Numerical simulation of single bubble growth considering contact angle through VOF method in saturated nucleate boiling condition

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1. Introduction

Two-phase heat transfer involving phase change within nuclear power plants is important for their performance and stability. In pressurized water reactors, maintaining the core in a subcooled state is essential to address thermo-hydraulic safety concerns that can arise due to a decrease in pressure within the core following accidents. For this reason, research is being conducted to comprehend the mechanism of nucleate boiling using computational fluid dynamics. Particularly in the nuclear industry, reactors require high and stable output along with efficient heat transfer. To facilitate significant heat transfer, attention must be given to the growth of bubbles generated by nucleate boiling.

Understanding the mechanisms behind bubble growth from nucleation and their departure from the heating surface is crucial. Hence, the aim of this study is to understand this mechanism using CFD, especially from the aspect of contact angle.

2. Background

2.1 Affecting factors for bubble growth

Studying the growth of individual bubble and their heat transfer characteristics is significant for understanding the mechanism of nucleate boiling. Factor such as contact angle is closely related with surface tension and it plays a significant role in bubble growth [4-7].

2.1.1 Contact angle

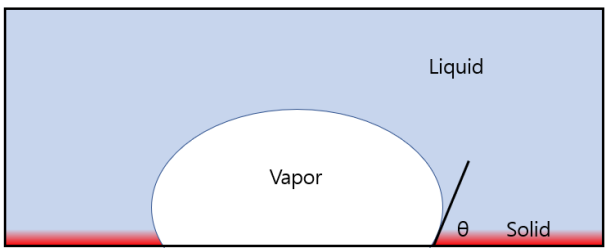

Fig. 1 Contact angle of bubble in nucleate boiling

In Fig. 1, the point where the three phases meet is defined as triple point. Here, the angle formed between the vapor and the solid phase is called the contact angle. The importance of contact angle lies in its direct relationship with surface tension. Surface tension is the intermolecular force acting between molecules at the surface of a liquid. This occurs because liquid molecules have attractive force each other within the liquid, but they interact differently near the surface of the liquid when in contact with a vapor, like a bubble [4].

The following is the Young-Laplace equation illustrating the relation between contact angle and surface tension in a bubble of radius, R:

$$(1)\ \Delta P = \frac{2\sigma}{R} = \frac{2\sigma\cos\theta}{a}$$

In equation (1), ΔP represents the pressure difference between the inside and outside of a bubble, σ denotes the surface tension at the vapor-liquid interface, and R signifies the radius of curvature of bubble. Through, equation (1), we can comprehend how changes in the size and shape of a bubble in a boiling situation lead to variations in pressure caused by surface tension which is affected by contact angle [4].

As the contact angle increases, the bubble growth rate, the time taken for bubbles to depart from the heating surface, and the diameter of the detached bubble all increase [1,2]. Additionally, the surface tension force in the vertical direction from the heating surface increases, causing a delay in the departure of bubble from the heating surface.

2.2 Governing equations

The equations that need to be considered for simulation are as follows: the equations of mass conservation, energy conservation, momentum conservation, and volume fraction conservation.

$$(3)\ \nabla \cdot (\rho u) = \dot{\rho}$$

$$(4)\ \frac{\partial \rho c T}{\partial t} + \nabla \cdot (u \cdot \rho c T) = \nabla \cdot (\lambda \cdot \nabla T) + h$$

$$(5)\ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (u \cdot \rho u) = -\nabla P + \nabla \cdot (\mu \cdot \nabla u) + S_s + S_g$$

$$(6)\ \frac{\partial \alpha_l}{\partial t} + \nabla \cdot (u \cdot \alpha_l) = \frac{\rho}{\rho} \alpha_l$$

The source term in equations (3) and (6) represents the mass variation during phase change processes, and the source term h in equation (4) signifies the energy

change during phase transition. The terms S_s and S_g in equation (6) correspond to the volumetric forces due to surface tension and gravity, respectively [1,2]. Additionally, to account for the effects of surface tension in Computational Fluid Dynamics(CFD), the Volume of Fluid(VOF) method with the Continuum Surface Force(CSF) model has been adopted. In the CSF model, the surface tension of the bubbles can be expressed as volumetric forces using the divergence theorem. The equation for this can be formulated as follows:

(7) $S_s = \sigma \frac{\alpha_l \rho_l \kappa_v \nabla \alpha_v + \alpha_v \rho_v \kappa_l \nabla \alpha_l}{0.5(\rho_l + \rho_v)}$

(8) $n_l = \nabla \alpha_l, n_v = \nabla \alpha_l$

(9) $\vec{n} = \frac{n}{|n|}$

(10) $\kappa_l = \nabla \cdot \vec{n}, \kappa_v = \nabla \cdot \overrightarrow{n_v}$

In the equations above, the symbols represent the following:

ρ represents density. σ is the surface tension coefficient. α is the volume fraction in the control volume. n stands for the surface normal. κ denotes curvature, which is expressed as the divergence of the gradient of α. l and v represent the liquid and vapor phases, respectively, including the states of the two phases. In regions where two distinct phases coexist, physical properties such as density, viscosity, and thermal conductivity are computed using the average volume fraction. This framework is used to model the behavior of multiphase flow, particularly during phase change processes, where the interplay between different physical phenomena is crucial.

