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Effect of dissolved gas on bubble growth on a biphilic surface: A diffuse-interface simulation approach

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ABSTRACT

In this paper, we numerically study pool boiling of a binary (water and nitrogen) mixture on a surface endowed with a combination of hydrophobicity and hydrophilicity (i.e., the so called *biphilic* surface). Here we adopt a numerical approach based on the phase field theory, where the vapor-liquid interface is assumed to be of a finite thickness (hence diffusive in nature) and requires no explicit tracking schemes. The theoretical modeling of two-phase heat and mass transfer in water diluted with nitrogen demonstrates the significant impact of impurities on bubble dynamics. The simulations show that locally high concentrations of nitrogen gas within the vapor bubble is essential to weakening the condensation effect, which results in sustained bubble growth and ultimately (partial) departure from the surface under the artificially enlarged gravity. Simply increasing the solubility of nitrogen in water, however, turns out to be counterproductive because possible re-dissolution of the aggregated nitrogen by the bulk water could deprive the bubble of vital gas contents, leading instead to continuous bubble shrinkage and collapse. Additionally, it is found that with the significant accumulation of nitrogen, the bubble interface is increasingly dominated by a strong interfacial thermocapillary flow due to the Marangoni effect.

1. Introduction

For a wide range of industrial applications (such as refrigeration and air conditioning systems, data centers, nuclear power plants, fusion reactors to name but a few) [1–3], thermal management entails the essential task of effective removal of excess heat. Recently, continuous technological progress towards device miniaturization drives exponential growth in power density, exceeding the capacity of most conventional single-phase heat transfer schemes (heat conduction and convection). Consequently, high-flux cooling solutions increasingly rely on two-phase heat transfer processes on account of their superior heat transfer efficiency [4], which takes full advantage of the significant latent heat involved in phase transition (e.g., boiling and condensation). In pool boiling heat transfer, in particular, repeated cycles of bubble nucleation, growth, and departure from the solid surface are capable of dissipating almost two orders of magnitude more heat—at a given surface superheat (defined as the excess temperature relative to the saturation temperature)—than would be possible with single-phase convection [5,6]. Such enhanced heat transport is attributable to a myriad of heat transfer mechanisms including heat conduction in the vapor phase, microconvection in the liquid phase, and release of latent heat of evaporation [7,8], of which a unified theory remains as yet elusive. Decades of extensive research notwithstanding [9–11], boiling phenomena still lack a proper unified mechanistic description, due largely to the inherent complexity embedded in the interactions between various interfacial subprocesses (some of which remain somewhat controversial). For instance, singularities such as fluid velocity slips and temperature gaps (discontinuities) might emerge over a macroscopic lengthscale at a moving contact line (where the three phases of liquid, vapor, and solid meet), which are responsible for possible non-integrable shear stress and extra thermal resistance [12,13]. As a result, boiling problems only admits a very limited number of analytical solutions (usually with considerable simplifications) [14–16]. Furthermore, the current knowledge with regard to the effects of surface characteristics (like roughness [17,18], texture

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Nomenclature

a	molecular attraction force
A	area
b	molecular volume
D	interfacial coefficient related to entropy
e	classical specific internal energy
e_T	full energy density
$\overrightarrow{\mathbf{e}}_g$	unit vector of the gravity force
E	interfacial coefficient related to internal energy
f	classical specific Helmholtz free energy
$\hat{F}$	generalized Helmholtz free energy
$\overrightarrow{F}$	body force vector
g	approximate shape function
$\tilde{G}$	dimensional artificial gravity
$\hbar$	Plank constant
$\overleftrightarrow{\mathbf{I}}$	identity tensor
k_B	Boltzmann constant
K	capillary coefficient
l	arc length
$\mathcal{L}$	auxiliary Lagrangian function
L	length
m	molecular weight
M_t	mean mass flow along the bubble interface
$\overrightarrow{\mathbf{n}}$	unit vector normal to the interface
p	thermodynamic pressure
r	r coordinate
R_g	dimensionless gravitational acceleration
R_f	dimensionless parameter defined in Eq. (15)
R_m	dimensionless parameter defined in Eq. (15)
R_P	dimensionless parameter defined in Eq. (15)
R_v	dimensionless parameter defined in Eq. (15)
s	classical specific entropy
$\hat{S}$	generalized entropy
t	time
$\overrightarrow{\mathbf{t}}$	unit vector tangential to the interface
T	temperature
$\hat{U}$	generalized internal energy
v	velocity
V	volume
z	z coordinate

Greek symbols

γ	interfacial energy
Γ	bubble outline
δ_{ij}	Kronecker delta
Δ	area ratio of the hydrophobic surface
ε	mean mass fraction inside the bubble
η	dynamic viscosity
ϑ_e	contact angle
λ	thermal conductivity
Λ	mobility coefficient
μ	classical chemical potential
$\hat{\mu}$	generalized chemical potential
$\overleftrightarrow{\Pi}$	generalized pressure tensor
ρ	density
σ	surface tension
τ_{ij}	viscous stress tensor
φ	volume fraction
Ω	ensemble

Subscripts

g	gas
i	component i of the binary system initial state
l	liquid
s	solid

Superscripts

l	liquid
v	vapor

[19–21], wettability [22–25], and thermophysical properties [26]) on boiling heat transfer is mostly empirical in nature—derived from experimental correlations—with few insights into the underlying mechanisms.

Given that only limited information can be garnered on the theoretical and experimental fronts, direct numerical simulation is gaining popularity for its potential in painting a more comprehensive physical picture—with details that are simply unavailable by other means—of boiling [27]. Depending on how the dividing interface between the liquid and vapor phases is modeled, however, continuum mechanics-based two-phase models often fall into two distinct groups:

(i) From a simple geometric perspective, the vapor and liquid phases can be viewed to be separated by a sharp interface of zero thickness. Under such an approximation, mass flow and heat transport in both phases need to be treated separately (that is, with their own governing laws of mass, momentum, and energy), which then has to be matched by imposing (discontinuous) boundary conditions at the interface. The accuracy of the overall depiction depends on the particular formulations (and assumptions) regarding various interfacial interactions, which sometimes rely on purely empirical parameters [27]. Moreover, within this mechanistic framework, a moving interface needs to be explicitly defined and tracked by means of interface-capturing techniques. Notable examples include the volume-of-fluid (VOF) method [28,29] and level-set (LS) method [30–32]. These schemes are usually accompanied by an auxiliary advection equation—the color function in the case of VOF schemes (that denotes the volume fraction of one phase) and the distance function relative to the interface in the case of LS schemes, for instance—to faithfully capture the interface. Another widely-used method is the front-tracking (FT) technique [33,34], which adopts, in addition to a fixed computational grid, a second Lagrangian moving mesh capable of following the motion of the interface.

(ii) Alternatively, the interface can be described through the prism of the phase field theory [35], in which phase change is taken as a smooth and continuous transition. Specifically, the liquid and vapor phases are treated as one continuous medium, and as a result, no explicit tracking of the interface is necessary. First introduced by van der Waals [36] (and later revisited by Cahn and Hilliard [37]), the concept of a diffuse interface endows the interface with *capillarity* (that is, surface tension) by amending the free energy functional with interfacial-gradient contributions scaled by a certain order parameter (candidates including the number density and component concentration). Despite being computationally onerous [38], the diffuse-interface method (DIM, also known as the second gradient method [39,40]) proves to be extremely versatile. On account of its firm foundation in