NUMERICAL SIMULATIONS OF DYNAMICS AND HEAT TRANSFER ASSOCIATED WITH A SINGLE BUBBLE IN THE PRESENCE OF NONCONDENSABLES

ABSTRACT
Under subcooled boiling conditions, the liquid may contain dissolved noncondensable gases. During phase change at the bubble-liquid interface, noncondensable gases will be injected into the bubble along with vapor. Due to heat transfer into subcooled liquid, vapor will condense in the upper regions of the bubble and the bubble interface is impermeable to noncondensables. As a result, noncondensable gases will accumulate at the top of bubbles. This existing gradient of noncondensable concentration inside bubble determines the saturation temperature gradient around the bubble surface. The nonuniform saturation temperature may cause a difference in surface tension which would give rise to thermocapillary convection in the vicinity of the interface. So far, this description is merely a hypothesis. It is felt that much inspection is in vital demand to clarify the uncertainty as to the role of noncondensables throughout this process. In this study, air is taken as noncondensable gas, and the aim is to investigate the effects of noncondensable air on heat transfer and bubble dynamics. The results from a numerical procedure coupling level set function with moving mesh method show the evidence of effects of noncondensable air imposed on heat transfer and the induced flow pattern is presented as well.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$C_g$</td>
<td>concentration or mass fraction of air</td>
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<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure</td>
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<td>$D$</td>
<td>diffusion coefficient</td>
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<tr>
<td>$g$</td>
<td>gravity vector</td>
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<tr>
<td>$g_e$</td>
<td>earth normal gravity</td>
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<tr>
<td>$H$</td>
<td>step function</td>
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<tr>
<td>$h$</td>
<td>grid spacing for the macro region</td>
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<tr>
<td>$h_{fg}$</td>
<td>latent heat of evaporation</td>
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<tr>
<td>$k$</td>
<td>thermal conductivity</td>
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<tr>
<td>$l_0$</td>
<td>characteristic length</td>
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<tr>
<td>$M$</td>
<td>molecular weight</td>
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<td>Marangoni number</td>
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<td>pressure</td>
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<td>$q$</td>
<td>heat flux</td>
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<td>$R$</td>
<td>universal gas constant</td>
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<td>$r$</td>
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<tr>
<td>$T$</td>
<td>temperature</td>
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<td>time</td>
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<tr>
<td>$t_0$</td>
<td>characteristic time</td>
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<tr>
<td>$\Delta T$</td>
<td>temperature difference</td>
</tr>
<tr>
<td>$\overline{u}$</td>
<td>velocity vector, $(u, v)$</td>
</tr>
<tr>
<td>$\overline{u}_{int}$</td>
<td>interfacial velocity vector</td>
</tr>
<tr>
<td>$u_0$</td>
<td>characteristic velocity</td>
</tr>
<tr>
<td>$x$</td>
<td>volume fraction</td>
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</table>

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Y height of computational domain
y vertical coordinate

Greek symbols

α thermal diffusivity
β_T coefficient of thermal expansion
δ_l thermal layer thickness
κ interfacial curvature
μ dynamic viscosity
ρ density
σ surface tension
φ level set function
ϕ contact angle

Subscripts

0 initial condition
g gas
int interface
l liquid
m mixture inside bubble
ref reference state
sat saturation
sub subcooling
sup superheat
v vapor
w wall