2.3 Numerical model

In the analysis of the growth of individual bubbles, heat transfer at the vapor-liquid interface is modeled using Lee's phase change model. Lee's phase change model (referred to as the Lee model) assumes phase change occurs under constant pressure and quasi-thermodynamic equilibrium conditions. In the Lee model, evaporation and condensation are induced by the vapor transport equation [3]. This approach is used to describe the mechanisms of heat and mass transfer during the growth of bubbles, especially focusing on phase change phenomena, and it provides insight into the intricate dynamics of the process. The vapor transport equation can be represented as follows:

(12) $\frac{\partial}{\partial t}(\alpha_v \rho_v) + \nabla \cdot (\alpha_v \rho_v \overrightarrow{V_v}) = \dot{m}_{lv} - \dot{m}_{vl}$

where vapor phase velocity $\overrightarrow{V_v}$ and $\dot{m}_{lv}$, $\dot{m}_{vl}$ are the rates of mass transfer. If the mass transfer rates $\dot{m}_{lv}$, $\dot{m}_{vl}$ in equation (12) are expressed differently based on temperature ranges, the equation would appear as follows:

(13) $\dot{m}_{lv} = coeff * \alpha_l \rho_l \frac{(T - T_{sat})}{T_{sat}} \rightarrow T_l > T_{sat}, evaporation$

(14) $\dot{m}_{vl} = coeff * \alpha_v \rho_v \frac{(T - T_{sat})}{T_{sat}} \rightarrow T_v < T_{sat}, condensation$

The energy source term related to the equation is obtained by multiplying the latent heat h to equation (13) and (14).

(15) $S_h = -\dot{m}_{lv} \times h_{lv}$

(16) $S_h = \dot{m}_{vl} \times h_{lv}$

The larger the value of coefficient, the more intense the heat and mass transfer at the phase interface, and the closer the interface temperature is to the saturation temperature. However, too large value of coefficient can lead to unstable interface morphology or even break up [1,4].

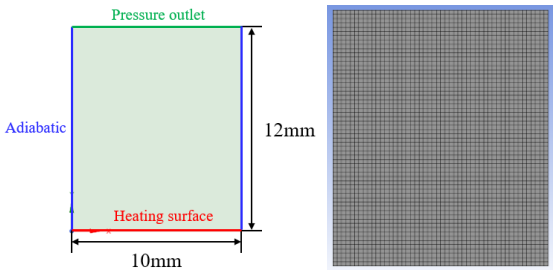

Fig. 2 Simulation domain and mesh distribution

Fig. 2 shows the geometry and mesh used for the simulation. The bottom of the geometry was set as the heating surface, and the sides were set as adiabatic walls. Similarly, the top of the geometry was set as a pressure outlet. The mesh was generated with a size of 40 micrometers, and all mesh sizes were set to be the same for use in simulation.

To investigate the behavior of individual bubble growth, the VOF(Volume Of Fluid) method in ANSYS FLUENT is employed for analysis. In consideration of surface tension during bubble growth, the CSF(Continuum Surface Force) model is applied in the simulation. Various source terms are implemented in the simulation using User-Defined Functions(UDFs). For detailed observation of bubble growth behavior, a small time step of 10^{-5}s is set. Additionally, to allow sufficient observation of bubble growth until detachment from the heating surface, the number of time steps is set to 4000-5000.

This setup allows for a comprehensive exploration of the intricate dynamics of bubble growth, considering factors like surface tension and various source terms, while ensuring the accuracy of the simulation through appropriate time step configurations.

3. Simulation results

This study aims to investigate how the behavior of bubble growth changes based on surface tension influencing bubble growth.

