$$

We are only interested in the second mode ($n = 2$) here. The analytical expression for the time period is obtained by $T_{th} = 2\pi/\omega_2$.

Figure 3.5 shows the transient change of the oscillating droplet shapes with $\nu = 3.333 \times 10^{-3}$ and $A = 1.0 \times 10^{-2}$. After assuming a spherical shape at $t = 700$, the droplet becomes an oblate spheroid at $t = 1,400$. The configuration turns into a prolate spheroid at $t = 2,500$. Such a series of oscillations can be also seen in Ref. [134]

The interfacial location is measured, and the results are shown in Fig. 3.6 as a function of time. The interfacial locations are recorded per 10 time steps. Under higher-interfacial tension [Fig. 3.6(a)], all cases attenuate with oscillation regardless of the kinematic viscosity. The higher the kinematic viscosity, the earlier attenuation occurs. For the lower-interfacial-tension case [Fig. 3.6(b)], the timescale of oscillation becomes qualitatively longer; this tendency agrees with the theoretical expectation by Eqs. (3.34) and (3.35). Only in the case of $\nu = 1.667 \times 10^{-2}$ does the interfacial location reach an equilibrium spherical shape without a series of oscillations, as shown in Fig. 3.5. The effect of viscous damping distinguishes rather than the effect of interfacial tension in this case.

The simulation parameters and evaluated errors in the oscillating period are summarized in Table 3.2. The error E is calculated as

$$E = \frac{|T_{th} - T_{sim}|}{T_{th}}, \tag{3.37}$$

where T_{sim} is the measured oscillation period. Note that, in the case of $\nu = 1.667 \times 10^{-2}$ and $A = 4.0 \times 10^{-4}$, we cannot measure the oscillation period since no oscillation occurred. The maximum errors are 2.4% for $A = 1.0 \times 10^{-2}$ and 10.8% for $A = 4.0 \times 10^{-4}$, respectively. Throughout, the accuracy is better when the kinematic viscosity is lower. It is found that the accuracy of the low-interfacial-tension case is difficult to assess via droplet-oscillation tests; however, the tests show that the present lattice Boltzmann model can be applied to unsteady two-phase-flow simulations.

Figure 3.5: Typical snapshots of shape change of an initially elongated drop.

Figure 3.6: Time history of the interfacial location of an oscillating droplet: (a) $A = 1.0 \times 10^{-2}$ and (b) $A = 4.0 \times 10^{-4}$.

3.3.3 Rayleigh–Taylor instability

To assess the validity of the body force implementation [Eqs. (3.20) and (3.21)], the Rayleigh–Taylor instability is selected as the next numerical test. The Rayleigh–Taylor instability is a fundamental interfacial instability that is induced when a heavy fluid is placed over a light one subjected to a slightly disturbed interface in a gravitational field [73]. The Rayleigh–Taylor instability has received considerable attention owing to its extensive applications, e.g., in the fundamental process of melt jet breakup [18, 82]. To our knowledge, this is the first time a color-fluid model has been applied to the three-dimensional Rayleigh–Taylor instability.

We refer to the computational setup adopted in [137]. A schematic diagram of the computational setup is illustrated in Fig. 3.7. The top and bottom boundaries are no-slip walls; the

Table 3.2: Parameters and evaluated errors of oscillating droplet tests.

ν	A	σ	$E\%$
3.333×10^{-3}	1.0×10^{-2}	2.27×10^{-3}	0.60
6.667×10^{-3}	1.0×10^{-2}	2.31×10^{-3}	0.83
1.667×10^{-2}	1.0×10^{-2}	2.44×10^{-3}	2.4
3.333×10^{-3}	4.0×10^{-4}	9.07×10^{-5}	2.7
6.667×10^{-3}	4.0×10^{-4}	9.24×10^{-5}	10.8
1.667×10^{-2}	4.0×10^{-4}	9.78×10^{-5}	–

lateral boundaries are periodic. As in the manner of [137], the single-mode initial perturbation is initially imposed as

$$h(x, y) = 0.05W \left[\cos\left(\frac{2\pi x}{W}\right) + \left(\frac{2\pi y}{W}\right)\right], \tag{3.38}$$

at the mid-plane, where W is the width of the computational domain. The body force in Eq. (3.21) for this problem is incorporated as

$$\mathbf{F}(\mathbf{x}, t) = -\left(\rho(\mathbf{x}, t) - \frac{\rho_r^0 + \rho_b^0}{2}\right)\mathbf{g}, \tag{3.39}$$

with $\mathbf{g} = (0, 0, -g)$. The gravitational acceleration g is chosen to satisfy $(Wg)^{1/2} = 0.04$ [96]. The computational domain is set to be $W \times W \times 4W$ with $W = 128$. The domain's size resulted in a $128 \times 128 \times 512$ lattice.

The Atwood number

$$\mathrm{At} = \frac{\rho_r^0 - \rho_b^0}{\rho_r^0 + \rho_b^0}, \tag{3.40}$$

is fixed at 0.5 throughout the simulations. The interface tension is neglected; thus, the perturbed interface is expected to always be unstable in the inviscid case. The kinematic-viscosity ratio is set to unity. Another dimensionless group is the Reynolds number, defined as

$$\mathrm{Re} = \frac{\sqrt{Wg}W}{\nu}. \tag{3.41}$$

We use three patterns of Reynolds numbers: $\mathrm{Re} = 512$, $1,024$, and $5,120$.

Figure 3.7: Boundary conditions for the Rayleigh–Taylor instability. (a) The computational domain is discretized into an $128 \times 128 \times 512$ lattice and the single-mode initial perturbation is initially imposed. (b) The top and bottom are no-slip boundaries and the lateral boundaries are periodic.

Figure 3.8 shows the interfacial evolution of the Rayleigh–Taylor instability. The dimensionless time is given by

$$t^* = \frac{t}{\sqrt{W/g}}. \tag{3.42}$$

In the initial stages by $t^* = 2$, the Reynolds number dependence on the interfacial configuration is small. We can see the edge of the spike rolled up at $t^* = 3$. At later stages ($t^* = 3, 4$), the higher the Reynolds number is, the more unstable the interface becomes. For the $\mathrm{Re} = 5,120$ case [Fig. 3.8(c)], the interface becomes especially complicated. The Kelvin–Helmholtz instability appears conspicuously as the Reynolds number increases.

The time history of the positions of the bubble front, spike tip, and saddle point are calculated and plotted in Fig. 3.9(a) (see Fig. 3.8 for the locations of the bubble front, spike tip, and saddle point). As can be seen in Fig. 3.9(a), the differences in the positions are very small in our simulations, unlike the interface structure shown in Fig. 3.8. [137] pointed out that, when $\mathrm{Re} > 512$, the Reynolds number dependence is negligible. The present simulation, using the forcing scheme in Eqs. (3.20) and (3.21), shows a similar trend, supporting their suggestion.

Using the same computational setup and the parameters of [137], three-dimensional Rayleigh–

Figure 3.8: Interface evolution of the single-mode Rayleigh–Taylor instability with (a) Re = 512, (b) Re = 1,024, and (c) Re = 5,120. The Atwood number [Eq. (3.40)] is fixed at 0.5 in all simulations.

Figure 3.9: Time history of the positions of the bubble front, spike tip, and saddle point. (a) Reynolds number dependence of the positions with Re = 512 (dash-dotted line), Re = 1,024 (solid line), and Re = 5,120 (dotted line). (b) Comparison of the present study (solid line) and previous works with the lattice Boltzmann [137, 138] and phase-field methods [139], where all simulations are performed with Re = 512.

Taylor simulations were carried out using the lattice Boltzmann [138] and phase-field methods [139]. [138] used the phase-field-based MRT lattice Boltzmann model; [139] directly solved the Navier–Stokes–Cahn–Hilliard equations. Here, we compare our results with previous works [137–139]. Figure 3.9(b) shows the time histories of the positions at Re = 1,024 and At = 0.5. Comparing the results, the time changes of the bubble front and the saddle point are almost the same, irrespective of the method used. For the spike-tip evolution, no significant difference is observed among the lattice Boltzmann simulations. At later stages, these simulations are found to penetrate more deeply than the phase-field simulation. The difference between the lattice Boltzmann and phase-field methods is considered to arise from the different wall-boundary conditions implemented.

3.4 Liquid jet breakup

3.4.1 Setup

Figure 3.10 illustrates a schematic diagram of the boundary conditions for liquid-jet-breakup simulations. This computational setup is the same as that of [88], except for the outflow boundary. In the initial state, the computational domain is filled with blue-particle-distribution functions, f_i^b, with zero velocity. The boundaries consist of an inflow boundary, a wall boundary, and an outflow boundary. A circular inflow boundary is implemented at the top within $(x - x_c)^2 + (y - y_c)^2 < (D_{j0}/2)^2$, where x_c and y_c are central locations on the x-y plane. The uniform velocity u_{j0} is implemented, with the corresponding equilibrium functions given at this site. No artificial disturbances are considered at the inflow boundary. A wall boundary is implemented on the top (except for an inflow-boundary site) and on the lateral sites. A free-slip condition [140] is implemented as a wall boundary condition. At the outflow, a convective boundary condition [141] is used, in which the following convective equation for the distribution functions

$$\frac{\partial f_i^k}{\partial t} + U_c \frac{\partial f_i^k}{\partial z} = 0, \text{ at } z = N, \tag{3.43}$$

is solved, where N is the node on the outflow boundary. Following [141], we set two ghost-nodes $N+1$ and $N+2$. The discretized form can be given by the first-order implicit scheme,

$$\begin{aligned} & f_i^k(x, y, N, t + \delta_t) \\ & = \frac{f_i^k(x, y, N, t) + \lambda f_i^k(x, y, N-1, t + \delta_t)}{1 + \lambda}, \end{aligned} \tag{3.44}$$

where $\lambda = U_c(t + \delta_t)\delta_t/\delta_x$. For the convective velocity normal to the outflow boundary U_c, several choices can be considered, e.g., the local velocity, the average velocity, and maximum velocity [142]. Through some numerical tests, we determine that the local velocity is suitable to the present system, that is,

$$U_c(x, y, N, t) = u_z(x, y, N-1, t), \tag{3.45}$$

Figure 3.10: Boundary conditions for a liquid-jet simulation. (a) The computational domain is discretized into a $8D_{j0} \times 8D_{j0} \times 20D_{j0}$ lattice. (b) A circular inflow boundary with a uniform velocity u_{j0} is implemented at the top within D_{j0}.

where $u_z(\mathbf{x}, t) = u_z(x, y, z, t)$ is the z-direction component of fluid velocity $\mathbf{u}$.

The body force in Eq. (3.21) for the liquid-jet simulations is set as

$$\mathbf{F}(\mathbf{x}, t) = \left(\rho(\mathbf{x}, t) - \rho_b^0\right) \mathbf{g}, \tag{3.46}$$

with $\mathbf{g} = (0, 0, g)$. Eq. (3.46) means that the gravitational force acts only in the dispersed phase [100].

3.4.2 Comparison with experiments

Using the lattice Boltzmann model developed in Sec. 3.2 and the boundary conditions provided in Sec. 3.4.1, we perform here numerical simulations of liquid-jet breakup. The parameters for this simulation are set to be exactly the same as in the experiments [88], and the results are compared. In the target experiments, a glycerin-water-mixture jet was injected into a silicon-oil pool. These test fluids were immiscible with each other. In [88], the lattice Boltzmann simulation was also carried out using the MRT color-fluid model based on the D3Q19 lattice.

Table 3.3: Conditions of the experiments and simulations.

	Experiment and present simulation	Previous simulation[1]
γ	1.4	1.4
η	4.2	1.0
Re	3.4×10^3	3.4×10^3
We	2.2×10^2	2.2×10^2
Fr	8.5	8.5

In the framework of linear theory, one can choose the following dimensionless groups to describe the problem [43]

$$\gamma = \frac{\rho_j}{\rho_c}, \tag{3.47}$$

$$\eta = \frac{\nu_j}{\nu_c}, \tag{3.48}$$

$$\mathrm{Re} = \frac{\rho_j u_{j0} D_{j0}}{\mu_j}, \tag{3.49}$$

$$\mathrm{We} = \frac{\rho_j u_{j0}^2 D_{j0}}{\sigma}, \tag{3.50}$$

$$\mathrm{Fr} = \frac{u_{j0}^2}{g D_{j0}}. \tag{3.51}$$

The conditions of the experiments and simulations are summarized in Table 3.3 and in the dimensionless groups in Eqs. (3.47)–(3.51). The parameters for the target experiments and the present simulation match exactly. In Table 3.3, only the kinematic-viscosity ratio η in the previous simulation differs from the others. This was because the previous D3Q19 MRT color-fluid model could not maintain the numerical stability when $\eta = 4.2$. Note that the present lattice Boltzmann model remains stable under the condition in Table 3.3.

According to the grid refinement study in [88], we determine the inlet diameter $D_{j0} = 25$ and the computational domain $8D_{j0} \times 8D_{j0} \times 20D_{j0}$. In this paper, the density of the dispersed phase $\rho_j (= \rho_r^0)$ and the inlet velocity u_{j0} are set to be 1.0 and 0.1, respectively. Other parameters can be determined using the relations of dimensionless groups [Eqs. (3.47)–(3.51)] in lattice units: $\rho_c = \rho_b^0 = 0.70$, $\sigma = 1.1 \times 10^{-3}$, $\nu_j = \nu_r = 7.4 \times 10^{-4}$, $\nu_c = \nu_b = 1.8 \times 10^{-4}$, and $g = 4.7 \times 10^{-5}$.

Figure 3.11 shows the interface evolution of the present simulation. Time is non-dimensionalized

Figure 3.11: Interface evolution of liquid-jet breakup under the same conditions as the target experiment: $\gamma = 1.4$, $\eta = 4.2$, $\mathrm{Re} = 3.4 \times 10^3$, $\mathrm{We} = 2.2 \times 10^2$, and $\mathrm{Fr} = 8.5$. The computational domain is set to be $200 \times 200 \times 500$.

by the inlet diameter D_{j0} and the inlet velocity u_{j0} as

$$t^* = \frac{t}{D_{j0}/u_{j0}}, \tag{3.52}$$

in the liquid-jet-breakup simulations. At $t^* = 3$, a mushroom-like head shape is created. At $t^* = 9$ to 15, the interface of the jet becomes unstable. Observation shows that this interfacial instability is triggered by the return flow of a mushroom head generated in an initial stage of jet injection. Such a characteristic flow pattern leads to the onset of interfacial instability, although no artificial spatial or temporal perturbation has been assumed in the initial or boundary conditions. At later stages ($t^* = 30$ and 72), the jet's leading-edge collapses, and the entrainment behavior, namely, the droplet formation from the side of the jet, is also observed. Finally, the liquid core becomes asymmetric, as can be seen at $t^* = 72$. Such a series of processes is similar to an experimental observation [88].

The history of jet penetration can be evaluated by both experiments and simulations. A comparison between experiments and simulations in terms of the position of the jet's leading-edge is provided in Fig. 3.12, where the position is normalized by the inlet diameter D_{j0}. Focusing on the results of lattice Boltzmann simulations, the time histories are almost the same until $t^* = 15$. Afterward, the differences in positions gradually increase and the present

Figure 3.12: Time history of jet penetration: the present simulation (solid line), previous simulation (dashed line) [88], and experimental result (square symbol) [88].

simulation results tend to be close to the experimental data. This is thought to be due to the influence of ambient viscosity. In the present simulation, the lower viscosity of the surrounding fluid facilitates the penetration of the jet. The simulation using the developed lattice Boltzmann model shows a better agreement with the experimental data than that using the previous D3Q19 model [88]. The enhanced numerical stability of the model enables us to simulate more realistic conditions.

3.4.3 Transition of breakup regimes

Recently, Saito et al. [82] have classified jet breakup regimes in liquid-liquid systems based on observations. This was an extension of Ohnesorge's classification for liquid-gas systems [45–47]. The classified breakup regimes are as follows: 0–dripping, I–varicose breakup, II–sinuous breakup, and III–atomization. Regime II was further divided into two sub-regimes: IIa–sinuous *without* entrainment, IIb–sinuous *with* entrainment. On the basis of the observations and phenomenological considerations, the flow-transition criteria were derived in Ref. [82]:

$$\mathrm{Oh} = 2.8\mathrm{Re}^{-1}, \tag{3.53}$$

Table 3.4: Simulation conditions for dimensionless numbers to be investigated.