INTRODUCTION

Nucleate boiling is a liquid-vapor phase-change process associated with bubble formation. As it is a very efficient mode of heat transfer, the boiling process has attracted the attention from many researchers in the last half century. Subcooled nucleate pool boiling exists when the bulk temperature in the liquid pool is less than the saturation temperature of the liquid at the given system pressure, and the temperature of the heating surface exceeds the nucleation temperature which is higher than the saturation temperature. In reality under subcooled boiling conditions, a certain amount of noncondensable gases is in existence inside the system. With increasing liquid bulk temperature, the solubility of noncondensables in water usually keeps decreasing. When subcooled boiling occurs, the evaporation process will carry noncondensable gases, which has not been compelled from the system, into bubbles with vapor, meanwhile the vapor will condense in the upper regions of the bubble and the bubble interface is impermeable to noncondensables. As a result, the noncondensables would accumulate at the top of bubbles. This gradient of noncondensable concentration inside bubble yields a nonuniform saturation temperature to be present along the bubble interface. Furthermore, the different surface tension arising from this temperature gradient may initiate thermocapillary convection. Studying the effects of thermocapillary convection under terrestrial situations is rather difficult, as the thermocapillary force may be over-shadowed by the gravity force. Therefore, studying a bubble growth when noncondensables are present is often carried out under microgravity.

In some studies attentions were directed toward the influences of gravity level, thermocapillary convection and noncondensable concentration on this heat transfer process. From the pool boiling experiments conducted in 1980s and 1990s under microgravity conditions with saturated and subcooled liquids, Straub [13] observed that under subcooled boiling a convection forms jet streams above the head of the bubbles, this flow does not actually contribute to the overall heat transfer itself and this flow is absent in saturated liquid. Those observation led the author a hypothesis: under subcooled boiling, noncondensable gases are carried along with the evaporating vapor into a bubble, at the portion of the interface exposed to subcooled liquid only vapor condense. As a result, noncondensable gases accumulate at the top portion of the bubble and reduce the partial pressure of vapor, therefore lower the saturation temperature. In this way, noncondensable gases can act as a source of thermocapillary flow in subcooled boiling. Marek and Straub [6] proposed that thermocapillary convection could enhance heat transfer. The author claimed Nu with thermocapillary convection can be as much as 3.5 times Nu without thermocapillary in the case of flow around a sessile and pending half-spherical bubble for Ma = 10^4. By a combined analytical and numerical approach the authors assumed a non-deformable, spherical bubble interface, and concluded that heat transfer can be increased dramatically if the bulk gas concentration exceeds a certain value, also the bubble becomes less sensitive to the accumulation of noncondensables with increasing subcooling. Henry et al. [2] performed experiments with 99.3% pure n-perfluorohexane under reduced gravity of 10^{-2}g_e. The authors claimed in the case of gas-saturated boiling the formed bubble is predominately a gas bubble and causes dry-out over a larger portion of the heater surface and lowers down the heat transfer from the wall. The authors believed the cause of the thermocapillary motion remains unclear, instead of dissolved gas suggested by Straub [13].

From the above-mentioned literature, some contradictions are still in existence and many questions remain unanswered. Since Straub proposed his hypothesis, some researchers have applied this theory to explain the observation in their own experiments. Unfortunately no current instruments are available to detect the small amount of noncondensables in the system during experiments and verify its feasibilities. Meanwhile, numerical simulation may provide a tool to complement experiments and aid in interpreting the physics. In literature related to numerical studies, many assumptions were made, such as: hemispherical bubble shape, stationary bubble, artificial temperature gradient or adiabatic interfacial conditions. The conclusions base on these
assumptions were not able to capture the physics accurately behind the scenes. In this study, air is taken as noncondensable gases and a numerical procedure which is capable to redistribute mesh and sustain the highly dense node concentration around the interface as the bubble grows, extends a model proposed by Son et al. [10] and also relaxes many assumptions is undertaken to simulate this complex phenomenon and study the effects of non-condensable air throughout this process.

NUMERICAL FORMULATION

To analyze the growth of a single bubble in subcooled nucleate boiling, we extend the numerical model originally developed by Son et al. [10]. In that model, the computational domain is divided into two parts: a micro region and a macro region. The micro region is a thin film that lies underneath the bubble whereas the macro region consists of the bubble and the liquid surrounding the bubble. Numerical simulations of fluid flow and heat transfer are carried out for a time-dependent system in both micro and macro regions. The computed shapes of the interface in the micro region and the macro region are matched at the outer edge of the micro-layer for a given contact angle. In the numerical analysis, a level-set function is solved to represent the macro region.

