Review on Dynamic Van der Waals Theory in two-phase flow

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Abstract: In this paper we review the Dynamic Van der Waals theory, which is a recent developed method to study phase separation and transition process in multiphase flow. Gradient contributions are included in the entropy and energy functions, and it's particularly useful and non-trivial if we consider problems with temperature change. Using this theory, we can simulate that, a droplet in an equilibrium liquid will be attracted to the heated wall(s) which was initially wetted, which is the main cause of the famous hydrodynamic phenomena-Leidonfrost Phenomena. After more than ten years development, this theory has been widely used to study the fluid flow in vaporing and boiling process, e.g. droplet motion. Furthermore, this theory has been combined with phase field model, which could be extended to solid-liquid phase transition. There has also been researches about constructing LBM scheme to extend to the Dynamic Van der Waals theory, using Chapman-Enskog analyze. In all, due to its rigorous thermodynamic derivation, this theory has now become the fundamental theoretical basis in the heated multiphase flow.

1. Introduction

In terms of physics and engineering, hydrodynamics is a subdivision for the description of fluids, which are usually combined with heat transfer and phase transition, and usually involving multiphase flow. For example, in the energy industry, performance forecasts, including reliability and safety, depend largely on "hot and flow" research techniques, from macro-scale to medium-scale to microscopic scale, to study oil recovery, fuel turbines, chemical batteries and power plants. Since the 1970s, a solution based on the Renault average Navier-Stokes (RANS) equation has developed a general-purpose computational fluid dynamics (CFD) to compute a combination of fluid flow and heat transfer. With the great development of supercomputers in the 1990s, methods including large eddy current simulation (LES) and direct numerical simulation (DNS) were more accurate, and computationally demanding methods are increasingly being used (Charles and Daivis, 2009; Xie et al., 2016). It is clear that the complex dynamic behavior of the interface-dominated system is needed, especially the behavior of the interfaces in these systems. On

the macroscopic length scale, the response of the interface leading material to the applied deformation, concentration gradient, or temperature gradient is usually described by a continuous model. There is a clearly recognizable interface in macroscopic free surface flow or thin films (such as films encountered in coatings), and we need to address the temporal evolution of the interface when modeling these systems. In the flow of red blood cells involving emulsions, finely divided polymer blends, microcapsule dispersions, or arterial blood flow, the dynamics of a single interface is usually not resolved at the macroscopic scale.

In order to construct such a coarse-grained macroscopic model, it is necessary to study the dynamics of each interface at a small length scale, that is, to track the temporal evolution of the interface of a single emulsion droplet or red blood cell or other small-length phenomenon. Therefore, in these systems, modeling interface dynamics is also very important. However, the macroscopic approach is developed with the assumption of continuity, which is not applicable anymore for certain physical problems, especially in the microscopic

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and mesoscale scale. The latest developments of computational techniques have been shifted to phase-field models, also known as diffue interface (DI) models, where the interface is modeled as a three-dimensional region and the values of all the properties of the material in one of its batch phases are constantly changing in other batch stages value. Diffuse interface method (DIM) has recently been more and more concerned by researchers and engineers, especially for those who are implementing multi-phase numerical simulation. Compared to a large variety of multiphase modeling methods, including the long-history sharp interface method, DI model shows the need for developing the governing equations of mass, momentum, and energy balance to address attractive features across the field, including interface and the nearby area. In DI model, the interface and the nearby area is being seen as a thin layer but with a thickness (infinite). Using this treatment, physical properties, including pressure, temperature and matter density will be continuous in space (Chen et al., 2001; Chen and Meiburg, 2002; Pecenko et al., 2011).

Different with the so-called sharp interface method, the phase field method is related to the study of multiphase processes whose characteristic length scales are comparable to typical interface thicknesses (e.g., coalescence and decomposition events involving emulsion flow in droplets or droplets). The framework begins by assuming that the free energy function of the square gradient term is included in the order parameter (for example, the population density and the component concentration field) (Kou and Sun, 2015; Kou and Sun, 2016a). From this function, the spatial distribution of these order parameters in the interface area is generated through an energy minimization theorem. This method leads to the natural extension of the van der Waals model of the phase transition and the general thermodynamics in the phase transition, assuming a simple pair of potential energy between pairs.

A popular description of the gas-liquid phase transition in a one-component fluid is the van der Waals theory. It is a mean field theory of hardball particles with long and attractive interactions, which is often used to describe the thermal equilibrium conditions. In addition, van der Waals introduced the Helmholtz free energy density gradient term in the 1893 pioneering paper to describe the gas-liquid interface. This gradient term has been applied a lot to statistically analyze the mechanism in non-uniform physical problems, including the paper of Ginzburg and Landau on type I superconductors, as well as the paper of Cahn and Hilliard on binary alloys. Its noted that the temperature T is always treated as a given parameter independent of the space in many existing published theories on phase transition and dynamic process. The Ginzburg-Landau theory is based on a free energy function with uniform T. Needless to say, there are various situations in which a phase change occurs in an uneven T or heat flow. In the fluid system, the wetting dynamics, the boiling process and the droplet movement are strongly influenced by the applied heat flux. In the liquid crystal of the first-order phase change and the binary fluid mixture, the Rayleigh-Bernard convection is very complex with phase separation. In some studies, the superfluidic transition can be influenced by the heat flux nonlinearity, which produces a sharp interface separating the superfluid and normal fluid. It is very difficult to understand this problem. We need to first construct a kinetic model to study the non-equilibrium effect, in which phase transition and fluid mechanics are inseparable coupling.

