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ABSTRACT

The use of computational fluid dynamics (CFD) tools is gaining popularity in the analysis of flow phenomenon in components used in air-conditioning and refrigeration systems. However, simulation of two phase (e.g., gas and liquid or oil and refrigerant) and phase changing (evaporation or condensation) flow is still unfeasible in many engineering problems. In this review, the development and status of direct numerical simulation of two-phase phase changing flow is discussed. The scope of this review is primarily focused on the boiling and evaporation methods that are most frequent in HVAC&R applications but generally relevant to all phase change simulations. The phase change method fundamentally depends on the properties and capabilities of its underlying multiphase methods and all studies of multiphase methods have been a naturally followed by their extension to phase change problems. Thus a comprehensive review on both multiphase and phase change numerical method is presented with a particular focus on the front capturing methods. Although developments of numerical methods for direct multiphase and phase change methods have shown promising results in solving simple phase change problems, applications to larger scale problems such as coiled tubes and heat exchangers unit still seems rough and has not been as successful. There are still major obstacles to overcome such as the mesh resolution requirement, higher order discretization schemes on unstructured grids, the nucleation sites, sharp interface properties and the associated accuracy and stability issue among others. Review of some large scale simulations and the underlying challenges are presented.

1. INTRODUCTION

The use of computational fluid dynamics (CFD) tools is gaining popularity in the analysis of flow phenomenon in components used in air-conditioning and refrigeration systems. They are used to study complex flows such as: air flow through slits in a fin, dehumidification on fin surface, refrigerant flow through smooth and enhanced tubes and flow through headers and tubes of a microchannel heat exchanger; to name a few. The analysis is further complicated by the flow being two phase (e.g., gas and liquid or oil and refrigerant) and changing phase (evaporation or condensation). For example, in a heat exchanger, there are both two-phase flow and phase changing process that occurs inside the header and the tubes. Often this causes mass flow rate and pressure mal-distribution along the tubes which results in degradation of the heat exchanger efficiency. Can we study such problem using CFD tools? What is the status of CFD development in simulation of such phase change problem?

Over the past few decades, study on the direct numerical methods for multiphase and phase change flow simulations have shown significant developments. They were widely used to study prototype problems such as droplets and thin film that can provide insights to the fundamental physics. Especially the front capturing methods simulations have shown promising results in solving phase change problems involving small number of droplets and simple flow conditions. Consequently application of these methods in the analysis of multiphase and phase change flow is also gaining attention in the air-conditioning and refrigeration research areas. However due to the inherent complexity of

multiphase and phase change problems, there exist no general method to implement using common CFD tools. There still exist gaps in both physical and numerical aspect that makes general and large scale application extremely difficult. In this paper, the development history and the current status of direct numerical simulation of multiphase, phase changing flow is reviewed and discussed. The reviewed literature is primarily focused on the boiling and evaporation methods that are most common in HVAC&R applications. However the numerical methods are generally relevant to all phase change simulations. The phase change method fundamentally depends on the properties and capability of its underlying multiphase methods and the developments of multiphase methods have been a naturally followed by their extension to phase change problems. Thus a background review on multiphase methods will be presented first followed by phase change methods. Then review of some large scale simulations and the underlying challenges are presented.

2. MULTIPHASE METHODS

In direct multiphase numerical methods, the interface between two different fluids should be recognized explicitly with sharp interfacial properties and should be free to move, deform, breakup and coalesce as how an actual interface would behave. The developments of various multiphase numerical methods have been driven by these principles and they are still the main challenges for direct multiphase methods.

