A critical comparison of smooth and sharp interface methods for phase transition

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A critical comparison of smooth and sharp interface methods for phase transition


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A B S T R A C T

In this study, the Local Front Reconstruction Method (LFRM) is extended to allow for the direct numerical simulation of flows with phase transition. The LFRM is a hybrid front tracking method without connectivity, which can easily handle complex topological changes. The expansion due to phase change is incorporated as a non-zero divergence condition at the interface. The energy equation is treated with two different approaches: smooth interface approach and sharp interface approach. The smooth interface approach uses a one fluid formulation to solve the energy equation with an interfacing source term accounting for phase change. This interfacial source term enforces the saturation temperature at the interface. However, in the sharp interface approach, the thermal properties are not volume-averaged near the interface and the saturation temperature is imposed as a boundary condition at the interface. A detailed mathematical formulation and numerical implementation pertaining to both approaches is presented. Both implementations are verified using 1D and 3D test cases and produce a good match with analytical solutions. A comparison of results highlights certain advantages of the sharp interface approach over the smooth interface approach such as better accuracy and convergence rate, reduced fluctuations in the velocity field and a physically bounded temperature field near the interface. Finally, both approaches are validated with a 3D simulation of the rise and growth of a vapor bubble in a superheated liquid under gravity, where a good agreement with experimental data is observed for the bubble growth rate.

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1. Introduction

Phase change phenomena, especially related to gas-liquid flows, are seen in many industrial systems, such as refrigeration systems, cooling systems, boilers, heat exchangers and nuclear reactors. Phase change is a relatively efficient mode of heat transfer because of the observed high heat transfer rates. Another advantage is that a large amount of energy can be stored in the form of latent heat making phase change important for thermal energy storage applications. A detailed understanding and accurate predictions of the phase change processes in such systems are important for their safe and efficient operation.

In addition to experiments, numerical simulations have become an important tool to study phase change phenomena. The advantage of Direct Numerical Simulations (DNS) is that, in contrast to the experiments, the complete details on temperature and velocity fields are available. This has facilitated the study of the transient and dynamic aspects of phase change.

The earliest attempt to simulate boiling flows can be traced back to Welch (1995). In this study, a 2D moving mesh finite volume method was developed. However, the method was limited to small topology changes of the interface. Since then, many different interface tracking techniques, such as Volume of Fluid (VOF), Level Set (LS), and Front Tracking (FT) methods, have evolved which can handle large deformation of the liquid–vapor interface.

Tsui et al. (2014) simulated boiling bubbles emerging from a planar film and a circular film using VOF. More recently, Sato and Ničeno (2013) used mass conservative VOF to simulate 3D nucleation and growth of a single bubble. In the VOF method, the interface is generally artificially smeared for the calculation of interfacial properties resulting in a higher numerical error for phase change calculations (Sato and Ničeno, 2013).

The LS method has been extensively used by Dhir's group (Dhir, 1998; 2001; Dhir and Purohit, 1978; Li and Dhir, 2007) to study different phase change phenomena such as nucleate boiling, film boiling from a horizontal cylinder and sub-cooled pool boiling. Apart from Dhir's group, Gibou et al. (2007) used the LS method to study film boiling and Tanguy et al. (2007) to simulate evaporation of a moving and deforming droplet. However, the LS method is a non-conservative approach and does not guarantee mass conservation for phase change calculations (Sato and Ničeno, 2013).

The smearing of the interface, as encountered in the VOF method, can be avoided by using the Front Tracking method, where the interface is directly tracked with a Lagrangian mesh. The Front Tracking method was first applied to study film boiling by Juric and Tryggvason (1998). They used an iterative procedure to set the correct temperature boundary condition at the interface. Subsequently, Esmaeeli and Tryggvason (2004) improved the method by eliminating the iterative algorithm and applied it to simulate 3D film boiling from multiple horizontal cylinders. Recently, Irfan and Muradoglu (2017) have developed an FT method to simulate the species gradient driven phase-change process.

Hybrid methods have been developed combining/modifyung these standard methods: Coupled Level Set and Volume of Fluid (CLSVOF) method, Level Contour Reconstruction Method (LCRM) and Local Front Reconstruction Method (LFRM). Film boiling simulations were carried out by Shin and Juric (2002) using LCRM. Tomar et al. (2005) developed a 2D CLSVOF method coupled with phase change and applied it to simulate film boiling. Shin and Abdel-Khalik (2007) studied the stability of an evaporating thin film of liquid on a heated cylindrical rod with parallel and cross vapor flow using improved LCRM. Recently, Shin and Choi (2016) further improved the energy formulation in LCRM and simulated a rising bubble with phase change. In this study, we use a hybrid front tracking method, the modified Local Front Reconstruction Method (Rajkotwala et al., 2018; Mirsandi et al., 2018), which offers better local and global mass conservation compared to other Front Tracking methods. The LFRM method is capable of dealing with breaking and merging of the interface and thus can be used to simulate complex topological changes like droplet collision (Rajkotwala et al., 2018). We extend the method to enable phase change simulations, which has not been done before.

The most important aspect of the phase change simulation methodology is the treatment of the variation of properties and of the jump conditions across the interface. These are broadly classified into two approaches: in the first approach, the governing equations are written in each phase separately and additional jump conditions are imposed at the interface to satisfy the conservation of mass, momentum and energy. This is known as the Jump Condition Formulation or Sharp Interface Approach. This approach has been coupled with VOF (Sato and Ničeno, 2013), LS (Gibou et al., 2007; Tanguy et al., 2007; Lee and Son, 2017) and LCRM (Shin and Abdel-Khalik, 2007; Shin and Choi, 2016).