	Re	Oh	$\mathrm{We} = (\mathrm{Re} \cdot \mathrm{Oh})^2$
Ref. case	3.4×10^3	4.4×10^{-3}	2.2×10^2
Case 1	4.6×10^2	4.4×10^{-3}	4.1
Case 2	3.4×10^3	3.0×10^{-3}	1.0×10^4

for Regimes I and II, and

$$\mathrm{Oh} = 22\mathrm{Re}^{-1}, \tag{3.54}$$

for Regimes II and III, where the Reynolds number Re is defined as in Eq. (3.49) and the Ohnesorge number Oh can be given by Eqs. (3.49) and (3.50) as $\mathrm{Oh} = \mathrm{We}^{1/2}/\mathrm{Re}$. By using the above transition criteria, one can predict the breakup regimes of an immiscible liquid-liquid jet from initial parameters. With the present lattice Boltzmann model, we assess here the potential for the reproducibility of the breakup regimes.

The simulation conditions are summarized in Table 3.4. The corresponding values on the dimensionless diagram are shown in Fig. 3.13. The description "Ref. case" represents the same condition as mentioned in Sec. 3.4.2. As can be seen, the simulation results provided in the previous section are in Regime II, where sinuous breakup with or without entrainment is expected. The other parameters, namely, density ratio γ, viscosity ratio η, and Froude1 number Fr, are set to be the same as in Table 3.3. In Case 1, Re is decreased by increasing the jet viscosity ν_j and decreasing jet velocity u_{j0} while Oh is fixed at the same value as in the Ref. case. As can be seen in Fig. 3.13, Case 1 is in Regime 0 or I. It is expected that the dripping- or varicose-breakup regimes will appear. In Case 2, Re is fixed at the same value as in the Ref. case while Oh is increased by decreasing the interfacial tension σ. Since Case 2 is in Regime III in Fig. 3.13, it is expected that atomization will appear. Note that it is impossible to change only *one* parameter in the experimental procedures; only the effect of a focused parameter can be taken into account in the numerical simulations.

Figure 3.14 shows the simulation results for Case 1 in Table 3.4. We set the inlet diameter and velocity to $D_{j0} = 15$ and $u_{j0} = 0.05$, respectively. The other parameters are as follows: $\sigma = 9.1 \times 10^{-3}$, $\nu_j = \nu_r = 1.6 \times 10^{-3}$, $\nu_c = \nu_b = 3.9 \times 10^{-4}$, and $g = 2.0 \times 10^{-5}$. At

Figure 3.13: Location of simulation parameters on the regime map proposed in [82].

$t^* = 17$, the swollen part is generated around the inlet. The mushroom-like head does not appear. The swollen part moves downward with the growth of the neck part at $t^* = 26$, and the corresponding part breaks up into a single droplet at $t^* = 30$. At this time, the following swollen part is generated on a liquid column. The formation of the swollen part, the growth of the neck part, and breakup into a single droplet are observed through simulation. In this case, the so-called satellite-droplet formation just after the primary-droplet formation is not observed. According to the experimental data in liquid-liquid systems [82], the average size of satellite droplet is about 0.3 times smaller than the nozzle diameter D_{j0}. To reproduce the satellite-droplet formation, the higher resolution would be required. The order of the droplet sizes has the same extent as the inlet diameter or is larger than it. This series of processes is a characteristic of the so-called pinch-off behavior, which is similar to the scenario considered in Rayleigh's breakup for a liquid column [64]. This corresponds to the varicose breakup or Regime I in Fig. (3.13). The characteristics of the varicose breakup regime are reproduced by the present lattice Boltzmann simulation.

Figure 3.15 shows the simulation results for Case 2 in Table 3.4. We set the inlet diameter and velocity to $D_{j0} = 30$ and $u_{j0} = 0.1$, respectively. The other parameters are as follows:

Figure 3.14: Simulation results of Case 1 in Table 3.4: $\gamma = 1.4$, $\eta = 4.2$, Re $= 4.6 \times 10^2$, We $= 4.1$, and Fr $= 8.5$. The computational domain is set to be $120 \times 120 \times 300$.

$\sigma = 3.0 \times 10^{-5}$, $\nu_j = \nu_r = 8.8 \times 10^{-4}$, $\nu_c = \nu_b = 2.1 \times 10^{-4}$, and $g = 3.9 \times 10^{-5}$. As in the Ref. case, a mushroom-like head appears at $t^* = 8$. Through $t^* = 18$–33, the jet continues penetration with active entrainment. The sizes of the generated droplets are much smaller than the inlet diameter, and the number of droplets is much greater than in the Ref. case and Case 1. Owing to the entrainment from a jet interface, the liquid column is fully covered, and it is difficult to identify this column in the snapshots shown in Fig. 3.15. The series of processes corresponds to the atomization or Regime III in Fig. (3.13). The characteristics of the atomization regime are also reproduced by the present lattice Boltzmann simulations.

Before summarizing the simulation results, let us mention the jet-breakup regime shown in Fig. 3.11 again. During the penetration, the jet maintains an axisymmetric configuration. This is reasonable because the computational setup described in Sec. 3.4.1 is exactly symmetric on the x-y plane. However, the jet column finally winds and becomes an asymmetric shape (see $t^* = 72$ in Fig. 3.11). In addition, the entrainment also can be seen in this case. This type of breakup regime corresponds to Regime IIb in Fig. (3.13). This implies that the physical balance among hydrodynamic forces, including inertia, viscous force, and interfacial-tension force can be naturally reproduced via the lattice Boltzmann simulation. This fact numerically supports the validity of the dimensionless diagram proposed in Ref. [82].

Figure 3.15: Simulation results of Case 2 in Table 3.4: $\gamma = 1.4$, $\eta = 4.2$, $\mathrm{Re} = 3.4 \times 10^3$, $\mathrm{We} = 1.0 \times 10^4$, and $\mathrm{Fr} = 8.5$. The computational domain is set to be $240 \times 240 \times 600$.

Finally, we summarize the simulation results in the dimensionless diagram of Fig. 3.13. Typical snapshots of liquid-jet breakup from Figs. 3.11, 3.14, and 3.15 are summarized in Fig 3.16. The characteristics of varicose breakup (Regime I), sinuous breakup (Regime II), and atomization (Regime III) are successfully simulated. On the breakup regimes, we can conclude that the lattice Boltzmann model developed in Sec. 3.2 under the boundary conditions described in Sec. 3.4.1 well reproduce the breakup characteristics expected by the regime map proposed in Ref. [82].

3.5 Summary

In this Chapter, a three-dimensional lattice Boltzmann model for immiscible two-phase flows was developed in the framework of a D3Q27 lattice. An MRT collision operator for the D3Q27 lattice [117,122] was introduced. The choice of relaxation parameters optimized by [118] greatly improved the numerical stability of the model. A generalized perturbation operator [108] and an enhanced equilibrium distribution function [111] were also successfully incorporated into the present D3Q27 model.

Using the formulated lattice Boltzmann model, three types of numerical tests were carried out:

Figure 3.16: Summary of the present results of liquid-jet-breakup simulations in the dimensionless diagram for liquid-liquid systems

a static droplet, an oscillating droplet, and the Rayleigh–Taylor instability. The static-droplet test shows that the measured pressure difference satisfied the Laplace law, and the interfacial tension agreed well with that predicted by Eq. (3.24) within a maximum error of 1.6%. The oscillating-droplet test was performed to compare the oscillation period with the analytical solution. For the high-interfacial-tension case, the error with the analytical solution was within 2.4%. Under low interfacial tension, a droplet reached equilibrium without oscillations in the most viscous case; the maximum error for the available data was 10.8%. The Rayleigh–Taylor simulations were performed with a computational setup and parameters that were strictly similar to those of [137]. The positions of the bubble front, spike tip, and saddle point were measured for comparison with previous works using the lattice Boltzmann [137,138] and phase-field methods [139]. The time changes of the bubble front and the saddle point were almost the same, irrespective of the method used. At later stages, a little difference between the lattice Boltzmann and phase-field simulations was observed for the spike-tip evolution owing to the difference in implementation of the wall-boundary conditions.

The developed model was applied to liquid-jet-breakup simulations. First, we chose the parameters to match the experimental conditions [88]. The five dimensionless groups were employed

to determine the physical properties in lattice units. The developed D3Q27 model maintained numerical stability throughout the simulations; the previous work using a D3Q19 color-fluid lattice Boltzmann model [88] failed to simulate stably under the same conditions. The present results showed that the characteristic interfacial evolution captured the experimental results. A mushroom-like head was formed at the early stages; later, the configuration of the liquid core transitioned from asymmetric to axisymmetric, and interface entrainment also naturally occurred. The time history of the jet's leading-edge was compared with that obtained by experiment. Quantitative comparisons agreed well with the experimental data.

By choosing the parameters based on the regime map for jet breakup in liquid-liquid systems [82], we performed simulations to evaluate the reproducibility of the regime map. In the varicose regime, pinch-off-type breakup, i.e., the droplet formation in the tip of the liquid column, occurred. Satellite-drop formation was not confirmed in the present simulation. In the atomization regime, entrainment from the liquid column was distinguished. The liquid column was fully covered with entrainment droplets, which were much smaller than the inlet diameter. In conclusion, the breakup regimes appearing in the simulations successfully reproduced the predicted regimes, including the varicose, sinuous, and atomization regimes.

Chapter 4

Hydrodynamic Melt-Jet Simulations

4.1 Literature review

Liquid–liquid-jet systems can be found in several fields, e.g., chemical processing [51, 53, 55] and CO_2 storage in oceans [57, 79]. In the nuclear engineering field, it is important to fully understand the interactions between melt and coolant when designing nuclear reactor safety. As a result, the dispersion of liquid metal in water has been extensively investigated in the literature [18,23,24,143], going all the way back to G.I. Taylor's classic experiment with mercury and water [144]. In these experiments, high-temperature melt and water are often used to simulate the core melt materials and coolant. Using the experimental facility at University of Tsukuba (UT), Matsuo *et al.* [26, 143] injected molten alloy with a melting point of 78 °C (U-Alloy78) into a water pool, using high-speed visualization to help understand the mechanism behind melt-jet breakup in water. The experiments of [2], called FARO-TERMOS (FT), are unique in that they used a liquid sodium coolant: they poured pure molten UO_2 into a pool of liquid sodium. The fragment size analysis showed that fine fragments were generated by interactions between the molten UO_2 and the liquid sodium, but they obtained little physical insight into the breakup behavior because liquid sodium is not transparent. In this paper, our simulation targets are these two melt-coolant experiments [2, 143]; we call them the UT and FT experiments, respectively.

The complexity of the phenomena involved in melt-coolant interactions means it is difficult to understand all the mechanisms simultaneously. Investigating the hydrodynamic interactions separately will thus help us to better understand the fundamental melt-jet breakup processes. Several researchers have already attempted to simulate jet breakup behavior using the volume-of-fluid method (see, e.g., [41,145,146]). Compared with macroscopic CFD methods, which are based on the Navier–Stokes equations, the LB method, which uses mesoscopic kinetic equations, has several advantages, such as making it easy to incorporate mesoscale physics like interfacial breakup and coalescence. In addition, the computational cost of simulating realistic fluid flows is far more reasonable than with particle-based methods (e.g., molecular dynamics).

The so-called BGK [147] approximation refers to this simplest form of the collision operator, which forces all populations to relax towards an equilibrium state with the same rate. Despite its simplicity and phenomenal popularity, the BGK LB method is known to suffer from numerical instability under high-Re (low-viscosity) conditions. One way to overcome this issue is to modify the collision operator [112]. For example, MRT collision operators [113–115] have been widely used, even for multiphase flows, to enhance numerical stability and accuracy and reduce spurious currents near the interface. Later, [148] proposed a new collision operator based on the relaxation of central moments (CMs), that can be obtained by shifting the lattice directions according to the local fluid velocity. Many studies have developed this approach to fully exploit the properties of CM-based schemes (see, e.g., De Rosis [149] and references therein). For multiphase flows, [150] first introduced CMs into the pseudopotential multiphase LB model. [151] also introduced CMs into the CG model with unit density ratio. Very recently, [152] formulated a CM-based LB scheme for coupled Cahn–Hilliard–Navier–Stokes equations. De Rosis has consistently adopted nonorthogonal CMs [153–157], which are characterized by straightforward derivation and easy practical implementation. Moreover, his analytical formulation is very general, as it can be extended to any lattice velocity space.

In this chapter, we present a three-dimensional CG LB model and apply it to hydrodynamic simulations of melt-jet breakup. We develop a lattice Boltzmann (LB) model for immiscible two-phase flow simulations with central moments (CMs). This successfully combines a three-dimensional nonorthogonal CM-based LB scheme [154] with our previous color-gradient LB

model [124]. Hydrodynamic melt-jet breakup simulations show that the proposed model is significantly more stable, even for flow with extremely high Reynolds numbers, up to $O(10^6)$. This enables us to investigate the phenomena expected under actual reactor conditions.

4.2 Methodology

The LB model presented here is based on our previous MRT CG model [124]. The most significant difference between the current and previous models is the introduction of De Rosis' nonorthogonal CMs [153, 154].

In the current three-dimensional LB model, the distribution functions move on a three-dimensional 27-velocity (D3Q27) lattice [140]. We adopt a lattice speed $c = \delta_x/\delta_t = 1$, where x and t are the lattice spacing and time step, respectively. The lattice velocities $\mathbf{c}_i = [|c_{ix}\rangle, |c_{iy}\rangle, |c_{iz}\rangle]$ are defined as follows:

$$\begin{aligned}
|c_{ix}\rangle =& [0, 1, -1, 0, 0, 0, 0, 1, -1, 1, -1, 0, 0, 0, 0, 1, -1, 1, -1, \\
& 1, -1, 1, -1, 1, -1, -1, 1]^\top, \\
|c_{iy}\rangle =& [0, 0, 0, 1, -1, 0, 0, 1, -1, -1, 1, 1, -1, 1, -1, 0, 0, 0, 0, \\
& 1, -1, 1, -1, -1, 1, 1, -1]^\top, \\
|c_{iz}\rangle =& [0, 0, 0, 0, 0, 1, -1, 0, 0, 0, 0, 1, -1, -1, 1, 1, -1, -1, 1, \\
& 1, -1, -1, 1, 1, -1, 1, -1]^\top,
\end{aligned} \tag{4.1}$$

where i $(= 0, 1, \ldots, 26)$ represents the lattice-velocity directions and the superscript "$\top$" is the transpose operator. Here, we employ Dirac's bracket notation, where the "bra" operator $\langle\cdot|$ denotes a row vector along one of the lattice-velocity directions and the "ket" operator $|\cdot\rangle$ denotes a column vector.

The model represents two immiscible fluids as red and blue fluids. Distribution functions f_i^k represent the fluids k, where $k = r$ and b denote "red" and "blue," respectively, and i is the lattice-velocity direction. The total distribution function is defined as $f_i = f_i^r + f_i^b$, and the

evolution is expressed by the following LB equation:

$$f_i^k(\mathbf{x} + \mathbf{c}_i\delta_t, t + \delta_t) - f_i^k(\mathbf{x}, t) = \Omega_i^k(\mathbf{x}, t), \tag{4.2}$$

where $\mathbf{x} = [x, y, z]$ and t are the position and time, respectively. The collision operator Ω_i^k is made up of three sub-operators [120]:

$$\Omega_i^k = (\Omega_i^k)^{(3)} \left[(\Omega_i^k)^{(1)} + (\Omega_i^k)^{(2)}\right], \tag{4.3}$$

where $(\Omega_i^k)^{(1)}$, $(\Omega_i^k)^{(2)}$, and $(\Omega_i^k)^{(3)}$ are the single-phase collision, perturbation, and recoloring operators, respectively. As in Ref. [109], the single-phase and perturbation operators are applied using the color blind distribution function f_i.

