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Brief communication

Direct three-dimensional numerical simulation of nucleate boiling using the level contour reconstruction method

Seungwon Shin [a,*], S.I. Abdel-Khalik [a], Damir Juric [b]

[a] George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, 801 Ferst Drive, N.W., Atlanta, GA 30332-0405, USA
[b] LIMSI-CNRS, BP 133, 91403 Orsay Cedex, France

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1. Introduction

The nucleate boiling process is known to be a very efficient mode of heat transfer. It is desirable to operate many engineering applications in this mode since high heat transfer rates and convection coefficients are associated with small values of the excess temperature. Despite its importance, nucleate boiling has not been fully numerically simulated until very recently because of the complexity of dealing with the phase change problem in addition to the interface method itself. Here we perform a full direct numerical simulation of nucleate boiling in a fully three-dimensional geometry using the Level Contour Reconstruction Method (Shin and Juric, 2002). Our work is aimed at predicting nucleate boiling heat flux values more accurately on a real surface by including the effect of nucleation site density in the numerical model. This has been achieved by changing the surface area for a single nucleate bubble corresponding to the wall temperature.

A large body of research in nucleate boiling deals with developing experimental correlations for heat transfer during the nucleate boiling process. Here we briefly review some of the heat transfer correlations developed for wall heat transfer in nucleate boiling. Tien (1962) obtained a

* Corresponding author. Tel.: +1 404 385 4364; fax: +1 404 894 8496.
E-mail address: seungwon.shin@me.gatech.edu (S. Shin).

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correlation using a hydrodynamic model of stagnation flow for saturated nucleate boiling on a flat surface. He found a heat transfer correlation through established analytical results in axisymmetric stagnation flow. His correlation is found to be in good agreement with measured data in the low heat flux region. Hara (1963) assumed that the heat flux is equal to the heat transferred from the surface to the liquid by conduction and the latent heat carried away by the bubble and found a correlation which is in fairly good agreement with experimental data. Mikic and Rohsenow (1969) included a more detailed mechanism such as the number of active nucleation sites, bubble departure diameter, frequency of bubble departure and natural convection effects in deriving their heat transfer correlation. Their correlation is also based on the idea that a departing bubble will remove heat from the heated surface by the action of a vortex ring created in its wake. Stephan and Abdelsalam (1980) used regression methods to correlate nearly 5000 existing experimental data points for nucleate boiling. Their correlation is valid for a wide variety of substances and geometries with fairly good accuracy. Kocamustafaogullari and Ishii (1983) found a constitutive relation for active nucleation site density for nucleate boiling which is in relatively good agreement with direct measurements available in the literature. They also showed a functional relationship between the heat transfer coefficient and other basic parameters. Recently, Sakashita and Kumada (2000) proposed a correlation for nucleate boiling consisting of heat flux, superheat, density of nucleation sites, and a group of physical parameters. In their model heat transfer by conduction in a thin surface layer is the primary heat transfer mechanism.

Phase change flows are among the most difficult challenges for direct numerical simulation especially for nucleate boiling due to the complexity in dealing with, among other physical phenomena, the wall contact problem. In addition to this they pose severe numerical challenges for interface methods since the complete phase change problem is highly dependent on the simultaneous coupling of unsteady mass, momentum and energy transport with the interfacial physics of surface tension, latent heat, interphase mass transfer, discontinuous material properties and complicated liquid–vapor interface dynamics.

Lee and Nydahl (1989) applied the axisymmetric Navier–Stokes and energy equations to model a boiling bubble in saturated nucleate pool boiling on a horizontal surface. They used a complex mapping of an interface to a plane where the bubble and wall boundaries lay along the constant coordinate lines. Although they accounted for the flow and temperature fields by solving the momentum and energy equations in the liquid, they had to assume that the bubble remained hemispherical in shape during its growth. They also included a microlayer evaporation effect which depended on an ad hoc determination of a microlayer thickness to match the predicted bubble growth with the experimental data reported in the literature.

Welch (1995) simulated a fully deformable, two-dimensional bubble using moving triangular grids. He used a semi-implicit finite volume moving mesh to capture the interface. He only considered small distortions of the interface because he had to use a dynamically restructured grid to simulate the deformable interfacial motion. He calculated bubble growth in nucleate boiling to show the capability of tracking the interface but could not simulate the full boiling cycle because the method was not capable of handling complex topology change.

