

Stochastic modeling of boiling-site interaction

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A stochastic model is proposed and kinetic equations are derived to describe the boiling process on a solid surface. The model considers bubble growth at discrete nucleation sites and accounts for interactions between adjacent sites. The model is valid for initial stages of nucleate boiling when vigorous surface boiling has not yet commenced. The interactions considered are the seeding with vapor of inactive sites by bubbles at neighboring active sites, and the deactivation of active sites by thermal interference from neighboring sites. The stochastic model is applied in Monte Carlo simulation, employing parameters obtained from experimental results, to predict bubble emission rates and heat fluxes from the surface. The numerical results predict the presence of many permanently inactive sites, the formation of active-site clusters, and the rise in the density of active sites with increase in overall heat flux. The description of the homogeneous nucleate boiling process in terms of dynamic percolation theory is presented.

I. INTRODUCTION

Nucleate boiling is commonly encountered in industrial processes. In nucleate boiling, initial vapor bubble generation occurs at discrete nucleation sites on a superheated wall. Poorly wetted and partly gas- or vapor-filled cavities or other surface irregularities serve as such nucleation sites. Several models have been proposed for describing bubble nucleation at such boiling sites, aimed principally at predicting the heat transfer from the surface. One of the major complications in modeling the surface heat removal by nucleate boiling has been the interaction between nucleation sites, whereby active nucleating sites either promote or hinder the emission of bubbles from adjacent sites.

Eddington, Kenning, and Korneichev [1] were the first to indicate that many nucleation sites failed to activate even though they satisfied the site activation condition:

$$R_{\text{cav}} = 2\sigma T_{\text{sat}} \sin\beta / \rho_v h_{LG} (T_w - T_{\text{sat}}), \quad (1)$$

where R_{cav} is the cavity radius, σ is the surface tension, ρ_v is the vapor density, h_{LG} is the heat of vaporization, T_w and T_{sat} are the wall and saturation temperatures, respectively, and β is the contact angle. They related this phenomenon to thermal interference of active sites with adjacent sites, hindering the nucleation at the latter. Such thermal interference might be due to the removal of superheated liquid from the surface by a rising bubble, and the consequent penetration of cooler liquid into the cavities. They also suggested that a bubble departing from a nucleation site could leave a residue of vapor at an adjacent site, thereby "seeding" an inactive site. The ex-

periments performed by Judd and Lavdas [2] corroborated the possibility of the above mechanisms of interaction between nucleation sites.

Kenning and Del Valle [3] presented a surface quenching model for boiling heat transfer which treated the interference between nucleating site by considering the overlap between adjacent sites. By applying geometrical considerations for various random and regular spatial site distributions, they predicted the effect of sites interaction on the heat transfer rate due to the reduction in boiling area, and the increased quenching frequency.

Chekanov [4], followed by Calka and Judd [5], assumed that in noninteracting sites the number of bubble emissions occurring at disjoint time intervals are independent random variables, and that the number of bubbles N generated during any time interval t is Poisson distributed with mean λt , i.e.,

$$P(N|t) = (\lambda t)^N e^{-\lambda t} / N!, \quad N=0,1,2,\dots \quad (2)$$

The latter assumption is valid if $P(1|\tau) = \lambda\tau + O(\tau)$ and $P(N > 2|\tau) = O(\tau)$, i.e., if the probability of one bubble emission during a small time interval τ is proportional to τ and the probability of more than one bubble emission during this time interval is negligibly small. It is known from the theory of stochastic processes [6] that under this assumption the time t for the departure of the ν th bubble is Γ distributed, i.e.,

$$f_{\nu}(t) = \lambda^{\nu} t^{\nu-1} e^{-\lambda t} / \Gamma(\nu), \quad \nu=0,1,2,\dots \text{ and } t \geq 0. \quad (3)$$

In particular, the time up to the first bubble emission

from a particular site is an exponentially distributed random variable:

$$f_1(t) = \lambda e^{-\lambda t}, \quad t \geq 0. \quad (4)$$

Suppose now that N bubbles must be emitted from the adjacent sites before a particular site may emit a bubble. Then, the time t , starting from a bubble emission in one site up to a bubble emission at an adjacent site, will be Γ distributed, with $\nu > 1$ in the case that the emission at one site accelerates the emission at the adjacent site (“attractive” interaction which occurs at short separating distances) and $\nu < 1$ in the opposite case (“repulsive” interaction which occurs at long separating distances). It is important to note that in this model the interference effects are taken into account only implicitly, since bubble emissions from adjacent sites are treated as statistically independent events; the stochastic model developed in the present work is free of such simplifying assumptions. In the case of no interference between the sites, the time from a bubble emission at one site and a bubble emission at an adjacent site will be distributed exponentially. Experimental investigations [4,5] have confirmed the suitability of the Γ distribution for describing site interactions, and revealed “attractive” interaction for short distances between sites and “repulsive” interaction for longer distances.