In the second approach, the jump conditions are expressed in the governing equations by introducing appropriate source terms using a (modified) Dirac delta function which is equal to zero everywhere in the domain, except at the interface. The interface is normally smeared out across 2 or 3 computational cells by defining a smoothed Heaviside or Dirac function to represent the spatial variation of physical properties across the interface, i.e. using a one fluid approach. This approach is commonly used because of its simplicity in implementation. Numerous studies can be found using this approach with VOF (Welch and Wilson, 2000; Ding et al., 2017; Tsui et al., 2014), LS (Li and Dhir, 2007), FT (Juric and Tryggvason, 1998; Esmaeeli and Tryggvason, 2004) and LCRM (Shin and Juric, 2002). However, the usage of this approach might result in a reduced accuracy when the interface is too close to a wall (Shin and Abdel-Khalik, 2007). Moreover, it is difficult to enforce the saturation temperature at the interface using a source term. This affects the accuracy of the results as the interfacial mass flux calculation is error prone if the temperature field is not accurate in the vicinity of the interface (Shin and Abdel-Khalik, 2007). Because a systematic comparison of the sharp and one fluid approaches is clearly missing in the literature, an attempt is made by this study to bridge this gap.

The outline of the paper is as follows: In Section 2, the formulation of the Navier–Stokes equation to accommodate jump conditions for phase change is described. The different forms of the energy conservation equation and closure equations are discussed based on the use of the sharp or smooth interface approach. In Section 3, the numerical methodology is explained with a special focus on the implementation details of the sharp interface approach. In Section 4, the methods are verified with the standard 1D tests, namely the Stefan problem and the sucking interface problem and with 3D bubble growth test. The errors are compared for both approaches. The section ends with a discussion of 3D bubble rise simulations. Finally, conclusions are presented in Section 5.

2. Mathematical formulation

In this study, we solve the flow equations using a one fluid approach whereas the energy equation is treated by both a smooth interface approach and a sharp interface approach. Although both approaches correspond to the same continuum limit, they use different numerical methods when dealing with the discontinuity at the interface while solving the energy equation. In the next sections, these differences will be explained in detail.

2.1. Mass conservation equation

We assume the liquid and the gas phases to be incompressible and single component. The mass density $\rho$ in the one fluid formulation is defined as

$$\rho = \rho_l I + \rho_\ell (1 - I),$$

where $\rho_\ell$ is the density of gas phase, $\rho_l$ is the density of liquid phase and $I$ is a Heaviside function which is one in gas phase and zero in the liquid phase.

Due to the phase transition, there is a difference in the gas and liquid velocities at the interface. The difference in the velocities is related to the evaporative mass flux where the relevant jump condition can be obtained by integration of the continuity equation across the interface, which is as follows:

$$\rho_l (u_l - u_f) \cdot n = \rho_\ell (u_\ell - u_f) \cdot n = \dot{m},$$

where $u_f$ is the interface velocity, and $\dot{m}$ is the evaporation rate at the interface. Note that in absence of phase transition, the velocity is continuous at the interface meaning $u_f = u_\ell = u_l$.

It is safe to assume a divergence-free velocity field everywhere except at the interface for low Mach number flows with low temperature variations in the gas phase as well as in the liquid phase. For flows with phase transition, the velocity field is not divergence-free at the interface because of fluid expansion/compression due to phase change. Thus, an interfacial source term which accounts for the expansion/compression has to be incorporated in the continuity equation. This term can be derived by taking the volume integral of the divergence of the velocity over the interface thickness.
In the smooth interface approach, the interfacial energy flux \( \dot{q} \) is incorporated in the energy equation by means of a source term:

\[
\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left[ \nabla \cdot (\mathbf{u}T) - T \nabla \cdot \mathbf{u} \right] = \nabla \cdot (k \nabla T) - \int_{A_f} \delta(x - x_f) \dot{q} dA_f.
\] (8)

The energy flux at the interface is related to the interfacial mass flux \( \dot{m} \) by the following equation:

\[
\dot{m} h = \dot{q}
\] (9)

where \( h = h_{\text{fg}} + (C_{\text{fg}} - C_{\text{lg}})(T_f - T_{\text{sat}}) \) with \( h_{\text{fg}} \) is the latent heat measured at the equilibrium saturation temperature \( T_{\text{sat}}(P) \), corresponding to the reference ambient system pressure and \( T_f \) is the interface temperature.

The final form of the energy equation is obtained by substituting above equation in (8):

\[
\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left[ \nabla \cdot (\mathbf{u}T) - T \nabla \cdot \mathbf{u} \right] = \nabla \cdot (k \nabla T) - \int_{A_f} \delta(x - x_f) \dot{m} h dA_f.
\] (10)

In the sharp interface approach, the jump conditions are imposed on the interface as a boundary condition, and hence, the interfacial source term is absent from the corresponding energy equation:

\[
\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left[ \nabla \cdot (\mathbf{u}T) - T \nabla \cdot \mathbf{u} \right] = \nabla \cdot (k \nabla T).
\] (11)

2.4. Additional equations

In the above presented equations, additional closure equations are required to calculate the interface temperature \( T_f \) and interfacial mass transfer \( \dot{m} \).