A more complete direct numerical simulation of nucleate boiling was performed by Son et al. (1999). They solved the equations governing conservation of mass, momentum and energy in the vapor and liquid phases. The vapor–liquid interface is captured by a level set method which can handle breaking and merging of the interface automatically. In analyzing the growth of a single

bubble, they divided the computational domain into micro and macro regions. The micro region contains the thin film that forms underneath the bubble whereas the macro region consists of the bubble and the liquid surrounding the bubble. They also assume axisymmetric and laminar flow, and constant properties in each phase. They derived the governing equation of microlayer thickness based on the radial location of the vapor–liquid interface which was obtained from the macro region and the lubrication theory developed by Wayner (1992) and Lay and Dhir (1995). They solve the macro region with proper boundary conditions and include a microlayer evaporation effect. They found that bubble growth predicted from their numerical analysis compared well with experimental data. But they still could not obtain a proper relation between heat flux and wall superheat. Their value was too small compared with experimental values because the number density of active nucleation sites strongly depends on the wall superheat which they did not include.

Most recently, Yoon et al. (2001) simulated a single bubble in both isothermal and nucleate pool boiling using a mesh-free numerical method (MPS-MAFL). This method is based on a particle method (MPS) which is combined with a gridless method (MAFL) for an arbitrary-Lagrangian–Eulerian calculation. All the calculations are carried out in two-dimensional coordinates except for the heat transfer estimation where they compute the liquid volume assuming an axisymmetric condition. They compare bubble growth rates in fairly good agreement with experiments but their heat transfer rate calculation is somewhat over-approximated and heavily dependent on experimental constants. They also calculate one cycle of bubble evolution but in reality since partial nucleate boiling is a cyclic process the computation should be carried out over several cycles to reach steady behavior from cycle to cycle.

Clearly, progress has been made in developing numerical methods for two-dimensional flows with deformable interfaces. However, many difficulties still remain in problems which require the direct simulation of three-dimensional multifluid flows including interface merging/breakup and phase change. In this work we perform a full direct numerical simulation in three-dimensional geometry using the state-of-the-art Level Contour Reconstruction Method (Shin and Juric, 2002; Shin et al., 2005). Our work here is explicitly aimed at predicting nucleate boiling heat flux values for a given wall temperature more accurately in three-dimensional space by including the effect of nucleate site density in the numerical model. In the next section we provide the direct simulation results and comparison to experimental correlation.

2. Results and discussion

The pertinent governing equations (see Shin and Juric, 2002 for the full description of the mathematical formulation) and boundary conditions can be made dimensionless by defining scales of length $l_0 = (\sigma/g(\rho_L - \rho_G))^{1/2}$ velocity $U_0 = (gl_0)^{1/2}$ temperature $\rho_G L_0/\rho_L c_L$ (measured from T_{sat}), and pressure $\rho_L U_0^2$ (measured from the reference ambient system pressure P_∞). The problem can then be characterized by the Reynolds, *Re*, Peclet, *Pe*, Jakob, *Ja* and Weber, *We*, numbers as well as the property ratios

$$Re = \frac{\rho_L U_0 l_0}{\mu_L}, \quad We = \frac{\rho_L U_0^2 l_0}{\sigma}, \quad Pe = \frac{k_L}{\rho_L c_L U_0 l_0}, \quad Ja = \frac{T_{sat} c_L}{L_0} \tag{1}$$

$$\frac{\rho_G}{\rho_L} = \rho^*, \quad \frac{k_G}{k_L} = k^*, \quad \frac{\mu_G}{\mu_L} = \mu^*, \quad \frac{c_G}{c_L} = c^* \tag{2}$$

Here σ is the surface tension, g is gravity, ρ is density, μ is viscosity, k is thermal conductivity, c is specific heat, T is temperature and L_0 is the latent heat.

The Level Contour Reconstruction Method (Shin and Juric, 2002) is a simplified front tracking method based on the method described in Unverdi and Tryggvason (1992) and Tryggvason et al. (2001) that eliminates logical connectivity and thus eliminates all of the associated algorithmic burden but retains the accuracy and advantages of explicit Lagrangian surface tracking. A primary advantage of this method is the ability to naturally and automatically handle interface merging and breakup in 3D flows.

As opposed to film boiling, nucleate boiling exhibits the formation of individual bubbles at the heated wall and thus also direct liquid contact with the heated wall. The detailed physics of this contact region regarding contact line motion is poorly understood and thus poses formidable difficulties in numerical simulations.

