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BRIEF REVIEW OF LATEST DIRECT NUMERICAL SIMULATION ON POOL AND FILM BOILING

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Despite extensive research efforts, the mechanism of the nucleate boiling phenomena is still not clear. A direct numerical simulation of the boiling phenomena is one of the promising approaches in order to clarify its heat transfer characteristics and discuss their mechanism. Therefore, many DNS procedures have been developed based on recent highly advancing computer technologies. This brief review focuses on the state of the art in direct numerical simulation of the pool boiling phenomena over the past two decades. In this review, the fundamentals of the boiling phenomena and the bubble departure and micro-layer models are briefly introduced, and then the numerical procedures for tracking or capturing interface/surface shape such as the front tracking method, level set method, volume of fluid treatments, and other methods (Lattice Boltzmann method, phase-field method and so on) are briefly reviewed.

KEYWORDS : Nuclear Hydraulics, Pool Boiling, Numerical Simulation, Inter Face Tracking/Capturing, Phase Change Model

1. INTRODUCTION

The boiling process consists of two phase-change processes, which is to say the evaporation process from liquid to vapor on a superheated wall or the condensation process from vapor to liquid in subcooled water. It is well known that nucleate boiling shows extensive heat transfer performance compared to single-phase flow. Therefore, boiling heat transfer is widely used in the mechanical, chemical and nuclear engineering fields. In the nuclear engineering field, the designs and safety assurances regarding boiling light water reactors (BWR) and pressurized light water reactors (PWR) strongly depend on the boiling heat transfer characteristics.

Despite extensive research efforts, the mechanism of the nucleate boiling phenomena is still unclear and so without any empirical correlation its mechanistic model has not been developed. Since the spatial scales of boiling phenomena vary from the thermal motion at the molecular scale to the convective motion governed by the macroscopic scale in the bulk fluid, the scale of the phenomena of interest should be clear when developing a mechanistic boiling model. The nucleation process especially is considered in the molecular scale and the molecules' motions are very fast, thus the non-thermal equilibrium state must be very important in this time scale. From the bubble growth process associated with the convective motion point of view, it is considered this non-equilibrium process will not be important because the time scale is rather long compared to the nucleation. In this sense, this brief review focuses mostly on the thermal equilibrium processes of boiling phenomena: it means the nucleation theory can be applied to determine the size of vapor embryo, and then its growth, departure and condensation processes will be considered.

On the other hand, a direct numerical simulation (DNS) of the boiling phenomena is one of the promising approaches in order to clarify the heat transfer characteristics of boiling phenomena and discuss their mechanism. With the advances in recent years of high performance computational technology, several DNS procedures to solve the conservation equations of mass, momentum, and energy for liquid and vapor phases simultaneously when an interface is continuously evolving at and near a heated surface have been developed. The solutions provide not only detailed physics associated with the thermal and hydrodynamic processes, but also the shape of the evolving interface.

In this review, the fundamentals of boiling phenomena and the bubble departure conditions and micro-layer models are briefly introduced, and then the numerical procedures for tracking or capturing interface/surface shape such as the front tracking method, volume of fluid treatments, level set method, and other methods are briefly reviewed.

2. BOILING PHENOMENA

2.1 General Fundamentals

The boiling phenomenon is described before a brief summary of several important experimental and numerical publications on boiling heat transfer is given. This brief summary mainly contains the aspects of pool boiling heat transfer and does not claim to be a comprehensive summary of all important publications on boiling heat transfer.

Several review articles by Dhir [1] and Manglik [2] have been published on boiling heat transfer. These review articles comprehensively summarized the major research achievements for many aspects of boiling heat transfer. The heat transferred between a heated wall and a bulk liquid can be expressed by the product of the heat transfer coefficient h, the heat transfer area S and the wall superheat ($T_{wall} - T_{sat}$).

$$Q = hS(T_{wall} - T_{sat}) \quad (1)$$

In order to increase the amount of thermal energy transport, the most efficient way is to increase the heat transfer coefficient. In this sense, the boiling heat transfer has a much higher heat transfer coefficient than that of single phase flow.

Nukiyama [3] published the memorable paper and one of the most cited papers in boiling research. He plotted the heat transferred to boiling water over a wide range of wall superheats and established the boiling curve qualitatively. The boiling curve of Nukiyama still gives us an important understanding for all boiling research and helps to distinguish the different phenomena in pool boiling. Van Stralen and Cole [4] describe the following regimes:

- **Nucleate boiling at moderate heat flux:**

In this regime, isolated bubbles grow at and depart from the heating wall without interacting with each other. The heat transfer in this regime is characterized by comparably high heat transfer rates at a moderate wall superheat. This is due to the large amount of heat that can be stored in the vapor phase (as latent heat), not in the liquid, and the agitation of the liquid by the bubbles which positively affects the single phase heat transfer in the vicinity of the bubbles. The range of this regime is limited by the onset of nucleate boiling (ONB) at small wall superheats. Below a minimum wall superheat no vapor embryo will be generated at the nucleation sites of the heating wall. At higher wall superheats this regime is limited by the onset of interaction between the bubbles which results from an increasing density of active nucleation sites.

