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Cluster dynamics and fictitious boiling in microchannels

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Abstract

Bubble nucleation could hardly be noted in microscale boiling systems even under high heat flux, denoting as the fictitious boiling phenomenon. We investigated in this work the role of perturbations on the dynamics of clusters, whence developing the physical interpretation of the fictitious boiling commonly observed in microscale boiling. Both the effects of internal and external perturbations were examined. The external perturbations could markedly depress the development of clusters, thereby correlating with the bubble-extinction characteristic noted in fictitious boiling. A pressure fluctuation model was proposed to provide a criterion to the occurrence of fictitious boiling. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Boiling; Microscale transport phenomenon; Bubble nucleation; Perturbation; Microchannal; Cluster dynamics; Pressure fluctuation model; Heat transfer

1. Introduction

Microscale transport processes had attracted worldwide research attention since the pioneering work of Tuckmann and Pease [1]. The characteristics of fluid flow and heat transfer in microchannels could be very different from that is in normal-sized channels [2–5]. Bowers and Mudawar [6] investigated flow boiling of R113 in minichannel and in microchannel. Lin et al. [7,8] noted that it is extremely difficult to generate bubbles even at a high heat flux from heater allocated in microchannels. Peng and Wang [9–11] conducted a series of works on the flow boiling in microchannels. These authors also noted the "bubble-extinction" behavior of microchannel boiling. That is, at a high heat flux that is sufficient to introduce vigorous nucleate boiling mode on a normal-sized heater, one could hardly observe vapor bubbles on a microchannel heater.

Peng and Wang [12] proposed the concepts of "evaporating space" and "fictitious boiling" to interpret the bubble-extinction behavior observed in microchannel boiling. The former concept stated that there exists a critical liquid space less than which normal bubbles could not form and grow. These authors proposed in the latter concept, that in microchannel the small bubble embryos would continuously form and collapse, thereby mimicking a boiling state. Conventional homogeneous vapor nucleation theory has been derived based on free energy change after bubble formation. A critical radius of bubble, r_C, is required to exceed for the bubble could subsequently grow and depart from the heated surface. Peng and Wang's "fictitious boiling" hypothesis acquires a mechanism effective only in

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Nomenclature

A	constant defined in Eq. (28)
a	coefficient in van der Waal's equation of state
b	coefficient in van der Waal's equation of state
C	integral constant in Eq. (12)
c	velocity of sound in Eq. (30)
C_0	number concentration of cluster in liquid
D	strength of perturbations
D_n	collision frequency
ΔG	free energy change
J_n	nucleation rate defined in Eq. (23)
K	Boltzmann constant
k	deactivatin coefficient
k_1	function defined in Eq. (10a)
k_2	function defined in Eq. (10b)
k_1^*	perturbed k_1 value in Eq. (18)
L	scale of microchannel
L_C	critical scale of microchannel
M	molecular weight
N	number of activated molecules in liquid of unit volume
N_0	total number of molecules in liquid of unit volume
N'	number of non-activated molecules in liquid of unit volume
n	number of activated molecules in cluster
p	pressure
p_v	pressure in cluster
p_∞	pressure in bulk liquid
R	gas constant
r	radius of cluster
r_C	critical radius of cluster
T	liquid temperature
t	time
t_C	time for cluster growth
t_R	time for pressure wave reflection
T_S	saturation temperature
t_S	time for initial phase of cluster growth
t'	dummy time
S	entropy
U_{FP}	potential energy defined in Eq. (21)
V	volume
V_C	volume of cluster
V_m	volume of activated molecule
Z_f	non-equilibrium factor in Eq. (23)
$\Gamma(t)$	white-noise perturbation
τ	characteristic time
λ	collision absorption coefficient
ρ	probability density function of random variable n
μ	chemical ptential
ν	proportional constant in Eq. (3)
ζ	proportional constant in Eq. (5)

microchannel that depresses the bubble embryos to be less than r_C in size. Peng et al. [13] provided a thermodynamic analysis to the inactivation of bubble growth.