There have been many investigations supposing a thin liquid film in the contact region which have produced models for microlayer evaporation and contact line dynamics, in particular the work of Son et al. (1999). There they coupled a separate microlayer equation, including various surface physics such as capillary, disjoining, and recoil pressure effects, with the macro governing equations. In their simulation, the contact line moves with fixed angle but the hysteresis of the contact angle as is found on real surfaces was not yet modeled. They found that the microlayer contributes about 20% to the total heat flux. They also found that the bubble growth period and departure size increase with increasing contact angle. The resulting Nusselt numbers and heat fluxes varied as $\Delta T^{0.4}$ and $\Delta T^{1.4}$, respectively. These values were too small compared to existing experimental values since a real surface has various size cavities where heat transfer depends strongly on the wall superheat. In their numerical experiment, they study the single bubble ebullition cycle within a relatively large computational domain without considering the effect of neighboring bubbles. They discussed the fact that the effect of cavity number density should be included in the numerical model in order to obtain more realistic data.

In nucleate boiling, bubbles trapped in cavities as nuclei grow to a certain size and depart from the heated surface. After bubble departure a certain time is needed to form a new bubble on the same active site. The location of nucleation is randomly distributed throughout the heated plate and the number density of nucleation, which is one of the most important parameters affecting the heat transfer in the boiling process, increases with wall superheat. We take into account the effect of the nucleation site density by changing the domain size of the simulation with proper boundary conditions in a horizontally periodic 3D domain. By decreasing the domain size, the bubble will be affected more closely by the boundary, in essence the neighboring bubbles, in the periodic simulation domain.

In our simulation, we neglect microlayer evaporation and contact line dynamics beneath the bubble even though this will influence the growth rate and heat transfer relation. We simply model the contact region as fixed in space. This is a crude approximation but could be applicable to certain cases where nucleation starts from a fixed cavity of a given size. We also assumed constant temperature of the heated surface.

Kocamustafaogullari and Ishii (1983) found a correlation between wall superheat and nucleation site density, N_{pn} [1/m^2], for water boiling on a variety of surfaces at pressures varying from 1 to 198 atm as

$$N^*_{\mathrm{pn}} = f(\rho^{\mathrm{R}}) R^{*-4.4}_{\mathrm{c}} \tag{3}$$

where

$$N^*_{\mathrm{pn}} = N_{\mathrm{pn}} D^2_{\mathrm{d}}, \quad R^*_{\mathrm{c}} = \frac{R_{\mathrm{c}}}{(D_{\mathrm{d}}/2)} \tag{4}$$

and

$$f(\rho^{\mathrm{R}}) = 2.157 \times 10^{-7} \rho^{\mathrm{R}^{-3.2}} (1 + 0.0049\rho^{\mathrm{R}})^{4.13} \tag{5}$$

The parameters D_{d}, R_{c}, and ρ^{R} are defined as

$$D_{\mathrm{d}} = 0.0012(\rho^{\mathrm{R}})^{0.9} \left(0.0208\phi \sqrt{\frac{\sigma}{g(\rho_{\mathrm{L}} - \rho_{\mathrm{G}})}} \right) \tag{6}$$

$$R_{\mathrm{c}} = \frac{2\sigma[1 + (\rho_{\mathrm{G}}/\rho_{\mathrm{L}})]/P_{\mathrm{L}}}{\exp[L_0 \Delta T_{\mathrm{sat}}/(R T_{\mathrm{w}} T_{\mathrm{sat}})] - 1} \tag{7}$$

$$\rho^{\mathrm{R}} = \frac{\rho_{\mathrm{L}} - \rho_{\mathrm{G}}}{\rho_{\mathrm{G}}} \tag{8}$$

where ϕ is the contact angle measured in degrees.

We have chosen to use the properties of water at atmosphere conditions thus our simulation parameters will be

$$\rho_{\mathrm{G}}/\rho_{\mathrm{L}} = 0.0006237, \quad \mu_{\mathrm{G}}/\mu_{\mathrm{L}} = 0.04353, \quad k_{\mathrm{G}}/k_{\mathrm{L}} = 0.03694, \quad c_{\mathrm{G}}/c_{\mathrm{L}} = 0.4847,$$
$$Re = 1334.2, \quad We = 1.0, \quad Pe = 0.0004268, \quad Ja = 0.6972$$

Tabulated in Table 1 are our simulation box sizes for each of three non-dimensional wall superheats, 15, 18, and 21 according to relation (3). The simulation box size of y in 2D or z in 3D has been taken sufficiently large to minimize the effect of the top boundary on the solution.