Sultan and Judd [7] demonstrated that the number density distribution of active sites on a heated surface may be approximated by a Poisson distribution. This assumption implies that the probability of one active site being present on a small surface element is proportional only to the surface element area, and that the probability for two or more active sites being located in this surface element is negligibly small. The active-site number density was found to depend on the heat flux; nevertheless, the overall site density does not depend on the heat flux. Thus, the overall site number density needs to be determined from experiment, and the site spatial distribution pattern on a given surface may be assigned by sampling from the Poisson distribution.

The site interaction phenomena in nucleate boiling processes exhibits stochastic features due to statistical variations in bubble formation rates and in the spatial distribution of nucleation sites on the surface. The generally accepted mechanism for nucleation site interaction has not as yet been developed. It is reasonable, however, to assume that this mechanism is also of a stochastic nature due to random effects associated with the vapor trapping process, which occurs when a cavity traps enough vapor to form a nucleus and statistical variations in the diameters of departing bubbles. This work attempts to formulate a phenomenological stochastic model of the phenomenon and to compare its predictions with the experimental results. The case considered will be that of a homogeneous liquid boiling on a plane horizontal solid surface.

II. KINETIC EQUATIONS FOR THE ACTIVE BOILING-SITE PROBABILITY DENSITY FUNCTION

Calka and Judd [5] found for boiling dichloromethane that the hindering effect between adjacent sites, presum-

ably caused by the thermal interference described above, extends up to a distance of $4D_b$ between the sites, where D_b is the mean bubble departure diameter. In this work, the thermal interference will be accounted for by letting a departing bubble delay nucleation at inactive sites for distances of up to KD_b from it by a time t_D , K and t_D being model parameters.

No information is available concerning the amount of vapor required in a site to initiate nucleation. It is also difficult to assess the amount of vapor retained in a site after a bubble departure and the amount of vapor transferred to an adjacent site by a bubble overlapping it. In the present study the probability that a site captures enough vapor to form a nucleus of radius $R_{\text{nuc}} = R_{\text{cav}} / \sin\beta$ as predicted by expression (1) is considered to be $1 - x_0$, where x_0 is a constant parameter of the model. Once a bubble begins to grow into a liquid with temperature $T_b < T_{\text{sat}}$, its rate of growth may be determined from the expression developed by Mikic, Rohsenow, and Griffith [8]:

$$\frac{dR^*}{dt^*} = \{t^* + 1 + \Theta[t^* / (t^* + \tau_w^*)]^{1/2}\}^{1/2} - (t^*)^{1/2}, \quad (5)$$

$$R^* = Ra / b^2, \quad (6)$$

$$t^* = ta^2 / b^2, \quad (7)$$

$$a = [\pi(T_w - T_{\text{sat}})h_{LG}\rho_v / (7T_{\text{sat}}\rho_L)]^{1/2}, \quad (8)$$

$$b = [12Ja^2\lambda_L / (\pi\rho_L c_L)]^{1/2}, \quad (9)$$

$$Ja = (T_w - T_{\text{sat}})\rho_L c_L / (h_{LG}\rho_v), \quad (10)$$

$$\Theta = (T_w - T_b) / (T_w - T_{\text{sat}}), \quad (11)$$

$$\tau_w^* = \tau_w a^2 / b^2, \quad (12)$$

where Ja is the Jacob number, R is the bubble radius, c_L is the liquid heat capacity, λ_L is the liquid thermal conductivity, ρ_L is the liquid density, and τ_w is defined below. Equation (5) above predicts the growth of a vapor bubble in a pure liquid due to heat transfer from the relaxation microlayer (surrounding the bubble dome) for nonuniform superheating. A more general expression derived by Stralen [9] combines the separate contributions of heat transfer from relaxation and evaporation microlayers with the Rayleigh solution. The resulting equation, however, differs only in its coefficients from Eq. (5) and may be easily incorporated into the stochastic model developed herewith. The bubble departure diameter may be determined from the following correlation [10]:

$$D_b = (4.65 \times 10^{-4} Ja_*^{5/4}) \{ \sigma / [g(\rho_L - \rho_v)] \}^{1/2}, \quad (13)$$