Ensembles of molecules having high energy that are bound without electronic coupling are called "clusters" [14–17]. A great number of bubble embryos, or clusters of activated molecules, should appear in the superheated liquid that correspond to the high heat flux achieved in microchannel boiling [18]. Information regarding the cluster dynamics in superheated liquid hence provides the basis to better understand the microscale transport processes, which is still largely lacking.

The clusters once being formed, would experience continuous disturbances during its subsequent development. Such a disturbance could be introduced either from the thermal fluctuations self-generated in the superheated liquid, or be imposed by certain external sources. We denoted herein the above-mentioned two kinds of disturbances, such as "internal perturbation" and "external perturbation", respectively. The number balance equation for activated molecules in clusters was first formulated. Then, the dynamics of clusters formed with internal or external perturbations were discussed. Finally, a pressure fluctuation model was proposed to provide the physical interpretation to the occurrence of fictitious boiling.

2. Clusters and clustering

2.1. Number balance of activated molecules in cluster

Consider a liquid system at temperature, T, and ambient pressure, p_∞. The temperature is considered to be higher than the corresponding boiling point temperature T_S at p_∞, the liquid is hence in a meta-stable state. Fig. 1 schematically depicts the cluster association/dissociation process.

Consider an ensemble containing N_0 molecules, including n activated molecules in the cluster, N activated molecules in the bulk liquid, and the remaining N' molecules (Fig. 2), or, $N_0 = n + N + N'$. Then, the number balance of activated molecules in the cluster could be stated as follows:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = \text{gain} - \text{loss}. \tag{1}$$

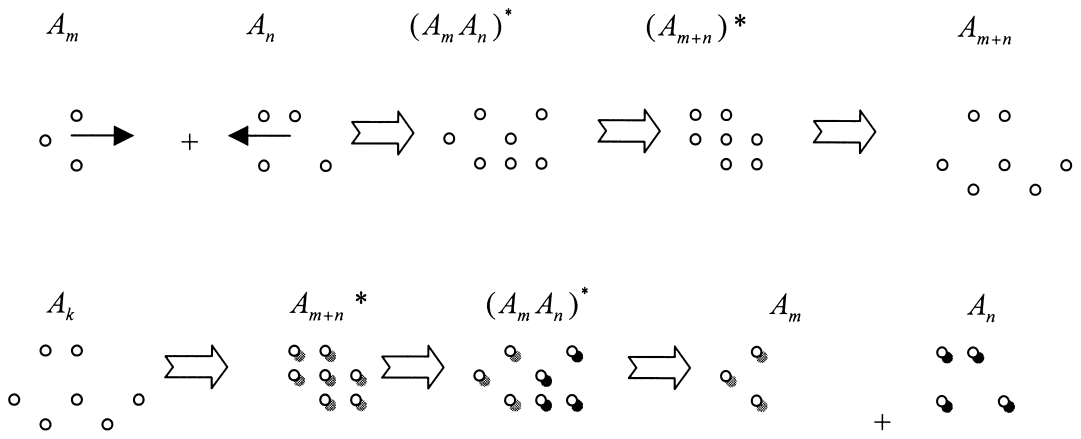

Fig. 1. Association and dissociation of clusters.

The increase in n comes from the collision between activated molecules in cluster and the activated molecules in the bulk liquid. That is,

$$\text{gain} = \lambda N \times n, \tag{2}$$

where λ is the collision adsorption coefficient and could be expressed as a function of superheated liquid [19]:

$$\lambda = \nu(T - T_s). \tag{3}$$

Conventional nucleation theory stated that

$$N = N_0 \exp(-\Delta G/KT), \tag{4}$$

where ΔG is the free energy of nucleation and could be approximately expressed as follows:

$$\Delta G = \zeta(T - T_S)n. \tag{5}$$

Then the first-order Taylor expansion of N in Eq. (4) could be stated as follows:

$$N = N_0\left[1 - \frac{\zeta}{KT}(T - T_S)n\right]n. \tag{6}$$

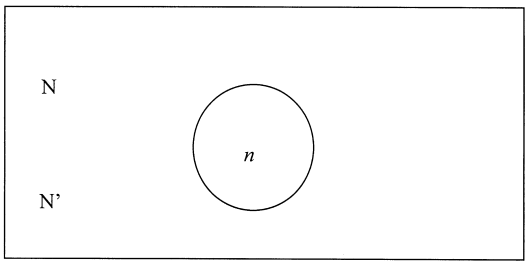

Fig. 2. Number balance model.