Fig. 1 describes the simulation geometry for both 2D and 3D cases. The computations are performed in a horizontally periodic domain. To allow vaporization, fluid is allowed to exit at the top boundary where the pressure is specified to be zero. The temperature field is initially zero everywhere with a constant temperature applied to the rigid bottom wall where a no-slip velocity boundary condition has been used. The hemispherical cap shaped initial seed bubble has been placed at the center of the bottom wall. The size of the initial nucleus should be big enough to initiate the boiling process so we have chosen the size of the initial nucleus as the approximate size of the departing bubble diameter. Fritz (1935) proposed an empirical relation for the departing bubble diameter as

Table 1
Box size and resolution for different wall superheat in simulation of nucleate boiling on a heated horizontal surface

T^*_{w}	$L^*_x \times L^*_y \times L^*_z$ (non-dimensional box size)	Resolution
15	$6.44 \times 6.44 \times 5.6$	$46 \times 46 \times 40$
18	$4.20 \times 4.20 \times 5.6$	$30 \times 30 \times 40$
21	$3.08 \times 3.08 \times 5.6$	$22 \times 22 \times 40$

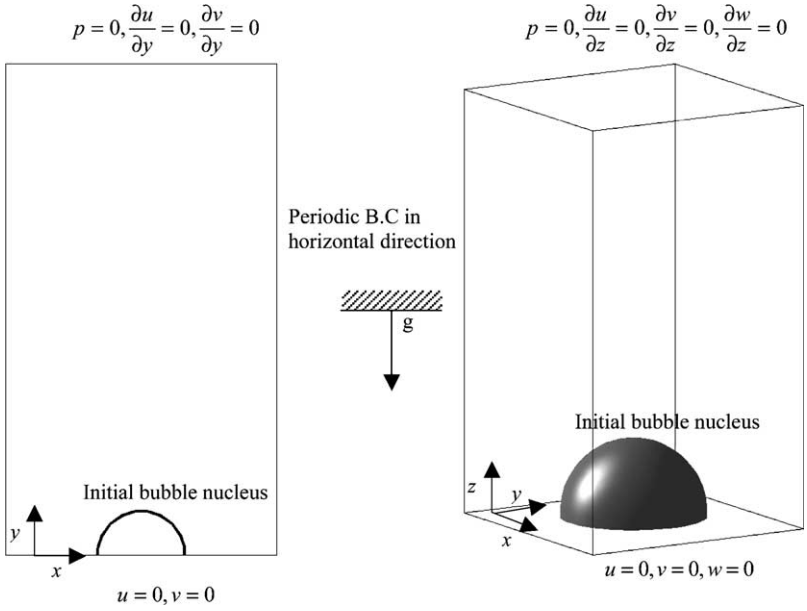

Fig. 1. Simulation geometry for 2D and 3D cases.

$$D_{\text{depart}} = 0.0208\phi\sqrt{\frac{\sigma}{g(\rho_{\text{L}} - \rho_{\text{G}})}} \tag{9}$$

by balancing buoyancy with the surface tension force acting on a static bubble. This bubble diameter can represent the appropriate length scale for the boiling process. Based on the assumption of a fixed contact line, we take the contact angle as 90° and this will lead us to the value of 1.0 as the radius of the initial seed bubble. For the 2D case, we used a radius of 0.5 to match the area ratio of the 3D simulation with non-dimensional wall superheat temperature of 21.

Before moving on to the three-dimensional simulations, we first tested our code with different grid resolutions for a two-dimensional case. From Fig. 2, we used the non-dimensional wall superheat of 21 as our test case and we can see that the interface converges with increasing resolution and the solution is almost converged at a grid resolution of 22×40.

We plot the Nusselt number along with time with non-dimensional wall superheat of 21 in Fig. 3(a). The Nusselt number is averaged over the bottom surface and we will denote this as *Nu*. As the boiling process is cyclic, we also averaged the Nusselt number, *Nu*, over one cyclic interval to get a cyclic averaged Nusselt number, Nu_{cyc}. To allow for a cyclic process the detached bubble is allowed to leave through the top boundary. The first cycle duration is calculated as the time taken between the arrival of the first and second bubbles at the top boundary and same procedure applied for next cycle. We also placed a line indicating the start and end points of each cycle in Fig. 3. As can be seen in Fig. 3(b), the Nusselt number is almost constant after the first cycle and is also converged at about a grid resolution of 22×40 (Fig. 2(b)).