where g is the acceleration of gravity and

$$Ja_* = \rho_L c_L T_{\text{sat}} / (r_G h_{LG}), \quad (14)$$

where Ja_* is the characteristic value of the Jacob number. Alternatively, D_b may be determined from experimental data. The mean waiting time between bubbles (i.e., from one bubble departure to the beginning of the next bubble growth) can be approximated as [10]

$$\tau_w = [\rho_L c_L / (\pi \lambda_L)] \{ R_{\text{cav}} (T_w - T_b) / [T_w - T_{\text{sat}} (1 + 2\sigma v_{LG} / R_{\text{cav}} h_{LG})] \}^2, \quad (15)$$

where v_{LG} is the specific volume change in vaporization. The above expression was obtained by determining the time necessary for the liquid in the vicinity of the nucleation site, which arrived from the bulk liquid following the previous bubble emission, to become supersaturated so that the condition expressed in Eq. (1) above is met. However, τ_w may also be assigned as a model parameter. The above empirical formula does not depend on the heat flux and may hence yield unsatisfactory results, particularly since the value of τ_w is employed in Eq. (5). The random waiting time t_w from bubble emission to the beginning of the next bubble growth, in the case of successful seeding and when there is no delay due to thermal interference, is distributed exponentially with the mean τ_w . It is not cumulative with the delay time t_D , i.e., if $t_w > t_D$, the time up to the beginning of the next bubble growth is t_w ; otherwise it is t_D .

The above assumptions imply that the interaction between sites only occurs upon the emission of a bubble from an adjacent site as suggested first by Judd [11]. This constitutes a certain approximation, since site seeding and thermal interference may occur during the bubble growth period; nevertheless, this approximation is reasonable because the overlap between sites is maximal when a bubble is about to be emitted, and because the thermal interference caused by liquid replacement occurs only when a bubble rises from the surface.

Following Judd and Hwang [12], the heat transfer rate from the surface is given as

$$Q_T = Q_{\text{NC}} + Q_{\text{NB}} + Q_{\text{ME}}, \quad (16)$$

where Q_{NC} , the rate of heat removal by nature convection, is given as

$$Q_{\text{NC}} = 0.18 A_{\text{NC}} \lambda_L [(g\beta\rho_L^2 / \mu_L)(C_L / \lambda_L)]^{1/3} (T_w - T_b)^{4/3}, \quad (17)$$

where A_{NC} is the surface area not covered by bubbles and β is the vapor volumetric expansion coefficient. The term Q_{NB} accounts for the quenching of the surface by fresh liquid upon the rise of a bubble:

$$Q_{\text{NB}} = \int_{W_r} Q_0 (\pi \rho_L C_L \lambda_L t_E)^{1/2} (T_w - T_b) K_R D_b^2 / 2 d\mathbf{r}, \quad (18)$$

where Q_0 is the rate of bubble emission per unit surface, t_E is the elapsed time between two successive bubble emissions from a particular site, and K_R is an empirical parameter representing the area in which the liquid is replaced (Judd and Hwang [12] recommended a value of $K_R = 1.8$) and $d\mathbf{r}$ is the surface element. The term Q_{ME} accounts for the heat removed by each departing bubble by microlayer evaporation:

$$Q_{\text{ME}} = \int_{W_r} Q_0 \rho_L h_{LG} V_{\text{ME}} d\mathbf{r}, \quad (19)$$

where V_{ME} is the average microlayer volume evaporated,

which may be found from experimental results. Thus the heat transfer flux can be expressed as a functional of the mean bubble emission rate Q_0 . The value of Q_0 can be calculated provided the probability density function of active boiling sites is known.

It is possible to derive a relatively simple kinetic equation for the active boiling-site probability density function by using averaged boiling rates, assuming that the system contains sufficiently many sites to allow this approximation. The sites will be categorized as active (A -type sites) if they emit bubbles continuously [i.e., with intervals $t_B = \max(t_w, t_D)$ between bubbles], inactive due to delay (D -type sites) if they are delayed by thermal interference from adjacent sites but have the requisite vapor seed to nucleate, and inactive (S -type sites) if they have recently emitted a bubble and no vapor seed was left. The corresponding probability density functions will be $f_A(\mathbf{r}, t)$, $f_D(\mathbf{r}, t)$ and $f_S(\mathbf{r}, t)$, normalized such that

$$\int_{W_r} [f_A(\mathbf{r}, t) + f_D(\mathbf{r}, t) + f_S(\mathbf{r}, t)] d\mathbf{r} = 1, \quad (20)$$

