

In the context of two-phase flow with phase change, two main difficulties are lay for developing a robust and accurate phase change model. As we know, the mass transfer occurs only in the cells containing interface, leading a discontinuity of the velocity field across the interface. Moreover, for large density contrasts between the two-phases, such singularity of the mass source induces numerical instability when solving the pressure-velocity equations near the interface region. The other difficulty comes from the boundary condition of the temperature at the interface. For most studies with low heat flux, the interface is imposed at the saturation temperature, which seems as a Dirichlet type boundary condition. In the following sections, we mainly review some work based on the VOF method or hybrid methods in terms of phase change.

The VOF method

Welch and Wilson [2000] firstly used the VOF method to capture the liquid-vapor interface in film boiling, they compared the results with Son and Dhir [1998] and Juric and Tryggvason [1998] using different interface capturing methods and found the results matching well. For a lower heat flux with smaller superheated temperature (ΔT_w , the difference between heated wall and saturated temperatures), the vapor bubble showed quasi-steady releasing behavior. However, when changing to a higher heat flux, the vapor bubble did not detached from the vapor film. A similar behavior was observed in the work of Juric and Tryggvason [1998].

Some researchers used smoothing techinique to smear mass source to improve the numerical stability. Yuan et al. [2008] used the VOF method to track liquid-vapor interface on non-orthogonal body-fitted coordinates. In order to overcome the discontinuous velocity field due to mass transfer at interface, the volume expansion or contraction due to mass exchange is moved from a mixture cell to the nearest vapor cell. Hardt and

Wondra [2008] developed one evaporation model compatible with interface-capturing schemes for vapor-liquid flow. They performed numerical simulations of film boiling and droplet evaporation using a VOF method. In their method, the evaporating mass flux is calculated from the interface temperature and the interfacial heat resistance. The mass source term filed is smeared, which is redistributed in some finite region around the interface, and smooths out the sharp discontinuity in velocity at the interface. The most notable feature of the model is that almost evaporation laws can be implemented, and the mass source terms can be compatible with different interface-capturing schemes such as the VOF and the level-set method. Based on Hardt's evaporation model, Kunkelmann and Stephan [2010] developed one phase-change model combined with algebraic VOF method in OpenFOAM and carried out a microlayer and contact angle model to simulate nucleate boiling on unstructured meshes. Magnini and Pulvirenti [2011] used a similar method to smear the mass source term into the neighbor cells and numerical study of vapor bubbles growing in quiescent superheated liquid was investigated.

Sun et al. [2014] developed a new phase-change model based on the VOF method in the FLUENT code. The model is suitable for the case in which one phase is unsaturated and the other is saturated. Tsui and Lin [2013] proposed a simple interface-reconstruction scheme (CISIT) based on the VOF method. The interface is represented by the contour surface of VOF value 0.5 and advanced in a conservative prediction-correction manner to ensure that the distribution of the VOF is a good approximation to the Heaviside function. Later, they (Tsui et al. [2014]) extended the method to calculate two-phase flow including heat and mass transfer due to phase change. They proposed an implicit way to solve the energy equation.

In the work of Fleckenstein and Bothe [2015], a numerical method for multi-component mass transfer with volume effects at moving interface has been performed. The central thought of this method is using spatial averaging techniques to solve Navier-Stokes equations combined with the VOF method accounting for volume effects. The simulation cases proved the method is able to capture volume effects with multi-components transfer. Strotos et al. [2016] studied the evaporation of suspended single or multi-component droplets using the VOF method. They estimated the local evaporation rate using Fick's law and compared the simulation results with experimental data. It is concluded the prediction of the overall evaporation rate for a wide range of cases was satisfactory. Georgoulas et al. [2017] performed an improved VOF method to numerically study heat transfer and phase change of bubble detachment in saturated pool boiling in Open-FOAM. The simulation results showed that the initial thermal boundary layer (ITBL) plays an important role in the bubble growth and detachment process. The contact angle equals 45° has significant effect on bubble detachment behavior. Samkhaniani and Ansari [2017] implemented a new solver named phaseChangeHeatFoam in OpenFOAM to simulate boiling and condensation based on the VOF method. He compared Lee and Tanasawa mass transfer models and found these two models had considerable difference in film boiling simulation. Moreover, the slight variation of saturation temperature was considered with the simplified Clausius-Clapeyron relation. Based on Gerris solver (Popinet [2013b]), which is an open-source solver similar to Basilisk solver, Zhang and Ni [2018] developed a new phase change model using the VOF method. A smoothed

mass transfer rate within a narrow region surrounding the interface is adopted in order to decrease the pressure oscillations for large density ratios. The saturated temperature is imposed at the interface using a ghost-cell approach. Reutzsch et al. [2020] proposed a new phase change model to investigate various phenomena with evaporation. Based on the VOF method, the basic idea of this model is to conduct the advection of the fluid and gaseous phase as well as a fully consistent phase change loop.