The assumptions in this study are the following: the process is two-dimensional and axisymmetric; the flows are laminar; the wall temperature remains constant; water at atmospheric pressure that serves as the test uid, the properties associated with water not affected by dissolved air; the thermodynamic properties of the individual phases are assumed to be insensitive to small changes in temperature and pressure except for surface tension.

The interface separating the two phases is advanced at the rate of the intercial velocity and is captured by solving the following equation for the level set function \( \phi \),

\[
\frac{\partial \phi}{\partial t} = - \overline{u}_{int} \cdot \nabla \phi, \tag{1}
\]

\[
\overline{u}_{int} = \overline{u} + \frac{m}{\rho}, \tag{2}
\]

A reinitialization equation is solved until steady state to ensure that \( |\nabla \phi| = 1 \),

\[
\frac{\partial \phi}{\partial t} = \text{sign}(\phi_c)(1 - |\nabla \phi|). \tag{3}
\]

Next, we present the governing equations of continuity, momentum, energy and species conservation for the macro region,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \overline{u}) = 0, \tag{4}
\]

\[
\rho (\frac{\partial \overline{u}}{\partial t} + \overline{u} \cdot \nabla \overline{u}) = -\nabla p + \rho \overline{g} - \rho \beta_T (T - T_{sat}) \overline{g} - \sigma \kappa \nabla H + \left( \overline{\tau} \cdot \nabla \sigma \right) \nabla \nabla H + \nabla \cdot \mu \nabla \overline{u} + \nabla \cdot \mu \nabla \overline{u}^T \tag{5}
\]

\[
p_c p_l \left( \frac{\partial T}{\partial t} + \overline{u} \cdot \nabla T \right) = \nabla \cdot \kappa \nabla T \quad \text{for } H > 0, \tag{6}
\]

\[
T = T_{sat}(p_f) = T_{sat,x_f=0} + \frac{\Delta H_{sat,x_f=0}}{M_{hf}} \quad \text{for } H = 0 \tag{7}
\]

\[
p_c p_l \left( \frac{\partial C_g}{\partial t} + \overline{u} \cdot \nabla C_g \right) = \nabla \cdot \rho D \nabla C_g \quad \text{for } H < 0 \tag{8}
\]

The fifth term of right hand side of momentum equation accounts for the surface tension variation along the interface, which has appeared in Murata and Mochizuki [7] and James and Lowengrub [3]. The vapor in the bubble was assumed to remain at the saturation temperature. As such, the energy equation in the vapor is not numerically solved, however, the saturation temperature variation caused by the partial pressure of vapor is taken into account by applying Clausius-Clapeyron equation. Additionally, \( \sigma \) is taken as a function of temperature (Lay and Dhir [5]), given as:

\[
\sigma = \sigma_{ref} \left[ 1 - \frac{1.22}{T_{critical}} (T - T_{ref}) \right] \tag{9}
\]

In the above equations, some relations are defined as follows,

\[
H = 1 \quad \text{if } \phi \geq +1.5h, \tag{10}
\]

\[
H = 0 \quad \text{if } \phi \leq -1.5h, \tag{11}
\]

\[
H = 0.5 + \phi/(3h) + \sin[2\pi\phi/(3h)]/[2\pi], \text{otherwise} \tag{12}
\]

where \( \rho_m \) and \( \rho \) are the density of the mixture inside bubble and the fluid density respectively. \( \rho_m \) can be determined as the following procedure: molar fraction \( x_g \) is easily gained from the

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concentration $C_g$ in the form of mass fraction from the previous time, then $T_{sat}$ is computed by solving Eq. (6). Next, a formula of vapor density as a function of $T_{sat}$ from Wagner et al. [14] is applied to obtain $\rho_v$, and hence $\rho_m$ is known based on the definition of $C_g$. $\mu$ is the fluid shear viscosity and $k$ is the thermal conductivity. The value of the level set is used to derive the properties in the thin region around the interface. This prevents numerical instability arising from discontinuity in the properties. Also, Eq. (12) is consistent with the assumption that the vapor temperature remains almost constant at $T_{sat}$.