- **Nucleate boiling at high heat flux:**

At high heat fluxes, more nucleation sites become activated and the density of growing bubbles increases. In this regime, the heat transfer rate is higher than in the case of isolated nucleation bubbles. However, as a larger area of the heating wall is covered by vapor, which has an insulating effect because of lower thermal conductivity, the required wall superheat increases, resulting eventually in a decreasing heat transfer coefficient. It should be noted that the maximum heat transfer coefficient lies at lower wall superheats than the maximum of the heat flux.

- **Transition to film boiling:**

If the critical heat flux (CHF) is reached, more places on the heater surface become covered with vapor. Eventually, a stable vapor layer (film) can be formed which completely separates the heater surface from the liquid. If the heat flux is kept constant or slightly increased at this point, the transition to a complete vapor film happens very quickly and the wall temperature jumps to a much higher value. If the local temperature of the heater is controlled rapidly and with high accuracy, a transition from a partial to a complete vapor film can be observed and results in a decreasing heat flux. A similar transition in the opposite direction can be observed when the heat flux or the temperature is decreased. If the heat flux is controlled the vapor film suddenly collapses and the wall superheat drops. If the wall temperature is controlled, the vapor film breaks up at many places as the temperature decreases resulting in an increasing heat flux.

- **Stable film boiling:**

As indicated by the name, this regime is characterized by a stable vapor film that separates the liquid phase from the heating wall. If the liquid-vapor interface approaches the wall, vapor generation is intensified and pushes the interface away from the wall until a stable position is reached. In this regime, droplets bounce off or hover above the heating wall without wetting it, i.e., so-called Leidenfrost effect.

2.2 Current Interests

One of the most important achievements of the experimental and numerical studies is the identification of the boiling heat transfer mechanisms. Although the transient heat transfer during boiling is still not fully understood, a very important contribution that distinguished different heat transfer mechanisms in the regime of nucleate pool boiling was discussed by Han and Griffith [5, 6]. There are two mechanisms of heat transfer during nucleate boiling: 1) the bulk convective heat transfer described that the superheated liquid entrained from the wall into the bulk liquid at each bubble departure and 2) a microlayer underneath the bubble was discussed by Cooper and Lloyd [7]. The microlayer is characterized by a very thin liquid film which has extensively high heat transfer rates. Recently, high tempo-spatial resolution experiments and numerical simulations have provided more detailed insights into the boiling process. Based on these results, Stephan and Kern [8] as well as Kim [9] describe the following mechanisms for the transport of heat from the wall into the fluid.

- **Enhanced convection:**

The liquid motion in the vicinity of a growing, departing, or rising bubble is induced by the bubble dynamics and enhances convective heat transfer rather than pure natural convection.

- **Transient conduction:**

During bubble growth, the superheated liquid layer becomes thinner due to a phase change. During the bubble departure regime, the superheated liquid layer is restored by conductive heat transfer from the heater into the liquid.

- **Microscale heat transfer at three-phase contact line:**

At the three-phase contact line, the heat transfer is almost governed by one-dimensional heat conduction through a very thin liquid film (the thickness is sub-micrometers) in which intermolecular forces become very important. In spite of the different conclusions on the importance of contact line heat transfer, Stephan and Kern [8] and Kim [9] report that the contact line heat transfer can make up to 20 to 30 % of the total heat consumed by a vapor bubble.

3. NUMERICAL SIMULATIONS

A direct numerical simulation (DNS) of the boiling phenomena is one of the promising approaches in order to clarify the heat transfer characteristics of boiling phenomena and discuss their mechanism. With the advances in recent years of high performance computational technology, several DNS procedures to solve the conservation equations of mass, momentum, and energy for liquid and vapor phases simultaneously when an interface is continuously evolving at and near a heated surface have been developed. The solutions provide not only detailed physics associated with thermal and hydrodynamic processes, but also the shape of the evolving interface.

Much of the numerical investigation focuses on either nucleate boiling at moderate heat flux (isolated bubbles) or stable film boiling. One of the key problems is the numerical description of two phase flow. Typically, there are several methods which are used for the simulation of boiling heat transfer.