Substituting Eqs. (3–6) into Eq. (2) yields the following expression for gain:

$$\text{gain} = \lambda N_0\left[1 - \frac{\zeta}{KT}(T - T_S)n\right]n. \tag{7}$$

Each activated molecule in the cluster might become deactivated that is controlled by the difference between its chemical potential and that in the bulk liquid. Restated,

$$\text{loss} = k \times n, \tag{8}$$

where k is the deactivation coefficient. The chemical potential $\mathrm{d}\mu = V\mathrm{d}p$, denoting the property difference between molecules under meta-stable state and those in the bulk liquid [20]. Restated, $k \propto |p_\infty - p_v|$.

Consequently, the number balance of activated molecules in cluster could be stated as follows:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = k_1 n - k_2 n^2, \tag{9}$$

where

$$k_1 = \lambda N_0 - k \tag{10a}$$

$$k_2 = \lambda N_0 \frac{\zeta}{k}\left(1 - \frac{T_S}{T}\right) \tag{10b}$$

For a superheated liquid considered herein, $T > T_S$, thereby $k_2 > 0$. On the other hand, k_1 could be positive or negative, depending upon the relative significance between association and dissociation processes.

A particular solution of Eq. (9) could be derived as follows:

$$n(t) = \frac{k_1}{2k_2} - \frac{|k_1|}{2k_2}\frac{C\exp(-|k_1|t) - 1}{C\exp(-|k_1|t) + 1} \tag{11}$$

where

$$C = \frac{\left|\frac{k_1}{k_2}\right| + \frac{k_1}{k_2} - 2n_0}{\left|\frac{k_1}{k_2}\right| + \frac{k_1}{k_2} + 2n_0} \tag{12}$$

and n_0 is the initial condition of n. Notably, $n(\infty) = 0$ for $k_1 \leq 0$ and $n(\infty) = k_1/k_2$ for $k_1 > 0$ ($k_1 = 0$ thereby denotes the critical point of the transcritical bifurcation).

For a non-positive k_1, the n_0 activated molecules in the cluster would finally die out. The inequality of $k_1 = \lambda N_0 - k \leq 0$ could be rearranged as follows:

$$\Delta T = T - T_S \leq \frac{k}{\nu N_0}. \tag{13}$$

The physical interpretation of Eq. (13) is that if superheated liquid is less than $k/\nu N_0$ and there is no external/internal perturbation, all clusters would collapse and the final steady state is $n = 0$. Otherwise, the cluster would form that contains k_1/k_2 activated molecules.

2.2. Cluster dynamics with internal perturbations

In this section, we considered the number balance of n, Eq. (9), evolves with a white-noise perturbation, $\Gamma(t)$. The white noise could be originated from the inhomogeneity self-generated in the superheated liquid, which satisfies the following two terms: $\langle\Gamma(t)\rangle = 0$ (zero-mean), and $\langle\Gamma(t')\Gamma(t)\rangle = 2D\delta(t - t') = 0$ (independent actions). D denotes the strength of white-noise perturbation and δ is the delta function. The corresponding Fokker–Planck equation for the probability density function, $\rho(n, t)$, for the stochastic variable n at time t, could be stated as follows:

$$\frac{\mathrm{d}\rho(n, t)}{\mathrm{d}t} = -\frac{\partial}{\partial n}\left[\left(k_1 n - k_2 n^2\right)\rho(n, t)\right] + D\frac{\partial^2\rho(n, t)}{\partial n^2}. \tag{14}$$

The initial condition is $\rho(n, 0) = \delta(n)$.