We now turn to 3D simulations of nucleate boiling on a horizontal surface. The computations are performed in a horizontally periodic hexahedral domain as discussed in Fig. 1. Here again the fluid is also allowed to exit the top boundary where the pressure is set to zero. We plot the

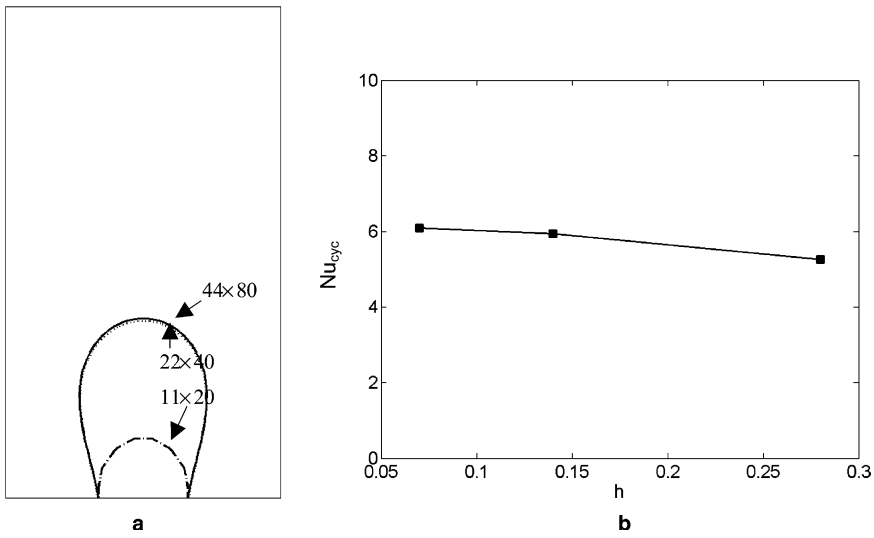

Fig. 2. Grid resolution test for a 2D nucleate boiling simulation with wall superheat temperature of 21. (a) Interface at each grid resolution has been plotted. Interface is almost converged at 22×40 resolution. (b) Space and cyclic averaged Nusselt number vs cell size. Even at a low resolution of 22×40 the difference in Nusselt number is small.

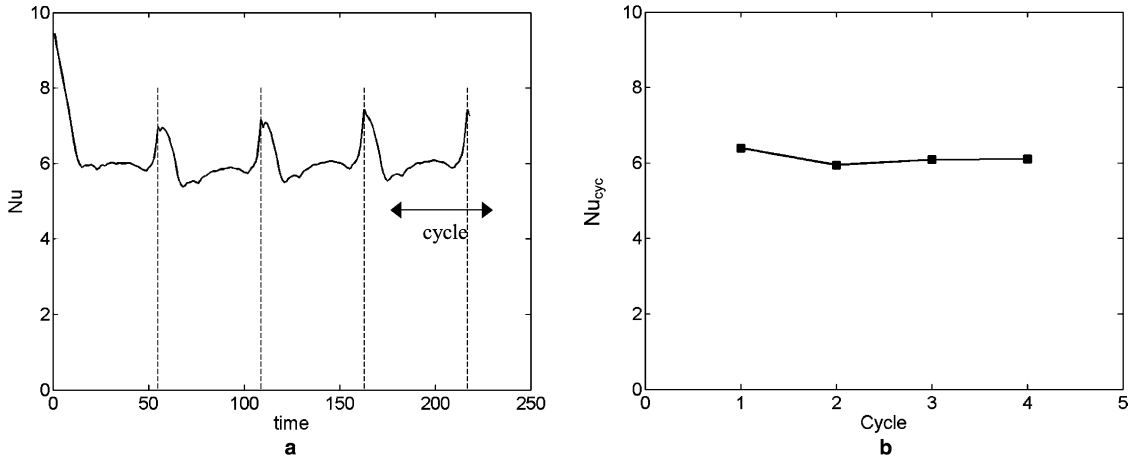

Fig. 3. Space and time averaged Nusselt number. The Nusselt number coefficient is almost constant after the first cycle.

interface evolution during 3D nucleate boiling with non-dimensional wall superheat temperature, $T_w^* = 21.0$ in Fig. 4. A single growing and rising bubble pinches off from a hemispherical cap shaped initial nucleus.