Malan et al. [2020] developed one novel phase-change model in open-source solver PARIS (Aniszewski et al. [2019]). The numerical methods adopted in PARIS are similar to Basilisk solver (Popinet [2013a]), the PLIC-VOF method is used to capture motion of gas-liquid interface. However, the VOF method cannot be applied directly to the VOF equation, due to the phase change source term makes the divergence of velocity not be zero at interface. In order to solve this problem, he proposed a novel geometric VOF advection method to deal with the discontinuity in the velocity that arises from phase change. The basic idea of the method is to split the VOF advection equation into two steps using time-fractional method. The first one is to construct one extended, divergence free liquid velocity domain; then shifting the interface to account for phase change. This method keeps the conservation of mass. Using this extended domain method, Scapin et al. [2020] investigated interface-resolved simulations of evaporating two-fluid flows. Different from Leon's method, they did not construct one sub-domain, but constructing a divergence-free extension of the liquid velocity field onto the entire domain. In Leon's study, they calculated mass transfer rate from temperature field. However, Scapin compute mass transfer rate using vapor mass fraction which would be solved by a standard convection-diffusion transport equation.

The CLSVOF method

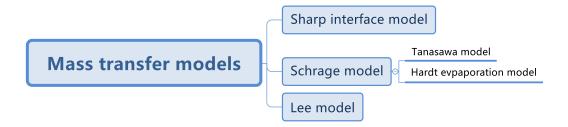
Sussman and Puckett [2000] first proposed a coupled level-set and volume-of-fluid method (CLSVOF) taking advantages of both the VOF the LS methods. The basic idea of this method is using the smooth LS function to estimate curvature and surface tension while the VOF method ensures exact mass conservation. Zhao et al. [2014] used an improved CLSVOF method to simulate free surface flow. The contribution of their method is the methodology for overset grid system of embedding, overlapping and moving structured grids. The CLSVOF method has also been applied in two-phase flow with phase change to evaluate the performance of proposed interface capturing method. For example, Tomar et al. [2005] used the coupled CLSVOF method to model the film boiling at near critical pressure for different excess temperatures in water and R134a liquid. The results showed the bubble release frequency is higher in R134a near critical condition but reduced considerably at far critical condition. However, they did not give validation case for phase-change model. Zeng et al. [2015] simulated single bubble condensation in subcooled flow using OpenFOAM based on CLSVOF method. The results showed that the initial bubble size, subcooling of liquid and system pressure would affect the bubble behaviour. The bubble will be pierced when the subcooling and initial diameter reach a certain value at the later condensing stage. As noted in Ningegowda and Premachandran [2014], all the CLSVOF methods adopted operator split advection except Yang

et al. [2006] who used a Lagrangian—Eulerian method for the advection of VOF function. Therefore, the CLSVOF is restricted on structured grid which will take more computational time to do twice and thrice interface reconstruction and re-initialization for 2D and 3D cases at each time step. In order to solve this problem, Ningegowda and Premachandran [2014] developed a new CLSVOF method with multi-directional advection algorithms for the phase change problems. Using this method, the interface reconstruction and re-initialization are carried out only once at each time step, which requires less computational time compared with the general CLSVOF method.

The VOSET method

Sun and Tao [2010] carried out a new hybird method, namely coupled volume-of-fluid and level set (VOSET) method. Unlike the CLSVOF method, this method is much easier to implement because it dose not need to solve volume fraction and level set advection equations both, just one volume fraction advection equation needs to be solved and the level set function is calculated by a simple iterative geometric operation. Ansari et al. [2016] used the VOSET method to study the bubble topology rising in a quiescent liquid for different Mo and Eo numbers. Guo et al. [2011] investigated vapor bubbles arising from a vapor film by VOSET method. The relationship between gas/liquid velocity in interfacial cell and volume change is obtained. The discontinuity of velocity due to the difference between mass-weighted velocity and volume weighted velocity caused by phase change is solved using this special treatment. Ling et al. [2014] performed simulation of 2D nucleate boiling using the VOSET method. A temperature interpolation method is presented to compute temperature field in interface cells.