where r is a position vector and W_r is the boiling surface area. Assume also that only binary interactions occur between sites and that the time correlation between the boiling rates at the interacting sites is small. These assumptions are justified when the site number density is sufficiently large and the duration of site interaction is small. Similar assumptions are made in derivation of the Boltzmann equation in rarefied gas dynamics (e.g., Lifshitz and Pitaevsky [13]). The time evolution of the probability density function of active sites $f_A(\mathbf{r}, t)$ is thus governed by the following kinetic equation which is similar to the Boltzmann equation in molecular gas dynamics:

$$\begin{aligned} \frac{\partial f_A(\mathbf{r}, t)}{\partial t} = & -f_A(\mathbf{r}, t) \cdot r_B \cdot x_0 \\ & - \int_{W_r} \Theta(KD_b - |\mathbf{r} - \mathbf{r}'|) f_A(\mathbf{r}, t) f_A(\mathbf{r}', t) r_B d\mathbf{r}' \\ & + f_D(\mathbf{r}, t) r_D, \end{aligned} \quad (21)$$

where Θ is the Heaviside step function, i.e., $\Theta(z) = 0$ if $z < 0$ and $\Theta(z) = 1$ otherwise. The first term on the right-hand side of Eq. (21) is the rate of site deactivation due to the lack of a vapor seed left after bubble departure, the second term is the rate of site deactivation by thermal interference from adjacent sites, and the third term is the rate of site activation which accounts for activation of delayed sites. Note that sites which lacked a vapor seed would be seeded during bubble emission from adjacent sites which would cause thermal interference, and hence would become D -type sites and not directly A type. The boiling rate at an active site r_B may be approximated as

$$r_B \cong 1 / [t_G + \max(\tau_w, t_D)], \quad (22)$$

where t_G is the bubble growth time. The rate r_D at which sites deactivated by thermal interference (but not lacking a vapor seed) are activated by the completion of the delay time t_D :

$$r_D \cong 1/t_D . \quad (23)$$

It must be noted that the calculation of interaction rates by using the boiling rates is in accordance with the above-mentioned concept that a site affects another only upon bubble emission. The rate of change of the probability density function of inactive sites $f_S(\mathbf{r}, t)$ is given by

$$\begin{aligned} \frac{\partial f_S(\mathbf{r}, t)}{\partial t} = & f_A(\mathbf{r}, t)r_B x_0 \\ & - \int_{W_r} \Theta(D_b - 2|\mathbf{r} - \mathbf{r}'|)(1 - x_0) \\ & \times f_S(\mathbf{r}, t)f_A(\mathbf{r}', t)r_B d\mathbf{r}' , \end{aligned} \quad (24)$$

where the first term is the rate of the deactivation of active sites due to lack of a vapor seed and the second term is the rate of seeding of S -type sites by adjacent boiling sites $[(1 - x_0)$ is the probability of successful seeding]. The rate of change of $f_D(\mathbf{r}, t)$ may be obtained from the requirement that the total number of sites be conserved:

$$\frac{\partial f_A(\mathbf{r}, t)}{\partial t} + \frac{\partial f_S(\mathbf{r}, t)}{\partial t} + \frac{\partial f_D(\mathbf{r}, t)}{\partial t} = 0 . \quad (25)$$

To find the steady-state solution of the above equations, set $\partial f_A / \partial t = \partial f_S / \partial t = \partial f_D / \partial t = 0$ and define

$$\int_{W_r} \Theta(D_b - 2|\mathbf{r} - \mathbf{r}'|)f_A(\mathbf{r}', t)d\mathbf{r}' = \pi D_b^2 \xi_A / 4 , \quad (26)$$

$$\int_{W_r} \Theta(KD_b - |\mathbf{r} - \mathbf{r}'|)f_A(\mathbf{r}', t)d\mathbf{r}' = \pi (KD_b)^2 \eta_A . \quad (27)$$