Although small confusion exists between some literatures, the multiphase numerical methods can be conventionally classified into the Lagrangian type method, Eulerian type method and hybrid methods (G. Tryggvason *et al.* 2001). Examples of Lagrangian type methods are boundary element method and boundary-fitted gird method and for Eulerian type method, also called the front capturing methods (G. Tryggvason *et al.* 2001) include volume of fluid method (VOF), level-set method (LSM), cubic interpolated polynomial method (CIP) and phase field method. For hybrid method, one of the most famous is the front tracking method. The Lagrangian type methods involves grid that follows the fluid and the interface (Ryskin and Leal 2006) and the boundary-fitted grid method uses separate, boundary-fitted grids for each phase (Feng *et al.* 1994). Although these methods have potentially higher accuracy in terms of interfacial physics, their applications are extremely limited to simple cases such as single or a few droplets with minor deformation. Thus recent trend for multiphase flow is focused on the front tracking methods and the front capturing methods. The front tracking method, which became largely popular from the work of Tryggvason *et al.* is a combination of fixed grid method for the flow governing equations and Lagrangian moving grid that represents the interface. Impressive work has been demonstrated by the their group (Unverdi and Grétar Tryggvason 1992; A. Esmaeeli and Grétar Tryggvason 2004b). However, as the need and expectation to solve more complex and general problem increase, the simplicity and compatibility in implementation of the methods in common CFD schemes have become more important. The front capturing methods are generally the easiest to implement and interface topological changes are naturally taken care of. This literature review is directed towards the front capturing methods and its extension to phase change methods. In particular, VOF and LSM which is one of the most actively researched method for evaporation and boiling problems. In order to facilitate the discussion in phase change methods, some basics on these two methods are described. Readers interested in further details on the front tracking method and front capturing methods should refer to Tryggvason *et al.* (2001) and Osher and Fedkiw(2001).

2.1 Volume of fluid method

Volume of fluid method is the most well-known and widely used direct multiphase methods. This method uses the volume of fluid function or so-called the color function, C that represents the phase fraction. The volume of fluid function in the cells completely occupied by one phase is unity whereas in the cells completely occupied by the other phase is zero. The fluid interface location is thus interpreted somewhere in the cells with color function value between these limits and the function is semi-discontinuous over the interface. The volume of fluid method has the advantage of accurately solving the interface advection equation without compromising the mass balance. However the volume of fluid method has its difficulty in sharp interfacial shape and properties such as curvature. In order to draw the interface shape using volume of fluid function, piecewise constant schemes or piecewise linear schemes (Youngs 1982) are applied to track a linear surface and its orientation. However implementation of these schemes is complicated especially in three dimensional cases.

In volume of fluid method, the density and viscosity are assigned as

$$\rho(\boldsymbol{x},t) = \rho_l + (\rho_g - \rho_l)C$$
$$\mu(\boldsymbol{x},t) = \mu_l + (\mu_g - \mu_l)C.$$

The volume fraction is advected with the velocity field by,

$$\frac{\partial C}{\partial t} + \boldsymbol{u} \cdot \nabla C = 0$$

where $\boldsymbol{u}$ is the velocity vector.

2.2 Level Set Method

The level-set method is closely related to the volume of fluid method. The difference is that the function representing the interface in the level set method is a continuous level set function. Most common level set function is the distance function. In this case, each cell has a distance function with positive or negative sign representing two different phases or fluids and the magnitude is the equal to the distance to the closest interface. Thus the zero level set contour defines the location of the interface. The level set method has advantages and disadvantages compared with volume of fluid method. While the calculation of curvature and the sharp interface location is simple and natural, the advection of the level set function is prone to numerical error causing mass loss. Successful implementations of the level-set methods have been demonstrated, for instance, by Sussman *et al.*(1994) and Koren and Venis (1999).

The advection equation of the level-set function $\emptyset$ is given by,

$$\frac{\partial \emptyset}{\partial t} + \boldsymbol{u} \cdot \nabla \emptyset = 0.$$

Typically level-set needs to be reinitialized after few time steps using,

$$\emptyset_\tau + sign(\emptyset_0)(|\nabla \emptyset| - 1) = 0$$

where *sign* is the sign of the distance function, 0 is the original level set value and τ is an artificial time step to solve the PDE.