- **Marker and Cell (MAC) method** [10] :

The interface is marked by many massless particles that are convectively transported with the Eulerian velocity field and can be used to reconstruct the interface position on a fixed mesh. However, it is sometimes difficult to determine the interface position precisely from the scattered particles after transporting the interface. As far as the author knows, the first boiling simulation based on the MAC method was done by Madhaven et al. in 1970. [11]

- **Front tracking (FT) method** [12]:

This method seems to be an advanced version of the MAC method, and is thus based on massless particles that follow the motion of the interface driven by the Eulerian velocity fields. The interfaceis tracked by a Lagrangian frame, and the interface position can be tracked precisely, but it is necessary to introduce some artificial rules to treat the break-up interface and also coalescence of interfaces during computation.

The original FT method has been further developed by Tryggvason and co-workers [12, 13] who applied it to the simulation of boiling flows [14, 15, 16, 17]. The method is very accurate in particular in terms of curvature calculation which is important for the simulation of very small bubbles. Tryggvason and co-workers used the model mainly for the simulation of film boiling [14]. Microscale heat transfer at the 3-phase contact line and the transient heat conduction in the solid wall are not taken into account.

- **Arbitrary Lagrangian-Eulerian (ALE) method** [47]:

This is based on a dynamic mesh that follows the motion of the interface. Thus, the interface coincides with a boundary of the computational domain at all times. According to this feature, the center of the control volume often may not coincide with the center of mass, and eventually the introduction of large artificial viscosity will be inevitable. If the boundary-fitted coordinate (BFC) system is used as the Eulerian frame for each velocity field, the precise interface can be represented. In this case, a re-meshing procedure is often required to fit the BFC of each phase to the phase interface; this procedure is quite a time consuming process for computation. Ramaswamy [98] firstly developed the ALE method coupling with FEM (Finite Element Method) and conducted the bubble growth and departure process including the contact angle evolution.

The latest ALE method is used by Fuchs [18] who simulated the transient heat transfer during pool boiling of binary mixtures. The work of Fuchs is based on the work of Kern and Stephan [19, 20] who calculated the quasi-steady heat flow at a growing bubble using a boundary-fitted mesh. An important advantage of the ALE method and boundary-fitted meshes in general is the possibility of treating the liquid-vapor interface as a boundary of the computational domain. This facilitates the calculation of the heat flux at the interface and therefore of the evaporation rate. Welch [21, 22] also used a numerical method very similar to ALE to simulate two-phase flows with phase change. However, microscale heat transfer at the three-phase contact line was not taken into account in its model.

- **Level-Set (LS) method** [23]:

This method uses a field that contains information about the distance of a numerical cell to the interface and which is convectively transported with the Eulerian velocity fields. The interface is represented by the zero-contour line of the level-set field. The criticism regarding LS method is a transport feature of the distance function because the distance is not a measure of physical property.

The LS method was used by Dhir and co-workers for various boiling configurations (a review of the advances was given by Dhir [24]). Already in the late 1990s, Son et al. [25, 26] numerically investigated film boiling and then Son et al. [27] investigated the heat transfer associated with a single bubble during nucleate pool boiling. Moreover, the bubble mergers [28], flow boiling [29], the effect of contact angle dynamics [30], film boiling on horizontal cylinders [31] and subcooled pool boiling [32, 33] were investigated. The model took the microscale heat and fluid flow at the 3-phase contact line into account. However, the transient heat conduction inside the solid wall was not modeled and the wall was also typically set to be a constant and uniform temperature. Recent works have been reported: [34~44]. Moreover, another version of the Level-set method was also developed [45, 46].

- **Volume-of-Fluid (VOF) method** [48]:

The most popular volume capturing procedure is based on the following transport equation of VOF (Volume of Fluid):

$$\frac{\partial F}{\partial t} + \mathbf{u} \cdot \nabla F = 0 \tag{2}$$

Here, F denotes the fraction of liquid or gas phase in the computational cell. $\mathbf{u}$ is the velocity vector. This uses a field that contains information about the volume fraction of one of the phases in a numerical cell and which is convectively transported with the Eulerian velocity fields. The volume fraction field has a piece-wise value at the position of the interface. There are some problems with the VOF method, such as the interface reconstruction between neighborhood cells and the precise calculation of interface curvature.