Define characteristic time $\tau = \sqrt{D/k_1}\mathrm{e}^{k_1 t}$. Let $\tau \ll 1$, that is, at the very beginning of cluster evolutions. Since the initial probability distributes very close to $n = 0$, $|n^2| \ll |n|$,and Eq. (9) has an analytical solution as follows:

$$\rho(n, t) = \sqrt{\frac{k_l}{2\pi D(\mathrm{e}^{2k_l t} - 1)}}\exp\left[-\frac{k_l n^2}{2D(\mathrm{e}^{2k_l t} - 1)}\right]. \tag{15}$$

If $\sqrt{D} \ll \tau \ll 1$, Eq. (15) could be simplified as follows:

$$\rho(n, t) = \frac{1}{\sqrt{2\pi\tau}}\exp\left[-\frac{n^2}{2\tau^2}\right]. \tag{16}$$

Eq. (16) represents a Gaussian distribution around $n = 0$.

In accord with Eq. (15), the time for the initial stage of relaxation process, t_N, could be identified as $D^{-1} \gg \exp(2k_1 t_s) \gg 1$.

At another extreme of $\tau \gg 1$, at the final steady state, the solution of Eq. (9) could be found as follows:

$$\rho(n,\infty) = \sqrt{\frac{k_1}{4\pi D}}\exp\left[-k_1\left(n - \frac{k_1}{k_2}\right)^2 \Big/ D\right]. \tag{17}$$

Eq. (17) also represents a Gaussian distribution with its mean value locating at $n = k_1/k_2$.

Fig. 3 schematically depicts the time evolutions of probability density function of random variable n. The presence of large internal perturbation would introduce a Gaussian distribution with great variance but its mean value is the same as that with no perturbation (Eq. (11)). The sole action of internal perturbation could not properly interpret the bubble-extinction behavior observe in microchannel boiling.

2.3. Cluster dynamics with external perturbations

In this section, the cluster dynamics with the existence of external perturbations were considered, which are originated from sources other than the system self-generated fluctuations. The external perturbations could stochastically affect the values of system parameters, like k_1. (Notably, as stated above, $k \propto |p_\infty - p_v|$. Consequently, any external perturbations that would yield a change in system pressure would influence the parameter k_1.) A form is assumed for the external perturbation as follows:

$$k_1^* = k_1 + \Gamma(t), \tag{18}$$

where $\Gamma(t)$ has the white-noise characteristics and $k_1 = \lambda N_0 - k$. The corresponding Fokker–Planck equation

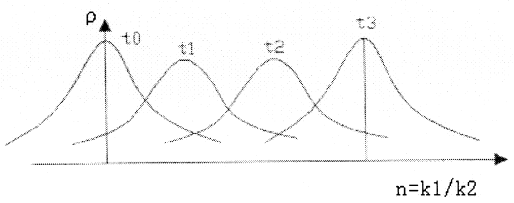

Fig. 3. Probability density function with internal perturbation.

for the probability density function for the stochastic variable n at time t, could be stated as follows:

$$\frac{\mathrm{d}\rho(n,t)}{\mathrm{d}t} = -\frac{\partial}{\partial n}\left[\left(k_1 n - k_2 n^2\right)\rho(n,t) + Dn\rho(n,t)\right] + D\frac{\partial^2 n^2 \rho(n,t)}{\partial n^2}. \tag{19}$$

The initial condition is $\rho(n,0) = \delta(n)$. The steady-state solution for Eq. (19) could be found as follows:

$$\rho(n,\infty) = \delta(n), \quad \text{for } k_1 \le 0; \tag{20a}$$

$$\rho(n,\infty) = Cn^{\frac{k_1}{D}-1}\mathrm{e}^{\frac{k_2 n}{D}} \quad \text{for } k_1 > 0. \tag{20b}$$

The parameter C in Eq. (20b) is the integral constant.