Korteweg proposed in 1901 the hydrodynamic equation of the binary fluid mixture, including the stress caused by the composition gradient. Then, in the presence of gradient stress, the diffusion interface between the two phases appears in the solution of the fluid mechanics equation. In this row, diffusion interface models in a variety of 2D numerical simulations have been proposed to describe the phase change and motion in single or binary component mixtures. Its extraordinary itself to have the numerical solution for single component flow. Note that the diffusion interface model or phase field model has been used for numerical analysis of dendritic instability in crystal growth. As a further series of studies, it has been studied that the critical dynamics in classical fluids, including the mass density and composition of the gradient contribution, are relevant even in a phase state where the correlation length near the critical point increases. The so-called model H of near-critical binary mixtures has recently been designed to describe the dynamics of thermal fluctuations but also to describe phase separation processes and steady states under shear flow. It is mentioned that the van der Waals liquid in Kawasaki has a long-distance hydrodynamic equation in which stress is non-local convolution, but is reduced to a well-known form in the critical dynamics of gradient approximation. At the same time, a set of non-linear hydrodynamic equations with gradient contribution was established in the early stage, and a simplified version similar to superfluidic conversion was used for critical dynamics and to study the nonlinear effects of heat flow.

In 2005, Prof. Onuki presented a theory that take into account the gradient contribution of both the entropy and energy, which is named by his as the dynamic van der Waals theory (Onuki, 2005; Onuki, 2007). They constructed hydrodynamic equations with gradient stresses and converted them numerically to check the droplet motion in the heat flow. A typical one of these findings is that the temperature within the droplets becomes uniform with heating, but under zero gravity. It has been observed that the interface region is quite close to the coexistence curve, $T = T_c x$ (p) , even in nonequilibrium, due to the strong latent heat transportation effect, but the pressure outside the droplet is uniform distributed. The subsequent theory will show similar results so its validated. Thus, the Malangoni effect due to uneven surface tension does not work in a one-component pure liquid, and even at very small impurity concentrations, the mixture can produce faster fluid and interfacial motions. This phenomena has been further recollected and studied in Onukis following work (Takae and Onuki, 2010). Based on that, a sequence of papers have been published, focusing on the temperature distribution and phase transition in vaporing or boiling process (Teshigawara and Onuki, 2008; Xu and Qian, 2012; Kou et al., 2016).

This review is structured as follows: In Section 2, the general form, including basic governing equations, as well as some physical derivation and explanation are presented.

Besides, a set of numerical tests are designed and their results will show the fundamental but complicated physical process including evaporation and bubble motion in superheated fluid flow. In Section 3 we discuss several numerical frameworks, which are all relevant to dynamic van der Waals theory or could be seen as its extensions. In Section 4 we discuss some potential future developments of the dynamic van der Waals theory, including multiscale schemes, which will make simulations of phase change and transition in fluid dynamics, especially coupled with heat transfer more effectively.

2. Theory

2.1 van der Waals Theory

The Helmholtz free density $f(n, T)$ for monoatomic molecules is written as following, as a function of the number density n and the temperature T,

$$f = k_B T_n \left[\ln \left(\lambda_{th}^d n \right) - 1 - \ln \left(1 - v_0 n \right) \right] - \varepsilon v_0 n^2 \quad (1)$$

in the above equation, $v_0 = a^d$ is the molecular volume and is the magnitude of the attractive potential with d being the space dimensionality. the internal energy density is given by:

$$e = \frac{d n k_B T}{2} - \varepsilon v_0 n^2 \quad (2)$$

and the entropy s per particle, and the pressure p are given individually by:

$$s = -k_B \ln \left[\frac{\lambda_{th}^d n}{(1 - v_0 n)} \right] + \frac{k_B (d + 2)}{2} \quad (3)$$

$$p = \frac{n k_B T}{(1 - v_0 n)} - \varepsilon v_0 n^2 \quad (4)$$

The chemical potential per particle changes as:

$$\mu - \mu_{cx} = \frac{M}{2} \frac{d^2 n}{dx^2} + \frac{d}{dx} \frac{M}{2} \frac{dn}{dx} \quad (5)$$

while the van der Waals pressure is expressed as:

$$p - p_{cx} = \frac{M}{2} n \frac{d^2 n}{dx^2} + \frac{d}{dx} \frac{M}{2} n \frac{dn}{dx} - M \left(\frac{dn}{dx} \right)^2 \quad (6)$$

Meanwhile, Van der Waals introduced the gradient free energy density:

$$f_{gra} = \frac{1}{2} M |\nabla n|^2 \quad (7)$$

and the surface tension is defined as:

$$\gamma = \int_{-\infty}^{+\infty} dx M \left(\frac{dn}{dx} \right)^2 \quad (8)$$

Obviously, M is the coefficient of the gradient term in the Helmholtz free energy defined in equilibrium as $M = CT + K$. The capillary pressure tensor C, which depends on the density of the density gradient, incorporates the total pressure tensor. The gradient term represents the contribution of the density

nonuniformity to the pressure tensor as a function of the density gradient and explains the energy required to form and maintain the density nonuniformity. The contribution of the gradient term to the pressure tensor is given by the coefficient M. The expression of the contribution of the density gradient to the equilibrium pressure is described by Felderhof (1977) and Anderson and Gerbing (1988). A key prediction of the van der Waals gradient theory is that the interface between the vapor and the liquid becomes wider as the critical temperature increases (Charles, 2014).