In this paper, we adopt the general MRT (GMRT) framework [158, 159] to describe the single-phase collision operator with nonorthogonal CMs, due to the simplicity of its relationship to the MRT and SRT collision operators. It should be noted that [159] propose a simplified version of De Rosis' nonorthogonal CMs [153, 154], showing a significantly reduced computational cost. In the GMRT framework, the single-phase collision operator can be written as

$$(|\Omega\rangle)^{(1)} = -\mathbf{M}^{-1}\mathbf{N}^{-1}\mathbf{KNM}\left(|f\rangle - |f^{(e)}\rangle\right) + |F\rangle, \tag{4.4}$$

where $\mathbf{M}$, $\mathbf{N}$, and $\mathbf{K}$ are the transformation, shift [158–160], and relaxation matrices, respectively. The density of the fluid k is given by

$$\rho_k = \sum_i f_i^k. \tag{4.5}$$

The total fluid density is given by $\rho = \sum_k \rho_k$, and the total momentum is defined as

$$\rho\mathbf{u} = \sum_i f_i\mathbf{c}_i + \frac{1}{2}\mathbf{F}\delta_t, \tag{4.6}$$

where $\mathbf{F}$ is the body force. Note that, in Eq. (4.6), the local velocity has been modified to incorporate the spatially varying body force [121]. To model the single-phase collision operator

[Eq. (4.4)], we use the nonorthogonal CMs proposed by De Rosis [154], namely,

$$\mathbf{NM} = \mathbf{T} = \begin{bmatrix} \langle |\mathbf{c}_i|^0 | \\ \langle \bar{c}_{ix} | \\ \langle \bar{c}_{iy} | \\ \langle \bar{c}_{iz} | \\ \langle \bar{c}_{ix}\bar{c}_{iy} | \\ \langle \bar{c}_{ix}\bar{c}_{iz} | \\ \langle \bar{c}_{iy}\bar{c}_{iz} | \\ \langle \bar{c}_{ix}^2 - \bar{c}_{iy}^2 | \\ \langle \bar{c}_{ix}^2 - \bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2 + \bar{c}_{iy}^2 + \bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}\bar{c}_{iy}^2 + \bar{c}_{ix}\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy} + \bar{c}_{iy}\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iz} + \bar{c}_{iy}^2\bar{c}_{iz} | \\ \langle \bar{c}_{ix}\bar{c}_{iy}^2 - \bar{c}_{ix}\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy} - \bar{c}_{iy}\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iz} - \bar{c}_{iy}^2\bar{c}_{iz} | \\ \langle \bar{c}_{ix}\bar{c}_{iy}\bar{c}_{iz} | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}^2 + \bar{c}_{ix}^2\bar{c}_{iz}^2 + \bar{c}_{iy}^2\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}^2 + \bar{c}_{ix}^2\bar{c}_{iz}^2 - \bar{c}_{iy}^2\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}^2 - \bar{c}_{ix}^2\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}\bar{c}_{iz} | \\ \langle \bar{c}_{ix}\bar{c}_{iy}^2\bar{c}_{iz} | \\ \langle \bar{c}_{ix}\bar{c}_{iy}\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}\bar{c}_{iy}^2\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}\bar{c}_{iz}^2 | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}^2\bar{c}_{iz} | \\ \langle \bar{c}_{ix}^2\bar{c}_{iy}^2\bar{c}_{iz}^2 | \end{bmatrix}, \tag{4.7}$$

where $|\bar{c}_{ix}\rangle = |c_{ix} - u_x\rangle$, $|\bar{c}_{iy}\rangle = |c_{iy} - u_y\rangle$, and $|\bar{c}_{iz}\rangle = |c_{iz} - u_z\rangle$. All the components of the vector $|\mathbf{c}_i|^0$ are equal to 1. The transformation matrix $\mathbf{M}$, whose components are constant, transforms the distribution functions into raw moments. The shift matrix $\mathbf{N}$, a lower-triangular matrix with components given by the macroscopic velocity $\mathbf{u}$, transforms the raw moments into CMs and can be written as $\mathbf{N} = \mathbf{T}\mathbf{M}^{-1}$. The practical forms of $\mathbf{M}$, $\mathbf{M}^{-1}$, $\mathbf{N}$, and $\mathbf{N}^{-1}$ are given in Ref. [161].

The relaxation matrix $\mathbf{K}$ is a diagonal matrix given by

$$\begin{aligned}\mathbf{K} = \mathrm{diag}[&s_0, s_1, s_1, s_1, s_{2\nu}, s_{2\nu}, s_{2\nu}, s_{2\nu}, s_{2\nu}, s_{2b},\\ &s_3, s_3, s_3, s_3, s_3, s_3, s_3,\\ &s_4, s_4, s_4, s_4, s_4, s_4, s_5, s_5, s_5, s_6],\end{aligned} \tag{4.8}$$

where the elements are the moments' relaxation times. If $s_0 = \ldots = s_i = \ldots = s_6$, the model reduces to the BGK (single-relaxation-time) model. The subscripts represent the orders (e.g., 2 means second-order). The parameters $s_{2\nu}$ and s_{2b} satisfy the following relations:

$$\nu = \frac{1}{3}\left(\frac{1}{s_{2\nu}} - \frac{1}{2}\right), \tag{4.9}$$

$$\zeta = \frac{1}{3}\left(\frac{1}{s_{2b}} - \frac{1}{2}\right), \tag{4.10}$$

where ν and ζ are the kinematic and bulk viscosities, respectively. Here, we use $s_0 = s_1 = 0$ and $s_{2b} = s_3 = s_4 = s_5 = s_6 = 1$.

For the single-phase collision operator, we use the following enhanced equilibrium distribution function [111] in three-dimensions [124]:

$$\begin{aligned}f_i^{(e)}(\rho, \mathbf{u}) =& \rho\left\{\varphi_i + w_i\left[\frac{3}{c^2}(\mathbf{c}_i\cdot\mathbf{u}) + \frac{9}{2c^4}(\mathbf{c}_i\cdot\mathbf{u})^2\right.\right.\\ &\left.\left. - \frac{3}{2c^2}\mathbf{u}^2 + \frac{9}{2c^6}(\mathbf{c}_i\cdot\mathbf{u})^3 - \frac{9}{2c^4}(\mathbf{c}_i\cdot\mathbf{u})\mathbf{u}^2\right]\right\} + \Phi_i.\end{aligned} \tag{4.11}$$

If $\Phi_i = 0$, Eq. (4.11) reduces to the standard form of an equilibrium distribution function up to third order. Using Eq. (4.11) improves the Galilean invariance of the variable density and

viscosity ratios under the assumption of a small pressure gradient [111, 125, 126].

The weights, w_i, are those of a standard D3Q27 lattice [119], as follows:

$$w_i = \begin{cases} 8/27, & |\mathbf{c}_i|^2 = 0, \\ 2/27, & |\mathbf{c}_i|^2 = 1, \\ 1/54, & |\mathbf{c}_i|^2 = 2, \\ 1/216, & |\mathbf{c}_i|^2 = 3. \end{cases} \tag{4.12}$$

In addition, for a D3Q27 lattice, we can derive

$$\varphi_i = \begin{cases} \bar{\alpha}, & |\mathbf{c}_i|^2 = 0, \\ 2(1-\bar{\alpha})/19, & |\mathbf{c}_i|^2 = 1, \\ (1-\bar{\alpha})/38, & |\mathbf{c}_i|^2 = 2, \\ (1-\bar{\alpha})/152, & |\mathbf{c}_i|^2 = 3, \end{cases} \tag{4.13}$$

and

$$\Phi_i = \begin{cases} -3\bar{\nu}(\mathbf{u}\cdot\nabla\rho)/c, & |\mathbf{c}_i|^2 = 0, \\ +16\bar{\nu}(\mathbf{G} : \mathbf{c}_i \otimes \mathbf{c}_i)/c^3, & |\mathbf{c}_i|^2 = 1, \\ +4\bar{\nu}(\mathbf{G} : \mathbf{c}_i \otimes \mathbf{c}_i)/c^3, & |\mathbf{c}_i|^2 = 2, \\ +1\bar{\nu}(\mathbf{G} : \mathbf{c}_i \otimes \mathbf{c}_i)/c^3, & |\mathbf{c}_i|^2 = 3, \end{cases} \tag{4.14}$$

where $\otimes$ is the tensor product, ":" represents tensor contraction, and $\bar{\nu}$ is the kinematic viscosity, which interpolates between the red and blue viscosities ν_r and ν_b via the following harmonic mean [109, 162, 163]:

$$\frac{1}{\bar{\nu}} = \frac{1+\phi}{2}\frac{1}{\nu_r} + \frac{1-\phi}{2}\frac{1}{\nu_b}. \tag{4.15}$$

Here, ϕ is the order parameter that distinguishes the two components in the multicomponent flow, defined as [102]

$$\phi = \left(\frac{\rho_r}{\rho_r^0} - \frac{\rho_b}{\rho_b^0}\right) \Big/ \left(\frac{\rho_r}{\rho_r^0} + \frac{\rho_b}{\rho_b^0}\right), \tag{4.16}$$

where the superscript "0" indicates the initial density value at the beginning of the simulation [111]. The order parameter value $\phi = 1, -1$, and 0 correspond to a purely red fluid, a purely blue fluid, and the interface between the two, respectively [120]. In the D3Q27 lattice framework, the tensor $\mathbf{G}$ in Eq. (4.14) is defined as

$$\mathbf{G} = \frac{1}{48}\left[\mathbf{u} \otimes \nabla\rho + (\mathbf{u} \otimes \nabla\rho)^{\top}\right]. \tag{4.17}$$

As established in Ref. [91], in order to obtain a stable interface, we must take the fluid density ratio γ into account, which is defined as follows:

$$\gamma = \frac{\rho_r^0}{\rho_b^0} = \frac{1-\alpha_b}{1-\alpha_r}. \tag{4.18}$$

The fluid pressures are given by an isothermal equation of state for the D3Q27 lattice:

$$p = \rho\left(c_s^k\right)^2 = \rho_k \frac{9(1-\bar{\alpha})}{19} c^2, \tag{4.19}$$

where $\bar{\alpha}$ interpolates between α_r and α_b as follows [109]

$$\bar{\alpha} = \frac{1+\phi}{2}\alpha_r + \frac{1-\phi}{2}\alpha_b. \tag{4.20}$$

In this paper, we set $\alpha_b = 8/27$, for which $c_s^b = 1/\sqrt{3}$ [88, 125].

The term $|F\rangle$ in Eq. (4.4) is a discrete forcing term that accounts for the body force $\mathbf{F}$. In the GMRT framework [158], it is

$$|F\rangle = \mathbf{M}^{-1}\mathbf{N}^{-1}\left(\mathbf{I} - \frac{1}{2}\mathbf{K}\right)\mathbf{N}\mathbf{M}\,|F'\rangle\,, \tag{4.21}$$

where $\mathbf{I}$ is the unit matrix, $|F\rangle = (F_0, F_1, \ldots, F_{26})^{\top}$, and $|F'\rangle = (F_0', F_1', \ldots, F_{26}')^{\top}$ is given by

$$|F'\rangle = w_i\left[3\frac{\mathbf{c}_i - \mathbf{u}}{c^2} + 9\frac{(\mathbf{c}_i \cdot \mathbf{u})\mathbf{c}_i}{c^4}\right] \cdot \mathbf{F}\delta_t. \tag{4.22}$$

Equations (4.21) and (4.22) reduce to the MRT forcing scheme [128] when we use $\mathbf{N} = \mathbf{I}$, and to

Guo *et al.*'s original forcing scheme [121] when we use a single-relaxation time (not necessarily required that $\mathbf{N} = \mathbf{M} = \mathbf{I}$).

To model the interfacial tension, we use the generalized perturbation operator derived in Ref. [108], based on the idea of continuum surface force (CSF) [129], and follow [105] to obtain the interfacial tension as follows:

$$(\Omega_i)^{(2)} = \frac{A}{2}|\nabla\phi| \left[w_i \frac{(\mathbf{c}_i \cdot \nabla\phi)}{|\nabla\phi|^2} - B_i \right]. \tag{4.23}$$

Equation (4.23) takes the correct form for an interfacial tension force in the Navier–Stokes equations when the lattice-specific variables B_i are chosen correctly. We have derived the following B_i values for the D3Q27 lattice framework:

$$B_i = \begin{cases} -(10/27)c^2, & |\mathbf{c}_i|^2 = 0, \\ +(2/27)c^2, & |\mathbf{c}_i|^2 = 1, \\ +(1/54)c^2, & |\mathbf{c}_i|^2 = 2, \\ +(1/216)c^2, & |\mathbf{c}_i|^2 = 3. \end{cases} \tag{4.24}$$

In this model, the interfacial tension can be given directly by

$$\sigma = \frac{4}{9} A \tau c^4 \delta_t, \tag{4.25}$$

where τ is the relaxation time and we have assumed that $A = A_r = A_b$. The parameter A controls the interfacial tension strength σ.

Although the perturbation operator $(\Omega_i^k)^{(2)}$ generates the interfacial tension, it does not guarantee the two fluids are immiscible. To promote phase segregation and maintain the interface, we apply the following recoloring operators [104, 106, 130]

$$(\Omega_i^r)^{(3)} = \frac{\rho_r}{\rho} f_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\theta_i) f_i^{(e)}(\rho, \mathbf{0}), \tag{4.26}$$

$$(\Omega_i^b)^{(3)} = \frac{\rho_b}{\rho} f_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\theta_i) f_i^{(e)}(\rho, \mathbf{0}), \tag{4.27}$$

where θ_i is the is the angle between $\nabla\phi$ and $\mathbf{c}_i$, defined by

$$\cos(\theta_i) = \frac{\mathbf{c}_i \cdot \nabla\phi}{|\mathbf{c}_i||\nabla\phi|}. \tag{4.28}$$

Here, we set the parameter β to 0.7 to reproduce the correct interfacial behavior with as narrow an interface as possible [108, 130, 164].

4.3 Static droplet tests

In this section, we carry out static droplet tests to evaluate whether the interfacial tension predicted by Eq. (4.25) is correct for various density ratios. We discretized the computational domain as a $100 \times 100 \times 100$ lattice and immersed a static red droplet of radius R in a blue fluid. The initial density fields for each phase were as follows:

$$\rho_r(x, y, z) = \frac{\rho_r^0}{2}\left[1 - \tanh\left(\frac{2(r-R)}{W}\right)\right], \tag{4.29}$$

$$\rho_b(x, y, z) = \frac{\rho_b^0}{2}\left[1 + \tanh\left(\frac{2(r-R)}{W}\right)\right], \tag{4.30}$$

where $W = 4$ and $r = \sqrt{(x-x_c)^2 + (y-y_c)^2 + (z-z_c)^2}$. Here (x_c, y_c, z_c) is the center of the computational domain. We set the kinematic viscosity ratio to be 1, with each phase's kinematic viscosity being 1/6, and set the parameters A in Eq. (4.25) to 0.01 and the initial droplet radius R to 25. We neglect gravity throughout the simulations and imposed periodic boundary conditions on all sides of the computational domain.

The three-dimensional Laplace equation is given by

$$\Delta p = \frac{2\sigma}{R}, \tag{4.31}$$

where Δp is the pressure difference across the droplet interface. We evaluated the pressure for each phase using Eq. (4.19) and measured it after 100 000 iterations via the procedure used by [106]. Table 4.1 summarizes the simulation parameters and resulting errors E, which were

Table 4.1: Static droplet tests for various density ratios.

γ	Theoretical (σ_{th})	Numerical (σ_{Lap})	$E\%$	$\lvert\mathbf{u}_{\text{max}}\rvert$
1	3.5556×10^{-4}	3.5697×10^{-4}	0.40	1.22×10^{-4}
10	3.5556×10^{-4}	3.5683×10^{-4}	0.36	4.23×10^{-5}
100	3.5556×10^{-4}	3.5669×10^{-4}	0.32	4.67×10^{-5}
1000	3.5556×10^{-4}	3.5696×10^{-4}	0.40	6.94×10^{-5}

calculated as [108]

$$E = \frac{|\sigma_{\text{th}} - \sigma_{\text{Lap}}|}{\sigma_{\text{th}}} \times 100, \tag{4.32}$$

where σ_{th} and σ_{Lap} are the interfacial tensions predicted by Eq. (4.25) and measured using the Laplace equation [Eq. (4.31)], respectively. Note that the droplets are always spherical at equilibrium, indicating that numerical stability was maintained for all density ratios. These tests confirm that the CM-based CG model described in Sec. 4.2 can predict the interfacial tension in static cases to within a maximum error of 0.40%. In addition, we measured the maximum spurious velocity $|\mathbf{u}_{\text{max}}|$ in the domain at equilibrium, finding a maximum value of 1.22×10^{-4} (Table 4.1). This value is smaller than that of our MRT-based CG model [124] ($|\mathbf{u}_{\text{max}}| = 5.8 \times 10^{-3}$ for $\gamma = 1.5$). These findings indicate that introducing the CMs into the single-phase collision operator can help to reduce the spurious velocity, contributing to enhance the numerical stability.

4.4 Jet breakup simulations

As mentioned in Sec. 4.1, we will now simulate the following two experiments using the method presented in Sec. 4.2:

- UT (University of Tsukuba) experiments [143] (see Sec. 4.4.1)
- FT (FARO-TERMOS) experiments [2] (see Sec. 4.4.2)

In the following simulations, we neglect temperature changes and do not take phase-change effects (e.g., vaporization, condensation, or solidification) into account, meaning that these are

Table 4.2: Conditions used for the UT experiment simulations, reproduced from Ref. [143].