3.1 Bubble growth behaviors

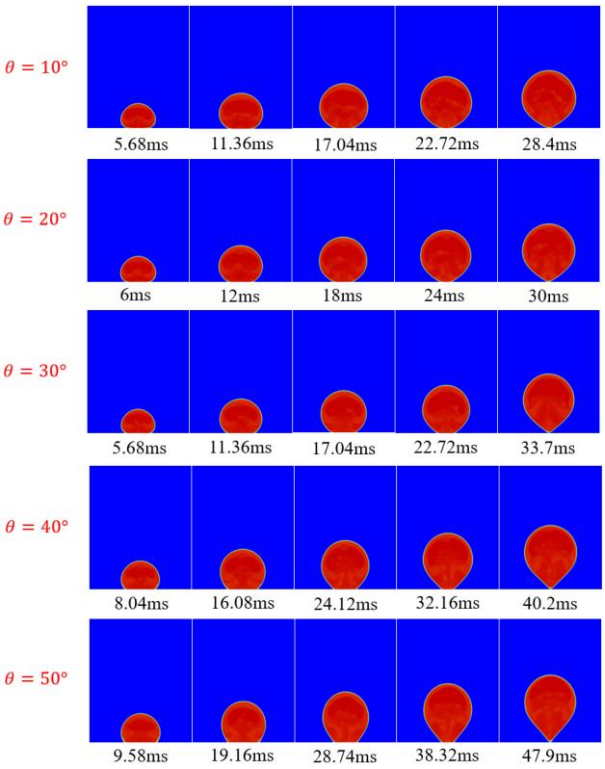

Fig. 3 Bubble growth behaviors at different contact angles

Fig. 3 illustrates the bubble growth behavior corresponding to contact angles ranging from 10 to 50 degrees. As the contact angle increases, the size of the bubble becomes larger, and the departure time also increases. When the contact angle is small, the liquid closely adheres to the vapor surface, leading to a reduced surface tension. Conversely, a larger contact angle implies less contact between the liquid and vapor, causing liquid molecules to approach each other more, leading to an increased surface tension. In summary, the contact angle directly influences surface tension, and this relationship is associated with bubble growth and stability. Large contact angle and higher surface tension force are shown to contribute to faster bubble growth and stability.

3.2 Effects of bubble parameters during growth and departure

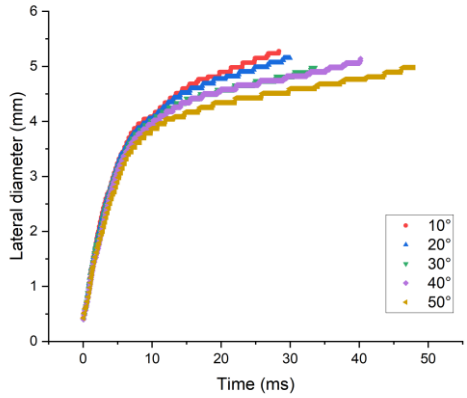

Fig. 4 Lateral diameter of bubble at each contact angle

Fig. 4 illustrates the bubble growth behavior as observed in Fig. 3, showing the bubble lateral diameter and departure time as the contact angle varies from 10 to 50 degrees. The point where the graph ends represents the bubble departure time.

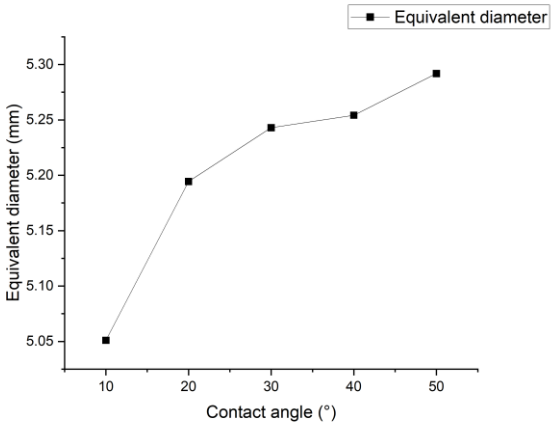

Fig. 5 Equivalent diameter at each contact angle

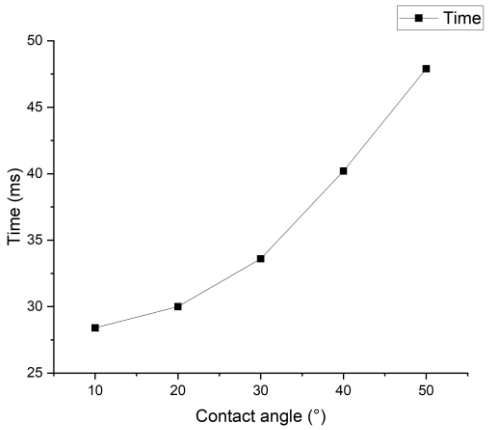

Fig. 6 Departure time at each contact angle

Figs. 5, 6 represent equivalent diameter and departure time, respectively. As you can see in Fig. 5 and 6, increasing contact angle leads to larger equivalent diameter and departure time. A smaller contact angle

leads to weaker interaction between the vapor and liquid, allowing the bubble to assume a more independent form. Additionally, from the perspective of bubble departure time, a smaller contact angle implies a higher likelihood of rapid growth and separation of the bubble.

4. Conclusion

This simulation aimed to investigate the influence of contact angle on bubble growth behaviors during nucleate boiling. The VOF method was applied to simulate the interface of bubble, and the simulation was conducted with varying contact angles. As the contact angle increased, the equivalent diameter and departure time of bubble increased. The results indicated that the contact angle plays an important role in determining the behavior of bubble growth during boiling processes.

To validate the accuracy of the simulation, it would be necessary to compare simulation result with experimental data from nucleate boiling with varying contact angles in future studies. This will contribute a more accurate understanding of the bubble growth mechanism.

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