Fig. 5 is plot of wall superheat vs Nusselt number. We can clearly see the marked difference between the 2D and 3D simulation results. The 3D simulation shows a more accurate relation between wall superheat and Nusselt number compared to existing experimental correlations than does the 2D simulation. This suggests that, even under the idealized conditions used in our simulations, the three-dimensional effect is very important for predicting the proper relationship

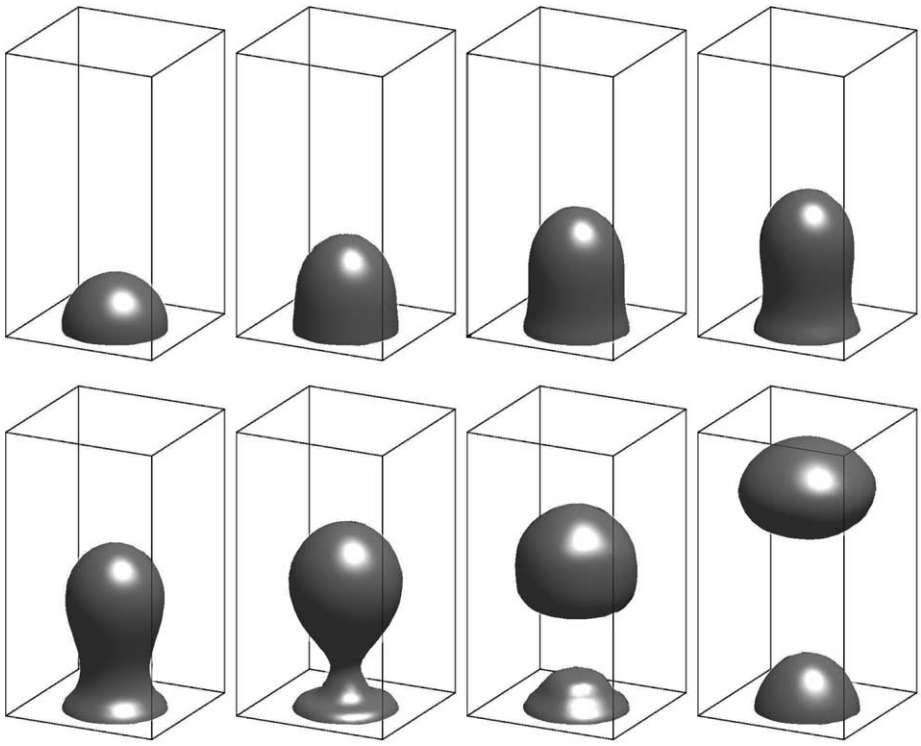

Fig. 4. Interface plots for a three-dimensional nucleate boiling simulation, $\rho_G/\rho_L = 0.0006237$, $\mu_G/\mu_L = 0.04353$, $k_G/k_L = 0.03694$, $c_G/c_L = 0.4847$, $T^*_w = 21.0$, $Re = 1334.2$, $We = 1.0$, $Pe = 0.0004268$, $Ja = 0.6972$, $22 \times 22 \times 40$ grid in a $3.08 \times 3.08 \times 5.6$ (non-dimensional) horizontally periodic domain. From a hemispherical cap shaped initial interface a single growing and rising bubble pinches off from the bottom.

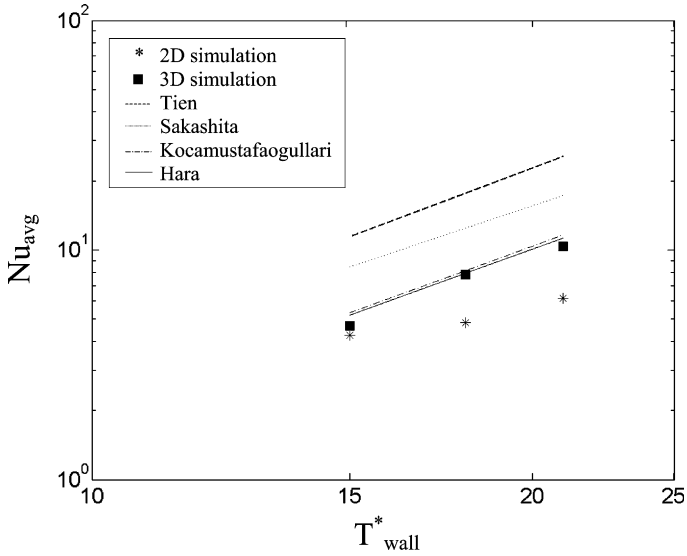

Fig. 5. Nusselt number vs wall superheat. Line plots are from experimental correlations of different authors.

between heat flux and the wall superheat for a realistic surface. The correlations from various authors are summarized in Table 2. Correlations which explicitly include nucleation site density have been chosen. In Fig. 6 we also plot the Nusselt number at the wall vs time with superheat temperature $T_w^* = 21.0$ for the three-dimensional case. The Nusselt number of our simulation is close to Kocamustafaogullari and Hara's correlation.