The governing equations are non-dimensionalized using the characteristic length, time and velocity scales, $l_0$, $t_0$ and $u_0$, respectively.

$$l_0 = \sqrt{\frac{\sigma}{g(\rho_l - \rho_v)}},$$

(13)

$$u_0 = \sqrt{gl_0} = \left[ \frac{\sigma g}{(\rho_l - \rho_v)} \right]^{1/4},$$

(14)

$$t_0 = \frac{l_0}{u_0} = \left[ \frac{\sigma}{g(\rho_l - \rho_v)} \right]^{1/4}. $$

(15)

The temperature is non-dimensionalized such that the wall temperature is 1 and the subcooled liquid temperature is 0. The concentration is non-dimensionalized by $C_{gl}$ in subcooled boiling cases.

The boundary conditions for the governing equations are,

At the wall $(y = 0)$,

$$u = 0, \quad v = 0, \quad \frac{\partial \phi}{\partial y} = -\cos \varphi, \quad T = T_w, \quad \frac{\partial C_g}{\partial y} = 0.$$  

(16)

At the top of computational domain $(y = Y)$,

$$\frac{\partial u}{\partial y} = 0, \quad \frac{\partial v}{\partial y} = 0, \quad \frac{\partial \phi}{\partial y} = 0, \quad T = T_l, \quad C_g = C_{gl}.$$  

(17)

At the planes of symmetry $(r = 0, R)$,

$$u = 0, \quad \frac{\partial v}{\partial r} = 0, \quad \frac{\partial \phi}{\partial r} = 0, \quad \frac{\partial T}{\partial r} = 0, \quad \frac{\partial C_g}{\partial r} = 0.$$  

(18)

\begin{table}[h]
\centering
\caption{Concentration of Air Inside Liquid}
\begin{tabular}{|c|c|c|c|c|}
\hline
Subcooling & 0°C & 1°C & 5°C & 7.5°C \\
\hline
$C_{gl}$ & 0 & 5.31E−7 & 2.486E−6 & 3.583E−6 \\
\hline
\end{tabular}
\end{table}

At the bubble interface,

$$\rho_m \nabla C_g = -C_g \frac{kVT}{h_{fg}}, \quad \text{for Condensation}$$  

(19)

$$\rho_m \nabla C_g = \frac{C_g - C_{gl}}{1 - C_{gl}} \frac{kVT}{h_{fg}}, \quad \text{for Evap.}$$  

(20)

Initially, the fluid velocity is set to be zero. The temperature profile is taken to be linear in the natural convection thermal boundary layer, and its thickness, $\delta_T$, is given by Kays and Crawford [4]:

$$\delta_T = 7.14(\nu \alpha_l / g \beta_{fg} \Delta T)^{1/3}.$$  

(21)

To determine $C_{gl}$, the thermodynamic equilibrium state at the top of computational domain is assumed. The partial pressure of vapor is the saturation pressure corresponding to the temperature of subcooled liquid. Therefore, the molar fraction of vapor and air are straightforward to obtain. Henry number is applied to divide the molar fraction of air in vapor side to get the molar concentration of air in liquid side which is converted into mass fraction: $C_{gl}$. $C_{gl}$ is assumed a constant for a fixed subcooling temperature, this may deviate from the reality, but it makes sense on a physical base.

\section*{Validation}

To validate this moving mesh method coupled with level set function, we studied a case of bubbles rising in a quiescent liquid and compared the results to those given by Ryskin and Leal [8] and Son [11]. A phase-change problem with an analytical solution was described in Son [12] and is used to test the capability of our method to include heat transfer. The numerical results for those two cases are reported in Wu \textit{et al.} [15]. In addition, the comparison between numerical simulations and experimental data will be addressed in another paper which is in preparation. This validation process lends support to latter numerical results in the next section.