	D_{j0} [mm]	u_{j0} [m/s]	γ [−]	η [−]	Re [−]	We [−]	Fr [−]
Case 1	7	2.10	8.3	0.54	6.1×10^4	2.3×10^2	64
Case 2	10	1.55	8.3	0.54	6.5×10^4	1.8×10^2	24
Case 3	15	1.73	8.3	0.54	1.1×10^5	3.3×10^2	20
Case 4	20	1.75	8.3	0.54	1.5×10^5	4.5×10^2	16

strictly hydrodynamic simulations. The computational setup is identical to the one presented in the last Chapter.

4.4.1 UT experiments

In the UT experiments [143], an alloy called U-Alloy78 (Osaka Asahi Co., Ltd.), with a melting point of 78 °C, was injected into a stagnant water pool under atmospheric pressure. We considered four cases with different nozzle diameters (D_{j0} = 7, 10, 15, and 20 mm) from Ref. [143] (see Table 4.2). In these four cases, the melt and water temperatures were set to 270°C and 70°C, respectively, and the physical properties were as follows: $\rho_j = 8\,183$ kg/m^3, $\nu_j = 0.24$ mm^2/s, $\sigma = 1.104$ N/m, $\rho_c = 981$ kg/m^3, and $\nu_c = 0.443$ mm^2/s. Note that they defined the jet velocity u_{j0} and inlet diameter D_{j0} as the contact velocity at the water surface and the nozzle diameter, respectively.

In this case, we discretized the computational domain into an $8D_{j0} \times 8D_{j0} \times 40D_{j0}$ lattice with $D_{j0} = 30$, resulting in a total of $240 \times 240 \times 1\,200 = 69\,120\,000$ grid points being used in the simulation. We set the inlet velocity u_{j0} to 0.05, the jet density $\rho_j = \rho_r^0$ to 1, and the coolant density $\rho_c = \rho_b^0$ to $1/\gamma$. We here mention the computational cost of the present simulations. For the simulations with 6 912 000 grids, it takes around 32 hours for 20 000 iterations with our MPI-parallelized code on an Intel Xeon based system (CPU: E5-2670v2 @2.5 GHz) with 600 cores. One way to reduce the cost may be using the reduced velocity model, such as D3Q15 or D3Q19 lattice models (see Refs. [154, 159]).

Figures 4.1–4.4 show comparisons of the UT experiments' results with those of our simulations

for Cases 1–4. The simulation parameters used are shown (in lattice units) in the captions. All the simulations (Table 4.2) were numerically stable, even for very low kinematic viscosities of $O(10^{-5})$. In all cases, the simulation results reproduce the qualitative interfacial behavior well, *i.e.*, many fragments are generated as the jets penetrate each other, both around the leading edge and the side regions. However, there are still some differences in interfacial behavior between the experiments and the simulations, particularly for smaller D_{j0} values (e.g., at $t = 0.15$ s in Fig. 4.1 and $t = 0.25$ s in Fig. 4.2). One reason for this is the effect of gas entrapment: in the experiments, some of the gas was trapped in the water pool when the jet came in contact with the water surface, and the simulations did not take this into account. In contrast, the simulated shape of the interface agreed relatively well with the experiments for larger D_{j0} values (Figs. 4.3 and 4.4) because little gas was trapped in these cases. For Case 4, the details of the generated fragments and the flow field are shown in Fig. 4.5. We can find that the liquid jet column has large velocity, while the generated fragments has small velocity. In the snapshot at upstream region [Fig. 4.5(b)], the fragments generate from the unstable liquid-jet interface. Most of the fragments in this region are stretched, which appear not to be spherical shapes. The velocity magnitude of stretched fragments is large, while that of spherical ones is small. In the snapshot at downstream region [Fig. 4.5(c)], most of the fragments are spherical shapes with low velocity magnitude.

In order to make a quantitative comparison, we compared the evolution of the jet's leading edge over time for each condition, and the results are summarized in Fig. 4.6. This shows that the simulation results agree well with the experimental data [143]. In all cases, the experimental observations are ahead of the simulation early on, but the simulation passes the experiment in the later stages. This is due to differences in the inlet conditions between the experiments and simulations: in the experiments, a given mass of melt material is injected, so the injection velocity u_{j0} may decrease over time (*i.e.*, is not constant), whereas the simulations assumed a constant injection velocity. This means that the simulations match the experiments particularly well in the early stages, during jet penetration.

Based on the evolution of the jet's leading edge over time, we can estimate the jet breakup length L, *i.e.*, the length of the continuous liquid column emitted from the nozzle [43,44]. This

Figure 4.1: Comparison of jet breakup behavior for Case 1 in Table 4.2 ($D_{j0} = 7$ mm), for the (a) UT experiment and (b) simulation. The simulation parameters used were as follows (in lattice units): $\sigma = 3.3 \times 10^{-4}$, $\nu_j = \nu_r = 2.5 \times 10^{-5}$, $\nu_c = \nu_b = 4.5 \times 10^{-5}$, $g = 1.3 \times 10^{-6}$, $\rho_j = \rho_r^0 = 1$, and $\rho_c = \rho_b^0 = 0.12$. The minimum spatial resolution in this case was $\Delta x = 0.23$ mm.

is one of the metrics that characterize jet breakup behavior. Here, we estimated it via the procedure used by previous melt-jet experiments [143, 165, 166]. Table 4.3 compares the jet breakup lengths from Ref. [143] and with those in our simulations; the error E here is defined as

$$E = \frac{|L_{\text{exp}} - L_{\text{sim}}|}{L_{\text{exp}}} \times 100, \tag{4.33}$$

where L_{exp} and L_{sim} are the breakup lengths obtained via the experiments and simulations, respectively. The simulation's accuracy improves as D_{j0} increases, the error dropping from 31.4% for Case 1 to 10.8% for Case 3. Thus, these simulations were able to predict the experimental jet breakup length L to within a maximum error of 31.4%.

Figure 4.2: Comparison of jet breakup behavior for Case 2 in Table 4.2 ($D_{j0} = 10$ mm), for the (a) UT experiment and (b) simulation. The simulation parameters used were as follows (in lattice units): $\sigma = 4.2 \times 10^{-4}$, $\nu_j = \nu_r = 2.3 \times 10^{-5}$, $\nu_c = \nu_b = 4.3 \times 10^{-5}$, $g = 3.4 \times 10^{-6}$, $\rho_j = \rho_r^0 = 1$, and $\rho_c = \rho_b^0 = 0.12$. The minimum spatial resolution in this case was $\Delta x = 0.33$ mm.

As another quantitative comparison, we also evaluated the fragment diameters. The fragment diameter d was determined by the following procedures:

1. Binarize the order parameter ϕ into 1 for the jet region and 0 for the others
2. Find the connected components (with 1) and regard them as fragments
3. Calculate each fragment's volume V
4. Convert the volume V into the equivalent spherical diameter by $d \equiv (6V/\pi)^{1/3}$

Figure 4.7 shows histograms of the measured diameters; we have excluded the continuous liquid column from the nozzle from the calculation. From the figure, we can find that the smaller the nozzle diameter is, the higher the observation frequency of the droplet is. Except for $D_{j0} = 7$

Figure 4.3: Comparison of jet breakup behavior for Case 3 in Table 4.2 ($D_{j0} = 15$ mm), for the (a) UT experiment and (b) simulation. The simulation parameters used were as follows (in lattice units): $\sigma = 2.3 \times 10^{-4}$, $\nu_j = \nu_r = 1.4 \times 10^{-5}$, $\nu_c = \nu_b = 2.6 \times 10^{-5}$, $g = 4.1 \times 10^{-6}$, $\rho_j = \rho_r^0 = 1$, and $\rho_c = \rho_b^0 = 0.12$. The minimum spatial resolution in this case was $\Delta x = 0.5$ mm.

mm [Fig. 4.7(a)], all the distributions have a long tail to the right, similar to a log-normal distribution.

Next, we compared the fragment diameters measured via the simulations with the experimental data and the predictions of hydrodynamic instability theories. We calculated the mass-median diameter as a fragment size metric, due to the shape of the distribution (Fig. 4.7). On the theoretical side, the first indicators we compared were the critical wavelengths of classical Rayleigh–Taylor (RT) and Kelvin–Helmholtz (KH) instabilities, $\lambda_{\mathrm{cr,RT}}$ and $\lambda_{\mathrm{cr,KH}}$. Assuming a

Figure 4.4: Comparison of jet breakup behavior for Case 4 in Table 4.2 ($D_{j0} = 20$ mm), for the (a) UT experiment and (b) simulation. The simulation parameters used were as follows (in lattice units): $\sigma = 1.7 \times 10^{-4}$, $\nu_j = \nu_r = 1.0 \times 10^{-5}$, $\nu_c = \nu_b = 1.9 \times 10^{-5}$, $g = 5.3 \times 10^{-6}$, $\rho_j = \rho_r^0 = 1$, and $\rho_c = \rho_b^0 = 0.12$. The minimum spatial resolution in this case was $\Delta x = 0.67$ mm.

two-dimensional stratified geometry, these are [73]

$$\lambda_{\mathrm{cr,RT}} = 2\pi \left[\frac{\sigma}{(\rho_j - \rho_c)g} \right]^{\frac{1}{2}}, \tag{4.34}$$

$$\lambda_{\mathrm{cr,KH}} = 2\pi \frac{\rho_j + \rho_c}{\rho_j \rho_c} \frac{\sigma}{u_{j0}^2}. \tag{4.35}$$

Here, we used the jet velocity u_{j0} as the scaling velocity, assuming that the ambient fluid was stationary in Eq. (4.35). The second theoretical indicator we compared was the critical Weber number $\mathrm{We}_{\mathrm{cr}}$, from which we obtained the critical droplet diameter d, as follows:

$$d = \mathrm{We}_{\mathrm{cr}} \cdot \frac{\sigma}{\rho_c u_{j0}^2}. \tag{4.36}$$

The value of $\mathrm{We}_{\mathrm{cr}}$ depends on the assumptions made, so several values have been proposed,

Figure 4.5: (a) Snapshot of detailed interface structure for Case 4 in Table 4.2 ($D_{j0} = 20$ mm). (b) Magnified snapshot for upstream region. (c) Magnified snapshot for downstream region.

such as 12 ([67]) and 18 ([26]). Previous studies [18, 19, 166] have pointed out that these theoretical quantities are related to the sizes of the fragments generated by jet breakup.

Figure 4.8 compares the simulated and experimental fragment sizes. The aforementioned hydrodynamic instability theories [Eqs. (4.34)–(4.36)] are also shown in the graph. The error bars indicate the 95% confidence intervals for the median diameter, which we used to express the widths of the droplet size distributions even though they were not necessarily Gaussian [82]. As in the experiment [143], the simulation results are in agreement with both the KH [Eq. (4.35)]

Table 4.3: Comparison of the jet breakup lengths observed in the experiments and simulations.

	Experiment [143] [mm]	Simulation [mm]	Error E (%)
Case 1	171	117	31.4
Case 2	264	337	27.8
Case 3	348	310	10.8
Case 4	440	382	13.0

Figure 4.6: Evolution of the jet's leading edge over time for (a) Case 1 ($D_{j0} = 7$ mm), (b) Case 2 ($D_{j0} = 10$ mm), (c) Case 3 ($D_{j0} = 15$ mm), and (d) Case 4 ($D_{j0} = 20$ mm).

and critical Weber number [Eq. (4.36)] theories. However, the RT instability [Eq. (4.34)] does not appear to be correlated with the numerical or experimental results. As in Figs. (4.1)–(4.4), the jet's interfaces appear to be very unstable at the jet-side region both in the experiments and simulations. Since there is velocity difference between the jet and the ambient fluid, KH instability may be one of the reasons of the onset of interfacial instability. In addition, fragments generated at the tip of the jet (also at the jet side in some cases) are considered to be fragmented into smaller drops again due to the limitation of the critical Weber number. These simulations thus support the breakup mechanism proposed based on the experimental observations. Table 4.4 compares the experimental and simulated median diameters; the error E is defined as

$$E = \frac{|d_{m,\mathrm{exp}} - d_{m,\mathrm{sim}}|}{d_{m,\mathrm{exp}}} \times 100, \tag{4.37}$$

where $d_{m,\mathrm{exp}}$ and $d_{m,\mathrm{sim}}$ are the experimental and simulated median diameters, respectively.

Figure 4.7: Fragment-diameter distribution histograms for (a) Case 1 ($D_{j0} = 7$ mm), (b) Case 2 ($D_{j0} = 10$ mm), (c) Case 3 ($D_{j0} = 15$ mm), and (d) Case 4 ($D_{j0} = 20$ mm). Here, d_m denotes the mass-median diameter.

The maximum error E was 41.9%, for Case 2.

4.4.2 FT experiments

The FT experiments were performed at the Joint Research Centre (JRC) in Ispra (Italy) by [2]. Around 100-kg-scale of UO_2 melt was poured into a liquid-sodium pool. Two experiments, called T1 and T2, were carried out, with release diameters of 50 mm and 80 mm, respectively. In this paper, we focus on the T1 experiment. A notable feature of the FT experiments is that sodium in not transparent, so these simulations will hopefully help us to better understand the phenomena involved.

For these simulations, we discretized the computational domain into an $8D_{j0} \times 8D_{j0} \times 20D_{j0}$ lattice. Table 4.5 summarizes the simulation conditions, together with the corresponding di-

Figure 4.8: Comparison of the experimental and simulated fragment sizes.

Table 4.4: Comparison of the mass-median diameters observed in the experiments and simulations.

	Experiment [143] [mm]	Simulation [mm]	Error E (%)
Case 1	4.54	2.85	37.2
Case 2	5.10	2.96	41.9
Case 3	5.23	4.91	6.0
Case 4	5.40	4.61	14.4

mensionless quantities, given by Eqs. (**??**)–(**??**). It should be noted that the Reynolds number in Table 4.5 (1.1×10^6) is extremely high from a multiphase LB perspective. The liquid–liquid-jet breakup flow-regime map [82] shown in Fig. 4.9 indicates we are in the atomization regime (Regime III) in this case. To examine the effect of grid resolution on jet breakup behavior, we considered two cases with different grids: a *coarse* case with $D_{j0} = 30$ and hence a $240 \times 240 \times 600$ lattice (= 34 560 000 grid points), and a *fine* case with $D_{j0} = 60$ and hence a $480 \times 480 \times 1\,200$ lattice (= 276 480 000 grid points). The resulting minimum spacings (in physical units) were $\Delta x = 1.67$ mm and $\Delta x = 0.83$ mm for the coarse and fine cases, respectively. For reference, the conditions of UT simulations presented in Sec. 4.4.1 are also shown in the same map.

Figure 4.10 shows the simulation results for the coarse case. The left hand side [Fig. 4.10(a)]

Figure 4.9: Flow regime region covered by the FT experiment together with the conditions our previous simulations ('o') [124]. Our current simulations ('×') involve substantially higher Re values compared with the previous ones.

Table 4.5: Conditions for the FT experiment simulations, reproduced from Ref. [2]. Here, we focus on their T1 experiment.

D_{j0} [mm]	u_{j0} [m/s]	γ [−]	η [−]	Re [−]	We [−]	Fr [−]
50	10	10.1	1.4	1.1×10^6	9.3×10^4	2.0×10^2

shows the time evolution of the jet interface in real units, while the right hand side [Fig. 4.10(b)] shows the calculated fragment size distribution at $t = 0.125$ s. The simulation parameters are given (in lattice units) in the caption. Even though the numerical conditions were somewhat extreme, numerical stability was maintained throughout the simulations These results show that using our CG LB model, based on nonorthogonal CMs, allowed Re to be increased significantly. In Fig. 4.10, most of the fragments are generated at the side of the jet due to entrainment, and they appear to be tiny compared with the inlet diameter D_{j0}. This is characteristic of the atomization regime (Regime III) [82]. This simulation therefore suggests that the jet state in the FT experiment should be similar to the atomization regime and, in fact, the debris collected in the T1 experiment was very fine (around 30–600 μm) [2]. That said, however, some unphysical points remain in terms of the fragment shapes and numerical dissolution. The

resulting fragments were not spherical but irregular, and the jet's leading edge faced numerical dissolution at the later stage compared to that at the initial stages. In addition, Fig. 4.10(b) shows that the fragment-diameter distribution appears to be log-normal, but this pattern is interrupted near the minimum resolution, which we believe is due to the low spatial resolution.