3. PHASE CHANGE METHODS

The development of multiphase numerical methods is naturally followed by the study of direct phase change problems and its methods. The phenomenon of boiling has very high efficiency in heat transfer and therefore it is commonly used in heat transfer processes. Thus, boiling is one of the most frequently studied problems in the field of direct multiphase phase change numerical method. Studies on other phase change phenomena such as condensation are based on similar model. Boiling from a heated solid surface involves natural convection, nucleate boiling, transitional boiling and film boiling. In order to accurately simulate these phenomena, the numerical method must generally include:

1. Accurate calculation of the heat flux across the interface driven by the difference in the temperature gradients.
2. Accurate calculation of the mass flux that results from the heat flux and the latent heat of evaporation at the saturation temperature.
3. The movement of the interface caused by both phase change and the fluid flow.
4. Stable and robust numerical method including phase change that can endure high property difference, high fluxes across sharp interface and large topological changes such as pinch-off and merging.

Based on these principles, numerous literatures have implemented and studied phase change methods and validated using prototype problems such as nucleate boiling and film boiling of single or a few bubbles.

3.1 Basics on the phase change model

When the phase change occurs, there are both mass transfer and heat transfer across the phase interface. The mass balance at the interface is given by (Oron *et al.* 1997)

$$j_m = \rho_g(\boldsymbol{u}_g - \boldsymbol{u}_i) \cdot \boldsymbol{n} = \rho_l(\boldsymbol{u}_l - \boldsymbol{u}_i) \cdot \boldsymbol{n},$$

which yields the velocity jump at the interface of

$$(\boldsymbol{u}_l - \boldsymbol{u}_i) \cdot \boldsymbol{n} = j_m \left(\frac{1}{\rho_l} - \frac{1}{\rho_g}\right),$$

where j_m is the mass flux per normal to the interface, $\boldsymbol{u}_l, \boldsymbol{u}_g, \boldsymbol{u}_i$ are the velocity vectors for liquid, gas and the interface and ρ_g, ρ_l are the density. The energy balance relation concerning only latent heat of phase change and heat conduction term gives the temperature gradient boundary condition for the interface as (Oron *et al.* 1997)

$$\left(-k_g \nabla T_g + k_l \nabla T_l\right) \cdot \boldsymbol{n} = j_m h,$$

where k_g, k_l, T_g, T_l are the thermal conductivity and the temperature field for each phase. The evaporation heat flux j_h at the interface can be given by a model such as (Tanasawa 1991) by to close the model.

$$j_h = \alpha(T_i - T_{sat})$$

$$\alpha = \frac{2\chi}{2 - \chi} \frac{h}{\sqrt{2\pi R}} \frac{\rho_g}{T_{sat}^{\frac{3}{2}}}$$

Here, α is the evaporation heat transfer coefficient, T_i is the temperature of the phase boundary, T_{sat} the saturation temperature, χ the evaporation coefficient, h the enthalpy of evaporation and R the gas constant for water. Note that the evaporation heat transfer coefficient may involves more complex factors that is not included in the above equation such as the effect of Laplace pressure caused by curved interface and Van der Waals forces between the solid and the liquid. Further interested readers can refer to the review article by Wayner (1999).

To implement these phase change effect, the mass flux can be added as a source term in the continuity equation in terms of heat flux and the latent heat of evaporation. It needs to be correctly applied in the spatial distribution near the interface such that it is positive on the gas phase and negative on the liquid phase. Juric and Tryggvason (1998) iteratively determined the velocity of the interface markers for the interface tracking method. For front capturing methods, Welch *et al.* (2000) and Tomar *et al.* (2005) implemented phase change by adding a mass source to the cell that is cut by the interface. Son *et al.* (1998), Luo *et al.* (2005) and Harts and Wondra (2008) have implemented a smeared-out heaviside function to avoid the instability related to the source term. In work by Gibou *et al.* (2007), they explicitly incorporate the velocity jump condition at the interface and derive the interfacial velocity field for the motion of interface instead from the mass conservation equation, giving sharp interfacial jump at the interface.