A standard way to derive these closures is assume that the phase transition occurs at a uniform temperature and the temperature depends only on the system pressure. Thus, the interface temperature is set to the equilibrium saturation temperature corresponding to the system pressure.

\[
T_f = T_{\text{sat}}(P_{\infty})
\] (12)

The corresponding mass flux is calculated from the energy jump condition as follows:

\[
\dot{m} = \frac{k_f \frac{\partial T}{\partial n} |_e - k_i \frac{\partial T}{\partial n} |_i}{h_{\text{fg}}}
\] (13)

This form of closure is used in many studies involving flow boiling (Mukherjee et al., 2011; Li and Dhir, 2007), film boiling (Shin and Juric, 2002; Welch and Wilson, 2000; Esmaeili and Tryggvason, 2004), pool boiling (Dhir, 2001) and evaporation (Irfan and Muradoglu, 2017).

A counter argument to the above assumption can be made that because of the pressure jump across the interface, the equilibrium saturation temperatures corresponding to those pressures cannot be equal i.e. \( T_{\text{sat}}(P_f) \neq T_{\text{sat}}(P_i) \). To test the validity of Eq. (12), Juric and Tryggvason developed a general expression of the deviation of the interface temperature from the saturation temperature using the entropy jump condition (Juric and Tryggvason, 1998). The impact of each term in this general expression was quantified using simulation of film boiling of hydrogen and it was concluded that \( T_f = T_{\text{sat}} \) is a valid assumption except when the interface comes close to the heated wall. Near the heated wall, the simple expression derived from kinetic theory of gases by Tanasawa (1991) was recommended.
A different approach to calculate the interfacial mass flux is using semi-empirical relations. For example, Schrage (1953) developed a model using kinetic theory of gases. In this model, the interfacial mass flux is calculated by relating the flux of molecules crossing the interface during phase change to the temperature and pressure of the phases. The empirical parameters in such models are generally calculated by comparing the mass flux to experimental data. This limits the general applicability of the model. A summary of such models is given in the recent paper by Kharangate and Mudawar (2017). To avoid introduction of empirical parameters in the method, the mass flux calculation from the energy jump condition, Eq. (13), is selected in this study.

3. Numerical methods

3.1. Fluid flow solver

The interface is represented by an unstructured mesh of triangular markers, which are formed by the connection of the Lagrangian points situated at the corners of these markers. The markers enable advection of the interface and surface tension calculation. \(\mathbf{F}_\tau\) is calculated on the Eulerian grid using the hybrid method of Shin et al. (2005), which combines the advantage of accurate curvature calculation (similar to the pull force model (Dikhuizen et al., 2010) in Front Tracking methods) and the proper balance of pressure jump and surface tension force at the discrete level (similar to the continuous surface model (Brackbill et al., 1992) in front capturing methods).

Subsequently, the governing equations are solved by a fractional step method to obtain the flow field at the next time step (Das et al., 2016). The method consists of two steps: In the first step, a projection of the velocity \(\mathbf{u}^{n}\) is calculated using information from the previous time step

\[
\mathbf{u}^{n+1} = \mathbf{u}^n + \frac{\Delta t}{\rho} \left[ \rho \nabla \cdot (\mathbf{u} \mathbf{u}) + \mathbf{u} (\nabla \cdot \mathbf{u}) - \nabla p + \mathbf{g} - \nabla \cdot \mathbf{F}_\tau \right].
\]

(14)

This equation is spatially discretized on a staggered grid using a finite volume approach. The convective term is discretised with a second order flux-delimited Barton scheme whereas the diffusion term with a second order central scheme (Rajkotwala et al., 2018). The convection term is treated explicitly and diffusion term is treated semi-implicitly. The term \(\rho \mathbf{u} (\nabla \cdot \mathbf{u})\) is evaluated by averaging the calculated divergence at the faces of velocity cells.

After the projected velocities are calculated, the velocity field is corrected in the pressure correction step to satisfy the continuity equation including interfacial mass flux.

\[
\nabla \cdot \mathbf{u}^{n+1} = \nabla \cdot \mathbf{u}^n - \nabla \cdot \mathbf{u}^{n+1}.
\]

(15)

The pressure equation is solved using a robust and efficient parallel Block-Incomplete Cholesky Conjugate Gradient (B-ICCG) solver (Das et al., 2016). The term \(\nabla \cdot \mathbf{u}^{n+1}\) is non-zero at the interface in case of phase change and is calculated using Eq. (6). The interfacial mass flux is calculated on the Lagrangian interface using Eq. (13) and distributed on the Eulerian grid using a discrete distribution function. In this study, we use a trilinear distribution function.

The calculation of the interfacial mass flux term on the Lagrangian mesh is done using the normal probe method of Udaykumar et al. (1996) as shown in Fig. 2. The right hand side of Eq. (13) is discretized using a first order approximation as follows:

\[
m = \frac{1}{\Delta n} \frac{1}{\Delta l} \left[ k_g (T_g - T_{sat}) - k_l (T_{sat} - T_l) \right].
\]

(16)

where \(T_l\) and \(T_g\) are found by interpolating the temperature using two normal probes which originate at the phase boundary and extend a distance \(\Delta n\) into the liquid and the gas. A tri-linear function is used for the interpolation of temperature on probing points from fixed grid points and the normal distance is usually taken equal to the grid step size (Shin and Juric, 2002; Esmaeeli and Tryggvason, 2004). The choice of tri-linear interpolation is motivated by the observation that there is a negligible difference in the results when a second order discretization is used (Esmaeeli and Tryggvason, 2004).

