# THE IMPORTANCE OF INITIAL THERMAL CONDITION FOR SIMULATION OF SINGLE VAPOR BUBBLE CONDENSATION

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## ABSTRACT

Accurate mass transfer model is essential for simulation of phase-change phenomena. However, there is no universal model to calculate the transferred mass during boiling or condensation yet. Among the existing models, the Fourier model seems promising. In this study, we investigate the limitation of this model via comparison of the numerical results with the experimental data. Our study confirms the great importance of the initial thermal boundary layer prescription for a simulation of single bubble condensation.

## 1. INTRODUCTION

Bubble condensation is an essential phenomenon for the description of heat and mass transfer in subcooled flow boiling. It is encountered in many industrial applications such as micro-reactors or micro channels where the bubble dynamics influences the cooling capacity and introduces challenges for robust operating condition. The size and the shape of vapor bubbles changes continuously during the condensation process, and this phenomenon significantly affects flow structure around each bubble. In order to understand the subcooled flow boiling, it is vital to obtain an extensive knowledge on the condensing bubbles behaviour.

Even though many experiments have been conducted on this topic [1], they are still limited to specific liquid properties or specific operating condition. Moreover, experimental studies based on visualization with high-speed videography or PIV capture the bubble shape evolution but seldomly provide detailed information on flow quantities such as temperature and pressure field. In the past decades the numerical solvers evolved to provide more detailed information on vapor condensation. The interface tracking and capturing methods such as Level-Set (LS) [2], Volume of Fluid (VoF) [3] and phase-field [4] can be employed for simulation of a single vapor bubble condensation. However, the main bottle-neck in numerical simulation is how to compute the transferred mass through the interface. Unfortunately, the mass transfer models are often semi-empirical correlations and can be rarely employed independent of their experiment counterpart.

The Lee mass transfer model is the most popular one [5]. It assumes that mass is transferred at a constant pressure in phase change flow system and the model is derived for a quasi-thermo-equilibrium state as:

$$\dot{m}^{\prime\prime\prime} = r_c \alpha_l \rho_l \frac{T - T_{sat}}{T_{sat}}, \text{ for condensation } (T < T_{sat})$$
 (1)

where the volumetric mass flux  $\dot{m}^{\prime\prime\prime}$  [kg/m<sup>3</sup>s] depends highly on the relaxation parameter  $r_c$ [s<sup>-1</sup>]. A wide range between 0.1 and 10<sup>6</sup> is proposed and successfully used for  $r_c$  in previous studies [6]. Tian et al [7] derived a correlation for relaxation parameter and showed the dependence of  $r_c$  to the temperature, physical properties, and phase volume fraction of the grid element.

Another widespread model is derived by Tanasawa [8] based on Schrage phase change model. Schrage computed the interfacial mass flux m'' [kg/m<sup>2</sup>s] using Hertz–Knudsen equation assuming a jump in the temperature and pressure across the interface  $T_{sat}(p_l) = T_l \neq T_{sat}(p_g) = T_g$ . It is given by:

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$$\dot{m}^{\prime\prime} = \frac{2}{2 - \gamma_c} \sqrt{\frac{M}{2\pi R}} \left[ \frac{\gamma_c p_g}{\sqrt{T_g}} - \frac{\gamma_e p_l}{\sqrt{T_l}} \right]$$
(2)

where R = 8.314 J/mol. K is the universal gas constant, M [kg/mol] is the molar mass and  $\gamma$  is the fraction of molecules transferred from one phase to the other. The subscripts c and e refer to condensation and evaporation, respectively.  $\gamma_c = 1$  means all vapor molecules hit the interface convert to liquid one. In numerical simulation, usually  $\gamma_c = \gamma_e$  is considered. Tanasawa assumed the interface is at saturation temperature and the mass flux varies linearly with temperature difference and the bulk temperature. He simplified Eq. 2 to:

$$\dot{m}'' = \frac{2\gamma}{2 - \gamma} \sqrt{\frac{M}{2\pi R}} \frac{\rho_g h_{lg} \left(T - T_{sat}\right)}{T_{sat}^{3/2}}, \quad \dot{m}''' = \dot{m}'' \frac{A}{V}$$
(3)

where  $h_{lg}$  [J/kg] is the latent heat. In both Eq. 2 and Eq. 3, the computed mass flux depends on empirical parameter  $\gamma$ . The  $\gamma = 0.1 - 1$  is suggested for dynamically renewing water surfaces such as jets and moving films and  $\gamma < 0.1$  for stagnant surfaces [9]. Samkhaniani and Ansari [10] manifested in vapor condensation simulation, the bubble life time is highly sensitive to the choice of  $\gamma$  and appropriate value must be selected for each simulation in comparison with experiment.

A wider list of available mass transfer models is given in ref. [11]. Almost all models suffer from dependence to a tuning parameter. In the present study, heat flux balance (Fourier) model is employed, stated as:

$$\dot{m}^{\prime\prime} = \frac{q^{\prime\prime}}{h_{lg}} = \frac{k_l \nabla T - k_g \nabla T}{h_{lg}}, \qquad \dot{m}^{\prime\prime\prime} = \dot{m}^{\prime\prime} \frac{A}{V}$$
(4)

where k [w/m. K] is the thermal conductivity, A is the interfacial area and V is the cell volume. The study objective is to investigate the model predictive capability in comparison with experiment and to identify its limitations.