3.2 Lagrangian type method

The early research of multiphase and phase change simulation was led by class of Lagrangian type multiphase methods. This is primarily due to ease of sharp interface representation in the Lagrangian type methods. Welch *et al.* (1995) were one of first to apply direct numerical method in simulating phase change problem. They used Lagrangian moving triangular grids which coincide with the interface and used to explicitly track the bubble. Son and Dhir (1997) also used moving coordinate system to simulate film boiling for two-dimensional and axisymmetric flow. In these methods the discretization of the governing equations of mass, momentum and energy for each phase is straightforward by coupling with matching jump conditions at the interface. However it is clear from the literatures that Lagrangian type methods are essentially limited to modest deformation especially for the case of phase change where interface motion also includes expansion and contraction.

3.3 Front tracking method

In order to overcome the limitation of Lagrangian type methods described earlier, Juric and Tryggvason (1998) simulated two and three dimensional film boiling flow by developing a hybrid method which use regular grid for flow equation and moving gird for tracking the interface. Their method employs a single-field formulation which

consists of one set of conservation equations of mass, momentum, and energy with variable fluid properties, which is valid for the entire flow field. In the formulation, the jump conditions at the interface are implicitly imposed by the interfacial source terms added to the governing equations with delta functions. Delta function creates smoothed out the interfacial properties over several grid points and is non-zero only at the phase boundary. This representation of the continuous flow field is combined with the Lagrangian surface segments of the interface. Later Esmaeeli and Tryggvason (2004a) have extended the front-tracking method to film boiling on horizontal cylinders while Al-Rawahi and Tryggvason (2002) combined with an immersed-boundary method to account for the velocity boundary conditions on irregular solid surfaces. They also carried out simulation of formation of several bubbles over sufficiently long times to capture the release cycles and to evaluate the quasi steady-state Nusselt number (A. Esmaeeli and Grétar Tryggvason 2004b). Although Tryggvason and co-workers have demonstrated the departure process of a bubble during film boiling, generally the Lagrangian method is not straightforward to implement for the interface with change in topology. Although they have demonstrated simulation of large deformation and break-up, the mechanism of interface break-up in Lagrangian scheme is difficult in nature and has to be manipulated. Shin and Juric (2002) explained their model or the merging and breakup of interfaces by incorporating eliminating logical connectivity of the Lagrangian interface segments and using characteristic interface function simpler to that of front capturing method to construct the interface.

3.4 Front capturing method

As the effort for large topological changes in Lagrangian scheme hit its limit, many researchers have turned to the front capturing methods. Welch & Wilson (2000) implemented phase change scheme with VOF method based on the Young's enhancement for discontinuous interfacial properties and studied Stefan problem and two-dimensional film boiling problem. Son and Dhir (1998) modified the level-set method to include the liquid-vapor phase change and their study of axisymmetric single nucleate boiling found good agreement with experimental data on interface movement. In subsequent works, Welch and Rachidi (2002) developed a conjugate heat transfer model with the solid wall with the previous VOF method to simulate saturated horizontal film boiling which was then extended by Agarwal *et al.*(2004) to include variable thermal properties. Other research work has been done to improve the numerical simulation such as application of higher order scheme for projection method (Luo *et al.* 2005) and in sphericosymmetric geometry (Ghosh *et al.* 2006). In recent studies Can and Prosperetti (2012) used level-set method with a high-order ghost fluid method and simplified assumption of vapor phase having time-dependent, spatially uniform pressure acting on the interface.