Then, Eqs. (21)–(24) yield

$$f_S^s(\mathbf{r}) = x_0 f_A^s(\mathbf{r}) / [\pi(1 - x_0)D_b^2 \xi_A / 4] \quad (28)$$

and

$$f_D^s(\mathbf{r}) = f_A^s(\mathbf{r})(r_B / r_D)[x_0 + \pi(KD_b)^2 \eta_A^s] , \quad (29)$$

where the superscript s denotes the steady-state solution. Defining the probability density function for the total number of sites, which depends solely on surface properties,

$$f_t(\mathbf{r}) = f_A(\mathbf{r}, t) + f_D(\mathbf{r}, t) + f_S(\mathbf{r}, t) , \quad (30)$$

one obtains from expressions (28) and (29)

$$\begin{aligned} f_A^s(\mathbf{r}) = & f_t(\mathbf{r}) / \{1 + [4x_0 / [\pi(1 - x_0)D_b^2 \xi_A^s] \\ & + (r_B / r_D)[x_0 + \pi(KD_b)^2 \eta_A^s]]\} . \end{aligned} \quad (31)$$

The obtained steady-state solution is realizable if the nonlinear integral equation (31) has a solution. The stability of this solution is considered in Appendix A. The dependence of the stability of the steady state on the relation between f_A^s and ξ_A^s , as given by expression (A10), indicates that it is the seeding effect which determines whether a steady state is attainable since only one parameter of the model, namely, the probability of successful seeding x_0 , enters these equations. The condition $f_A^s(\mathbf{r}) > \xi_A^s(\mathbf{r})$ implies that in the stable steady-state nucleate boiling, the active-site distribution is inhomogeneous, such that dense clusters of active sites surrounded by nonnucleating regions must appear.

Consider now the steady-state solution in the homogeneous case, i.e., when $f_A^s(\mathbf{r}) = \xi_A^s(\mathbf{r}) = \eta_A^s(\mathbf{r})$. The stability analysis indicates that this steady state would be stable. Equation (31) yields a quadratic equation for $f_A^s(\mathbf{r})$, having the following solution:

$$f_A^{s,h} = -(1 + x_0 r_B / r_D) + \{ (1 + x_0 r_B / r_D)^2 + 4K^2 r_B [\pi D_b^2 f_t - 4x_0 / (1 - x_0)] / r_D \}^{1/2} / (2\pi K^2 D_b^2 r_B / r_D) . \quad (32)$$

The above solution is real and positive only if $f_t > 4x_0 / [\pi(1 - x_0)D_b^2]$. Thus, the steady state in the homogeneous case requires a minimum density of sites to sustain nucleation; otherwise, the steady-state boiling would proceed in an inhomogeneous mode, so that active-site clusters and nonactive zones would form. Again, the seeding interaction is seen to play a crucial role in the possibility of attaining a steady-state solution, since when $x_0 = 0$, i.e., when the seeding probability is 1, Eq. (32) always has a positive solution. Yet another possible steady-state solution is the trivial $f_S^{s,h} = f_t$ and $f_A^{s,h} = f_D^{s,h} = 0$ corresponding to the extinction of nucleation.

Let us further consider the addition of an independent seeding mechanism to Eqs. (21) and (24):

$$\begin{aligned} \frac{\partial f_A(\mathbf{r}, t)}{\partial t} = & -f_A(\mathbf{r}, t)r_B x_0 \\ & - \int_{W_r} \Theta(KD_b - |\mathbf{r} - \mathbf{r}'|)f_A(\mathbf{r}, t)f_A(\mathbf{r}', t)r_B d\mathbf{r}' \\ & + f_D(\mathbf{r}, t)r_D + f_S(\mathbf{r}, t)r_R \end{aligned} \quad (33)$$

$$\begin{aligned} \frac{\partial f_S(\mathbf{r}, t)}{\partial t} = & f_A(\mathbf{r}, t)r_B x_0 \\ & - \int_{W_r} \Theta(D_b - 2|\mathbf{r} - \mathbf{r}'|)(1 - x_0)f_S(\mathbf{r}, t) \\ & \times f_A(\mathbf{r}', t)r_B d\mathbf{r}' - f_S(\mathbf{r}, t)r_R , \end{aligned} \quad (34)$$

where

$$r_R = 1/t_R \quad (35)$$

is the independent vapor seed regeneration rate. To find the stable steady-state solution to the homogeneous case with independent vapor seed regeneration, one needs to solve a polynomial equation of third order for $f_A^{s,h}$; however, in case when $r_R \gg r_B$, the following solution is obtained:

$$f_A^{s,h} = \{ -(1+r_B x_0/r_D) + [(1+r_B x_0/r_D)^2 + 4f_t r_B \pi (KD_b)^2]^{1/2} \} / [2r_B \pi (KD_b)^2] . \quad (36)$$

The linear stability analysis shows that the stationary is stable provided that $r_R \gg r_B$. The latter condition corresponds to fast independent vapor seed generation, so that the significance of seeding interaction is diminished. The above solution always obeys $0 < f_A^{s,h} < f_t$, and hence is realizable. Notably, the creation of a vapor seed in a site by an independent molecular mechanism is known [9] so that the addition of an independent vapor regeneration term is physically reasonable. It is of interest to note that the developed stochastic model can be reformulated in terms of dynamic percolation theory [14] as described in Appendix B.