Once the flow field is solved, the interface is advected, i.e. the Lagrangian points are moved. The equation of motion for marker points is

\[
\frac{dx_f}{dt} = \mathbf{u}_n \cdot \mathbf{n}_f
\]

(17)

where \(\mathbf{u}_n\) is the normal velocity. The equation of this normal velocity, derived from Eq. 2, reads

\[
\mathbf{u}_n = \mathbf{u} \cdot \mathbf{n} - \frac{m}{\left( \frac{1}{\rho_l} + \frac{1}{\rho_g} \right)}
\]

(18)

In the above equation, the normal velocity at the interface has two components; one due to fluid advection (the first term) and another one due to phase change (the second term). The first term is interpolated from the Eulerian grid (Cubic spline interpolation is used) and the second term is directly calculated on the Lagrangian mesh using normal probe method of Udaykumar et al. (1996) as explained before. The equation is integrated in time using the fourth order Runge–Kutta method.

Due to the advection of Lagrangian points, the mesh quality decreases, a reconstruction procedure is required to overcome this. In this study, we use the modified LFRM (Rajkotwala et al., 2018; Mirmandi et al., 2018). Finally, the physical properties are updated using local cell phase fractions in each cell. From the calculated phase fractions, the average mass density and viscosity are calculated in each grid cell by algebraic and harmonic averaging, respectively. The local phase fraction can be calculated by geometric analysis using the position of the interface (Dijkstraizen et al., 2010) which
is exact and computationally more efficient than solving the Poisson equation.

3.2. Energy solver

At each time step, the energy equation is solved using the updated velocity and physical properties. However, the form of energy equation varies with the numerical approach as explained in Section 2.3. In both approaches, the convective term and the diffusion term are discretised with a second order flux-delimited Barton scheme (Rajkotwala et al., 2018) and a second order central scheme, respectively. The time step restriction is relaxed by treating the diffusion term implicitly. The discretization of term $\rho C_v T (\nabla \cdot \mathbf{u})$ for cell $(i, j, k)$ uses the temperature in the cell center times the divergence that is also naturally defined in the cell center.

The main differences in the two approaches lie in the treatment of the interface source term and the calculation of thermal properties. The specific details of the two approaches are given in following sections.

3.2.1. Smooth interface approach

The treatment of the interface source term in the energy conservation Eq. (8) is similar to that in mass conservation Eq. (6), i.e. the interfacial mass flux will be calculated on the Lagrangian interface using Eq. (13) and distributed on the Eulerian grid using a discrete distribution function. In this study, we use a trilinear distribution function. From the updated phase fractions, the average volumetric heat capacity and conductivity are calculated in each grid cell by algebraic and harmonic averaging, respectively.

3.2.2. Sharp interface approach

In the sharp interface approach, the saturation temperature is imposed as a boundary condition at the interface. This is handled at the discrete level by use of irregular stencils in the discretization of diffusion terms. The thermal properties are treated sharply, i.e. the cell centers lying in the liquid and gas phase are assigned corresponding phase properties. Thus, the first step in this approach is phase-wise flagging of all cells and calculation of the stencil length.

As shown in Fig. 4, the cells are marked with four different flags: “gas” (cell center in gas phase), “liquid” (cell center in liquid phase), “I-gas” (gas cell adjacent to interface) and “I-liquid” (liquid cell adjacent to interface). As the interface is represented using a triangulated mesh, the exact location of the interface is known and can be used for the flagging of the cells. This is done by identifying the triangles which intersect the grid lines (i.e. the lines passing through neighboring cell centers) as shown in Fig. 3. A fast triangle intersection algorithm (Pant et al., 2001) is used, which uses the side product of the line with the edges of the triangle.

The dot product of the line with the normal of the triangle indicates whether a cell center is to be flagged as I-gas or I-liquid cell. Once the interface cells are flagged, the cells which are completely filled with gas (gas fraction $f = 1$) are flagged as gas cells and the rest of the cells are flagged as liquid cells. Next, the normalized distance of the interface (normalized by the grid size) with respect to the closest cell center in the gas phase is calculated (e.g. $\xi_{i0}$ and $\xi_{j0}$ in Fig. 4). This is done by calculating the intersection point of the triangle (plane containing triangle) and the line passing through the neighboring cell centers. These distances are stored in a linked-list data structure where path to the data is given by flag of “I-liquid” cells.

Subsequently, the thermal properties are assigned to the cells based on cell flags, i.e. cells with “gas” or “I-gas” flags are given gas properties and cells with “liquid” or “I-liquid” flags are given liquid properties. As mentioned previously, the convection term is explicitly calculated using the Barton scheme. The temperature gradient in the convection term can be computed in the sharp formulation (Sato and Nishida, 2013) or conventional form (similar to smooth approach). Similar to Shin and Choi (2016), we found that the sharp energy formulation for the convection term gives similar accuracy of the solution as the conventional form. Therefore, the conventional form is used for the discretization of the convection term.

The diffusion terms are discretized by a second order central difference scheme. The complete discretized energy equation is represented as a set of algebraic equations as follows:

$$A_C T_C + \sum_{n_b} A_{nb} T_{nb} = B_C$$

where $T$ is temperature, the subscript ‘C’ indicates cell center and ‘nb’ indicates the six neighbouring cells. The coefficients $A_C$ and $A_{nb}$ depend on thermal properties, grid size and time step size and $B_C$ contains all explicit terms. For all the interface cells, the saturation temperature is imposed as a boundary condition by changing the coefficients and $B_C$ term. The implementation is based on the immersed boundary method of Das et al. (2016, 2018) and Deen et al. (2012).

In Fig. 4, I-liquid cell C has two neighbour I-gas cells $X_n$ and $Y_n$. While calculating the temperature at I-liquid cell C, the saturation temperature is imposed at the interface by changing the value of coefficients of the neighbouring I-gas cells $X_n$ and $Y_n$. A quadratic fit (between $S_1 - C - X_p$ and $S_2 - C - Y_p$) is used to modify the coefficients. However, when the interface is very close to C, a linear fit (between $S_1 - X_p$ and $S_2 - Y_p$) is used to modify the coefficients.