As mentioned above the general front capturing method has the disadvantage of implicit representation of interface somewhere between fixed grid points. In many studies using front capturing method, the well-known Continuous Surface Force(CSF) model proposed by Brackbill *et al.*(1992) is used that spread the interface over a few computational cells (Samuel W.J. Welch and Wilson 2000; Tomar *et al.* 2005). Such feature is undesirable especially for phase change problems where mass and heat fluxes at the interface and the curvature property are of critical importance. In relatively latest studies, the ghost fluid method (Frederic Gibou *et al.* 2002; D. Q. Nguyen *et al.* 2001; M. Kang *et al.* 2000; Ronald P Fedkiw *et al.* 1999) has been widely applied as a remedy to the diffused interface issue. The level set method with ghost fluid approach for interfacial jump condition was first implemented for phase change problem by Nguyen *et al.* (2001) and then further developed by Gibou *et al.* (2007). Ghost fluid method utilizes artificial fluid cell which implicitly induces the proper jump condition along the interface. It has been shown to remove spurious oscillations and minimize numerical smearing normally induced by discontinuous interfacial properties such as pressure and velocity. However the introduction of velocity jump condition and interfacial velocity separate from fluid velocity has stability issue in its computation and some extrapolation techniques are required. The ghost fluid method has also been adapted to other numerical methods for multiphase and phase change simulation. For example Marianne *et al.* (2006) utilized variation of VOF method and ghost fluid method to induce sharp interface and compared with CSF model.

Another issue, particularly with the level set formulation, is that the total mass conservation is not satisfied in both level set advection and redistribution step. Several efforts have been reported to tackle this issue. Sussman *et al.* (1998) modified the level set formulation by introducing another iterative procedure for better mass conservation and Chang *et al.* (1996) proposed a correction to the level set function by a normal motion proportional to its local curvature and the deviation of the total mass. This correction procedure had to be stabilized by adding a certain constant and to be iterated by several steps. Subsequently, Son (2001) improved his previous phase change method to achieve mass conservation during the whole calculation procedure by adding volume-correction step.

Further efforts to enhance the mass conservation have been made by combining two front capturing methods. In order to incorporate advantages of both the volume of fluid method and level-set method, conservation of mass and accurate curvature property a coupled level-set and volume of fluid (CLSVOF) method was introduced by Bourlioux 1995) This method was further developed by Sussman and Puckett (2000) for computing incompressible two-phase flows. In this method, the interface is reconstructed from the volume of fluid function and the interface normal is evaluated from the smooth LS function. The reconstructed interface is used to calculate the fluid volume fluxes and to reinitialize the LS function for mass conservation. Tomar *et al.* (2005) utilized this method in the simulation of film boiling and bubble formation. They studied refrigerant R134a and the effect of saturation pressure and the superheat. Enright *et al.* (2002) came up with hybrid particle – level set method (HPLS) using Lagrangian particle and level set method to correct interface advection and conserve mass.

4. APPLICATIONS AND CHALLENGES

Even though the study of direct multiphase phase change method has shown significant progress and results over the past decade, the application of these methods has been limited largely to the scale of formation of a single or a few bubbles from thin film, prescribed nucleation sites or off the wall location. It is now possible to simulate a few hundred bubbles depending on the simplicity of the flow conditions and available computational resource(G. Tryggvason *et al.* 2005). However, they are still much simpler than common engineering problems often encountered in real world.

In engineering problems:

1) Nucleation sites and film boiling appear naturally and randomly.
2) Number and location of sites depend on the material properties, surface roughness and the operating conditions of the system.
3) Scale of bubble, droplet or film formation is typically very small compared to other length scales.
4) Contact angle and the slip condition on the surface have to be determined.

Numerically, the most obvious problem is that the large total mesh size forces trade-off between resolutions requirement for accuracy of the solution and computational time. There are numerous efforts devoted to develop techniques to overcome this problem such as adaptive grid meshing but they are not as much efficient to resolve the issue, especially in the case of phase change problems involving industrial case complexity. For general implementation, difficulty of implementing high order schemes such as the 5^{th} order WENO scheme in unstructured grid coordinate is another issue. Also, there are very little experimental data available to validate volume of fluid or level set simulation results for the direct multiphase phase change methods.