To investigate the effect of spatial resolution, we then carried out a fine simulation, in which there were twice as many grid points in each direction. We used the same dimensionless quantities (Table 4.5) as in the coarse case. Figure 4.11 shows the results of this simulation, with the simulation parameters again shown (in lattice units) in the caption. Compared with Fig. 4.10(a), the interfacial behavior seen in Fig. 4.11(a) is clearly different in terms of the fragment sizes and shapes: they are smaller and nearly spherical, and fragmentation now occurs around the jet's leading edge and side. The fragment-diameter distribution in Fig. 4.11(b) is also smoother than that in Fig. 4.10(b), resembling a log-normal distribution. Adopting a higher-resolution computational domain also improved the numerical dissolution issue, as more physically reasonable results were obtained. In both cases (coarse and fine), the atomization regime appeared, implying that the grid resolutions used in this paper were sufficient to simulate the qualitative behavior of the entire jet. However, we can also observe that finer grids will be required to perform quantitative evaluations.

4.5 Summary

we have extended the previous CG LB model [124] by introducing nonorthogonal CMs in three dimensions [154] within the GMRT framework [158, 159]. Static droplet tests showed that our model can predict the interfacial tension for a range of density ratios (up to 1 000) to within a maximum error of 0.40% and also that it can greatly reduce the spurious velocity. We also applied our model to hydrodynamic melt-jet breakup simulations, targeting two different experiments, namely, the UT [143] and FT [2] experiments. Numerical simulations under corresponding conditions, including those equivalent to an actual reactor, demonstrated that our model was more stable. In particular, our model allowed the Reynolds number to be

Figure 4.10: FT simulation results for the coarse (low-resolution) case, showing the (a) interfacial behavior and (b) fragment-diameter distribution. The inlet diameter was set to $D_{j0} = 30$ (in lattice units), and the computational domain was discretized into a $240 \times 240 \times 600$ lattice (= 34 560 000 grid points). The simulation parameters were as follows (in lattice units): $\sigma = 1.6 \times 10^{-5}$, $\nu_j = \nu_r = 1.4 \times 10^{-6}$, $\nu_c = \nu_b = 9.9 \times 10^{-7}$, $g = 4.1 \times 10^{-7}$, $\rho_j = \rho_r^0 = 1$, and $\rho_c = \rho_b^0 = 0.099$. The minimum spatial resolution in this case was $\Delta x = 1.67$ mm.

increased significantly, up to $O(10^6)$. The UT simulations predicted the jet breakup length and median fragment-diameter to within maximum errors of 31.4% and 41.9%, respectively. The results of the FT simulation suggested that the jet in the experiment was in the atomization regime.

Figure 4.11: FT simulation results for the fine (high-resolution) case, showing the (a) interfacial behavior and (b) fragment diameter distribution. The inlet diameter was set to $D_{j0} = 60$ (in lattice units), and the computational domain is discretized into a $480 \times 480 \times 1\,200$ lattice ($= 276\,480\,000$ grid points). The simulation parameters used were as follows (in lattice units): $\sigma = 3.2 \times 10^{-5}$, $\nu_j = \nu_r = 2.8 \times 10^{-6}$, $\nu_c = \nu_b = 2.0 \times 10^{-6}$, $g = 2.0 \times 10^{-7}$, $\rho_j = \rho_r^0 = 1$, and $\rho_c = \rho_b^0 = 0.099$. The minimum spatial resolution in this case was $\Delta x = 0.83$ mm.

Chapter 5

Boiling Heat Transfer on a Particle

5.1 Literature review

Since a pioneering work of Nukiyama [167], boiling phenomena have been investigated via theoretical, experimental, and numerical works [168]. Due to its important role in investigating the mechanism and heat transfer characteristics of boiling, numerical simulations of boiling phenomena have been carried out since late 1990s. In these Navier–Stokes-based simulations, a level-set method [169], a front-tracking method [170], and a volume-of-fluid method [171] are often used to track the liquid-vapor interfaces. Since then, a lot of numerical studies have been conducted to investigate boiling phenomena (see review papers. [172–175] for detail). However, most of them assumes an initial vapor phase, that is, those methods cannot simulate nucleation in boiling.

Forced convective boiling on a sphere (or cylinder) has been theoretically and experimentally investigated. That is because the heat transfer coefficient from a particle to liquids is quaite important for assessmen of the fuel-coolant interactions during nuclear accidents. Liu and Theofanous [176] carried out experiments on film boiling from spheres in single- and two-phase water flows. The effects of water flow velocity, water subcooling, sphere superheat, sphere diameter, and sphere material on the film boiling heat transfer were investigated. They also performed an analysis of film boiling, and provided generalized correlation of film boiling heat

transfer coefficient, where several existing correlations (*e.g.* Epstein–Hauser [177] and Dhir–Prohit [178]) were considered.

In recent years, several kinds of lattice Boltzmann (LB) methods for multiphase flows have been applied to simulating liquid-vapor phase transitions. Among the LB models, the pseudopotential model and the phase-field model are widely used [97]. In most of the phase-field LB models, an interface tracking equation is solved to capture the liquid-vapor interface and a source term is incorporated into the continuity equation or the Cahn–Hilliard equation to define the phase transition. This implies that the rate of the liquid-vapor phase transition is an *artificial input*. The pseudopotential LB method [100] becomes most widely used for simulating multiphase flows. The most distinct feature of the method is that the phase separation is achieved via an interparticle potential. In the case considering temperature change, the liquid-vapor phase transition is driven by the equation of state. Hence no artificial phase-change terms need to be added to the temperature equation [97]. After the first attempt by Zhang and Chen [179], many researchers proposed thermal LB models based on the pseudopotential LB approach and those models simulate nucleate boiling without artificial terms [180–186]. Most of their models have the feature in common that a thermal LB equation with a temperature distribution function is used to mimic the macroscopic temperature equation. However, the forcing term included in the thermal LB equations introduce a spurious term into the macroscopic temperature equation [187], and such a forcing term lead to significant errors in the simulation of thermal flows [188]. Furthermore, in temperature-based thermal LB equations, another error term proportional to $\nabla \cdot (T\nabla\rho/\rho)$ appears in the macroscopic temperature equation, that can be seen in Refs. [189, 190]. This term yield considerable errors in multiphase flows with density varying. According to Li et al. [187], solving the temperature equation using the classical finite-difference method enables us to be free of the aforementioned problems.

Besides, the original pseudopotential LB method generally also suffers from the problem of density ratio. Recently, Lycett-Brown et al. [191] introduced the cascaded LB method [148] to a pseudopotential multiphase scheme to enhance stability at high density ratio. Later, Lycett-Brown and Luo [192] improved their cascaded multiphase LB model based on their original forcing scheme [193]. The basic philosophy of this improved forcing scheme is introducing

artificial terms in the pressure tensor to counteract the lack of thermodynamic consistency in the original pseudopotential model [158]. The cascaded collision operator relaxes the so-called central moments [148, 153, 194, 195], instead of raw moments used in the multiple-relaxation-time (MRT) method [114, 196]. Their model shows the excellent numerical stability in the simulation of binary collisions of water droplets in the air, whose density ratio up to 1000 [192], which cannot be simulated by the LB model with the MRT collision operator.

In this chapter, we develop the numerical method to simulate a series of boiling phenomena, including nucleation, growth, coalescence, and departure of vapor bubbles. The phase-change lattice Boltzmann model is adopted as the solver. Simulations are performed in two dimensions. Convection boiling heat transfer on a cylinder is investigated with the developed numerical method. Several heat transfer coefficient correlations are compared and validated from the present numerical simulations.

5.2 Methodology

In this paper, fluid field and temperature field are solved by the lattice Boltzmann method and the finite difference method, respectively. This kind of approach can be found in Refs. [187, 197, 198].

5.2.1 Central-moment lattice Boltzmann model

Let us consider an Eulerian basis $\boldsymbol{x} = [x, y]$ and the D2Q9 velocity space [140]. The lattice Boltzmann equation predicts the space and time evolution of the particle distribution functions $|f_i\rangle = [f_0,\, f_1,\, f_2,\, f_3,\, f_4,\, f_5,\, f_6,\, f_7,\, f_8]^\top$ collide and stream on a fixed square grid along the generic link $i = 0 \ldots 8$ with velocity

$$\begin{aligned} |c_{ix}\rangle =& [0,\, 1,\, -1,\, 0,\, 0,\, 1,\, -1,\, 1,\, -1]^\top, \\ |c_{iy}\rangle =& [0,\, 0,\, 0,\, 1,\, -1,\, 1,\, -1,\, -1,\, 1]^\top. \end{aligned} \tag{5.1}$$

Let us employ the symbols $|\bullet\rangle$ and $\top$ to denote a column vector and the transpose operator, respectively. The BGK LB equation reads as follows:

$$f_i(\boldsymbol{x}+\delta_t\boldsymbol{c}_i, t+\delta_t) = f_i(\boldsymbol{x},t) + \omega\left[f_i^{\mathrm{eq}}(\boldsymbol{x},t) - f_i(\boldsymbol{x},t)\right] + G_i(\boldsymbol{x},t), \tag{5.2}$$

where the time step is $\delta_t = 1$. As usual, the LBE can be divided into two steps, *i.e.* collision:

$$f_i^{\star}(\boldsymbol{x},t) = f_i(\boldsymbol{x},t) + \omega\left[f_i^{\mathrm{eq}}(\boldsymbol{x},t) - f_i(\boldsymbol{x},t)\right] + G_i(\boldsymbol{x},t), \tag{5.3}$$

and streaming:

$$f_i(\boldsymbol{x}+\delta_t\boldsymbol{c}_i, t+\delta_t) = f_i^{\star}(\boldsymbol{x},t), \tag{5.4}$$

where the superscript $\star$ denotes post-collision quantities here and henceforth. The dependence on the space and the time will be implicitly assumed in the rest of this section. The term G_i accounts for external body forces $\boldsymbol{F} = [F_x, F_y]$ and its role will be elucidated later. The fluid density ρ and velocity $\boldsymbol{u} = [u_x, u_y]$ are computed as

$$\rho = \sum_i f_i, \;\; \rho\boldsymbol{u} = \sum_i f_i\boldsymbol{c}_i + \frac{\boldsymbol{F}}{2}\delta_t, \tag{5.5}$$

respectively. The second term of the right-hand side of Eq. (5.3) is the BGK collision operator, that forces all the populations to relax with the same rate ω to a discrete local equilibrium f_i^{eq}. Following the works by Malaspinas [199] and Coreixas [200, 201], the equilibrium distribution can be expanded into a basis of Hermite polynomials $\mathcal{H}^{(n)}$ as

$$f_i^{\mathrm{eq}} = w_i\rho\left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{1}{2c_s^4}\mathcal{H}_i^{(2)} : \boldsymbol{u}\boldsymbol{u} + \frac{1}{2c_s^6}\left(\mathcal{H}_{ixxy}^{(3)}u_x^2u_y + \mathcal{H}_{ixyy}^{(3)}u_xu_y^2\right) + \frac{1}{4c_s^8}\mathcal{H}_{ixxyy}^{(4)}u_x^2u_y^2\right], \tag{5.6}$$

with $w_0 = 4/9$, $w_{1\ldots4} = 1/9$, $w_{5\ldots8} = 1/36$ and $c_s = 1/\sqrt{3}$ is the lattice sound speed. Notice that the maximum order of the expansion is equal to four in the D2Q9 space. Moreover, the model recovers the classical second-order truncated equilibrium is $\mathcal{H}^{(3)}$ and $\mathcal{H}^{(4)}$ are neglected.

The pivotal idea to design any CMs-based collision operator is to shift the lattice directions by

the local fluid velocity [148]. Therefore, it is possible to define $\bar{\boldsymbol{c}}_i = [|\bar{c}_{ix}\rangle\,,\,|\bar{c}_{iy}\rangle]$, where

$$
\begin{aligned}
|\bar{c}_{ix}\rangle &= |c_{ix} - u_x\rangle\,,\\
|\bar{c}_{iy}\rangle &= |c_{iy} - u_y\rangle\,.
\end{aligned}
\tag{5.7}
$$

Then, one must choose a suitable basis of moments. Let us adopt the basis

$$
\mathsf{T} = \begin{bmatrix}
\langle|\boldsymbol{c}_i|^0| \\
\langle\bar{c}_{ix}| \\
\langle\bar{c}_{iy}| \\
\langle\bar{c}_{ix}^2 + \bar{c}_{iy}^2| \\
\langle\bar{c}_{ix}^2 - \bar{c}_{iy}^2| \\
\langle\bar{c}_{ix}\bar{c}_{iy}| \\
\langle\bar{c}_{ix}^2\bar{c}_{iy}| \\
\langle\bar{c}_{ix}\bar{c}_{iy}^2| \\
\langle\bar{c}_{ix}^2\bar{c}_{iy}^2|
\end{bmatrix}\,,
\tag{5.8}
$$

Let us collect pre-collision, equilibrium and post-collision CMs as

$$
\begin{aligned}
|k_i\rangle &= [k_0,\,\ldots,\,k_i,\,\ldots,\,k_8]^\top\,,\\
|k_i^{\mathrm{eq}}\rangle &= [k_0^{\mathrm{eq}},\,\ldots,\,k_i^{\mathrm{eq}},\,\ldots,\,k_8^{\mathrm{eq}}]^\top\,,\\
|k_i^\star\rangle &= [k_0^\star,\,\ldots,\,k_i^\star,\,\ldots,\,k_8^\star]^\top\,,
\end{aligned}
\tag{5.9}
$$

respectively. The first two quantities are evaluated by applying the matrix T to the corresponding distribution, that is

$$
\begin{aligned}
|k_i\rangle &= \mathsf{T}\,|f_i\rangle\,,\\
|k_i^{\mathrm{eq}}\rangle &= \mathsf{T}\,|f_i^{\mathrm{eq}}\rangle\,,
\end{aligned}
\tag{5.10}
$$

where $|f_i^{\mathrm{eq}}\rangle = [f_0^{\mathrm{eq}},\,\ldots f_i^{\mathrm{eq}},\,\ldots f_8^{\mathrm{eq}}]^\top$. By adopting $n = 4$, equilibrium central moments are

$$
|k_i^{\mathrm{eq}}\rangle = \left[\rho,\,0,\,0,\,\frac{2}{3}\rho,\,0,\,0,\,0,\,0,\,\frac{\rho}{9}\right]^\top\,,
\tag{5.11}
$$

Notably, only three equilibrium CMs assume values different from zero. It is of interest to notice that the discrete equilibrium CMs have the same form of the continuous counterpart when the full set of Hermite polynomials is considered. The post-collision central moments can be written as

$$|k_i^\star\rangle = (\mathsf{I} - \mathsf{K})\,\mathsf{T}\,|f_i\rangle + \mathsf{K}\,\mathsf{T}\,|f_i^{\mathrm{eq}}\rangle + \left(\mathsf{I} - \frac{\mathsf{K}}{2}\right)\mathsf{T}\,|\mathcal{F}_i\rangle\,, \tag{5.12}$$

where I is the 9×9 unit matrix and

$$\mathsf{K} = \mathrm{diag}[1,\, 1,\, 1,\, 1,\, \omega,\, \omega,\, 1,\, 1,\, 1], \tag{5.13}$$

is a 9×9 relaxation matrix with $\omega = \left(\frac{\nu}{c_s^2 \delta_t} + \frac{1}{2}\right)^{-1}$, ν being the fluid kinematic viscosity.

