International Journal of Heat and Mass Transfer 110 (2017) 921–939

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

A mechanistic model for embryo size prediction at boiling incipience: 'Work of formation' based approach

Janani Srree Murallidharan [a], B.V.S.S.S. Prasad [a], B.S.V. Patnaik [b,*]

[a] Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai, 600036, India
[b] Department of Applied Mechanics, Indian Institute of Technology Madras, Chennai, 600036, India

ARTICLE INFO

Article history:
Received 28 October 2016
Received in revised form 6 February 2017
Accepted 3 March 2017
Available online 3 April 2017

Keywords:
Boiling
Nucleation
Gibb's free energy
Embryo
Phase-change

ABSTRACT

The initial size of the embryo, which is formed at the inception of boiling, plays a vital role in the accurate prediction of component scale wall boiling phenomenon. Embryo size predictions are typically calculated using the classical theory of nucleation. However, in recent times, the predictive capability of this theory was found to have limitations. Hence, there is need for a more fundamental and mechanistic model to overcome some of the drawbacks. In this paper, we propose a 'work of formation' based model for the embryo formation. This model is mechanistic and includes a Van der Waals based real gas treatment for the vapour. It also incorporates Lewins surface tension model that is a function of the boiling-nucleus size. The present model also accounts for the boiling occurrence in the presence of undissolved nanobubbles on the surface. The embryo formation model has been extensively tested for both low and high pressures, horizontal and vertical test section orientation, and for different surfaces and fluids. The energy required for the embryo formation was found to be higher, when the initial gas bubble is intact compared to when the gas bubble diffuses into the embryo. Some of the contradictory claims on the suitability of classical theory of nucleation to nanosurfaces have been tested. From the present embryo formation model, the physics of nucleation such as, the effect of pressure fluctuations and energy dissipation mechanisms involved in the formation is explained.

1. Introduction

Boiling and condensation influences a wide spectrum of industrial systems. The design and safety of such systems is highly dependent on the precise understanding associated with the phase change process. To be able to better design the safety standards, several plausible scenarios need to be addressed. To this end, computational techniques can play a prominent role in building models with phase-change that can accurately mirror the physics. The Eulerian-Eulerian multiphase model (*EEMF*), is one of the popular choices for the computational framework in such component-scale systems. The heterogeneous nature of boiling occurring at the wall is modeled through the 'wall heat flux partitioning' model (*WHFP*). A detailed study of this framework for high pressure subcooled flow boiling conditions was recently discussed in Murallidharan et al. [1]. In that study, the wall bubble departure diameter (D) was identified as the most important parameter that needs to be modeled mechanistically and accurately. For a better prediction of D, it is essential to accurately obtain the initial size of the bubble nucleus that forms on the wall. Correlations such as Benjamin and Balakrishnan [2]'s nucleation site density model, Kirichenko [3]'s models, Wang and Dhir [4]'s model were analyzed in Ref. [1], and it was found that, the 'radius of cavity' term played a crucial role. In general, the classical theory of nucleation is used to determine the cavity size (or) embryo size [5]. The formulation of the classical theory, as shown in Eq. (1), is obtained by combining the Clausius - Clayperon equation and the Young's Laplace equation as follows:

$$T_l - T_{sat}(P_l) > \frac{2\sigma_{lv} T_{sat} \Delta v_{lv}}{h_{lv} r_{\min}} \quad (1)$$

where T_l and T_{sat} is the superheated liquid and saturation temperature respectively, σ_{lv} is the surface tension, Δv_{lv} is the difference in specific volume between vapour and liquid, h_{lv} is the latent heat of vaporization and r_{min} corresponds to the radius of the bubble embryo. However, the classical theory is only elementary and does not take into account key parameters such as, the wall contact angle and wall roughness [6]. Based on the current state of literature (presented in Section 2) it can be seen that an accurate and comprehensive framework to model nucleation is required. In this work, we propose a embryo formation model which is more mechanistic

* Corresponding author.
E-mail address: bsvp@iitm.ac.in (B.S.V. Patnaik).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2017.03.011
0017-9310/