1 Mass transfer models



1.1 The sharp interface model

The sharp interface model is based on the Rankine Hungoniot jump conditions under energy conservation. The sharp interface model is widely used by many investigators to calculate the interfacial phase change (Gibou et al. [2007]). In this model, heat transfer at the interface is assumed to be consumed by latent heat of the fluid. The heat flux $(\dot{q}(w/s))$ near the interface estimated by applying Fourier's law can be written as:

$$\dot{q} = \mathbf{n} \cdot (\lambda_l \nabla T_l - \lambda_v \nabla T_v) = \dot{m} L_h \tag{1}$$

where **n** is the normal vector to the interface, λ is the conductivity of fluids. $\dot{m}(kg/(m^2s))$ is the mass flux (counted as positive from liquid to vapor) due to the phase change across the interface. L_h is the latent heat.

The volumetric mass source term $S(kg/(m^3s))$ is defined by $S_v = -S_l = \dot{m}|\nabla \alpha_l|$. The subscript v and l denote the vapor and liquid phase, respectively. In one computational cell, $|\nabla \alpha_l|$ is one at interface and zero elsewhere, which is obtained from

$$|\nabla \alpha_l| = \frac{1}{V} \int |\nabla \alpha_l| dv = \frac{A_{\Gamma}}{V}$$

where A_{Γ} is the interfacial area and V the cell volume. α indicates the volume fraction. Juric and Tryggvason [1998] used the sharp interface model to simulate film boiling flow and found the generated vapor bubbles do not readily pinch off from the vapor layer. They claimed the reason is that the computations are two-dimensional and this will not appear in three-dimensional cases. Welch and Wilson [2000] constructed the interface geometry associated with Young's method, aiming to derive mass flux through calculating the discontinuous normal component of normal vector of heat flux vector. Esmaeeli and Tryggvason [2004a], Esmaeeli and Tryggvason [2004b] used the method of Udaykumar (Udaykumar et al. [1996]) to calculate the heat source using a first order finite difference approximation. They added mass source and heat source in governing equations to investigate the behavior of film boiling. Gibou et al. [2007] proposed a new algorithm for multiphase flows with phase change based on the sharp interface method. The new algorithm used the ghost fluid method to impose interface's boundary conditions to satisfy the jump conditions. Akhtar and Kleis [2013] studied boiling flow simulations using adaptive octree grids. A phase change model based on the sharp interface model associated with the mixture formulation was developed.

Son et al. [1999] simplified the Eq. 1 by assuming saturation temperature at vapor side, therefore, the mass transfer is considered only the temperature gradient on the liquid side. The volumetric mass source term then can be rewritten as

$$S_v = -S_l = \frac{\lambda_{eff}(\nabla T \cdot \nabla \alpha_l)}{L_h} \tag{2}$$

where λ_{eff} is effective thermal conductivity and calculated as the average of the liquid and vapor phases, weighted by their respective volume fractions. Nichita and Thome used a similar formulation for the source term and can be found in Ganapathy et al. [2013]. This simplification is also used by Luo et al. [2005] to simulate multiphase incompressible flow with phase change.

However, this simplification is less accurate. For example, in film boiling, the liquid is saturated and vapor is superheated, the bubble growth rate is not relevant to the liquid thermal conductivity λ_l in the growing process of a vapor bubble. However, in Eq. 3, λ_{eff} contains the effect of λ_l which not matching the physical phenomena. In order to overcome this problem, Sun et al. [2012] proposed an alternative simplified from based on neglect of heat conduction in saturated phase, and linear temperature profile is in unsaturated phase, namely

$$S_v = -S_l = \frac{2\lambda_l(\nabla T \cdot \nabla \alpha_l)}{L_h} \tag{3}$$

In overall, the sharp interface model based on the Rankine-Hungoniot jump conditions keep the sharp physical feature at interface. However, it should be noted that this model does not account for kinetic energy contributions. The $|\nabla \alpha_l|$ limits the mass transfer along the interface due to this only non-zero at the interface. The model can be used in boiling flow and condensations.