\section*{RESULTS AND DISCUSSIONS}

In this section, the numerical results including saturated and subcooled boiling, pure water as well as systems containing dis-
solved air as test fluid under various gravity levels are presented. The saturated cases are regarded as a reference state by comparison to which the effects of subcooling and concentration of air could be manifested clearly. All the numerical results are taken from the computation of the first cycle.

**EARTH NORMAL GRAVITY, \( g/g_e = 1 \)**  
Numerical simulations of single bubble dynamics during saturated and subcooled nucleate boiling for a wall superheat of 8°C, contact angle of 54° and system pressure of 1.013 × 10^5 Pa are performed with different initial mass fraction of air inside bubble (i.e. \( C_{g,0} = 0, 0.2 \) and 0.4). The initial mass fraction of air inside bubble is reasonably made for the recognition of the fact that the bubble embryo starts with trapped air from wall imperfection in reality. For saturated boiling, zero concentration of air is assumed in liquid side. The growth rate of the bubble is adopted as the primary means of comparing the effects of different parameters. The actual volume of the bubble is first computed, thereafter it is converted into an equivalent diameter of a sphere.

Figure 1 shows the growth rate of the bubble with four different initial mass fraction of air inside bubble and varying subcooling of 0°C, 1°C, 5°C and 7.5°C respectively. The higher concentration of air inside bubble would lower saturation temperature, as a result, the departure diameter becomes larger and the growth period is shortened. For instance, initial \( C_{g,0} = 0.2 \) and 0.4 would decrease saturation temperature by 3.83°C and 8.34°C respectively. For subcooling of 1°C, the bubble detaches from the wall at a size which is smaller than its maximum size. This bubble shrinkage near the point of departure is caused by the negative total heat transfer to the bubble, i.e., condensation heat transfer is larger than the sum of evaporation heat transfer around the bubble and from the microlayer, as described in Singh [9]. For subcooling of 5°C and 7.5°C, in all cases, the bubble grows to a maximum size and then begins to shrink. This shrinkage is due to the large condensation heat transfer that occurs at the upper portion of the bubble. As a result, the bubble never achieves the bubble departure size. Eventually a balance is reached in evaporation and condensation rate, and the bubble remains attached to the heating surface. Figure 2 reveals the total heat transfer through bubble interface for four different subcooling. The positive initial higher heat transfer rate accounts for the rapid bubble growth at their early stage. As a bubble approaches to its departure, heat transfer drops to and below zero for subcooling of 0°C and 1°C respectively. For subcooling of 5°C and 7.5°C, heat transfer around zero after 0.1 s is in accord with the very small change in bubble size.

Figures 3 and 4 demonstrate the calculated flow field and temperature profile for two different subcooling during bubble growth process. Since no obvious difference takes place between cases of various contents of air in the system for the same subcooling, only one set of data is presented. From the numerical simulation, it can be seen that the growing bubble pushes out the liquid. The location where the vapor-liquid interface contacts the wall is observed to move outward and then inward as the bubble grows and departs. The highest heat transfer rate occurs at the base of the bubble. The nonuniform velocity inside bubble results in a noticeable vortex. The isotherm that terminates at the base condenses over most of the interface. The liquid that has just condensed around the interface flows downward toward the wall and thins down the thermal layer near the base of the bubble. This in turn leads to saddle points in the isotherms. The isotherm
distribution is quite different from the case for low subcooling as shown in Figures 3. The neighboring contours from concentration distribution represent a difference of one tenth between the maximum and minimum values. The highest concentration of air occurs at the top of the bubble and the concentration of air keeps decreasing downward. At the bottom of bubble where the highest heat transfer occurs, the influx composed of the lowest mass fraction of air throughout the system will dilute concentration there.