Table 2
Experimental correlations for nucleate boiling

Tien (1962)	$q = 61.3\, Pr_L^{0.33} k_L \Delta T n^{1/2}$ $Nu = 61.3 (RePe)^{-0.33} n^{1/2}$
Hara (1963)	$q = (C_1 C_2)^{3/4} (4\pi C_2/3)^{-1/2} (\rho_L c_L k_L)^{3/4} (\rho_G L_0)^{-1/2} \Delta T^{3/2} n^{3/8}$ $C_1 = 5.5,\ C_2 = 0.056$ $Nu = (C_1 C_2)^{3/4} (4\pi C_2/3)^{-1/2} (PeU_0)^{-0.25} \Delta T^{1/2} n^{3/8}$
Kocamustafaogullari and Ishii (1983)	$q = 14 k_L (\rho_L c_L/\rho_G L_0)^{0.5} Pr_L^{-0.39} D_b^{-0.25} \Delta T^{1.5} n^{3/8}$ $D_{bF} = 0.0208\phi \sqrt{\frac{\sigma}{g(\rho_L - \rho_G)}}$ $D_b = 0.0012 \left(\frac{\rho_L - \rho_G}{\rho_G}\right)^{0.9} D_{bF}$ $Nu = 14 (RePe)^{0.39} D_b^{*-0.25} \Delta T^{0.5} n^{3/8}$ $D_b^* = 0.0012 (1/\rho^* - 1)^{0.9} (0.0208\phi)$
Sakashita and Kumada (2000)	$q = 0.5 k_L (\sigma/\mu_L \alpha_L)^{0.35} Pr_L^{-1/12} (\rho_L c_L/\rho_G L_0)^{1/3} \Delta T^{4/3} n^{3/8}$ $Nu = 0.5 Re^{1/3} Pe^{-1/6} We^{-1/4} \Delta T^{1/3} n^{3/8}$

Correlations which explicitly include nucleation site density have been chosen.

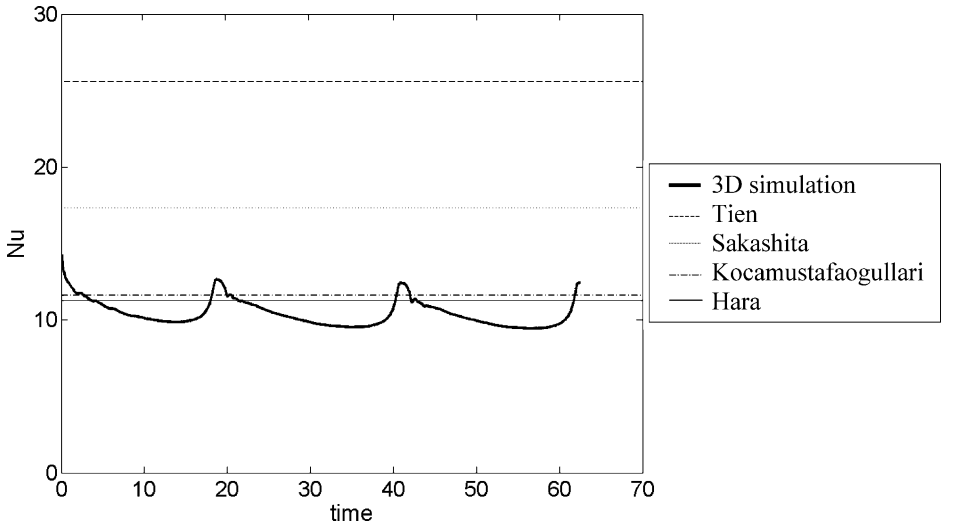

Fig. 6. Nusselt number plot at wall superheat temperature $T_w^* = 21.0$. The Nusselt number from the simulation is in good agreement with Kocamustafaogullari and Hara's correlation.