Once all the coefficients are modified, the temperature is computed by solving the resulting modified system of linear equations using a parallel B-IICG solver (Das et al., 2016).

3.3. Summary of the solution algorithm and the time step size restriction

The solution procedure can be summarized as follows:

1. Calculate the mass flux $n$ using temperature field at time level $n$, Eq. (16).
2. Update the hydrodynamic properties (based on interface position of time level $n$)
3. Calculate the surface tension force $F_s$
4. Update the velocities and pressure to time level $n+1$ using fractional step method, Eqs. (14) and (15).
5. Advect the interface to the next time level $n+1$, Eq. (17).
6. Update the phase flag using updated interface.
7. Update the thermal properties (based on interface position of time level $n+1$)
8. Update the temperature field to time level \( n+1 \) either using smooth interface approach, Eq. (10) or sharp interface approach, Eq. (11).

9. Advance to time level \( n+1 \).

The time step size is restricted by CFL condition and the stability criteria due to surface tension as follows:

\[
\Delta t = \min \left( \frac{c_{\text{CFL}} \Delta x}{a_{\text{max}}}, \frac{\rho_T \Delta x^3}{2 \pi \sigma} \right)^{1/2}
\]

(20)

where \( c_{\text{CFL}} \) is the dimensionless safety factor.

**4. Results and discussion**

4.1. Stefan problem

4.1.1. Problem definition

The Stefan problem is a well-known test case to verify the phase change problems, which is schematically shown in Fig. 5. As seen in the figure, the vapor and liquid phases are separated by a vertical interface. The temperature of the left wall (next to the vapor phase) is kept above the saturation temperature. The liquid starts vaporizing and the interface moves towards the right. A free flow boundary condition is applied at the right boundary for the liquid to flow out. However, the liquid temperature stays fixed at the saturation value. Because the vapor remains stationary, diffusion is responsible for heat transfer from the wall to the interface. The analytical solution is given in literature (Welch and Wilson, 2000; Irfan and Muradoglu, 2017).

The energy equation needs to be solved only in the vapor phase, and is given by

\[
\frac{\partial T}{\partial t} = \alpha_g \frac{\partial^2 T}{\partial x^2}
\]

(21)

where \( x \) varies from 0 to \( x_I(t) \), with \( x_I(t) \) the position of the interface at time \( t \).

The above equation is solved with the following boundary conditions:

\[
T(x = 0, t) = T_w \quad \text{and} \quad T(x = x_I(t), t) = T_{\text{sat}}
\]

(22)

The heat flux at the interface is computed using energy jump condition:

\[
\dot{q}_I = -k_g \frac{\partial T}{\partial x}\bigg|_I
\]

(23)

The analytical solution for the interface location is given by

\[
x_I(t) = 2 \beta \sqrt{\alpha_g t}
\]

(24)

where \( \beta \) is the solution of the transcendental equation

\[
\beta \exp \beta^2 \operatorname{erf} \beta = \frac{C_{\text{lg}} (T_w - T_{\text{sat}})}{h_{\text{lg}} \sqrt{\pi}}
\]

(25)

where \( h_{\text{lg}} \) is latent heat of vaporization.
The analytical solution of temperature in the gas phase is given by

\[
T_g(x, t) = T_W + \left(\frac{T_{sat} - T_W}{\text{erf} \beta}ight) \text{erf} \left(\frac{x}{2\sqrt{\alpha \beta t}}\right)
\]  

(26)

4.1.2. Problem setup

The test parameters are chosen from Irfan and Muradoglu (2017). The properties of the fluids are summarized in Table 1. The wall temperature \(T_W\) is set to 12 K. As the problem is one-dimensional, the computational domain is replicated as 1D by choosing 5 cells in Y and Z directions respectively. The length ‘L’ along X is taken as 1 m. Three grid sizes are selected: coarse \((4 \times 10^{-4} \text{ m})\), medium \((2 \times 10^{-4} \text{ m})\) and fine \((1 \times 10^{-4} \text{ m})\). The analytical solution is evaluated using MatLab. The problem is initialized with an interface at \(x_{t,0} = 0.1\) m. The temperature and velocity fields are initialized using the analytical solution corresponding to \(x_{t,0}\).

4.1.3. Smooth interface approach

The Stefan problem is solved using the smooth interface approach for different grid sizes. The temperature variation along the domain length and the evolution of the interface location and liquid velocity with time are given in Fig. 6. The solution agrees well with the analytical solution and converges upon grid refinement. However, it can be seen in Fig. 6(a) that the temperature at the interface is not completely maintained at the saturation temperature (especially on the coarse grid). This is a well-known problem of this technique (Shin and Abdel-Khalik, 2007; Shin and Choi, 2016) as the interface temperature is implicitly enforced to be the saturation temperature by a source term, which also leads to velocity fluctuations in the domain (Fig. 6(c)).

4.1.4. Sharp interface approach

Similarly, the Stefan problem is solved using the sharp interface approach for 300 s for different grid sizes. The temperature variation along the domain length is given in Fig. 7 (a). The solution agrees well with the analytical solution and converges upon grid refinement. The variation of the interface location (Fig. 7(b)) and liquid velocity (Fig. 7(b)) with time is compared to the analytical solution and a very good agreement is observed.