The derivation of exact kinetic equations adhering to the described model is encumbered by history-dependent terms. Nevertheless, in the boiling process, sites are affected either by delays which have a duration τ_D or by waiting times t_w which are exponentially distributed, so that it is reasonable to assume that the boiling process depends only on its recent history. Referring to the boiling process with discretized time units, the state vector \mathbf{X}_n describing the state of the ensemble of N nucleation sites after n time intervals may then be assumed to depend only on the last k state vectors $\mathbf{X}_{n-1}, \mathbf{X}_{n-2}, \dots, \mathbf{X}_{n-k}$. Thus, the model described above specifies a transition probability

$$P(\mathbf{X}_n | \mathbf{X}_0, \mathbf{X}_1, \dots, \mathbf{X}_{n-1}) \\ = P(\mathbf{X}_n | \mathbf{X}_{n-k}, \dots, \mathbf{X}_{n-2}, \mathbf{X}_{n-1}) .$$

This is a k -dependent Markov chain. By defining $\mathbf{Y}_n = (\mathbf{X}_n, \mathbf{X}_{n+1}, \dots, \mathbf{X}_{n+k-1})$ one obtains a stochastic process which holds the Markovian property, i.e., $P(\mathbf{X}_n | \mathbf{X}_0, \mathbf{X}_1, \dots, \mathbf{X}_{n-1}) = P(\mathbf{Y}_n | \mathbf{Y}_{n-1})$. In the relevant model, this transition probability does not change with time, so that a steady-state solution may be expected to exist as a solution of the system of linear algebraic equations $\mathbf{Y} = \mathbf{P}\mathbf{Y}$ [6].

III. MONTE CARLO SIMULATION PROCEDURE

Even the simplified stochastic model formulated above in terms of the nonlinear integrodifferential equations (21), (24), and (25) above is clearly very difficult to solve analytically. Hence, a numerical simulation procedure is proposed herewith, exploiting the possibility described above to approximate the process as a discrete time Markov process. This representation is achieved by including the history-dependent terms of the stochastic process of boiling-site evolution into the vector of state variables. Mathematically this reduction can be described as transformation of the k -dependent Markov chain into the ordinary Markov chain. The numerical model is based essentially on the results of the comprehensive studies of the mechanism of boiling-site interaction performed by Judd [11]. The N nucleation sites are arranged on the regular square lattice, the area of which is determined as N divided by the site number density. At each nucleation site the vapor trapping process is simulated according to

the described above model. With the probability $1-x_0$ a site captures enough vapor to form a nucleus and becomes an active site.

At each active site a bubble grows during a time interval Δt according to Eq. (5). Since the τ_w values employed were rather large, the solution of the bubble growth equation (5) was approximated by the solution appropriate to inertially controlled growth [8] applicable when the vapor density is very small and relatively small evaporation will cause substantial bubble growth:

$$R^* = t^* . \quad (37)$$

Once the bubble attains a diameter D_b , the bubble departs, leaving at the site a vapor nucleus with probability $1-x_0$. With probability x_0 a nucleus fails to form at an active site and it becomes an inactive site. A time interval t_w required to elapse until the next bubble starts to grow at the same site is sampled from an exponential distribution with τ_w as a mean, and a time counter t_E is set equal to t_w . Upon the bubble rise from the surface, with the probability $1-x_0$ the inactive sites overlapped by it succeed in trapping enough vapor to form a nucleus and to become active sites. The departing bubble can also cause a delay t_D in the nucleation of inactive sites within a radius of KD_b away from the boiling site. Since, as noted above, this delay is not cumulative with t_w or the delays caused by other sites, t_D is added to t_E in the inactive sites only if it exceeds t_E . The seeding interaction is recorded upon the bubble departure at each site overlapped by the departing bubble with probability $1-x_0$. Contributions to heat transfer rates Q_{NB} and Q_{ME} by the departing bubble are then calculated, according to expressions (17) and (18).

Following the above stochastic model, in order to allow for independent generation of a vapor seed in inactive sites so as to prevent the extinction of the boiling process as described above, after every time interval Δt with the probability $1-x_0$ the inactive site succeeds in trapping enough vapor to form a nucleus and become an active site. Since a deactivated site might be reactivated by a molecular mechanism [9,15], the introduction of this source into the kinetic equation is physically reasonable. Certainly site seeding by this homogeneous nucleation can occur when the surface and liquid are both superheated and vigorous surface boiling has not yet commenced.