1.2 The Schrage model

Based on Hertz-Knudsen equations (Knudsen and Partington [1935]), Schrage [1953] firstly developed one mass transfer model. The premise of this model, assuming vapor and liquid is saturated but allows jump conditions occur at the interface. According to kinetic gaseous theory, high kinetic molecules would cross the interface due to the temperature deviation on the interface. A ratio γ , between numbers of molecules changing phase and transferring across the interface, is defined to express evaporation and condensation processes as follows:

$$\gamma_e = \frac{\text{number of molecules obtained by vapor phase}}{\text{number of molecules from liquid to vapor}} \quad \text{for evaporation}$$

$$\gamma_c = \frac{\text{number of molecules absorbed by liquid phase}}{\text{number of molecules from vapor to liquid}} \quad \text{for condensation}$$
 (5)

The mass flux is determined by the deviation between vapor-liquid or liquid-vapor mass flux.

$$\dot{m} = \frac{2\gamma}{2 - \gamma} \sqrt{\frac{M}{2\pi R}} \left[\frac{p_v}{\sqrt{T_{v,sat}}} - \frac{p_l}{\sqrt{T_{l,sat}}} \right]$$
 (6)

where M is molecular weight, R the universal gas constant (8.314J/mol K) and γ the evaporation or condensation coefficients. Similar to Lee model, Scharge model also needs to specify γ according to experimental data. Marek and Straub [2001] adopted γ with 0.1 and 1, respectively, in simulation of jets and moving films. Hardt and Wondra [2008], Kunkelmann and Stephan [2009] and Magnini and Pulvirenti [2011] recommended $\gamma=1$ for film boiling. Kharangate et al. [2015] recommended $\gamma=0.1$ and concluded larger γ would do influence numerical stability. Kartuzova and Kassemi [2011] suggested a low value of $\gamma=0.01$ considering turbulent phase change flow.

Furthermore, based on Scharge model, some investigators developed several simplified phase-change models. For example, Tanasawa [1991] assumes for small deviation of interfacial temperature, mass flux has linear property with temperature jump between the interface and vapor phase. This model can be written as the form:

$$\dot{m} = \frac{2\gamma}{2 - \gamma} \sqrt{\frac{M}{2\pi R}} \frac{\rho_g L_h (T - T_{sat})}{T_{sat}^{3/2}} \tag{7}$$

Samkhaniani and Ansari [2017] implemented this model to simulate bubble condensation in OpenFOAM. This simplified model is available for most phase-change problems except for micro scales, where interfacial jump conditions need to be considered. Silvi et al. [2020] used Tanasawa model to model two-phase annular flow boiling inside a tube.

The volumetric mass source term for the Schrage and Tanasawa model is given by $S_v = -S_l = \dot{m} |\nabla \alpha_l|$.

The Schrage model considers both physical kinetic energy effects. One proper phase change coefficient needs to be defined in the model. The other challenge in the Schrage model is $|\nabla \alpha_l|$, limiting the mass source only at the interface. The Schrage model has been used to investigate boiling flow and evaporating falling films.

1.3 The Lee model

Lee [1980] proposed a very simple phase-change model for studying evaporation and condensation processes. In this model, the phase change is driven by deviation of temperature between phases and keep the interface saturated temperature (T_{sat}). The volumetric mass source term is given by:

$$S_v = -S_l = R_i \alpha_l \rho_l \frac{T - T_{sat}}{T_{sat}}$$
 for evaporation: $T > T_{sat}$ (8)

$$S_l = -S_v = R_i \alpha_v \rho_v \frac{T - T_{sat}}{T_{sat}} \quad \text{for condensation: } T < T_{sat}$$
 (9)

where R_i is an empirical value called mass transfer intensity factor with unit s^{-1} , which has different values considering different phase change problems. Extremely large values of R_i result in a numerical instability, while excessively small values of R_i cause a significant deviation between interfacial temperature and saturation temperature. An optimum of R_i depends on many factors, such as mesh size, computational time step. Therefore, it's necessary to determine R_i first. A wide range of R_i from 0.1 to $10^8 s^{-1}$ has been reported in literature. For instance, R_i is defined as $0.1s^{-1}$ by some authors (Lee and Nydahl [1989], Wu et al. [2007], De Schepper et al. [2009], Alizadehdakhel et al. [2010]). However, R_i is specified as $100s^{-1}$ in the work of Yang et al. [2008] and Goodson et al. [2010]. Gorl et al. [2015] gave large R_i as $5000s^{-1}$ in their simulation. In turbulent flow, R_i has larger value. Da Riva et al. [2012] used R_i value from 7.5×10^5 to 5×10^6 in their study on the condensation of turbulent flow in a horizontal circular minichannel. In addition, Chen et al. [2014] eliminated T_{sat} from numerator of the source term to simplify the expression, which can be regarded as introducing one similar factor $r_i = \frac{R_i}{T_{sat}}$ in the calculation. Chen et al. [2020] proposed one expression to approximately compute the value of R_i , using this expression, the initial guess of R_i does not need anymore.