4.1.5. Error comparison

As the grid is refined, the results of both methods approach the analytical solution. To compare the accuracy of both approaches, the temperature distributions for grid size \(L/\Delta x = 100\) obtained at time \(t = 219.02\) s are shown in Fig. 8. As discussed before, an undershoot below the saturation temperature is observed in case of the smooth approach, which is not physical in nature, whereas for the sharp approach the interface is at saturation temperature. The L2 norm of the error in the temperature at time \(t = 219.02\) s at different grid sizes is calculated using the following expression

\[
\epsilon_T = \sqrt{\frac{\sum_{j=1}^{N_x} (T_{num, j} - T_{ana, j})^2}{N_x}}
\]  

(27)

where \(T_{num}\) is the temperature obtained from simulation, \(T_{ana}\) is the temperature obtained from the analytical solution and \(N_x\) is the number of grid points along domain length \(L\).

The convergence of the L2 norm of the error in the temperature with decreasing grid size is shown in Fig. 9. The error is lower for the sharp interface approach than for the smooth interface approach. Also, the average order of convergence for the sharp interface approach (1.24) is higher than for the smooth interface approach (1.05). The reason for the reduced order of convergence can be the boundary condition treatment and mass flux calculation (i.e. first order temperature gradients calculation and linear interpolation of temperature field onto Lagrangian mesh and mass flux onto Eulerian grid).

4.2. Sucking interface problem

4.2.1. Problem definition

The sucking interface problem is also a benchmark case used to verify phase change models. The schematic of the test case can be seen in Fig. 10. In this test case, a vapor layer is attached to the left wall of the domain while the rest is filled with liquid as the same
species as vapor. The vapor phase is at saturation temperature $T_{sat}$, and stays at rest throughout the simulation. The liquid temperature is higher than the saturation value, therefore phase change occurs at the interface. This causes the interface to move towards the right and a flow develops in the liquid phase. The heat of vaporization, absorbed at the interface due to phase change, comes from the liquid, which results in the formation of the thermal boundary layer at the interface. The analytical solution is given in literature (Welch and Wilson, 2000; Irfan and Muradoglu, 2017).

The energy equation needs to be solved only in the liquid phase, given by

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \alpha \frac{\partial^2 T}{\partial x^2}$$

(28)

with $x_{i}(t)$ the position of the interface at time $t$.

The above equation is solved with the following boundary condition:

$$T(x = x_{i}(t), t) = T_{sat}$$

(29)

The analytical solution for the interface location is given by

$$x_{i}(t) = 2\beta \sqrt{\alpha_{g}t}$$

(30)

where $\beta$ is the solution of the transcendental equation

$$\beta - \left( \frac{T_{\infty} - T_{sat}}{C_{p_{g}}k_{l} \sqrt{\alpha_{g}}} \right) \exp \left( -\frac{\beta^2 \rho_{l} g \sqrt{\alpha_{g}}}{m_{g}} \right) = 0.$$  

(31)

where $h_{lg}$ is latent heat of vaporization.
4.2.2. **Problem setup**

The physical properties used in this test case are given in Table 1. The wall temperature $T_w$ is set equal to saturation temperature $T_{sat}$. Similar to the Stefan problem, the computational domain is replicated as 1D by choosing 5 cells in Y and Z directions respectively. The length ‘L’ in the X-direction is taken as 1 m. Three grid sizes are selected: coarse ($2 \times 10^{-2}$ m), medium ($1 \times 10^{-2}$ m) and fine ($5 \times 10^{-3}$ m). The analytical solution is evaluated using MatLab. The problem is initialized with an interface at $x_{T,0} = 0.1$ m. The temperature and velocity fields are initialized using the analytical solution corresponding to $x_{T,0}$.

The analytical solution for the temperature in the liquid phase is given by

$$T_l(x, t) = T_\infty - \frac{T_\infty - T_{sat}}{\text{erfc} \left( \frac{\beta \rho_s \sqrt{\alpha_l}}{2 \sqrt{\alpha_l t}} \right)} \text{erf} \left( \frac{x}{\sqrt{\alpha_l t}} \right) + \frac{\beta (\rho_s - \rho_l)}{\rho_l} \sqrt{\frac{\alpha_s}{\alpha_l}}.$$

4.2.3. **Smooth interface approach**

For the smooth interface approach, a good agreement with the analytical solution is observed for the temperature variation and the evolution of interface location as shown in Fig. 11. The overall agreement in the liquid velocity variation with the analytical solution is good. Significant fluctuations of the velocity are observed which are due to implicit enforcement of the saturation temperature at the interface using source term as explained before.

4.2.4. **Sharp interface approach**

The results obtained using the sharp interface approach are given in Fig. 12. The results converge to the analytical results as the grid is refined. The minor oscillation in the velocity is caused by the mass flux source term in the pressure correction equation.

4.2.5. **Error comparison**

To compare the accuracy of both approaches, the temperature distributions for grid size $L/\Delta x = 200$ at time $t = 219.02$ s are shown in Fig. 13. Similar to the Stefan problem, the convergence of both methods is compared by calculating the error in the temperature at time $t = 219.02$ s at different grid sizes as shown in...
4.3. 3D bubble growth under zero gravity condition

4.3.1. Problem definition

In this verification test case, a simulation of a 3D spherical bubble in a super-saturated liquid under zero gravity is carried out. As shown schematically in Fig. 15, a gas bubble is placed in the middle of the domain and is surrounded by super saturated liquid. Similar to the sucking interface problem, the gas phase is at saturation temperature $T_{sat}$ and stays at rest throughout the simulation. The phase change at the interface causes growth of the bubble, which will push the liquid out of the domain. The heat of vaporization comes from the liquid, and thus, a thermal boundary layer is formed in the liquid phase near the interface. The analytical solution is given in literature (Scriven, 1959; Sato and Níčeno, 2013).