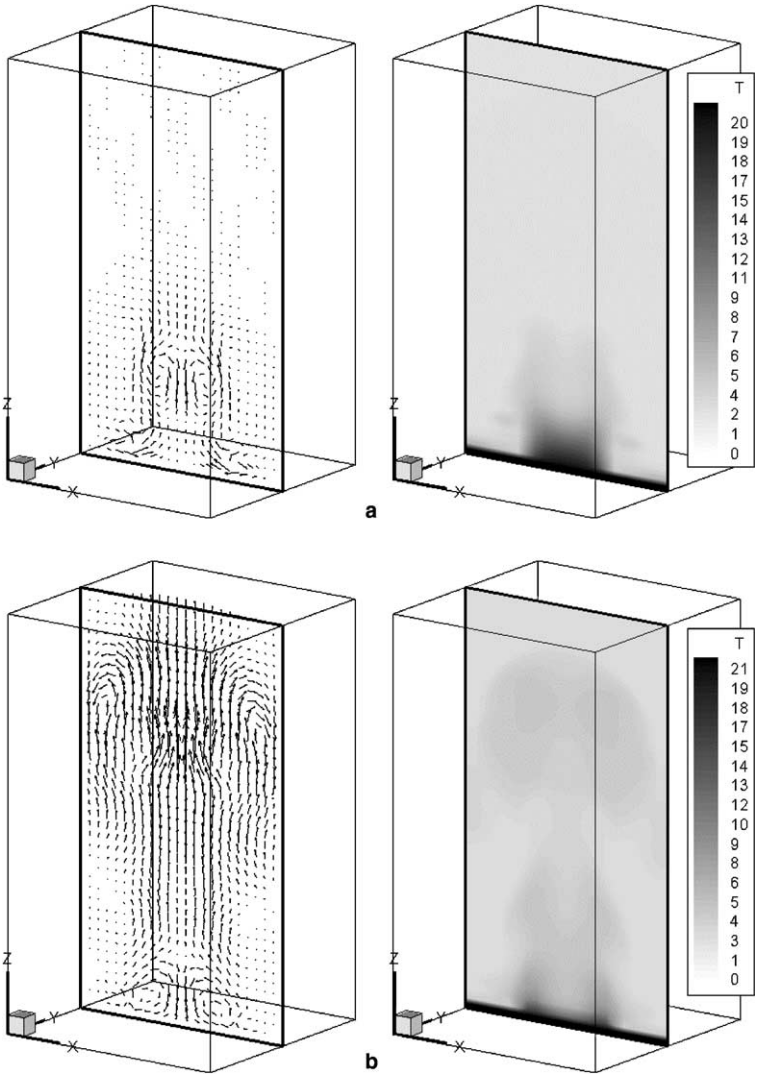

Fig. 7. (a) Velocity vectors and temperature profile for the vertical center plane of the second frame in Fig. 4. (b) Velocity vectors and temperature profile for the vertical center plane of the eighth frame in Fig. 4.

Fig. 7(a) shows temperature and velocity vectors for a vertical center plane of the second frame in Fig. 4. During this early period of bubble growth, the vapor evaporated near the wall region is seen to be pushed inward and this will lead to the symmetric vortex at the upper region of the bubble. The temperature profile also indicates that the hot wall temperature is pushed up by evaporated vapor convection near the contact line but this will become quite uniform by the vortex placed at the top side of the nucleus. The temperature and velocity profile during later period of nucleate boiling can be seen in Fig. 7(b). Fig. 7(b) shows the temperature and velocity vectors of the eighth frame in Fig. 4. Here we can see the large vortex that is generated around the detached bubble and there is also a small vortex inside the remaining bubble. These vortices

mix the entire flow field to keep the temperature field at nearly saturation level except near the heated wall.

3. Conclusion

The complex transport and coupled interface dynamics of nucleate boiling have been simulated in three-dimensions using the Level Contour Reconstruction Method. Our work is aimed at predicting nucleate boiling heat flux values more accurately on a real surface by including the effect of nucleation site density in the numerical model. This has been achieved by changing the surface area for a single nucleate bubble corresponding to the wall temperature.

The three-dimensional simulations demonstrated more accurate agreement with published Nusselt number correlations than did the two-dimensional simulations. The results for Nusselt number lie close to existing experimental correlations. We found that complete three-dimensional simulation, including the effect of neighboring bubbles, is very important for predicting the proper relationship between heat flux and the wall superheat in a realistic surface. For simplicity and to isolate our focus in this paper, we did not incorporate models for microlayer evaporation and contact line dynamics which are essential to the heat transfer mechanism and ultimately we would need to use increased resolution and implement accurate contact line dynamics and microlayer modeling to obtain more reliable data.

Detailed structure of the velocity and temperature distributions during nucleate boiling has also been obtained. Although more work needs to be done in comparing numerical and experimental results over broader ranges of operating conditions, numerical simulations hold the promise to complement experimental investigations and provide information that is hard to measure by experiment. Therefore, by understanding this small scale information it is hoped that progress can be made toward the long-term goal of providing quantitative predictions for linking operating conditions to large scale aspects of nucleate boiling heat transfer.

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