In order to overcome the solution's dependency on R_i in the Lee model, Rattner and Garimella [2013] also proposed a new phase change model that includes the computing time interval for predicting the phase change amount. The heat flux can be calculated by using three different parts, as follows:

$$\dot{q} = \begin{cases} -min(\dot{q}_1, \dot{q}_2, \dot{q}_3) & \text{for evaporation} \\ min(\dot{q}_1, \dot{q}_2, \dot{q}_3) & \text{for condensation} \end{cases}$$
(10)

In Eq. 10, $\dot{q}_1, \dot{q}_2, \dot{q}_3$ are expressed by:

$$\dot{q}_1 = \frac{(\rho c_p)_{eff}(T - T_{sat})}{\Delta t}$$

$$\dot{q}_2 = \begin{cases} \frac{\alpha_l \rho_l L_h}{\Delta t} & \text{for evaporation} \\ \frac{\alpha_v \rho_v L_h}{\Delta t} & \text{for condensation} \end{cases}$$

$$\dot{q}_3 = \frac{L_h}{\Delta t} \left(\frac{1}{\rho_v} - \frac{1}{\rho_l}\right)^{-1}$$

here c_p is the specific heat under constant pressure condition. $(\rho c_p)_{eff}$ is effective coefficient calculated as the average of the liquid and vapor phases, weighted by their respective volume fractions. \dot{q}_1 is defined to force the interface to the saturation temperature at every time step, recovering the physical equilibrium condition. To ensure the physical results, \dot{q}_2 gives a constraint on the range of \dot{q}_1 , because it is not practicable for the mass of fluid condensed in a mesh cell exceed the mass of vapor present in that cell in each time step. \dot{q}_3 guarantees the phase change model satisfying the Cournat-Friedrichs-Lewy (CFL) condition.

The mass flux can be calculated using the following Eq. 11:

$$\dot{m_v} = -\dot{m_l} = \frac{\dot{q}}{L_h} \tag{11}$$

Pan et al. [2016] used one similar Ratter model to simulate flow boiling, however, they just considered the \dot{q}_1 and neglected the other two heating sources. Kim et al. [2017] used the Ratter model to compare with different phase change models and validating the models using one-dimensional stefan problem. Luo et al. [2020] used the Ratter model to investigate annular flow boiling in a rectangular microchannel.

Overall, the Lee model is a simplified saturation model which very depends on the value of mass transfer intensity. It's necessary to attempt and choose the optimum value for different physical problems, however, there is no exact physical explanation on the mechanism of this phase change model. Unlike the Schrage model, which just allows the mass transfer along the interface, the Lee model allows for phase change both along the interface and within the saturated phase (Kharangate and Mudawar [2017]). The Lee model can be widely used to simulate full scale flow boiling and flow condensation processes, but with reduced accuracy.

1.4 Other methods to calculate mass transfer

There are other methods to simulate phase change. Krepper et al. [2007] proposed one simple method to compute mass flux in order to simulate subcooled boiling, as follows:

$$\begin{cases} \dot{m}_{l} = max \frac{h_{i}(T_{sat} - T)A_{\Gamma}}{L_{h}} & \text{for subcooled liquid} \\ \dot{m}_{v} = max \frac{h_{i}(T - T_{sat})A_{\Gamma}}{L_{h}} & \text{for superheated liquid} \end{cases}$$
(12)

where h_i is the heat transfer coefficient, calculated according to Ranz et al. [1952]. Jeon et al. [2011] used the same method to study the bubble condensation in subcooled boiling flow. It was found that the condensing bubble has many different aspects compared with adiabatic bubble. In the work of Chen et al. [2009], they applied a similar model but different in calculating mass flux, the cell temperatures near interface are used for vapor and liquid, namely $\dot{m} = \frac{h_i(T_v - T_l)A_\Gamma}{L_h}$. Sun et al. [2014] computed the mass flux at interface through the heat exported from interface and neighboring cell for the condensation process, or the heat imported in interface and neighboring unsaturated cell for the evaporation process. Zhang et al. [2001] added a large artificial source term to the enthalpy equation to force interface temperature saturated, the heat and mass source terms are computed using the updated temperature filed.

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