Following every time interval Δt , the surface area available for heat transfer by natural convection A_{NC} is calculated by deducting the areas occupied by the bubbles located on the surface from the overall surface area, and rate of heat removal by natural convection Q_{NC} is calculated accordingly from expression (17). The rates of heat removal Q_{NB} and Q_{ME} in the expression for the total heat flux (16) are calculated from expressions (18) and (19) after the steady state is attained. Then the values Q_{NB} and Q_{ME} are calculated as a time average of (18) and (19) over the time interval $50 \Delta t$.

Thus, the value of time interval Δt is used only for calculating the heat transfer by natural convection and for the regeneration of vapor seed in stagnant inactive sites. Δt is not employed for calculating site interaction; rather, the site interactions are calculated upon bubble emissions, and hence the time intervals τ_w and t_D affect both the precision of the simulation and the nature of the process. The overall time period simulated should naturally be much longer than the time intervals Δt , τ_w , and t_D , so as to obtain a solution involving long-time effects.

In choosing a plane surface element for simulation, as described above, it is assumed that the surface element is located on an infinitely large surface. Hence, periodic boundary conditions are applied to sites on the boiling surface, whereby the site distribution pattern recurs in the two axes of the plane so that sites close to two opposing boundaries of the computational domain are allowed to interact with each other. These are the usually employed boundary conditions in Monte Carlo lattice simulation (see, e.g., Binder and Heermann [16]).

The interactions between sites during the time interval Δt are taken into account by selecting the affected sites in random order, so as to avoid a situation where certain sites will never nucleate merely because other sites will always be allowed to nucleate before them and thus permanently prevent their boiling, by a thermal interference mechanism.

IV. NUMERICAL RESULTS AND DISCUSSION

The above simulation procedure has been implemented for describing site interactions in the boiling of dichloromethane, in accordance with the experiments conducted by Judd and Hwang [12]. The physical properties are accordingly taken to be those of dichloromethane, at a pressure of 0.5 atm. The liquid bulk temperature was chosen such that $T_{\text{sat}} - T_b = 11.3^\circ\text{C}$. According to Judd and Hwang [12], the overall site density may be estimated as $\sim 1 \times 10^6$ sites/m² (corresponding to lattice spacing 10^{-3} m), and the microlayer volume, bubble departure radius, and surface temperature are taken as a function of the overall heat flux and liquid bulk temperature (see Table I). The simulation time interval Δt was taken as 0.01 s, so that it was much smaller than the mean time between bubble emissions at a single site. The attaining of a steady state was assumed when the expectations of the total boiling rate and the number of active sites were invariant with time; hence, the mean values of these parameters were calculated over periods of $50 \Delta t$. A steady state was always obtained following one such period. The number of sites in the simulation was varied in the range

between 600 and 900, and the dimensions of the simulated boiling surface area were found from this number and the overall site number density. Numerical results presented in Table II were obtained by using the following values of parameters: $\tau_w = 0.02$ s, $t_D = 0.03$ s, $K = 4$, $K_R = 1.8$, $N = 600$, and the threshold value for site nucleation $x_0 = 0.6$. The coefficients K and K_R have a geometrical meaning and their values were taken to be the same order of magnitude as those reported in the literature. The values of the time parameters τ_w and t_D determine the overall boiling rate and are therefore limited to a range of values such that the boiling rate obtained would be of the same order as the experimental value.

As seen in Table II, the simulation results are of the same order of magnitude as the experimental values. For $Q_T/A_T = 7 \times 10^5$ W/m², under the same conditions as above only without interaction between the sites, the active site density was 1×10^6 sites/m² (i.e., all the sites present were active), and the average bubble emission frequency was 102 bubbles/site s (see Fig. 2). Thus, the stochastic model is successful in accounting for the presence of permanently inactive sites.

While the simulation predicts an increase in the active-site number density with a rise in the overall heat flux, it underestimates the extent of this trend. Also, the simulation did not predict the increase of the bubble emission rate with the rise in the overall heat flux. In the simulation, the reason for the increase in the active site number density when increasing Q_T/A_T was the decrease in the bubble departure diameter D_b . It appears that the latter does not suffice to describe the enhancement of the boiling process when increasing Q_T/A_T , so that possibly parameters such as τ_w and t_D need to be decreased. The discrepancies between the experimental and calculated heat transfer rates may also be attributed to the failure to predict the changes in the bubble emission rates in the active sites.