2.2 Gradient theory and equilibrium conditions

Gradient contributions to the entropy and the internal energy in van der Waals theory could be included into:

$$S_b = \int dr \left[n s (n, e) - \frac{1}{2} C |\nabla n|^2 \right] \quad (9)$$

$$\varepsilon_b = \int dr \left[e + \frac{1}{2} K |\nabla n|^2 \right] \quad (10)$$

in which the two coefficients C and K are often selected as $K = 0$ and C is a parameter.

The gradient term represents the decrease in entropy and the increase in energy due to the inhomogeneity of n. They are particularly important in the interface area. We then define the local temperature T by:

$$\frac{1}{T} = \left(\frac{\partial}{\partial e} S_b \right)_n = n \left(\frac{\partial s}{\partial e} \right)_n \quad (11)$$

where n is fixed in the derivatives. This definition of T is analogous to that in a microcanonical ensemble. We will use it even for inhomogeneous n and e in nonequilibrium. We also define a generalized chemical potential per particle including the gradient contributions by:

$$\hat{\mu} = -T \left(\frac{\delta S_b}{\delta_n} \right)_{\hat{e}} = \mu - T \nabla \cdot \frac{M}{T} \nabla n + \frac{M'}{2} |\nabla n|^2 \quad (12)$$

Now, regarding S_b as a functional of n and $\hat{e}$, we consider small changes of n and $\hat{e}$ and which yield an incremental change of S_b.

$$\delta S_b = \int dr \left(\frac{1}{T} \delta_e - \frac{\hat{\mu}}{T} \delta_n \right) - \int da \frac{M}{T} (\vec{v} \cdot \nabla n) \delta_n \quad (13)$$

In the Ginzburg-Landau theory, we furthermore minimize W with respect to n to obtain:

$$\hat{\mu} = k_B T v = const \quad (14)$$

We can then find the stress based on van der Waals pressure as:

$$\Pi_{ij} = p \delta_{ij} - CT \left[n \nabla^2 n + \frac{(\nabla n)^2}{2} \right] \delta_{ij} + CT \nabla_i n \nabla_j n \quad (15)$$
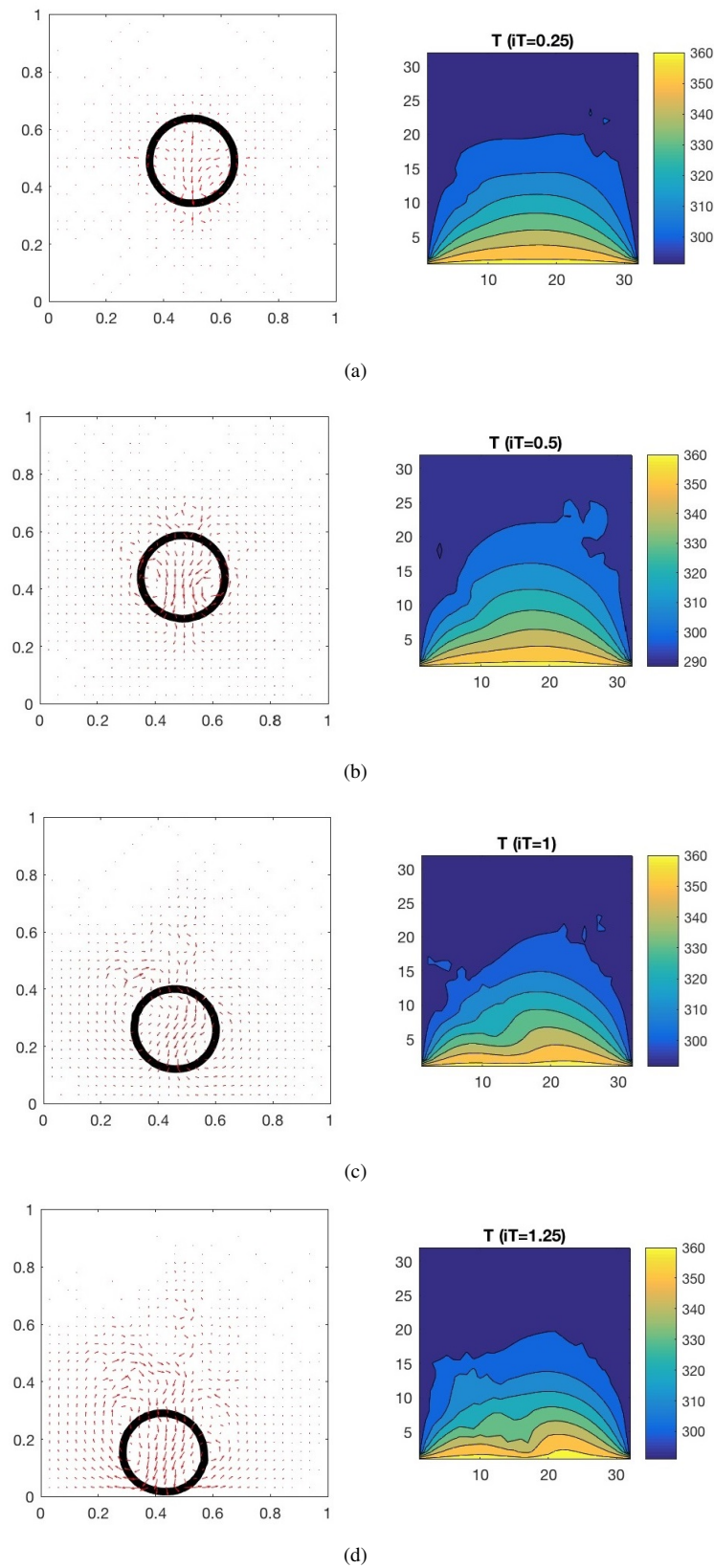
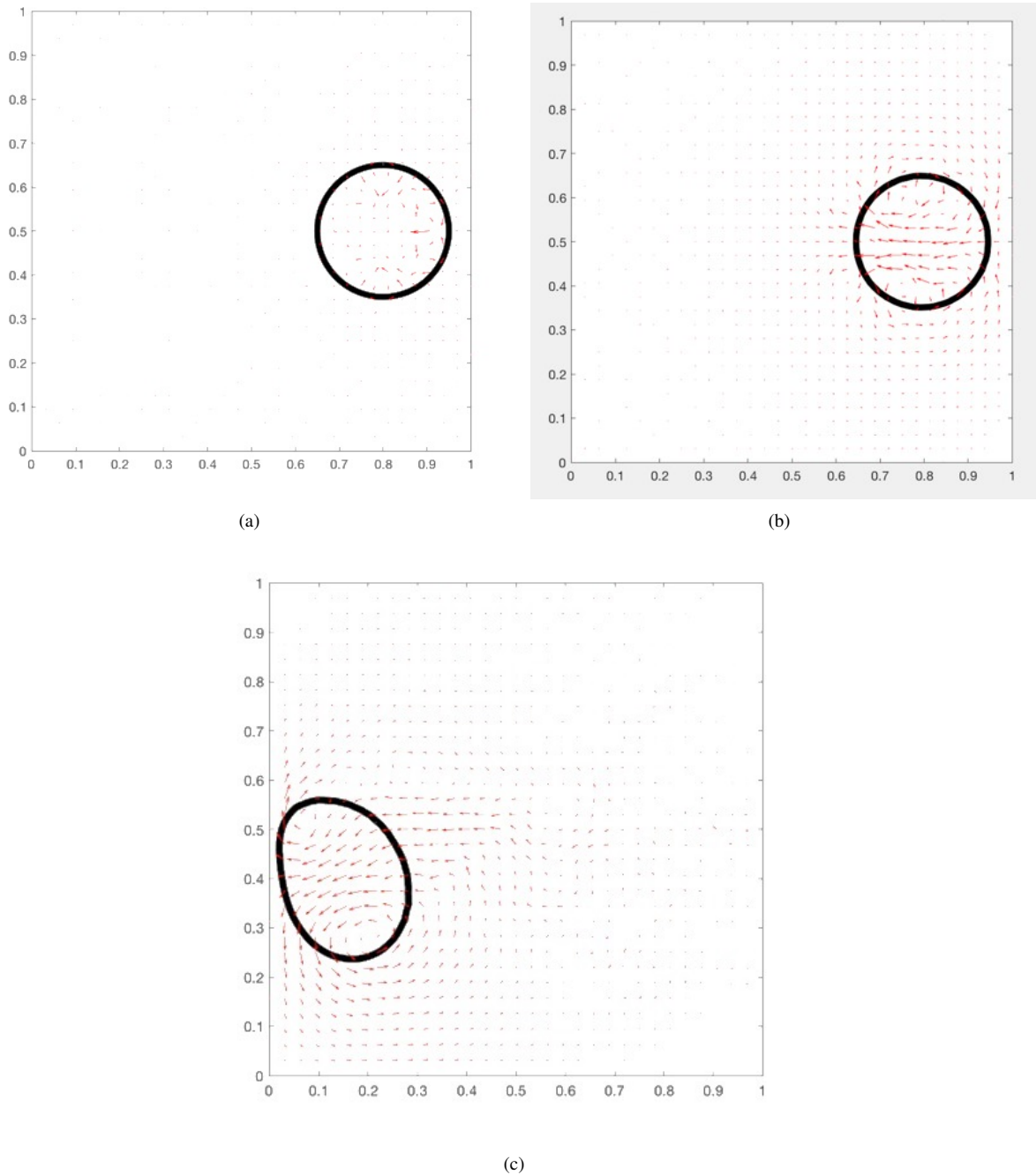**Fig. 1.** Simulation results of cases under only temperature gradient.

(a)

(b)

(c)

Fig. 2. Simulation results of cases under only temperature gradient (in horizontal direction).

2.3 Generalized hydrodynamic equations

A fluid mechanics equation was proposed by Onuki that takes into account gradient entropy and energy (Onuki, 2007). They have the same form as the compressible fluid in the preceding literature except that the stress tensor contains the gradient contribution. The guiding principle is derived from the nonnegative determinism of entropy generation in bulk areas. We assume that the fluid is in a solid container with a controlled boundary temperature and that the velocity field v disappears at the boundary. We include, in the following, the gravity g exerted in the axial downward direction. The continuum equation could be written as:

$$\frac{\partial}{\partial t}\rho = -\nabla\left(\rho\vec{v}\right) \tag{16}$$

where $= mn$, thus we could transfer it to:

$$\frac{\partial}{\partial t}n = -\nabla\left(n\vec{v}\right) \tag{17}$$

Afterwards, the momentum and energy equation could be written as:

$$\frac{\partial}{\partial t}\rho\vec{v} = -\nabla\cdot\left(\rho\vec{v}\vec{v}\right) - \nabla\cdot\left(\Pi - \sigma\right) - \rho g e_z \tag{18}$$
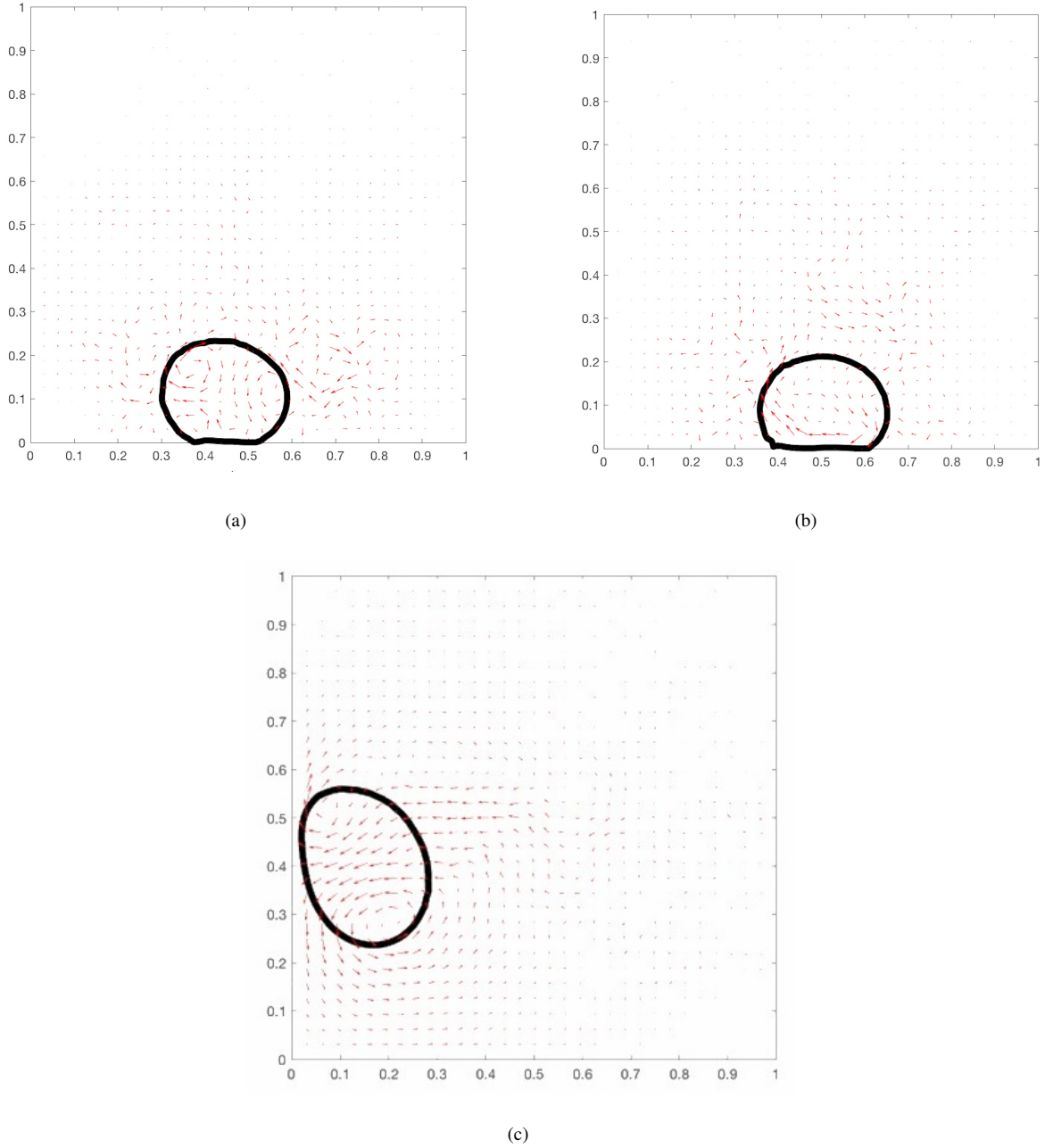
(a)

(b)

(c)

Fig. 3. Simulation results of Leidonfrost effect.

$$\frac{\partial}{\partial t} e_T = -\nabla \cdot (\rho \vec{v}\vec{v}) - \nabla \cdot (\Pi - \sigma) - \rho g v_z \qquad (19)$$

2.4 Numerical cases

First, we calculate the droplet motion under temperature gradient and without gravity. From the left figure, we can see the initial state, with a droplet in the centre of a domain.

We draw the velocity quiver at the same time to show the trend of droplet motion.

From the figures above, we can see that the droplet is driven to the warm walls, and with a bounce back process

and effect back the heat transfer process. The velocity caused by droplet motion may bring heat or cold and disturb the temperature field. It can be reasonable, as the surface tension is inverse proportional to the temperature. So if the temperature is higher, the surface tension is lower, and the surface tension is higher in a lower temperature. As a result, droplet surface in the warm part will be less tight than that of the cold part, and this difference in surface will drive the drople move to the warmer part. Besides, due to the different tension, the droplet shape will be changing throughout the whole process.

To avoid the misunderstanding of gravity effect, the left wall is the warm wall here. We can see that with the temperature rise, there will be velocity emerging inside the bubble,

and then it will move to the warm wall. This is the same as references.