Define the potential function U_{FP} as $U_{\mathrm{FP}} = -D\ln\rho(n,t)$, then we could obtain the following expressions:

$$U_{\mathrm{FP}}(n) = \ln\delta(n) \quad \text{for } k_1 \le 0; \tag{21a}$$

$$U_{\mathrm{FP}}(n) = k_2 n - k_1 n + D\ln n - D\ln N \quad \text{for } k_1 > 0. \tag{21b}$$

Notably, there are two qualitative changes in ρ distribution occurring at $k_1 = D$ and 0. Fig. 4 schematically illustrates such an occurrence. For $k_1 > D$, a maximum probability for cluster exists at a size of $n = (k_1 - D)/k_2$. For $0 < k_1 < D$, maximum probability point is at $n = 0$, denoting that most molecules are not in the associated state (cluster). However, there still exist possibility to have some clusters at a greater size in the system. At $k_1 < 0$, $n = 0$ behaves as the only attractor in the system. Regardless of the size of the initial clusters, eventually they would all dissociate into individual molecules. Imposing external perturbations would have a distinct influence to cluster dynamics as compared with internal perturbations. Restated, external perturbation could yield the collapse of clusters, thereby correlating with the observations of bubble-extinction characteristics in microchannel boiling.

For the criterion of $k_1 < D$ for most activated molecules in a dissociated state, the superheated liquid could be found as follows:

$$\Delta T = T - T_{\mathrm{S}} \le \frac{K + D}{\nu N_0}. \tag{22}$$

Apparently, when compared with Eq. (13), the external perturbation would yield the greater superheated liquid to form stable clusters of the smaller size $((k_1 - D)/k_2)$.

3. Fictitious boiling in microchannels

In the above-mentioned discussions the action of external perturbation should mainly correspond to the bubble-extinction behavior observed in microchannel boiling. We proposed herein that the pressure wave generated accompanied with cluster formation corresponding to the source of external perturbations. Kwak et al. [15] estimated the pressure difference between that in the cluster and that in bulk liquid, giving an as high as 280 atm during the initial phase of cluster growth. Many clusters form and grow in the superheated liquid. The pressure waves would hence generated from many points and propagate outwards. For a normal-sized channel such a pressure wave would transmit outward from the cluster and rapidly dissipate. However, in a microchannel the wall may reflect the generated pressure waves back to the clusters, acting as random external perturbations imposed to the clusters (Fig. 5). Such an occurrence could stochastically affect the values of system parameters, like k_1. (Notably, as stated above, $k \propto |p_\infty - p_v|$. Consequently, any external perturbations that would yield a change in system pressure would influence the parameter k_1.)

The cluster growth is mainly achieved by absorption of activated molecules onto the existing clusters [14].

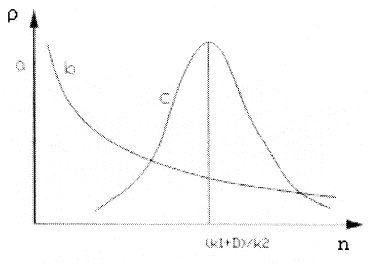

Fig. 4. Probability density function with external perturbation.

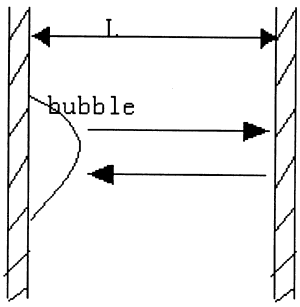

Fig. 5. Pressure wave transmits in microchannal.

According to conventional nucleation theory, the nucleation rate per unit volume could be stated as follows:

$$J_n = N_0 D_n Z_f \exp\left(-\frac{\Delta G}{KT}\right), \tag{23}$$

where D_n and Z_f are the collision frequency of liquid molecules with cluster surface, and the non-equilibrium factor, respectively. Notably, J_n is the product of the gain term in Eq. (2) and the concentration of clusters in superheated liquid (C_0); restated, $J_n = C_0 * \text{gain}$. Typically, $D_n Z_f = 10^7\ s^{-1}$ [21]. Hence, $\lambda C_0 = 10^7\ s^{-1}$.