Now, let us define the forcing term G_i. Specifically, we employ the expression adopted by Huang et al. [202]:

$$G_i\left(\boldsymbol{u}\right) = w_i \left(\frac{\boldsymbol{F}}{c_s} \cdot \mathcal{H}^{(1)} + \frac{[\boldsymbol{F}\boldsymbol{u}]}{2c_s^2} \cdot \mathcal{H}^{(2)} + \frac{[\boldsymbol{F}\boldsymbol{u}\boldsymbol{u}]}{6c_s^3} \cdot \mathcal{H}^{(3)}_{[xyy],[xxy]} + \frac{[\boldsymbol{F}\boldsymbol{u}\boldsymbol{u}\boldsymbol{u}]}{24c_s^4} \cdot \mathcal{H}^{(4)}_{[xxyy]}\right), \tag{5.14}$$

where the square bracket in Hermite coefficient denotes permutations. Notice that the popular formula by Guo [121] is recovered if $\mathcal{H}^{(3)}$ and $\mathcal{H}^{(4)}$ are neglected. The central moments of the present discrete force term can be computed as

$$|R_i\rangle = \mathsf{T}\,|G_i\rangle\,, \tag{5.15}$$

with $|R_i\rangle = [R_0,\, \ldots R_i,\, \ldots R_8]^\top$, and read as follows:

$$|R_i\rangle = \left[0,\, F_x,\, F_y,\, 0,\, 0,\, 0,\, \frac{F_y}{3},\, \frac{F_x}{3},\, 0\right]^\top, \tag{5.16}$$

Some considerations should be drawn regarding these results. The same expressions of $|R_i\rangle$ can be achieved when the continuous Maxwell–Boltzmann distribution are considered [158, 203]. This is consistent with a recent paper by De Rosis and Luo [204], where it is argued that the central moments of the discrete distribution collapse into the continuous counterpart when the full set of Hermite polynomials is considered. Moreover, $|R_i\rangle$ can be achieved by

disregarding the velocity-dependent terms in Eq. (15) of Ref. [156]. Again, this is consistent with Ref. [204], where the velocity terms vanishes when the maximum $\mathcal{H}$ is adopted to construct central moments. Finally, present findings are different from and simpler than those in Ref. [202] [see Eq. (9)] due to the adoption of a different basis. In the following, we report the post-collision central moments:

$$|k_i^\star\rangle = \left[\rho,\, \frac{F_x}{2},\, \frac{F_y}{2},\, \frac{2}{3}\rho,\, (1-\omega)\, k_4,\, (1-\omega)\, k_5,\, \frac{F_y}{6},\, \frac{F_x}{6},\, \frac{\rho}{9},\, \right]^\top, \tag{5.17}$$

One can immediately appreciate that the present scheme is highly intelligible and the resultant algorithm is very concise. Then, the post-collision populations are reconstructed as

$$|f_i^\star\rangle = \mathsf{T}^{-1}\, |k_i^\star\rangle\,, \tag{5.18}$$

with $|f_i^\star\rangle = [f_0^\star,\, \ldots f_i^\star,\, \ldots f_8^\star]^\top$, that are eventually streamed.

5.2.2 Pseudopotential and thermodynamic consistency

In the pseudopotential lattice Boltzmann model, the interaction force to mimic the molecular interactions plays as important roll in phase separation, which is given by [100, 192]

$$\boldsymbol{F}_m(\boldsymbol{x}) = -\mathscr{G} c_s^2\, \psi(\boldsymbol{x}) \sum_{i=0}^{N} w(|\boldsymbol{c}_i|^2)\, \psi(\boldsymbol{x}+\boldsymbol{c}_i)\, \boldsymbol{c}_i, \tag{5.19}$$

where ψ is the interaction potential, $\mathscr{G}$ is the interaction strength, and $w(|\boldsymbol{c}_i|^2)$ are the weights. The number of discrete velocities N used in the force calculation need not to be equal to the number of lattice velocities. We consider the case of $N = 24$ (pseudo D2Q25 lattice) for calculation of the interaction force. The weights can be defined as $w(0) = 247/140$, $w(1) = 4/21$, $w(2) = 4/45$, $w(4) = 1/60$, $w(5) = 2/315$, and $w(8) = 1/5040$ [107, 205, 206]. This treatment means that the interaction force is discretized with the 6th-order isotropic gradient [107].

The Taylor series expansion of Eq. (5.19):

$$\boldsymbol{F}_m(\boldsymbol{x}) = -\mathscr{G}c_s^2(\psi\nabla\psi + \lambda\psi\nabla\nabla^2\psi) + O(\nabla^5), \tag{5.20}$$

where λ depends on the lattice geometry (for our case, $\lambda = 2/7$). With some manipulations, one can rewrite

$$\begin{aligned}\boldsymbol{F}_m(\boldsymbol{x}) &= -\mathscr{G}c_s^2(\psi\nabla\psi + \lambda\psi\nabla\nabla^2\psi) + \cdots \\ &= -\frac{\mathscr{G}c_s^2}{2}\nabla\psi^2 - \lambda\mathscr{G}c_s^2[\nabla(\psi\nabla^2\psi) - \nabla^2\psi\nabla\psi] + \cdots \\ &= -\frac{\mathscr{G}c_s^2}{2}\nabla\psi^2 - \lambda\mathscr{G}c_s^2\nabla\psi\nabla^2\psi + \lambda\mathscr{G}c_s^2[\nabla\cdot(\nabla\psi\nabla\psi) - \frac{1}{2}\nabla|\nabla\psi|^2] + \cdots\end{aligned} \tag{5.21}$$

To incorporate a non-ideal equation of state (EOS) p_{EOS} into the pseudopotential lattice Boltzmann model, the following potential form should be chosen as [207–209]

$$\psi(\boldsymbol{x}) = \sqrt{\frac{2(p_{\mathrm{EOS}} - \rho c_s^2)}{\mathscr{G}c_s^2}}, \tag{5.22}$$

where $\mathscr{G}$ is only required to guarantee the term inside the square root to be positive [100, 208].

Although the potential form of Eq. (5.22) is consistent with the EOS, there still remains the problem of thermodynamic inconsistency; Eq. (5.16) cannot satisfy thermodynamic consistency. To overcome this problem we here derive the corrected forcing term $|\mathcal{R}_i'\rangle$, where the macroscopic velocity in Eq. (5.14) is replaced by the following modified velocity [210, 211]:

$$\boldsymbol{u}' = \boldsymbol{u} + \frac{\sigma\boldsymbol{F}_m}{(\omega^{-1} - 0.5)\delta_t\psi^2}. \tag{5.23}$$

where σ is a constant to tune thermodynamic consistency, and τ is the relaxation time. By substituting Eq. (5.23) into Eq. (5.14), we can obtain the corrected forcing term. Through this procedure, one can find that $R_{3,4,5,6,7,8}$ are needed to be changed. However, we here drop the

$O(F^3)$ terms. This reads as

$$R_3 = \frac{4\sigma(F_{m,x}^2 + F_{m,y}^2)}{\psi^2\delta_t}, \tag{5.24}$$

$$R_4 = \frac{2\sigma(F_{m,x}^2 - F_{m,y}^2)}{(\omega^{-1} - 0.5)\psi^2\delta_t}, \tag{5.25}$$

$$R_5 = \frac{2\sigma F_{m,x}F_{m,y}}{(\omega^{-1} - 0.5)\psi^2\delta_t}, \tag{5.26}$$

$$R_8 = \frac{4\sigma(F_{m,x}^2 + F_{m,y}^2)}{3\psi^2\delta_t}, \tag{5.27}$$

where $|\boldsymbol{F}_m|^2 = F_{m,x}^2 + F_{m,y}^2$. As can be seen, only the terms R_3 and R_8 have been changed compared with the original forcing term in Eq. (5.16). When we choose $\sigma = 0$, Eq. (5.27) clearly reduces to Eq. (5.16), which is identical to the original consistent forcing scheme [158]. Due to this modification, we can rewrite the post-collision central moments as follow:

$$k_3^\star = \frac{2\rho}{3} + \frac{2\sigma(F_{m,x}^2 + F_{m,y}^2)}{\psi^2}, \tag{5.28}$$

$$k_4^\star = (1-\omega)\, k_4 + \omega\frac{2\sigma(F_{m,x}^2 - F_{m,y}^2)}{\psi^2}, \tag{5.29}$$

$$k_5^\star = (1-\omega)\, k_5 + \omega\frac{2\sigma(F_{m,x}F_{m,y})}{\psi^2}, \tag{5.30}$$

$$k_8^\star = \frac{\rho}{9} + \frac{2\sigma(F_{m,x}^2 + F_{m,y}^2)}{3\psi^2}, \tag{5.31}$$

where we set to $\delta_t = 1$. Comparing to Eq. (5.17), the underlined terms have been appeared in Eq. (5.31) to tune the thermodynamic consistency.

Through the Chapman–Enskog multiscale analysis, the Navier–Stokes equation can be derived as

$$\partial_t\, \rho\boldsymbol{u} + \nabla\cdot\rho\boldsymbol{u}\boldsymbol{u} = -\nabla(c_s^2\rho) + \nabla\cdot[\rho\nu\,(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^\top) + \rho(\nu_b - \nu)(\nabla\cdot\boldsymbol{u})\,\mathsf{I}] + \boldsymbol{F} - 2\sigma\mathscr{G}^2c_s^4\nabla\cdot(\nabla\psi\nabla\psi). \tag{5.32}$$

If we consider only the iterparticle force as the external force, Eq. (5.32) can be rewritten as

$$\partial_t \rho \boldsymbol{u} + \nabla \cdot \rho \boldsymbol{u}\boldsymbol{u} = -\nabla \cdot \mathsf{P} + \nabla \cdot [\rho\nu\,(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^\top) + \rho(\nu_b - \nu)(\nabla \cdot \boldsymbol{u})\,\mathsf{I}], \tag{5.33}$$

where

$$\mathsf{P} = \left(\rho c_s^2 + \frac{\mathscr{G} c_s^2}{2}\psi^2 + \lambda \mathscr{G} c_s^2 \psi \nabla^2 \psi + \frac{\lambda \mathscr{G} c_s^2}{2}|\nabla\psi|^2\right)\mathsf{I} + (-\lambda \mathscr{G} c_s^2 + 2\sigma \mathscr{G}^2 c_s^4)\nabla\psi\nabla\psi \tag{5.34}$$

It is obvious that the pressure tensor has been modified to be thermodynamically consistent.

5.2.3 Energy equation and non-ideal EOS

Now let us derive the energy equation about temperature T. If we assume that the thermal diffusion is governed by the Fourier law, the energy equation about the internal energy e can be given by

$$\rho \frac{\mathrm{D}e}{\mathrm{D}t} = \nabla \cdot (\lambda \nabla T) - p\,(\nabla \cdot \boldsymbol{u}) + \Phi, \tag{5.35}$$

where λ is the thermal conductivity, $\mathrm{D}/\mathrm{D}t \equiv \partial/\partial t + \boldsymbol{u} \cdot \nabla$ is the material derivative, and $\Phi = \boldsymbol{\Pi} : \nabla \boldsymbol{u}$ is the viscous heat dissipation [212]. The second term in Eq. (5.35) describes the pressure work. Meanwhile, for the internal energy and temperature, we have the following thermodynamic relation:

$$\mathrm{d}e = c_v \mathrm{d}T + \left[T\left(\frac{\partial p}{\partial T}\right)_v - p\right]\mathrm{d}v, \tag{5.36}$$

where c_v is the specific heat at constant volume and $v = 1/\rho$ is the specific volume. Dividing Eq. (5.36) by $\mathrm{d}t$ and replacing $\mathrm{d}/\mathrm{d}t \to \mathrm{D}/\mathrm{D}t$ yields

$$\begin{aligned} \rho \frac{\mathrm{D}e}{\mathrm{D}t} &= \rho c_v \frac{\mathrm{D}T}{\mathrm{D}t} + \rho\left[T\left(\frac{\partial p}{\partial T}\right)_v - p\right]\frac{\mathrm{D}v}{\mathrm{D}t} \\ &= \rho c_v \frac{\mathrm{D}T}{\mathrm{D}t} + \left[T\left(\frac{\partial p}{\partial T}\right)_\rho - p\right](\nabla \cdot \boldsymbol{u}), \end{aligned} \tag{5.37}$$

where we use the continuity equation:

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\,(\nabla\cdot\boldsymbol{u}), \quad \frac{\mathrm{D}v}{\mathrm{D}t} = \frac{1}{\rho}\,(\nabla\cdot\boldsymbol{u}). \tag{5.38}$$

Note that we replaced we replaced the subscript $v \to \rho$ in Eq. (5.37). Substituting Eq. (5.37) into Eq. (5.35) results in

$$\rho c_v \frac{\mathrm{D}T}{\mathrm{D}t} = \nabla\cdot(\lambda\nabla T) - T\left(\frac{\partial p}{\partial T}\right)_\rho \nabla\cdot\boldsymbol{u} + \Phi. \tag{5.39}$$

In this paper, we neglect the viscous heat dissipation, *i.e.*, $\Phi = 0$. Finally, the practical form of the energy equation about temperature is now given by

$$\frac{\partial T}{\partial t} + \boldsymbol{u}\cdot\nabla T = \frac{1}{\rho c_v}\nabla\cdot(\lambda\nabla T) - \frac{T}{\rho c_v}\left(\frac{\partial p_{\mathrm{EOS}}}{\partial T}\right)_\rho \nabla\cdot\boldsymbol{u}, \tag{5.40}$$

where we replaced $p \to p_{\mathrm{EOS}}$. To solve Eq. (5.40), we use the fourth-order Runge–Kutta scheme for time; the fifth-order WENO (weighted essentially non-oscillatory) scheme [213, 214] for the convection term[1]; the sixth-order isotropic central difference [107, 205, 215] for the other spatial derivation.

Although the derivation in this paper is based on the internal energy, Eq. (5.40) is identical with the energy equation in Ref. [187], who began with the local entropy balance [216]. On the other hand, Eq. (5.40) is different from the Gong et al.'s one [217]. See Ref. [218] for mode details on this discussion, where we can find a comprehensive explanation on the issue of energy equation for phase-change LB model.

As can be seen in Eqs. (5.19) and (5.40), the coupling between the pseudopotential LB model and the finite-difference scheme is established via a non-ideal EOS. The realistic EOS widely used in the multiphase lattice Boltzmann simulations includes van der Waals, Carnahan–Starling, Peng–Robinson, etc. We adopt the Peng–Robinson EOS in this simulations, which is

[1] We stress that some *upwind*-type schemes should be adopted for the convection term. Otherwise, the non-physical oscillation will appear for convection-dominant cases.

given by [208]

$$p_{\text{EOS}} = \frac{\rho RT}{1 - b\rho} - \frac{a\varphi(T)\rho^2}{1 + 2b\rho - b^2\rho^2}, \tag{5.41}$$

where $\varphi(T) = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{T/T_c})]^2$ with the acentric factor ω. The critical properties can be obtained as follows: $a = 0.4572R^2T_c^2/p_c$ and $b = 0.0778RT_c/p_c$. We set $b = 2/21$, $R = 1$, and the acentric factor $\omega = 0.344$ (for water). The value of a is closely related to the interface width; the larger the value a is, the thinner the interface becomes [211]. To keep the interface thinner as possible, we set $a = 3/49$ as in Refs. [187, 217, 219]. Then, the critical density, temperature, and pressure can be calculated as $\rho_c = 2.657$, $T_c = 0.1094$, $p_c = 0.08936$, respectively.

By reducing a in Eq. (5.41), the achievable reduced temperature decreases. In case of $a = 3/49$, which we will use for phase-change simulation, the minimum reduced temperature is $T_r \sim 0.8$. In general, the small value of a leads to numerical stability for high density ratios (e.g., 2/49 [208], 0.02267 [186], and 1/49 [220] have been used in the literature). By multiplying a reducing parameter δ to EOS as, $p'_{\text{EOS}} = \delta p_{\text{EOS}}$, one can achieve higher density ratio [220,221], which is not targeted here.

5.3 Validation study

5.3.1 Laplace's law

To validate the surface tention obtained by the present lattice Boltzmann model, the static bubble test is conducted. From the Laplace law for two-dimensional case, the pressure difference between inside and outside of bubble can be given by

$$\Delta p = \frac{\gamma}{R}, \tag{5.42}$$

where γ and R is the bubble diameter. In the computational domain discretized into $200\delta_x \times 200\delta_x$, a stationary bubble with various radius R was initially placed. All the boundary con-

dition is set to be periodic boundary conditions. At the equilibrium state, we measured the pressure difference for three reduced temperature values, $T_r = 0.86$, 0.90, and 0.95. Fig. 5.1 shows the results. As can be seen, the measurements result well fitted with tye Laplace law, that is, the pressure difference was proportional to $1/R$.

Figure 5.1: Laplace's law for several reduced temperatures.

5.3.2 Thermodynamic consistency

To check the thermodynamic consistency of the present lattice Boltzmann model, the additional static bubble test is conducted. We use the same computational setup as the last Laplace tests. Following Li et al. [211], we set the initial bubble to $R = 50$. The analytical solution was obtain via Maxwell equal area rule, *i.e.*, by numerical integration of the EOS.

Fig. 5.2 shows the comparison of simulation results with analytical solution of Maxwell construction. As reference, the case with the original forcing scheme [158] is shown in the figure. From the Fig. 5.2, we can see that the present model well describe the analytical solution of Maxwell construction by setting $\sigma = 0.66$, whereas the case with the original forcing scheme ($\sigma = 0$) does not agree with the analytical solution. Based on such characteristics, we confirmed that this model can perform thermodynamically-consistent phase-change simulation.

Figure 5.2: Simulation of two-dimensional circular bubble with $\nu = 0.1$. Line: Maxwell's equal rule area. Symbol: lattice Boltzmann simulation with $\sigma = 0$ and $\sigma = 0.66$. The case of $\sigma = 0$ corresponds the original consistent scheme [158].