Furthermore, we want to show the Leidenfrost effect, which means that a gas layer near the hot wall to keep the droplet suspension. The trick here is to find a proportional gravity acceleration coefficient, to show the balanced effect of surface tension (caused by temperature gradient) and gravity. So, we set the top wall a warmer boundary, to attract droplet against gravity. Again, the droplet is attracted to the warm walls, but under gravity it will again drop down. So, there will be a very thin gas layer in the bottom and cause a bounce back of the droplet.

In these figures, its easy to get that the droplet is driven by both the gravity and surface tension difference. As we care more on the bounce-drop balance process, we focus on the droplet moving already to the bottom part and try to capture the balance process. It can be read from these figures that the droplet will show a process of flattened first, driven by gravity and then bounce back, driven by temperature difference and then iterations. Due to the balance between surface tension and gravity, the shape of droplet varies significantly and intensely.

3. Recent developments and Extensions

3.1 Phase Filed Model coupled with Equation of State

The phase field model is used to replace the boundary condition at the interface with the evolution of the auxiliary field (phase field) acting as the initial parameter by the partial differential equation. This phase field has two different values (for example, +1 and -1) in each phase, and there is a smooth change between the two values in the area around the interface, and then the region has a finite width diffusion. In general, hydrodynamics and elasticity will be both included in single component system. It can be used to study problems including liquid-liquid or solid-liquid phase transitions, and recently it has been developed further to study gas-liquid phase transitions. In the case of a first-order phase change, the velocity field is caused around the interface even in the presence of a density difference between the two phases, even if no shear flow is applied. As an application, they present two simulation results in the case of melting, where the solid domain is placed on the heated wall in one case and in another case is suspended in the warmer liquid under shear flow in (Onuki, 2007). They have found that the solid region moves or rotates as a result of elasticity, releasing latent heat. We also checked the liquid-liquid phase of the high viscosity domain to a less viscous liquid on the heating wall, which caused an uneven velocity field in the projected portion of the domain. In these phase transitions, in the presence of a heat flow in the surrounding liquid, the interfacial temperature is almost equal to the coexistence temperature Tcx (p) leaving the heating wall (Takae and Onuki, 2010; Liu et al., 2016).

Researchers has developed the phase field model of fluids based on the van der Waals theory (Takae and Onuki, 2010). It can handle uneven evaporation and condensation, occupying latent heat. The purpose of this kind of method is to include

hydrodynamics and elasticity on the basis of clear thermo-dynamics. Therefore, such model could be applied to solid-liquid phase and liquid-liquid phase change (Lamorgesea et al., 2017).

Kou et al. (2016) proposed a general diffuse reflection interface model with realistic state equation (such as the Peng Robinson equation of state). Based on the NVT-based framework principle, a multi-component two-phase fluid flow is described. The NPT-based framework is used to simulate the real fluid. The proposed model uses Helmholtz free energy rather than Gibbs free energy in the NPT-based framework. Different from the traditional routines, they combine the first laws of thermodynamics with the relevant thermodynamic relations to obtain the entropy equilibrium equation, and then derive the transport equation of Helmholtz free energy density. In addition, by using the second law of thermodynamics, they have obtained a set of uniform equations that describe the partial miscibility of the two fluids and the bulk phase. The relationship between the pressure gradient and the chemical potential gradient is established. This relationship leads to a new formula for the momentum balance equation, indicating that the chemical potential gradient is the main driving force of fluid motion. In addition, they demonstrate that the proposed model satisfies the total (free) energy dissipation over time. For the numerical simulation of the proposed model, the key difficulty is due to the strong nonlinearity of the Helmholtz free energy density and the tight coupling between the molar density and the velocity. In order to solve these problems, they proposed a novel convex and concave splitting of Helmholtz free energy density and deal well with the coupling relationship between molar density and velocity by very careful physical observation (Kou et al., 2015; Kou and Sun, 2016a).

For comprehensive binary mixtures, Liu et al. (2016) proposed a new scheme of diffuse interface model based on the mass, momentum and energy conservation, as well as the second thermodynamic law. The analysis and numerical analysis show that the model can well describe the phase equilibrium of the actual binary mixture (carbon dioxide / ethanol considered in this paper) by adjusting the attraction parameters between the two component model molecules. They also show that the calculated surface tension of the different concentrations of CO_2 + ethanol mixture is consistent with the measured values in the literature when the mixed capillary coefficients are used as the geometric mean of the capillary coefficients for each component. Simulated three different cases of two droplets in the shear flow with the same or different concentrations, indicating that the higher the surface tension of CO_2 at higher concentrations, the easier the droplet deformation.

In many cases, the van der Waals force model of the single component system and the Cahn-Hilliard or phase field model of the binary incompressible flow are inappropriate. One such situation is the binary system near the critical point of the phase diagram, such as carbon dioxide or water at elevated pressure and temperature. The above application, that is, the solvent used as a solvent in the vicinity of the critical value in chemical analysis and synthesis, is an example. This compressible binary mixture has not been extensively studied

using this method. Onuki studied the properties of very dilute binary mixtures. Instead of modeling the mixture as a single fluid, the Helmholtz free energy density extends through the van der Waals theory to the two-component fluid. Solute density assumptions are very small, depending on the density of the solvent. No governing equation for the binary system was given (Kou and Sun, 2013; Liu et al., 2016; Kou and Sun, 2016b).