Consider the radius of cluster as r at time t. In an increment of time dt the radius of cluster increases by dr see Fig. 6). Then the number of activated molecules absorbed onto the cluster increases by $J_n n 4\pi r^2\,dt$. Based on number balance of activated molecules, the change of radius with time could be stated as follows:

$$\frac{dr}{dt} = J_n n V_m, \tag{24}$$

where V_m is the volume of activated molecule. Take $r(0) = 0$, then the radius of cluster would increase linearly with time. The volume of cluster hence becomes,

$$dV_c = 4\pi (J_n n V_m)^3 t^2\,dt. \tag{25}$$

The change in bulk liquid volume would be $dV = -dV_C$. Assume that the bulk liquid follows the van der Waal's equation of state:

$$\left(p + \frac{a}{V^2}\right)(V - b) = RT. \tag{26}$$

Then, the pressure fluctuation introduced by volume change dV could be stated with the assistance of Eq. (25) as follows:

$$dp = At^2\,dt \tag{27}$$

where

$$A = \left[-\frac{RT}{(V-b)^2} + \frac{2a}{V^3}\right]\frac{4\pi}{M}(J_n n V_m)^3. \tag{28}$$

Consequently, the pressure difference inside and outside the cluster could be estimated as follows:

$$p_v - p_\infty = \frac{A}{3}t^3. \tag{29}$$

While the clustering process occurs in a short time scale, the pressure difference described in Eq. (29) could be taken as the magnitude of pressure wave therein generated.

The velocity of pressure wave propagation, c, could be estimated as follows:

$$c = \sqrt{\left(\frac{dp}{d(1/V)}\right)_S} = \sqrt{\left(\frac{V}{V-b}\right)^2 RT - \frac{2a}{V}}. \tag{30}$$

In a microchannel of size L, the time for the pressure wave to be reflected by the wall back to cluster would be estimated as follows:

$$t_R \approx \frac{2L}{c}. \tag{31}$$

The time required for a vapor embryo to develop during the initial phase (t_C) is approximately 10 μs [20]. As discussed in the preceding section, the imposition of external perturbation, like pressure wave discussed herein, could markedly affect the parameter k_1, whence depress the development of clusters. Consequently, if t_R were less than the time for cluster to form and grow, the pressure wave would have a chance to be reflected back and to depress its growth. The criterion for the occurrence of fictitious boiling could be thereby stated as follows:

$$L < \frac{1}{2}ct_C. \tag{32}$$

Take water at 120°C and 1 MPa as an example. The corresponding velocity c is estimated as 477 m/s. The critical scale of microchannel could be estimated on the basis of Eq. (32) as $L_C = 2.4$ mm. Restated, if the channel size is less than approximately 2.4 mm, the fictitious boiling phenomenon would emerge.

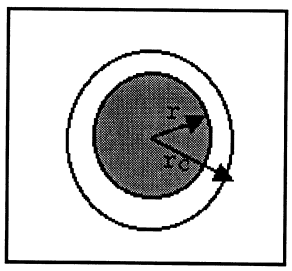

Fig. 6. Growing model of cluster.

4. Conclusions

In this work the role of perturbations on the dynamics of clusters was investigated, from which a physical interpretation of the fictitious boiling phenomena commonly observed in microscale boiling was proposed. The number balance of cluster was first formulated. A transcritical bifurcation corresponds to

the formation of cluster of finite sizes. Both the effects of internal perturbations and external perturbations on cluster dynamics were examined. The presence of external perturbations but the internal perturbations could depress the development of clusters, thereby correlating with the bubble-extinction characteristic noted in fictitious boiling. A pressure fluctuation model was proposed to provide a criterion to the occurrence of fictitious boiling. The pressure waves being reflected from the channel wall are the external perturbations to clusters. A criterion for the occurrence of fictitious boiling was also proposed.

Acknowledgements

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