**Figure 3.** Flow field, temperature profile and concentration distribution under conditions of wall superheat = 8°C, liquid subcooling = 1°C, contact angle = 54°, pressure = 1.013 × 10^5 Pa, \( g/g_e = 1 \), \( C_{g,0} = 0.4 \), \( C_{g,l} = 5.31E^{-7} \).

**Figure 4.** Temperature distribution, velocity field and concentration profile for initial mass fraction of air = 0.4 under conditions of wall superheat = 8°C, liquid subcooling = 5°C, contact angle = 54°, pressure = 1.013 × 10^5 Pa, \( g/g_e = 1 \), \( C_{g,0} = 0.4 \), \( C_{g,l} = 2.486E^{-6} \).

**MICROGRAVITY, \( g/g_e = 0.01 \)** This section presents the results for the cases where the gravity levels are 1% of earth normal gravity. Under these conditions, not only is the size of the bubble an order of magnitude larger, but also the time periods are much longer.

Figure 5 shows the growth rate of the bubble with two different initial mass fraction of air inside bubble and two different liquid temperature under conditions of wall superheat of 8°C, contact angle of 54° and system pressure of 1.013 × 10^5 Pa. The trends of bubble growth are similar to cases of earth normal grav-
The liquid with 5°C subcooling shrinks the bubble to approximately an half in size from a saturated bubble. After maintaining a quasi-steady state under subcooled boiling conditions, the bubble with the presence of air inside the system remains at a diameter of 12.1mm, while it maintains a size of 10.9mm with the absence of air. At the same time, these effect brought by air are not pronounced in saturated boiling. Figure 6 demonstrates the total heat transfer rate across the interface for subcooling of 0°C and 5°C. This plot indicates that the subcooling affects the heat transfer rate under microgravity much more substantial than it does under earth normal gravity if Figure 2 is also in consideration, since the much more larger interfacial area is involved.

Figure 7 displays the calculated flow field and temperature profile during bubble growth process under saturated boiling conditions. By comparison to its counterpart under earth normal gravity, a vortex in liquid side is in more violent and distorted pattern. In Figures 8 and 9, the isotherms represent dimensionless temperature of 0.01 (i.e. 95.13°C), 0.1, 0.2, 0.3, 0.3846 (i.e. 100°C), 0.5, till 0.9. An interesting observation of a protruding profile of 95.13°C is made above the head of bubble in Figure 9. The differences between Figure 8 and 9 lay in two aspects, saturation temperature and surface tension. An extra numerical study considering only saturation temperature variation and uniform surface tension is conducted to determine which factor is responsible for this flow pattern in Figure 9. In that study, the growth rate, flow field and temperature distribution resemble what is depicted in Figure 8. This leads us to conclude that thermocapillary
Figure 8. Temperature distribution and velocity field under conditions of wall superheat = 8°C, liquid subcooling = 5°C, contact angle = 54°, pressure = 1.013 $\times 10^5$ Pa, $g/g_e = 0.01$, $C_{g,0} = 0.0$, $C_{g,l} = 0$.

flow at the early stage of bubble growth drives the fluid flowing from the bubble base toward its top in the vicinity of the interface, enlarges the evaporation interfacial area and yields a larger bubble. It is also interesting to notice that this temperature distribution bears much similarity to experimental presentation in Abe and Iwasali [1], although different test fluids are applied in their study.

CONCLUSIONS

A numerical procedure coupling the level set function with the moving mesh method has been employed to simulate nucleate boiling with different mass of air inside the system, various subcooling and varying gravity level.

The effects of noncondensables and subcooling on the bubble behaviors are more pronounced under microgravity than they do under earth normal gravity conditions.

The effects of noncondensables on saturated cases are insignificant by comparison to subcooled cases. The higher content of air inside the system increases the bubble size and shortens the growth period.

Under microgravity, the flow becomes more violent and convection dominant, as a result, temperature distribution is more distorted and dramatic.
ACKNOWLEDGMENT

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REFERENCES