From another point of view, In the D.I. model, the interface is modeled as a three-dimensional region of finite thickness, where the sequence parameters continuously change from a value in a body phase to its neighboring value. The model begins with a free energy function with a nonlocal contribution, expressed in the initial order of the squared gradient of the sequential parameters. The spatial distribution of density or concentration in the interface area is then determined by minimizing the free energy. When a pair of simple intergranular potentials are assumed, the natural extension of the van der Waals force model is obtained (Shen and Yang, 2015). Assuming the simple constitutive relationship of the flux of the material in a very viscous binary mixture, the theory of Cahn-Hilliard joint decomposition can be obtained. For systems that can not ignore the flux of fluxes, a reversible force called the Korteweg force must be added to the Navier-Stokes equations proportional to the chemical potential gradient. For systems that are not in equilibrium, the force is nonzero and is responsible for the strong convection observed when the mixture is separated, and is not present in the system where the chemical potential is uniform. Like the Gibbs fractal surface model, the diffuse reflection interface model has been widely used in the mixing and delamination of binary mixtures, buoyancy-driven separation of droplets, droplet breakage and coalescence, Marangoni effect and flow of nanometer and microchannels (Lamorgese et al., 2017). Diffuse interface models resolve the steep but smooth transition of an order parameter for a two-phase system at the fluid interface. Ideas to describe both phases of an inhomogeneous system in one unifying framework originate from van der Waals (1873) (Widom and Rowlinson, 1970; Rowlinson, 1979) and Cahn & Hilliard (1958). Derivations of diffuse interface equations for single and binary fluid systems from a nonequilibrium thermodynamics framework have been presented, amongst others, by Anderson et al. (1998), Jacqmin (1999) and Onuki (2007) (Nold, 2016).

3.2 Boiling and droplet motion

The dynamic van der Waals theory is more applicable in simulations of physical process with heat transfer and phase change, thats why its widely used in numerical researches on boiling and droplet motions. Several new continuum mechanics modeling frameworks are developed for liquid-vapor flows, especially in boiling and evaporation process, concentrating mostly on the fluid flow belonging to van der Waals type, using new schemes combining entropy function and other thermodynamic variables. Generally, it can be shown that the energy stability of such schemes in discretized style, which will lead to an unconditionally stable property and accuracy

up to 2nd order. A set of benchmark problems and their analytical solution have developed and generally used for validation. Large variety of simulations have been carried out to demonstrate the large capability and usage of the algorithm based on dynamic van der Walls theory (Tryggvason et al., 2011; Liu et al., 2015; Taylor and Qian, 2016).

In a one-component fluid, the temperature of the bubbles (or droplets) of the thermal capillary (Marangoni) is almost impossible to vary. Generally, we can see the interface as an isothermal fluid layer where the temperature is saturated (Amijo and Barnard, 2010). Meanwhile, we need to take into account the fact that evaporation and condensation might occur on both sides in the same time, and the bubbles may be displaced. At the HYLDE equipment of CEA-Grenoble and the ISL DECLIC plant, we observed that two different fluids were affected by the temperature gradient under gravity. Experiments and subsequent analyzes are carried out near the critical point of gas-liquid, benefiting from the critical universality. In order to better understand the phenomenon, has been carried out 1D numerical simulation. After applying the temperature gradient, two schemes can be demonstrated. At the beginning, there will be a temperature change around and in the bubble due to the difference in compressibility and the so called piston effect, which means that along with the expansion of the thermal boundary layer, the fast adiabatic bulk thermalization will be induced. Different distribution of temperature will result in a different physical process of evaporation, as well as condensation, and such phenomena might vary the bubble shape and drive the bubble/droplet motion. After a long time, or at the near-steady state, there will a temperature gradient in the liquid and such gradient is the main cause of droplet/bubble motion to the hot wall. The temperature in bubble/droplet will have no such gradient. Bubble velocity in such process has been studied and compared with existing theories in Nikolayevs work (Nikolayev et al., 2017). They derive a set of hydrodynamic equations based on the thermodynamic theorem which contains the stress caused by density gradient. The so-called gradient effect is used again. Such governing equations can be further developed and wider applied in phase transition process in non-uniform temperature distribution (Nikolayev et al., 2017).

Droplet movement has been extensively researched due to its wide application potential in chemical and biology engineering, as well as petroleum industry. Various physical processes involving droplet movements can take into account both phase change (including both evaporation and condensation process) and associated phenomena including velocity slip and substrate cooling/ heating. The hydrodynamic and thermal properties of fluid flow will be automatically resolved using the phase method (such as phase field method) coupled with dynamic van der Waals theory. Besides, in many other methods, the rate of evaporation and condensation is set previously, but here such rate is obtained through calculation, which is another advantage. The numerical results will show that the wettability increasing direction on solid substrate is the main direction. Professor Qian investigated the movement of vaporized droplets in a one-component fluid on a solid substrate with a wettability gradient. Another result we can

obtain is that the relative contribution of phase transition and boundary velocity on contact line is mainly decided by the slip length. We can see two examples of the droplet migration and the energy dissipation process from Kou and Sun (2016c).

Recently, there has been a simple kinetic model for the evolution of a droplet in a cell, based on the Van der Waals equation of state, to investigate the behavior of liquid-vapor undergoing adiabatic expansion during isochoric and rapid heating. The evolution of the two phase fluid between the molecular and hydrodynamic scales is studied at different time steps, focusing on out-of-equilibrium and surface effects. Researcher have found a formula for the temperature difference between the gas and the droplets and they check it with numerical calculations. Afterwards, the formula is applied to delimit the thermalized and non-thermalized expansion regimes. The growth rate of liquid fraction is proportional to the estimation value, while a limit of droplet evaporation rate is derived in case of rapid expansion. Also, there has been discussion on the range of experimental situations (Armijo and Barnard, 2010). Onuki himself also proposed the boiling process, which could be divided into nuclear boiling, membrane boiling and their transition state.