The analytical solution for the bubble radius $R$ as a function of time is given by

$$R = 2\beta \sqrt{\frac{k_l}{\rho_l C_{pl}}} t,$$

where $k_l$, $C_{pl}$, and $\rho_l$ are the thermal conductivity, the specific heat capacity and the density of liquid, respectively, and $\beta$ is the "growth constant": $\beta$ is obtained by solving the following implicit equation

$$\frac{\rho_l C_{pl} (T_\infty - T_{sat})}{\rho_g (h_{lg} + (C_{pl} - C_{pg}) (T_\infty - T_{sat}))} = 2\beta^2 \int_0^1 \exp \left(-\beta^2 \left(1 - \zeta\right)^{-2} - 2 \left(1 - \frac{\rho_g}{\rho_l}\right) \zeta - 1\right) d\zeta. \quad (34)$$

where $C_{pg}$ and $\rho_g$ are the specific heat capacity and the density of gas, respectively, $h_{lg}$ is the latent heat and $T_\infty$ is the super saturation temperature of the liquid.
Fig. 17. Final bubble shape at time $t = 83.68$ s for the coarsest grid.

The analytical solution for the temperature field at time $t$ is given by

\[
T = \begin{cases} 
T_{\infty} - 2\beta^2 \left( \frac{\beta}{\rho_l} \frac{(C_{pl} - C_{pg})(T_{\infty} - T_{sat})}{\rho g} \right) \\
\frac{1}{T_{sat}} \int_{r=1}^{R} \exp \left( -\beta^2 \left( (1 - \xi)^{-2} - 2(1 - \frac{\rho_l}{\rho g})\xi - 1 \right) \right) d\xi & r > R \\
T_{sat} & r \leq R 
\end{cases}
\tag{35}
\]

4.3.2. Problem setup

The properties of the fluids are the same as in the previous test cases. A bubble of radius $R_0 = 0.15$ m is initialized in the center of a cubic domain with size 1 m$^3$. The temperature and velocity fields are initialized using the analytical solution corresponding to $R_0$. The surrounding liquid temperature is set to $T_{\infty} = 12$ K. A constant pressure ($P = 0$ bar) and zero heat flux ($\frac{dT}{dn} = 0$ K/m) boundary conditions are applied to all walls. Three grid sizes are selected: coarse ($4 \times 10^{-2}$ m), medium ($2 \times 10^{-2}$ m) and fine ($1 \times 10^{-2}$ m).

4.3.3. Results and comparison

The bubble growth is simulated for time 70 s starting from the initial bubble of radius $R_0$. The evolution of the computed radius with time is shown in Fig. 16. The results closely agree with the analytical solution and grid convergence can be observed with decreasing grid size. The final shape of the bubble at the end of the simulation is shown in Fig. 17. The figure shows that the spherical shape of the bubble is retained by both approaches even at the coarsest grid. The sphericity parameter $\Psi$ for the final bubble
shape can be calculated using the following expression

\[ \Psi = \frac{\pi \frac{1}{2} (6V_b) \frac{1}{2}}{A_b} \]  

(36)

where \( A_b \) and \( V_b \) are bubble area and volume respectively. At the coarse grid, the area and volume of the bubble time \( t = 83.68 \) s for the sharp interface approach are 1.6127 m² and 0.1925 m³, respectively and the corresponding sphericity \( \Psi = 0.9999 \). Similarly, the area and volume of the bubble time \( t = 83.68 \) s for the smooth interface approach are 1.8465 m² and 0.2359 m³, respectively and the corresponding sphericity \( \Psi = 0.9999 \). In both cases, the sphericity is very close to 1 confirming that the spherical shape of the bubble is retained by both approaches even at the coarsest grid.

The temperature distribution in the center plane obtained by the sharp interface approach is shown in Fig. 18. For both coarse and fine grids, the temperature distribution is radially symmetric. The temperature profile in the thermal boundary layer is not fully resolved for the coarse grid, which is indicated by the discontinuities in the temperature distribution near the interface region. However, these discontinuities are not present in the fine grid result indicating that the thermal boundary layer is fully resolved.

Similar observations can be made for the temperature distribution of the bubble growth obtained by the smooth interface approach (Fig. 19). However, an important difference in the temperature distribution obtained by the two approaches is that the bubble does not remain at the saturation temperature in the smooth interface approach. The bubble is at temperature \( T = 10.089 \) K and \( T = 10.012 \) K for the coarse and the fine grid, respectively. This (small) non-physical deviation in temperature occurs in the smooth interface approach due to the implicit forcing of the interface to the saturation temperature. As expected, this non-physical deviation is not observed in the results obtained by sharp interface approach. For further comparison, the temperature variation along radial direction \( t = 53.68 \) s obtained by both approaches for the coarsest and finest grid is shown in Fig. 20. It can be seen that both methods converge towards the analytical solution with grid refinement. Also, the non-physical deviation from saturation temperature in case of the smooth interface approach is clearly visible.

Finally, the velocity distribution in the center plane for the finest grid obtained by both approaches is shown in Fig. 21. Ideally, the vapor phase in the bubble should be at rest. However, a small vertical velocity field is observed in the results indicating the presence of parasitic currents. However, the magnitude of these currents is in the range of \( 10^{-6} \) m/s and, hence, does not affect the temperature field. In the velocity distribution corresponding to both approaches, a similar magnitude and pattern of parasitic currents is observed which is the expected behaviour since the surface tension term is treated in a similar manner in both approaches. This finding suggests that the parasitic currents are not influenced by how the temperature field is calculated.