The VOF method is categorized into two methods depending on whether interface reconstruction is required: 1) no interface reconstruction methods such as SOLA-VOF [48] (based on a Donor-Acceptor method), FCT-VOF [49]. and CICSAM (Compressive Interface Capturing Scheme for Arbitrary Meshes) [50], 2) interface reconstruction methods such as SLIC (Simple Line Interface Calculation) [51] and PLIC (Piecewise Linear Interface Calculation) [52]. The PLIC method generally gives a highly accuracy solution with requiring some geometric calculation [53]. The typical procedure of using PLIC is as follows: 1) Calculation of the interface slope or the normal vector of it, 2) Reconstruction of the interface while maintaining the interface continuity, 3) Transport of VOF. Moreover, several procedures have been proposed, such as the simple calculation of the interface slope [54] and LVIRA (Least Square Volume-of-fluid Interface Reconstruction Algorithm) [55] as a second-order procedure. As for the interface reconstruction method, the Newton-Rapthon method is often used as an iteration procedure for interface reconstruction but a faster method has also been proposed [56]. Regarding VOF transport, the operator-splitting method and multi-dimensional method are often used. More accurate procedures such as the Stream method [57] and GPCA (Geometrical Predictor-corrector Advection) [58] have been proposed. However, the advance procedure of VOF transport with high accuracy seems to not work well. Procedures based on PLIC have been proposed such as MARS (Multi-interface Advection and Reconstruction Solver) [59], the unstructured grid version [60], CLSVOF (Coupled Level-set and Volume-Of-Fluid) [61] based on the combination of PLIC and Level-set methods [62], and so on.

The well-known problem of the VOF procedures is how to remove or suppress the "Spurious Velocity" caused by the surface tension calculation; many studies have been conducted on this problem. Since most VOF procedures based on the CSF (Continuum Surface Force) [63] do not show high accuracy of the curvature calculation by using the VOF values in the neighboring cells, more accurate methods have been proposed to strongly suppress the spurious velocity such as the method by using the estimator function [64] and the second order approximation of the local interface shape, PROST (Parabolic Reconstruction of Surface Tension) [65]. Recently, RDF (Reconstructed Distance Function) [66], based on the reconstruction of the distance function for the curvature calculation, was proposed. To suppress the spurious velocity, in addition to the development of the highly accurate curvature calculation procedure, the forces between the pressure and the surface tension at the interface cell must be satisfied, so Francois et al. developed the very effective procedure named "Balanced-force Algorithm" [67].

The VOF method has been used for the simulation of boiling flows so far. Welch and Wilson [68] implemented a model for phase change in a VOF method and simulated 1D test cases and film boiling. Welch and Rachidi [69] extended the model by the transient heat conduction in the solid wall and simulated film boiling. Aus der Wiesche [70] used the VOF method to simulate nucleate pool boiling of water. Recently, Hardt and Wondra [71] proposed a method for implementing phase change in a VOF or LS approach and performed simulations of film boiling and droplet evaporation using a VOF method. Kunugi [72] conducted the subcooled pool and flow boiling problem by MARS and Ose and Kunugi [73, 74] conducted the subcooled pool boiling simulation and validated the numerical results by their visualization experimental data aided by the ultra-high tempo-spatial resolution video camera system [75]. Some recent works on boiling simulation based on the VOF methods have been reported [76~79] and results using the commercial code have also been reported [80, 81, 82]. However, none of the aforementioned models based on the VOF method include any sub-model for evaporation at the 3-phase contact line. In this sense, Kunkelmann [83] implemented the VOF solver of the open-source CFD package OpenFOAM [84] which solves incompressible two-phase flow problems. Detailed information on the numerical method can be found in [85

~87]. The model takes into account the microscale heat transfer at the 3-phase contact line and the conjugate heat transfer between solid and fluid. Kunkelmann performed 2D simulations [83]. Recently, Kunkelmann et al. [87] states that the extension of the model to 3D simulations was straightforward, and the calculation of the local evaporation rate and the local coupling between LS and VOF have been implemented for unstructured meshes [88].

In addition to the aforementioned methods, the Lattice Boltzmann Method (e.g. Hazi and Markus [89] and Succi [90]) and the Phase Field Method (e.g. Jamet and co-workers [91]) which is often called as the Diffuse Interface Method because of no physical basis regarding the potential function, have to some extent been used for the simulation of boiling flows [92~94]. Cellular automata [95] was also tried to apply to the boiling problem. However, these methods still seem to be strongly limited to very fundamental research. Moreover, Koshizuka et al. [96] developed the moving-particle semi-implicit (MPS) method which was a macroscopic, deterministic particle method (Lagrangian mesh-free method) and was applied to nucleate pool boiling [97].

4. SUMMARY

The numerical modeling of boiling phenomena has progressed tremendously within the last decades. Nevertheless, each of the models mentioned above has several shortcomings which restricted its use to a specific boiling configuration. In particular, the simulation of boiling in complex geometries has been beyond the research of these models In this sense, 3D simulations that definitely require adaptive mesh refinement at the liquid-vapor interface in order to keep the computational cost at a reasonable level would be strongly required. Although the use of unstructured meshes could be required depending on the complexity of the geometry, the accuracy of the numerical solutions by using the unstructured mesh system must be carefully discussed.

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