For industrial applications, CFD simulation requires a package consisting of pre-processing, solver and post-processing. Therefore as mentioned as earlier, numerical methods that are simple and more general are need for implementation in common CFD packages. This resulted in the VOF based implementation becoming the most popular in common CFD packages (e.g., ANSYS FLUENT, ANSYS CFX, CD-adapco STAR-CD, OpenCFD Ltd OpenFOAM). There are only a handful of studies using direct multiphase or phase change simulations on large scale application for example on tube or channel of length longer than a hundredth of it diameter or on a small heat exchanger component. Yang *et al.* (2008) simulated flow boiling of R141B in a horizontal coiled tube using the VOF multiphase flow model in commercial CFD software package FLUENT (Fluent Inc. 2006) with a user defined evaporation model. They have performed validation with corresponding experiments. However their total mesh of 118,800 hexahedral grids (in cross-section area, 135) is very rough compared to the simulations of prototype problems that has been used to as validation models for the numerical methods and is difficult to considered the accuracy. Chen Fang *et al.* (2010) implemented phase change model and a model for interphase mass transfer and capillary force in FLUENT to study the mechanism of vapor-venting heat exchangers. Again, the mesh resolution of 191,400 computation nodes is not large enough to capture accurate interfacial physics. Several other studies have been performed for large scale phase change simulation implemented in FLUENT. Sandra *et al.* (2009) who coupled FLUENT VOF method with in-house developed codes for the mass and energy transfer phenomena during flow boiling process to simulate the flow boiling process of a hydrocarbon feedstock in the tubes of a convection section heat exchanger of a steam cracker. Ye *et al.* (2011) studied the fluid flow and heat transfer in a plate-fin unit used for rapid heat storage/release by phase change material (PCM). They developed correlations and conducted to

validate with the experimental data. Wu *et al.* (2007) also used FLUENT with a phase-change model for the mass transfer to investigate the refrigerant flow boiling in a horizontal serpentine round tube. Srinivasan *et al.* (2010) simulated the immersion quench cooling process using the commercial code AVL-FIRE. Mass transfer effects are modeled based on different boiling modes such as film or nucleate boiling regime prevalent in the system.

In above simulations, many disregarded the accuracy of sharp interfacial properties. Implementation of phase change method in a CFD package with the detailed techniques reviewed earlier is not an easy task. Recently, efforts are increasing to apply advanced multiphase phase change methods. Nichita (2010) in his thesis implemented coupled level-set volume of fluid method in FLUENT with dynamic contact angle model to study static bubble, bubble rising in a stagnant liquid and boiling heat transfer. Kunkelmann and Stephan (2009) implemented and validated of a nucleate boiling model in the volume-of-fluid solver of OpenFOAM (OpenFOAM Foundation 2011), an open-source CFD package. Their implementation includes the contact line evaporation, which can typically not be resolved by the numerical grid, and the conjugate heat transfer between solid and fluid. For validation, the sucking interface problem and the growth of a spherical bubble have been simulated. In both studies, however, the application is yet limited to validation of the implementation using the prototype problems.

5. CONCLUSIONS

A comprehensive review on the development and status of direct numerical simulation of two-phase phase changing flow is discussed with the scope primarily focused on boiling and evaporation methods that are most common in HVAC&R applications. The review shows the trend of research in direct multiphase phase change simulations is evolving toward simple but effective and accurate representation of interfacial properties and motion.

Although developments of numerical methods for direct multiphase and phase change methods, especially the front capturing methods for CFD simulations have shown promising results in solving simple phase change problems, applications to common HVAC problems still needs much more study. There are still major obstacles to overcome such as the mesh resolution requirement, high order discretization schemes in unstructured grids, the nucleation sites, sharp interface properties and the associated accuracy and stability issue among others.

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