There has also been researches on an extended thermodynamics (ET) theory of dissipative dense gases. In particular, the ET theory with six fields has been studied, where the shear viscosity and heat conductivity is ignored. Two nonequilibrium temperatures is emerged. Its generally viewed that the translational modes and the internal modes are the two main cause of the merge, which will help us understand the origin of dynamic pressure more clearly. Furthermore, the characteristic velocities is evaluated associated with the hyperbolic system and the fluctuation-dissipation is addressed by its relation to the bulk viscosity. The fluid flow based on dynamic van der Waals theory is taken as an example in such research.

Teshigawara and Onuki (2008) focused on the evaporation of a hydrophilic drop on an isothermal substrate. The total evaporation rate is counted in their research its found that the rate is doubled in region compared to that on the interface of contact line. It could be further concluded that the evaporation occurs mainly near the contact line, especially in large time scale, which is the same as results from other thermodynamical theory. Meanwhile, the accuracy should be more concerned in this method as in some cases, the edge evaporation rate is even higher than the total one, which is questioned (Xie et al., 2016).

3.3 Other extentions

The vapor condensation on the planar liquid surface caused by the reflection of weak shock waves was studied by three different simulation methods. The first is based on the molecular dynamics (MD) simulation of Lennard-Jones fluid, which should provide a reference solution. The second method is based on the diffusion interface model (DIM), consistent with the thermodynamic properties and transport properties of the Lennard-Jones fluid. The third method is based on a hybrid model (HM), where the liquid is described by pure fluid mechanics, and the steam is described by the Boltzmann equation. The two phases are connected by kinetic boundary conditions. The results show that DIM can not accurately predict the rate of condensation when vapor phase dilution, but it becomes more accurate when the gas phase becomes thicker. Assuming the unit condensation factor, HM reproduces MD with almost ideal vapor condensation accuracy (Barbante and Frezzotti, 2016). Besides, there has also been simulaitons using the dynamic van der Waals theory and coupling with Navier-Stokes equations in nanotubes (Grjeu et al., 2013).

Meanwhile, the dynamic van der Waals theory is used to simulate the single vapor bubble growth when the bulk liquid is heated (Chaudhri et al., 2014). For one component van der Waals fluid, the expansion dynamics of bubbles arising in pool boiling regime has been widely studied, where the contact line motion and the effect of substrate wettability are the main focus. It was found that the substrate wettability could control the apparent contact angle as well as the bubble growth rate (total evaporation rate), and thats how we can determine the line speed. It has also been obtained that an approximate expression could be derived from the theory, which is in good accordinane with the simulation result. Its indicated that the movement velocity of contact line velocity is mainly determined by three factors, (1) interface shape, the effect is even higher when the bubble growing in a slow rate (2) constant apparent contact angle and (3) constant bubble growth rate. Thus, the contact line velocity is sensitive to substrate wettability through a significant contact angle, where the latter is also the main cause of bubble growth. The hydrophobic surface produces a thinner bubble shape than the hydrophilic surface , as well as a higher evaporation rate, which results in a faster contact line speed. Such results are connected with the vapor film formation and further boiling process (Xu et al., 2012; Taylor and Qian, 2016).

There is also a lattice Boltzmann scheme that allows simulating the thermodynamic mechanical equations of multiphase fluids, including the contribution of interface free energy (Sofonea et al., 2004). This is an example of LBM that correctly reproduces the quality, momentum, and energy equations established by Onuki in the second phase of the Chapman-Enskog extension. Assuming the simple constitutive relationship of the flux of the material in a very viscous binary mixture, the theory of Cahn-Hilliard joint decomposition can be obtained. The phase-field method has been used to simulate the mixing of conventional mixtures, the junction decomposition in conventional mixtures and the various heterogeneous problems of van der Waals liquids, the phase separation effect on heat transfer and nucleation (Gonnella et al., 2007; Gan et al., 2012).

In conclusion, the uncertainties and challenges need to be highlighted in Drp. Significant progress is necessary to transform micro-tomography and conceptual model from the current researchch problem into a robust computational big data tool for multi-scale scientific and engineering problems in earth science related fields.

4. Conclusion

Multicomponent and multiphase fluid flows are very im-

portant in both real life and scientific research, while their modeling is still in an early stage. As a result, for researchers who want to do numerical simulation, its always a problem to select. One main focus in energy research is the phase transitions, in which the fluctuations of the temperature T are often assumed to be small, and for some extreme conditions, such as in macroscopic level, are generally neglected. Meanwhile, the physical process of varying temperature is still attracting so much attention that we may consider phase transition and other thermodynamical-releveant phenomena. A popular example is that in applied heat flux, the wettability may be deeply affected by the temperature gradient (Garrabos et al., 2001). Besides, the boiling processes remain largely unexplored, which is very common seen in chemistry or energy industry (Beysens et al., 1999). To treat such problems, Onuki (2005) proposed to consider with the gradient contribution of entropy and energy, with which the temperature is defined as a functional of the order parameter and the energy density. Based on that, a family of thermal and hydraulic governing equations have been derived, and thats called dynamic van der Waals theory. This theory is non-trival for its concerning on gradients, as well as a very convincing physical origin, and with which we can perform better numerical simulation on phase change and transition process with better efficiency and accuracy.

Acknowledgements

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