Furthermore, we investigated the viscosity dependency of the present model against the thermodynamic consistency. Fig. 5.3 shows the comparison of simulation results with analytical solution under variable kinematic viscosities. We found that the present forcing scheme well approximate the thermodynamic consistency for wide range of kinematic viscosities. Thus, it is possible to investigate the phase-change behavior of various Reynolds numbers while maintaining thermodynamic consistency.

5.4 Forced convection boiling on a cylinder

5.4.1 Setup

Computational setup is described in Fig. 5.4. The domain is filled with the saturated liquid. The periodic boundary conditions are imposed at the side boundaries. The gravitational acceleration acts on the whole computational domain. We set the velocity boundary and convective boundary conditions at the inflow and outflow boundaries, respectively. At the inlet boundary, we impose the constant velocity u_0. According to Zou and He [222], the unknown populations

Figure 5.3: Simulation of two-dimensional circular bubble with variable kinematic viscosities. Line: Maxwell's equal rule area. Symbol: lattice Boltzmann simulation with $\nu = 0.1$, $\nu = 0.01$, and $\nu = 0.001$. We can see the present forcing scheme can achieve thermodynamic consistency independent of kinematic viscosity.

after the streaming step, f_3, f_5, and f_8, are specified as follows:

$$\begin{aligned}
\rho_{\text{in}} &= \frac{f_0 + f_1 + f_2 + 2(f_4 + f_6 + f_7)}{1 - u_0}, \\
f_3 &= f_4 + \frac{2}{3}\rho_{\text{in}} u_0, \\
f_5 &= f_6 - \frac{1}{2}(f_1 - f_2) + \frac{1}{6}\rho_{\text{in}} u_0, \\
f_8 &= f_7 + \frac{1}{2}(f_1 - f_2) + \frac{1}{6}\rho_{\text{in}} u_0.
\end{aligned} \tag{5.43}$$

The convective boundary condition is imposed at the outflow boundary [141].

$$\frac{\partial \phi}{\partial t} + U_c \frac{\partial \phi}{\partial y} = 0, \text{ at } y = N, \tag{5.44}$$

where N is the outflow boundary node. Following Ref. [141], we added two additional ghost nodes, $N+1$ and $N+2$. The discretization form can be given by the first-order implicit scheme

$$\phi(x, N, t + \delta_t) = \frac{\phi(x, N, t) + \lambda \phi(x, N - 1, t + \delta_t)}{1 + \lambda}, \tag{5.45}$$

where $\lambda = U_c(t+\delta_t)\delta_t/\delta_x$. There are several possibilities for such as the local, average, or maximum velocity. After conducting some numerical tests, we determined that the local velocity was most suitable for the current system, namely

$$U_c(x, N, t) = u_y(x, N-1, t), \tag{5.46}$$

where $u_y(\boldsymbol{x}, t) = u_y(x, y, t)$ is the component of the fluid velocity $\boldsymbol{u}$ in the z direction. The variables f_i, ρ, $\boldsymbol{u}$, and $\boldsymbol{F}$ are also convected with Eq. (5.44).

Figure 5.4: Boundary conditions for the boiling simulations.

As in Fig. 5.5, the cylindrical domain is modeled via the second-order interpolated bounce-back scheme [223, 224], which is similar treatment by Hatani et al.'s condensation simulation [225]. In the interpolated bounce-back scheme, the populations at fluid node $(\boldsymbol{x}_f, t)$ are calculated

$$\begin{aligned}\tilde{f}_{\bar{i}}(\boldsymbol{x}_f, t) =& q(1+2q)f_i(\boldsymbol{x}_f + \boldsymbol{c}_i, t) + (1-4q^2)f_i(\boldsymbol{x}_f, t) \\ &- q(1-2q)f_i(\boldsymbol{x}_f - \boldsymbol{c}_i, t) + 3w_i[\boldsymbol{c}_i \cdot \boldsymbol{u}(\boldsymbol{x}_w, t)] \text{ for } q < \frac{1}{2},\end{aligned} \tag{5.47}$$

$$\begin{aligned}\tilde{f}_{\bar{i}}(\boldsymbol{x}_f, t) =& \frac{1}{q(1+2q)}f_i(\boldsymbol{x}_f + \boldsymbol{c}_i, t) + \frac{2q-1}{q}f_i(\boldsymbol{x}_f - \boldsymbol{c}_i, t) \\ &- \frac{2q-1}{2q+1}f_i(\boldsymbol{x}_f - 2\boldsymbol{c}_i, t) + \frac{3w_i}{q(1+2q)}[\boldsymbol{c}_i \cdot \boldsymbol{u}(\boldsymbol{x}_w, t)] \text{ for } q \geq \frac{1}{2},\end{aligned} \tag{5.48}$$

where $q = |\boldsymbol{x}_f - \boldsymbol{x}_w|/|\boldsymbol{x}_f - \boldsymbol{x}_b|$ is the fraction of each link, being $\boldsymbol{x}_w$ the exact position of a wall node. We only consider the stationary cases; the velocity at the solid boundary $\boldsymbol{u}(\boldsymbol{x}_w)$ is set

to be zero. Thus, the last terms in Eqs. (5.47) and (5.48) can be dropped. In the cylindrical region, we set superheat temperature T_w, which is higher than the saturated temperature T_{sat}.

In the following simulations, the reduced temperature is set to be $T_r = 0.86$, which corresponds to the water-vapor system under around 7 MPa. The physical properties (kinematic viscosity, Prandtl number, thermal conductivity, specific heat, surface tension) under $T_r = 0.86$ were reproduced from the steam table for saturated condition [226]. We assumed that specific heat ratio for each phase is unity. The computational domain is discretized into $W \times H = 600\delta_x \times 1350\delta_x$. The circular region with $D = 30\delta_x$ was set up, in which the center of the cylinder localed at the $(0.5W, 0.2H)$.

The investigated parameters are the Reynolds and Jacob numbers, defined as follows:

$$\mathrm{Re} = \frac{u_0 D}{\nu_l}, \tag{5.49}$$

$$\mathrm{Ja} = \frac{c_{p,v}\Delta T}{h_{fg}}, \tag{5.50}$$

where ν_l, $c_{p,v}$, $\Delta T = T_w - T_{sat}$, and h_{fg} are, respectively, the kinematic viscosity for liquid phase, specific heat at constant pressure for vapor phase, wall superheat degree, and latent heat. We set $u_0 = 0.05$ and h_{fg} is automatically determined via the EOS. The Reynolds number was adjusted by the kinematic viscosity; the Jacob number was adjusted by the wall superheat[2]. In the initial $3000\delta_t$ run, the energy equation [Eq. (5.40)] was neglected.

5.4.2 Boiling regimes

Figure 5.6 shows the simulation results for Ja = 0.33. The white circular region describes the cylinder. In each figure, the convection is given from the bottom. For both Reynolds number cases, nucleation, growth, and detach of the vapor bubble can be seen. A series of boiling process can naturally arise with the present method, but there can be found some differences between them. From Fig. 5.6, the vapor mainly generated from the upper side of the cylinder at $t = 2\,000\delta_t$. The neck part of the vapor became thinner and bubbles were formed. From

[2]The specific heat can also be taken as the input parameter in the present simulations.

Figure 5.5: Schematic diagram of interpolated bounce-back scheme.

Fig. 5.6 (b), the interface was more unstable compared with Fig. 5.6 (a). At $t = 4\,500\delta_t$ in Fig. 5.6 (b), the generated bubble broke up into two smaller bubbles We can see that the upstream region keeps to contact with liquid, whereas the wake region contacts with vapor. In this Jacob number, the film boiling cannot be observed from the interfacial shape.

Figure 5.6: Snapshots of boiling behavior on a cylinder for Ja = 0.33. (a) Re = 30, (b) Re = 3 000.

Figure 5.7 shows the simulation results for higher Jacob number case: Ja = 1.35. The drastic vaporization can be seen at $t = 1000\delta_t$, regardless of the Reynolds number. For Re = 30, the cylinder was covered with vapor all the time. Obviously, this kind of boiling regime is the film

boiling. For Re = 3 000, in contrast, the cylinder partially contacted with the liquid (*e.g.*, at $t = 6\,000\delta_t$). However, the the Jacob number is sufficiently large, the cylinder was quickly covered with the vapor. Thus, we cannot identify what this boiling regime is; so we should quantify the behavior by heat flux.

Figure 5.7: Snapshots of boiling behavior on a cylinder for Ja = 1.35. (a) Re = 30, (b) Re = 3 000.

We then compare the interfacial shape with Liu–Theofanous' boiling regime sketch. From the simulation result in Fig. 5.8, the vapor was streched into downstream region due to the forced convection. Fluctuation of the interface is observed. A cone-like shape appeared. Totally, the present simulation seems to qualitatively agree with the model of 'completely saturated'.

5.4.3 Heat flux and boiling curve

The average heat flux can be calculated as

$$\bar{q}(t) = \frac{1}{W}\int_0^W q(\boldsymbol{x})\mathrm{d}s, \tag{5.51}$$

Figure 5.8: Comparison of boiling regime obtained from the simulation with the sketch reproduced from Liu and Theofanous [176].

where W is the circumference length, and the local heat flux is given by

$$q(\boldsymbol{x}) = -\lambda(\boldsymbol{x})\frac{\partial T}{\partial n}|_{\text{wall}}, \tag{5.52}$$

where λ is the thermal conductivity and n is the normal direction.

Figure 5.9 represents the time history of the average heat flux on the cylinder for Re = 30. For higher Jacob number case, some peaky behavior was observed only at the initial stages; however, it seems to converge to a certain value.

Figure 5.9: Average heat flux on a cylinder surface with Re = 30. (a) Ja = 0.33, (b) Ja = 1.35.

More drastic difference can be found from Fig. 5.10, which represents the average heat flux for Re = 3 000. For lower Jacob number case, the qualitative tendency was similar to those for Re = 30. On the other hand, for higher Jacob number case, very intense fluctuation of heat flux values were observed. That is because the cylinder intermittently repeated contact with vapor and liquid. When it contacted with the liquid, higher heat flux was observed; when it contacted with the vapor, lower heat flux was observed.

By averaging the heat flux during steady state, we can calculate the averaged heat flux in time. When the heat flux is plotted against the superheat (Ja), the obtained curve describes the boiling curve.

Figure 5.10: Average heat flux on a cylinder surface with Re = 3 000. (a) Ja = 0.33, (b) Ja = 1.35.

Figures 5.11 and 5.12 the caluculated boiling curve for Re = 30 and Re = 3 000. The error bars on the plots describe the standatd deviation. Looking at the behavior of the *average* value, both well reproduce the existing boiling curves [167]. That is, thile the degree of heating is small, the heat flux rises and reaches the maximul point (critical heat flux: CHF). Then, after reaching the minimul point (minimum heat flux: MHF), the heat flux decreases and starts to rise again. Such well known characteristics of boiling curve was successfully reproduced with the present lattice Boltzmann method.

From Fig. 5.12, we can find the *deviation* is extremely large as the Jacob number increases. After reaching the CHF point, the tendency strongly appears. As mentioned in the last section,

this is due to the ntermittent contact with vapor and liquid. From the boiling curve evaluation, it is thought that film boiling occurs when Ja is 0.5 or more, but according to this analysis it is in contact with the liquid. The larger the Reynolds number, the more unstable the interface, suggesting the possibility of contact with the solution in the time-space manner even in the film boiling region.

Figure 5.11: Boiling curve for Re = 30

Figure 5.12: Boiling curve for Re = 3000

5.4.4 Comparison with film boiling heat transfer correlations

Finally, we compare the present simulation results with the existing film boiling heat transfer model. All the folm boiling heat transfer correlations in this section have been reduced for the saturated condition; the term related subcooling degree has been dropped. To find the original expression, refer to the original paper [176–178].

The first corerlation is the one proposed by Dhir and Purohit [178]:

$$\mathrm{Nu} = 0.8\left(\mathrm{Ar}^{\frac{1}{4}}\mathrm{Pr}^{\frac{1}{4}}\mathrm{Ja}^{-\frac{1}{4}} + \mathrm{Re}^{\frac{1}{2}}\right), \tag{5.53}$$

where Ar is the Archimedes number. If the second term in Eq. (5.53) is neglected, the equation is reduced to the saturated correlation for pool boiling heat transfer coefficient. That is, they considered that the forced convection effect is simply added to the pool boiling heat transfer.

The corerlations of Epstein–Hauser [177] and Liu–Theofanous [176], respectively, have similar forms as follows:

$$\mathrm{Nu} = 1.13\left(\frac{\rho_l}{\rho_v}\right)^{\frac{1}{4}}\left(\frac{\nu_l}{\nu_v}\right)^{\frac{1}{2}}\mathrm{Pr}^{\frac{1}{4}}\mathrm{Ja}^{-\frac{1}{4}}\mathrm{Re}^{\frac{1}{2}}, \tag{5.54}$$

$$\mathrm{Nu} = 0.5\left(\frac{\rho_l}{\rho_v}\right)^{\frac{1}{4}}\left(\frac{\nu_l}{\nu_v}\right)^{\frac{1}{2}}\mathrm{Pr}^{\frac{1}{4}}\left(\frac{1}{\mathrm{Ja}} + \frac{1}{2}\right)^{\frac{1}{4}}\mathrm{Re}^{\frac{1}{2}}. \tag{5.55}$$

There are mainly two differences between Epstein–Hauser and Liu–Theofanous correlations: coefficients 1.13 and 0.5 and the definition of Jacob number. Actually, Liu–Theofanous' spesific latent heat was defined as $h'_{fg} = h_{fg} + 0.5c_{p,v}\Delta T$.

Figure 5.13 compares the calculated Nusselt number with the above correlations [Eqs. (5.53)–(5.55)]. The higher Reynolds number, the higher the Nusselt number as a whole. The film boiling regime in the simulations apprear $\mathrm{Ja} > 0.6$. The Dhir–Prohit correlation proved to be overestimated for both results.

For low Reynolds number case from Fig. 5.13 (a), the simulation results approaches between Epstein–Hauser and Liu–Theofanous correlations. It is thought that the case of low value is

close to the condition of theoretical analysis because the cylinder is always covered with vapor.

For high Reynolds number case from Fig. 5.13 (b), all the correlations overestimates the simulation results. Among them, the Liu–Theofanous correlation was closest to the simulaton results of film boiling. Although there still remains a difference between the simulation results and Liu–Theofanous correlation, the slopes were in good agreement. It was found that the Liu–Theofanous correlation can predict the heat transfer coefficient best within the scope of this simulation condition.

Here, we consider the cause of the difference between the existing correlations. The first point is that this simulation does not consider radiation heat transfer. If radiation is taken into account, the heat transfer coefficient will increase. The first point is the matter of temperature boundary layer and resolution. Especially for high Reynolds number, the simulation can not resolve the temperature boundary layer.

Figure 5.13: Comparison of the simulation results with semi-empirical correlations [176–178]. (a) Re = 30 and (b) Re = 3 000

5.5 Summary

The pseudopotential lattice Boltzmann model for phase change is developed to simulate a series of boiling two-phase flows. To keep numerical stability even at high Reynolds number, central-moments-based formulation is adopted. The model is then applied to convection boiling on a cylinder. Two cases of Reynolds number, 30 and 3000, are investigated. We found that the present model can well reproduce the overall behavior of boiling curve. Also, a series of boiling process, nucleation, growth, departure of vapor bubbles were observed from simulations. The obtained heat flux is nondimensionalized to Nusselt number in order to compare with the semi-empirical correlations. It was found that the Liu–Theofanous correlation can predict the heat transfer coefficient best within the scope of this simulation condition.

Chapter 6

Melt-Coolability Assessment

In this chapter, we outline the heat transfer model for melt fuel cooling performance evaluation, and evaluate the actual machine cooling performance based on the parameters decided based on the experiment result.

6.1 Concept of the heat transfer model

The heat transfer model used in this chapter is based on the crude mixed heat transfer model pmjet developed by Moriyama et al. [37] for LWR conditions, and was improved by Abe et al. [36] and Matsuo et al. [26] for SFR conditions. This simply models the coolability of the melt jet in the premixing region. Therefore, it is considered that the influence of parameters such as particle size on the cooling behavior is physically and prospectively given well. The outline of this model is shown again Fig. 1.1 and described below. See *e.g.* Refs. [26, 36] for details. Here we basically take the conservative-side assumptions from melt-coolability points.