Nomenclature

A	interface area (m^2)
D	bubble departure diameter (m)
G	Gibb's free energy (J)
h	latent heat of vaporization (J/kg)
K	Boltzmann constant
n	number of moles of species (moles)
P	pressure (bar)
Q"	heat flux (W/m^2)
r	radius (m)
S	entropy (J/K)
T	temperature (K)
U	internal energy (J)
V	volume (m^3)
v	specific volume (m^3/mole)
W	expansion work (J)

Greek symbols

Δ	difference operator
η	diffusivity (m^2/s)
θ	contact angle (°)
μ	chemical potential (J/mole)
ρ	density (kg/m^3)
v	specific volume (m^3/mole)
σ	surface tension (N/m)
Ω	incipience of surface tension
∞	planar surface value

Subscripts and superscripts

b	base
c	cavity
cr	critical point
g	gas
gl	gas-liquid
i	chemical species
j	interface
l	liquid
ls	liquid property at saturation temperature
lv	liquid-vapour
min	minimum
O	before boiling
sat	saturated
v	vapour
vg	vapour-gas
vs	vapour property at saturation temperature
$wall$	value at the wall
$*$	after boiling
/	non-dimensionalised parameter w.r.t. critical point

Abbreviations

CHF	critical heat flux
D-RGC	diffused – real gas core
EEMF	Eulerian-Eulerian Multiphase model
I-RGC	intact-real gas core
LSR	liquid saturation ratio
ONB	onset of nucleate boiling
OSV	onset of significant void
WHFP	wall heat flux partitioning

and is based on 'work of formation'. Additionally, the proposed model is applicable for component scale boiling models, interface tracking, DNS based studies etc. Currently in these studies, the initial embryo size is arbitrarily chosen and is based on mesh resolution [7]. It will be shown that, the proposed embryo formation model provides a mechanistically accurate alternative.

2. Background literature

2.1. Nucleation theories

All existing nucleation theories can predominantly be classified as – phenomenological, kinetic and molecular. The phenomenological models compute the energy involved in the formation of a nucleus, primarily using the Gibb's free energy function [8,9]. Computing the formation energy of the nucleus is based on the assumption that, both vapour and liquid are a continuum, and can be represented through the macroscopic properties such as, temperature, pressure and surface tension. Kinetic methods focus on computing rate of nucleation using models such as, the Boltzmann statistics of equilibrium cluster distribution and by using empirical coefficients such as the monomer evaporation coefficient [10]. The molecular based nucleation deals with very small length scales and accounts for atomic behavior (e.g.: molecular interaction potential) as well as interface movement (e.g.: density functional approach [11]). Models based on kinetic and molecular nucleation theories use small length scales (molecular) and considerable statistical empiricism (kinetic methods) and hence have only limited experimental support. In fact among the various nucleation theories there is a seven orders of magnitude difference between micro and macro length scales [12]. Moreover, all of them cannot be used to solve the problem at the same level due to length and time scale issues and other computational constraints. From the categories stated above, the phenomenological approach of free-energy based nucleation can span various length scales without significant computational demand and mesh resolution. Furthermore, it can easily be implemented alongside existing boiling modules of general purpose computational fluid dynamics (CFD) solvers. More importantly, the Gibb's free energy based approach is based on the fundamentals of continuum thermodynamics. Hence it is most suited for easy application to the component scale modeling of boiling.

2.2. Free-energy based nucleation

The study of nucleation using Gibb's free energy was first proposed by Volmer and Weber (see [13]). Lu and Peng [14] modeled the dynamic evolution of nucleation for different types of cavities such as inside, outside, and twice-nucleation. They have concluded that, the structure of the cavity (cavity size) and surface characteristics strongly influence the type of nucleation. However, their study was not validated against experiments and was not tested for different operating conditions. They have treated the newly formed nucleus as a cluster of atoms and used the kinetic equations of nucleation for modeling its distribution and rate of growth. Their study did not account for the presence of pre-existing gas nuclei at the wall, although they are usually observed in reality. Wu et al. [15] improved upon this study and modeled nucleation near a wall by introducing a temperature gradient in the vicinity of the wall. Validations were performed by comparing the predictions of heat flux variation vs. wall superheat with that of the experiments. They have studied the variation in the free-energy of the system for various temperature gradients and contact angles. However, no direct validation of predicted embryo size