4.4. Bubble rise with phase change

4.4.1. Problem definition

A 3D simulation of the rise and growth of a vapor bubble in superheated liquid under gravity is carried out. This test case serves as a validation case for both approaches. The hydrodynamic part of the current method has already been validated with the simulation of the rise of a bubble under gravity in isothermal conditions (Rajkotwala et al., 2018). The rise of the bubble with phase
change is more complicated as the vapor bubble not only rises due to buoyancy but at the same time expands due to boiling at its surface. The evolution of the growth of an ethanol bubble is calculated and compared to the experimental data of Florschuetz et al. (1969).

### 4.4.2. Problem setup

The simulation settings are taken from the study by Shin and Choi (2016). The thermodynamic properties of the working fluids, i.e. liquid ethanol and ethanol vapor, are selected at the system pressure of 101.3 kPa and are given in Table 2. The liquid superheat $\Delta T$ is set to 3.1 K. A spherical bubble of radius 210 $\mu$m is initialized in a $5 \times 5 \times 5$ mm$^3$ cubic domain. The initial position of the bubble is (2.5,2.5,3) mm; i.e. it is located along the central axis of the domain but at the height of 3 mm from the bottom face.

<table>
<thead>
<tr>
<th>Property</th>
<th>Gas</th>
<th>Liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>1.435</td>
<td>757.0</td>
</tr>
<tr>
<td>$\mu$ (Pas)</td>
<td>$1.04 \times 10^{-5}$</td>
<td>$4.29 \times 10^{-4}$</td>
</tr>
<tr>
<td>$k$ (W/mK)</td>
<td>0.020</td>
<td>0.154</td>
</tr>
<tr>
<td>$C_p$ (J/kgK)</td>
<td>1830</td>
<td>3000</td>
</tr>
<tr>
<td>$h_{fg}$ (J/kg)</td>
<td>$9.63 \times 10^5$</td>
<td>-</td>
</tr>
<tr>
<td>$\sigma$ (N/m)</td>
<td>0.018</td>
<td>-</td>
</tr>
<tr>
<td>$T_{sat}$ (K)</td>
<td>351.45</td>
<td>-</td>
</tr>
</tbody>
</table>

### Table 2
Ethanol vapor and liquid properties.
The temperature is initialized with the analytical solution for the zero gravity condition (Eq. (35)) corresponding to the initial bubble size. A moving window concept (Rajkotwala et al., 2018) is used in this simulation such that the bubble retains its initial position with respect to the domain. A free slip boundary condition is applied at the side walls and an outflow condition is applied at the remaining walls. The simulations are carried out for grid dimensions of 250 × 250 × 250 and 500 × 500 × 500 corresponding to a grid size of 20 and 10 μm, respectively.

4.4.3. Results and comparison

In Fig. 22, it can be seen that the bubble shape changes from spherical to ellipsoidal and bubble shape is well preserved by both approaches. As expected, a region of low superheat can be seen at the trailing edge of the bubble and the thermal boundary layer on the top and side of the bubble is thinner than at the bottom of the bubble. Also, a winding vortex can be seen at the side of the bubble.

The evolution of the non-dimensional bubble radius with time obtained by both approaches is compared to experimental data in Fig. 23. At a fine grid, the results obtained by both approaches agree well with the experimental data. At a given instant in time, the bubble radius obtained by the smooth interface approach is larger than in the sharp interface approach. This is because the temperature of the bubble is not maintained at the saturation temperature in case of the smooth interface approach. In the current case, it is lower than the saturation temperature giving rise to additional mass flux at the interface. Note that this is not apparent in Fig. 22(b) as the temperature range is modified to be same as Fig. 22(a).

5. Conclusion

In this paper, we have extended the Local Front Reconstruction Method to allow for phase transition using two different approaches to solve the energy equation. Both phases are assumed to be incompressible; however, the expansion due to phase change is incorporated by modifying the divergence-free velocity field condition at the interface. This modification requires the addition of a source term in the continuity equation which is related to mass flux generated due to phase transition. The derivation of this modified continuity equation was presented in Section 2.1.

The energy equation has been treated with two different approaches: the smooth interface approach and the sharp interface approach. The smooth interface approach uses a one fluid formulation to solve the energy equation with an interfacing source term accounting for phase change. In the smooth interface approach this interfacing source term is used to enforce the saturation temperature at the interface. In the sharp interface approach, the thermal properties are not volume-averaged near the interface, and the saturation temperature is imposed as a boundary condition at the interface. Thus, a different form of energy equation is required for both approaches as explained in Section 2.3. Based on a literature study and relevance of application of the method, we chose to keep the interface at saturation temperature and a model based on the energy jump condition at interface was selected.

Finally, both approaches were verified with two 1D phase change problems: the Stefan problem and the sucking interface problem. The obtained results closely agree with the analytical solution, and the error comparison showed the sharp interface method to be more accurate with a better order of convergence than the smooth interface approach. A 3D bubble growth in a superheated liquid under zero gravity was also simulated. The bubble growth rate agreed well with the analytical solution for both approaches upon grid convergence. A symmetric temperature distribution was seen during the whole simulation time, and the impact of the parasitic currents on the simulation was found to be negligible. However, a small unphysical rise in the temperature of the bubble was observed in the results of the smooth interface approach. This is an artifact of the implicit forcing of the saturation temperature at the interface and is a serious drawback of the smooth interface approach. In addition to the verification tests, a 3D validation simulation of the rise and growth of an ethanal vapor bubble in superheated liquid ethanol was carried out, and a good agreement was obtained between the calculations and experiment for the growth rate of the bubble.

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Supplementary material

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