- To perform analysis targeting SFRs, the physical properties of MOX fuel (or UO_2) and sodium are used, referring Refs. [61, 62].
- The diameter of the jet ($D_j(z)$) decreases linearly with respect to the direction of penetration of the jet until it reaches the jet break-up length (L_{brk}) which is the disappearance

distance of the core.

$$\frac{dD_j(z)}{dz} = -\frac{D_{j0}}{L_{brk}}. \tag{6.1}$$

- The particles emerging from the surface of the jet are spherical and have a single particle size.
- The generated particles settle at solidification at the terminal velocity (V_s) immediately after production.

$$V_s = \sqrt{\frac{4}{3c_f}}\sqrt{\frac{(\rho_m - \rho_c)}{\rho_c}D_p g}. \tag{6.2}$$

- Ignore the heat transfer between the jet and the coolant and consider only the heat transfer between the generated particles and coolant.
- Consider *film boiling* heat transfer as a boiling regime; neglect radiation heat transfer from conservative side.
- In the initial unsteady process from the time the jet begins to penetrate until it reaches the jet breakup length, the shape of the jet is equal to the steady state and the tip position varies with time according to the jet velocity; that is, in the initial unsteady process, the shape of the jet is treated as a truncated cone.
- Particles generated at a certain location settle while cooling, and are excluded from the calculation when they reach the bottom of the coolant pool ($z = H$).
- In the initial state, the coolant has reached the saturation temperature; neglect the coolant subcooling from conservative side.

To perform the present analysis, the following three physical quantities must be identified by some correlations.

- Jet breakup length
- Droplet diameter
- Heat transfer coefficient

Figure 6.1: Schematic of the melt-coolability assessment model.

6.2 Correlations

Here we choose the correlations and provide the physical consideration for why we chose them. As the reactor conditions, we assume $D_{j0} = 55$ mm and $u_{j0} = 5$ m/s. Figure 6.2 briefly sumarrizes the model outline with the adopted correlations. See below for detail of the adopted correlations.

6.2.1 Jet breakup length

Combining these asumptions and the physical properties from Refs. [61, 62] enables us to evaluate the flow regime of the expected reactor condition as shown in Fig. 6.3. The numerical simulation results obtained in this dissertation are also included in Fig. 6.3 for reference. The calculated Reynolds number and Ohnesorge number are $\mathrm{Re} = 6.0 \times 10^5$ and $\mathrm{Oh} = 2.7 \times 10^{-4}$. The operating diagram in Sec. 2 indicates that the flow regime of the melt jet breakup is the atomization regime, which means that the entrainment (fragmentation from the jet side) would be the dominant mechanism.

The Epstein–Fauske [38] correlation given by

Figure 6.2: Adopted correlations used for melt-coolability assessment.

$$\frac{L_{\mathrm{brk}}}{D_{j0}} = \frac{1}{2E_0}\left(\frac{\rho_j}{\rho_c}\right)^{\frac{1}{2}}, \tag{6.3}$$

is adopted to give the jet breakup length. The entrainment coefficient E_0 is set to 0.05 from the conservative side. Moreover, the experimental results in Sec. 2 showed that the jet's diameter decreases *almost* linearly with respect to the direction of penetration of the jet until it reaches the jet break-up length.

6.2.2 Melt drop diameter

To predict the generated droplet's diameter, we use the critical Weber number Although the value itself has room for selection (*i.e.* 12 [67], 18 [26], etc.), $\mathrm{We}_{\mathrm{crit}}$ 18 was used here, that is

$$D_p = \frac{\sigma}{\rho_l V_j^2}\mathrm{We}_{\mathrm{crit}} = \frac{\sigma}{\rho_l V_j^2}18, \tag{6.4}$$

Figure 6.3: Assumptions and simulation conditons. From mapping on the flow-regime diagram, the regime is evaluated as atomization regime.

$$D_p = \min\left(\frac{\sigma}{\rho_l V_j^2}18,\ D_{j0}\right) \tag{6.5}$$

Note that the surface solidification effect [30] is not considered in the present calculation.

6.2.3 Heat transfer coefficient

To give the heat transfer coefficient from the melt particle to coolant, we give the correlation of film boiling heat transfer. From the findings in Sec. 5, Liu–Theofaunous correlation [176] without subcooling term (for saturated condition) is adopted.

$$\mathrm{Nu} = 0.5\left(\frac{\rho_l}{\rho_v}\right)^{1/4}\left(\frac{\nu_l}{\nu_v}\right)^{1/2}\mathrm{Pr}^{1/4}\left(\frac{1}{\mathrm{Ja}}+\frac{1}{2}\right)^{1/4}\mathrm{Re}^{1/2}. \tag{6.6}$$

The simulations in Sec. 5 indicated that the Liu–Theofanous corelation was most conservative, and the correlation's tendency relatively agreed with the numerical simualtions compared with Dhir–Purohit [178] and Epstein–Hauser [177] correlations. Also, it should be noted that the

Table 6.1: List of the present sensitivity analyses. 'Ref.' denotes the reference case. Cases 1–3 and 4–6 investigate the sensitivity of melt particle diameter and pool depth, respectively.

	D_{j0} [mm]	u_{j0} [m/s]	L_{brk} [m]	d_p [mm]	H [m]
Ref.	55	5	1.74	0.39	3
Case 1	55	5	1.74	0.78	3
Case 2	55	5	1.74	2.0	3
Case 3	55	5	1.74	3.9	3
Case 4	55	5	1.74	0.39	1.5
Case 5	55	5	1.74	0.39	7.5
Case 6	55	5	1.74	0.39	10

Liu–Theofanous correlation is on the most conservative side among them.

6.3 Calculations and sensitivity analysis

We do two types of sencitivity analysis. First, the melt drop diameter is considered, and then the pool depth. The list of sensitivity analysis is shown in Table 6.1. We begin with the result of Ref. case, where the values of jet breakup length L_{brk}, drop diameter d_p, and heat transfer coefficient h are evaluated using Eqs. (6.3), (6.5) and (6.6), reaspectively. Cases 1–3 and 4–6 investigate the sensitivity of melt particle diameter and pool depth, respectively. Note that for Case 4, the jet breakup length is larger than pool depth ($L_{brk} > H$); thus the melt jet reach the bottom before completely breakup.

By using the present melt-coolability calculation model, the particle mass in the coolant and on the floow can be evaluated. Furthermore, heat transfer calculation enables us to specify whether the generated drop is *melt* state or *solidified* state. Fig. 6.4 shows the calculation results for Ref. case. The solid line denotes the total mass, that is, the mass of jet column, particles in the coolant, and those on the floor. As in Fig. 6.4, the total mass increases linearly, because the inlet flow rate is constant (*i.e.*, D_{j0} = const., u_{j0} = const.). All particles in the coolant, denoted by dotted line, continued to rise to around 7 s and then became constant. At this time, all particles on the floow, denoted by the broken line, started to increase. This means

Figure 6.4: Calculation results for Ref. case.

that the particles reached to the floor owing to settlement around 6 s. We can also find the melt-state particle, denoted by chain line, in Fig. 6.4 even though the amount is quite small. Note that the Ref. case does not have the melt particle on the floor; all of the particle has been cooled down in the coolant region.

In the evaluation of vapor explosion (*e.g.*, [37]), the presence of melt drop in the bulk coolant (or premixing region) may be of interest to investigate, but, our focus here is on the melt coolability; whether the particles cool down or not to reach the floor is the present interest. Therefore, from now on we focus on the mass on the floor.

First, we show the sensitivity analysis of the drop diameter. Based on the Ref. case, we set two (Case 1), five (Case 2), and ten times (Case 3) the diameter (see Table 6.1). Fig. 6.5 shows the sensitivity analysis results. The larger the particle size, the faster the time to reach it. Only for the largest particle diameter (Case 3), the particles reached the bottom in the molten state. In other words, we found that all the particles settled down onto the floor after completely cooled, except for Case 3.

Next, we investigate the sensitivity of pool depth. Based on the Ref. case (3 m), we set the pool depth as 1.5 m (Case 4), 7.5 (Case 5), and 10 m (Case 6) (see Table 6.1).

Figure 6.5: Sensitivity analysis of the drop diameter.

To quantify the melt coolability, we define the following mass ratio:

$$\Gamma = \frac{m_{melt}}{m_{total}}, \tag{6.7}$$

where m_{melt} and m_{total} are the mass of melt state and total mass, respectively. In Fig. 6.7, the calculated melt mass ratio Γ for Cases 3 ($d_p \times 10$) and 4 ($H = 1.5$ m) are described. For both cases, Γ quickly became a steady state with a quite small value: ~ 0.009 for Case 3 and ~ 0.005 for Case 4. However, we can see there are large differences between Case 3 and Case 4. For Case 3 ($d_p \times 10$), the time series of Γ began with very high value (0.94) at the early stages (around 2.0 s), and then decreased drastically. This means that a large amount of particles would reach the floor in melt state, although the time is not so long. On the other hand, for Case 4, the highest Γ was at most 0.17 (that is, 17% of the particles were in melt state). Comparing Cases 3 and 4, Case 3 would be more dangerous from the point of coolability. The present sensitivity analyses indicate that the melt drop diameter is more important factor to be treated carefully than the pool height. This implies that if the melt jet breaks up into particles fine enough, the melt particles cooled down sufficiently.

Figure 6.6: Sensitivity analysis of the pool depth.

6.4 Summary

To assess the melt coolability, we used the simplified melt coolability model, where several correlations were to be identified. Three physical quantities, the jet breakup length, the melt drop diameter, and the heat transfer coefficient, were modelled through the appropriate correlations. The correlations were specified based on the experimental and numerical findings in the present dissertation.

By using this model with the physical properties of SFR systems, we conducted sensitivity analyses. The particle diameter and pood depth were investigated. The present sensitivity analyses indicate that the melt drop diameter is more important factor to be treated carefully than the pool height. This implies that if the melt jet breaks up into particles fine enough, the melt particles cooled down sufficiently.

Figure 6.7: Melt mass ratio on the floor for Case 3 and Case 4.

Chapter 7

Conclusion

7.1 Liquid-liquid jet experiments

A detailed experimental study to understand the jet fragmentation is presented. The study mainly focuses on hydrodynamic interaction of jet breakup. The experiments were carried out in an immiscible liquid-liquid system. The indices of refraction in the two liquids were matched, so that the vertical plane of jet flow was clearly visualized using laser-induced fluorescence (LIF). The jet breakup length obtained by image processing is compared with the existing correlations. Then, the breakup regimes were organized on a dimensionless operating diagram, with the derived correlations representing the criteria for regime boundaries of a liquid-liquid system based on the observation and analysis results. The experimental data were extrapolated to the expected reactor conditions.

7.2 Liquid-liquid jet simulations

In order to investigate parameter ranges that can not be observed by experiments, we proposed a numerical method and conducted numerical simulations. A three-dimensional color-fluid lattice Boltzmann model for immiscible two-phase flows was developed in the framework of a

three-dimensional 27-velocity (D3Q27) lattice. This model was applied to liquid-jet-breakup simulations. The reproducibility of the regime map for liquid-liquid systems was confirmed.

7.3 Hydrodynamic melt-jet simulations

We improved the numerical method to investigate the hydrodynamic jet flow in the reactor-equivalent condition. This successfully combined a three-dimensional nonorthogonal central-moment-based lattice Boltzmann scheme with the color-gradient lattice Boltzmann model. Hydrodynamic melt-jet breakup simulations showed that the proposed model is significantly more stable, even for flow with extremely high Reynolds numbers, up to $O(10^6)$. This enabled us to investigate the phenomena expected under actual reactor conditions.

7.4 Boiling heat transfer on a particle

Heat transfer from particles generated from molten jet to coolant was numerically investigated. The problem was set as forced convection boiling around the cylinder to simplify the actual situation. We used the phase-change lattice Boltzmann method with some improvements on the numerical stability. A series of pool boiling process, such as nucleation, growth, coalescence, and departure of vapor bubbles were successfully simulated. The simulation results were compared with existing film boiling heat transfer correlations.

7.5 Melt-coolability assessment

Appropriate physical models for melt-jet breakup in coolant were identified by integrating the experimental and numerical simulation results. The correlations required for the melt-coolability assessment were determined, which are supported by the experimental or numerical evidences. The sensitivy analysis showed the coolability performance of the melt jet in coolant under various conditions. The particle diameter and pood depth were investigated. The present

sensitivity analyses indicate that the melt drop diameter is more important factor to be treated carefully than the pool height. This implies that if the melt jet breaks up into particles fine enough, the melt particles cooled down sufficiently.

It is believed that the results obtained in this article, based on the phenomenological discussion supported by the detailed experiments and simulations, provide fundamental knowledge with which to assess melt-jet breakup and fragmentation under the conditions that would pertain to accident conditions.

Publication list

Included papers

1. **S. Saito**, A. De Rosis, A. Festuccia, A. Kaneko, Y. Abe, K. Koyama, Color-gradient lattice Boltzmann model with nonorthogonal central moments: Hydrodynamic melt-jet breakup simulations, , *Physical Review E*, Vol. 98, Iss. 1, p. 013305, 2018.

2. **S. Saito**, Y. Abe and K. Koyama, Lattice Boltzmann modeling and simulation of liquid jet breakup, *Physical Review E*, Vol. 96, Iss. 1, p. 013317, 2017.

3. **S. Saito**, Y. Abe and K. Koyama, Flow transition criteria of a liquid jet into a liquid pool, *Nuclear Engineering and Design*, Vol. 315, pp. 128–143, 2017.

4. **S. Saito**, Y. Abe, A. Kaneko, T. Kanagawa, Y. Iwasawa and K. Koyama, Simulation of a liquid jet using the lattice Boltzmann model for immiscible two-phase flow, *Japanese Journal of Multiphase Flow*, Vol. 29, Iss. 5, pp. 431–441, 2016 (in Japanese).

5. **S. Saito**, Y. Abe and K. Koyama, Visualization and measurement of jet breakup behavior using LIF, *Transactions of the JSME (in Japanese)*, Vol. 81, Iss. 832, 2015.

Papers not included in the thesis

1. Y. Abe, K. Fujiwara, **S. Saito**, T. Yuasa, and A. Kaneko, Bubble dynamics with aerosol during pool scrubbing, *Nuclear Engineering and Design*, Vol. 337, pp. 96–107, 2018.

Book chapter

1. Y. Abe and **S. Saito**, Vapor explosion between high-temperature molten liquid droplet and water pool, in: Boiling: Research and Advances, pp. 682–705, Elsevier, 1st Ed., June 2017.

Conference proceedings

1. **S. Saito**, K. Ebihara, A. De Rosis, K. Kawasaki, A. Kaneko, Y. Abe and K. Koyama, "A numerical study on convective boiling heat transfer simulating a melt particle in a coolant," *Proceedings of the 11st Korea-Japan Seminar on Nuclear Thermal Hydraulics and Safety (NTHAS11)*, Busan, Korea, 2018.

2. **S. Saito**, Y. Abe, K. Ebihara, A. De Rosis, A. Kaneko and K. Koyama, "A coupled lattice Boltzmann-finite difference approach for boiling two-phase flow with high density ratios," *Proceedings of the 16th International Heat Transfer Conference*, No. 22464, Beijing, 10-16 August 2018.

3. **S. Saito**, Y. Abe, A. Kaneko, A. Festuccia, A. De Rosis, and K. Koyama, "Numerical simulations of hydrodynamic process of melt jet breakup with two-phase lattice Boltzmann method," *Proceedings of the 26th International Conference on Nuclear Engineering*, ICONE26-81663, London, England, July 2018.

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6. **S. Saito**, Y. Abe, A. Kaneko, T. Kanagawa, Y. Iwasawa, E. Matsuo, K. Ebihara, H. Sakaba, K. Koyama, H. Nariai, "Experimental Study on Jet Instability and Breakup Behavior in Liquid-Liquid System," *Proceedings of the 23rd International Conference on Nuclear Engineering*, ICONE23-1886, May 17-21, 2015.

7. **S. Saito**, Y. Abe, Kaneko, A., T. Kanagawa, Y. Iwasawa, E. Matsuo, K. Ebihara, H. Sakaba, K. Koyama and H. Nariai, "Visualization and Measurement of Jet Breakup Behavior with Interfacial Fragmentation using LIF and PIV," *Proceedings of the 9th Korea-Japan Symposium on Nuclear Thermal Hydraulics and Safety (NTHAS9)*, N9P0025, November 16-19, 2014.

8. **S. Saito**, Y. Abe, A. Kaneko, Y. Iwasawa, E. Matsuo, K. Ebihara, H. Sakaba, K. Koyama, and H. Nariai, "Influence of Hydrodynamic Interaction on Jet Breakup and Fragmentation Behavior," *Proceedings of the 22nd International Conference on Nuclear Engineering*, ICONE22-30028, July 7-11, 2014.

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