#### 2. MATHEMATICAL MODEL

The two-phase flow is treated as incompressible and immiscible Newtonian fluid. The Interface between two phases is resolved using volume-of-fluid method (VoF) extended with contour-based reconstruction method. The reconstruction part is essential for accurate mass flux rate and interface curvature calculation. This improves surface tension representation in CSF model and reduces the parasitic current up to one order. The two-phase Navier-stokes equation in single formulation is solved within PIMPLE loop. The solver is extensively applied for simulations of boiling [12,13] and recently upgraded to OpenFOAM-6.

The governing equations are:

- Mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla . \left( \rho \mathbf{u} \right) = \dot{m}^{\prime \prime \prime} \tag{5}$$

- Momentum conservation

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla . \left(\rho \mathbf{u} \mathbf{u}\right) - \nabla . \left[\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)\right] = -\nabla p + \rho \mathbf{g} + \kappa \sigma \nabla \alpha_l$$
(6)

- Energy conservation

$$\frac{\partial \rho c_p T}{\partial t} + \nabla . \left( \rho c_p T \mathbf{u} \right) - \nabla . \left( k \nabla T \right) = \dot{m}^{\prime \prime \prime} h_{lg}$$
<sup>(7)</sup>

- Interface transport equation

$$\frac{\partial \alpha_l}{\partial t} + \nabla . \left( \alpha_l \mathbf{u} \right) = \dot{m}^{\prime \prime \prime} \frac{\alpha_l}{\rho}$$
(8)

Where  $\alpha_l = V_l/V_{cell}$  is liquid volume fraction, the physical properties  $\theta \in [\rho, c_p, k, \mu]$  are estimated with linear interpolation in the interfacial region  $\theta = \theta_l \alpha_l + \theta_g (1 - \alpha_l)$ . In the present study, the volumetric mass transfer  $\dot{m}^{\prime\prime\prime}$  is calculated with Fourier model (Eq. 4).

### **3. VAPOR BUBBLE CONDENSATION**

The rising of a single vapor bubble at saturated temperature ( $T_{sat} = 380.2$  K at 0.13 Mpa) surrounded by a quiescent subcooled water ( $T_{inf} = 355.2$  K) is simulated similar to [6,10]. The computational domain size is  $2D_0 \times 4D_0$  and filled with  $100 \times 200$  uniform hexahedral cells. The grid is generated with OpenFOAM mesh generator *blockMesh*. The initial diameter of vapor bubble is set to  $D_0 = 1.008$  mm. The bubble centre is located at the position (x, y) = ( $D_0, D_0$ ) in the initial state. The thermophysical properties are for vapor ( $\rho = 0.754$  kg/m<sup>3</sup>, k = 0.0259 W/m. K,  $c_p = 2110.7$  J/kg. K) and for liquid ( $\rho =$ 953.1 kg/m<sup>3</sup>, k = 0.68 W/m. K,  $c_p = 4224.4$  J/kg. K). The surface tension  $\sigma = 0.057$  N/m and latent heat  $h_{lg} = 2237$  kJ/kg are specified. At the boundaries, the dynamic pressure (p = 0) and temperature ( $T = T_{sat}$ ) are fixed and the velocity gradient and volume fraction gradient are zero.

The bubble shape sequence is compared with experiment [14] in the Figure 1, the result shows qualitatively good agreement. The vapor bubble condenses while moving upward and accelerates as it becomes smaller.



Figure 1: Top: experimental study [14], Bottom: present numerical simulation with Fourier model ( $\delta \sim 0.2D_0$ )

There is a thin thermal region around the interface where the temperature smoothly changes from saturated temperature to subcooled temperature. As shown in Figure 2(left), the initial temperature profile in Eq. 9 is radially applied inside this region:

$$T(r) = ar^{2} - b\sqrt{(r)} + c, a = \frac{T_{Sat} - T_{Inf}}{\delta^{2}}, b = 2a\left(\frac{D_{0}}{2} + \delta\right), c = a\left(\frac{D_{0}}{2} + \delta\right)^{2}$$
(9)

Where *r* is the distance to the bubble centre and  $\delta$  is the thickness of this region. For quantitative comparison, the bubble life time is plotted against experiment data in Figure 2(right). For  $\delta \sim 0.2D_0$  bubble evolution coincides well with the experimental data. It shows the bubble life time is controlled by this thin thermal layer. A thicker thermal boundary layer around the interface slows down the process and prolongs the bubble lifetime.

#### **4. CONCLUSION**

The present study reveals the importance of sub-millimetre region around the interface on the bubble condensate rate. It is the most influencing parameter in simulation using Fourier model. Unfortunately, experimental studies do not provide any information about this thermal boundary layer. Therefore, a comparison with experimental data without knowing the exact temperature field in this tiny region in

the beginning of a simulation is a trial-and-error process, so an accurate prescription of the temperature distribution is rather difficult. This also might explain the discrepancy between tuning parameters in Lee and Tanasawa model in literature. Those terms impose a constrain on the condensation rate to cope with the unknown initial temperature field in thermal boundary layer.

In future work, we aspire to identify a correlation for estimating this thermal region thickness based on some experimental or analytical studies.



Figure 2: Left) The initial temperature profile, Right) vapor bubble life time, Exp. is taken from [9]

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