A steady state was attained in the simulation only when the vapor nucleus was allowed to be regenerated independently of site interactions; otherwise, the boiling process extinguished. This is in agreement with the above theoretical analysis based on the simplified stochastic model. It is well known [15] that the rate of homogeneous nucleation is not sufficient to predict the experimentally observed boiling rates. On the contrary, the rate of heterogeneous nucleation from the active nucleation sites allows us to predict the experimentally observed boiling rates. However, the results obtained with the aid of the model described above suggest that the classical kinetic homogeneous nucleation mechanism might be essential to support the quasistationary heterogeneous nucleation and to prevent the extinction of the boiling process at the early stage.

Moreover, as predicted by the above analysis, in the steady-state nucleation sites were either active or permanently inactive. It seems that the permanently inactive sites have no chance to nucleate due to the thermal interference from highly active sites in their vicinity. A plot of the active-site locations on a surface (Fig. 1) indicates that many active sites were arranged in clusters, mostly pairs, such that members of a cluster are located

TABLE I. Nucleation parameters for dichloromethane boiling at 0.5 atm, $T_{\text{sat}} - T_b = 11.3^\circ\text{C}$.

Q_T/A_T (W/m ²)	$T_w - T_b$ ($^\circ\text{C}$)	D_b (mm)	V_{ME} (m ³)
2.5×10^4	38	2.4	2.8×10^{-11}
4.0×10^4	38	1.8	1.4×10^{-11}
6.0×10^4	38	1.4	1.3×10^{-11}

TABLE II. Simulation results vs experimental [12] results ($K=4$, $K_R=1.8$).

Q_T/A_T (10^{-4} W/m 2)		Q_{NC}/A_T (10^{-4} W/m 2)		Q_{ME}/A_T (10^{-4} W/m 2)		Active-site density (10^{-5} sites/m 2)		Bubble emission rate [(bubbles/active site)/s]	
Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.
6.0	6.2	1.0	2.6	2.2	1.4	1.5	1.2	30	30
4.0	5.7	1.2	2.6	1.0	1.3	0.80	0.8	24	30
2.5	5.1	1.8	2.6	0.3	0.9	0.23	0.6	12	25

within a distance of order D_b from each other. Such cluster members may seed each other with vapor. The formation of active nucleation sites clusters has been experimentally observed by Sultan and Judd [7].

Sensitivity analysis of the model parameters indicated a relatively modest effect of the threshold value x_0 ; since an allowance was made for independent vapor seed generation, the effect of seeding by site interaction was weak, and thus changing x_0 did not change the number of active sites but changed the rate of boiling at the active sites. The simulation results were also insensitive to an increase of the number of sites beyond 900; increasing N from 900 to 1800, even when the range of thermal interference was large ($K=4$), did not change the percentage of active sites or the boiling rate by more than 10%. The effect of τ_w was extensive, causing changes by several times in bubble emission rates. The values of τ_w predicted by correlation (15) were not compatible with the use of Eq. (5), and hence τ_w was chosen such that fitting of the experimental results was obtained. Notably the change of τ_w in the range from 2×10^{-4} to 0.5 s caused the very moderate decrease of the fraction of active sites from 12 to 7%.

The effect of changing the delay time interval t_D is demonstrated in Fig. 2. Increasing t_D above 0.003 s

caused the percentage of active sites to decrease. The rate of bubble emission per active site decreased as well while increasing t_D up to 0.015 s (close to the value of τ_w). Further increasing t_D caused this rate to increase, until some asymptotic value was attained. The changes observed may be attributed to the increased thermal interference as t_D increased, so that more sites were permanently deactivated. Nevertheless, above some value of t_D , nucleation at the few sites which remained active was less suppressed by adjacent sites and hence was more vigorous. Eventually, only isolated sites remained active and could no longer be affected by changes in t_D , hence the asymptotic behavior at higher t_D values.

Since in the model the effect of the overall heat flux was accounted for by changing the bubble departure diameter D_b , a calculation was performed in which a varying heat flux was applied by letting D_b be a normally distributed random variable. For a system with $t_D=0.03$ s, $\tau_w=0.02$ s, $x_0=0.6$, $K=4$, $K_R=1.8$, 1×10^6 sites/m 2 , and D_b normally distributed with mean 1.4 mm and standard variation 0.14 mm, 13% of the sites were active, emitting an average 23 bubbles/s active site; in similar

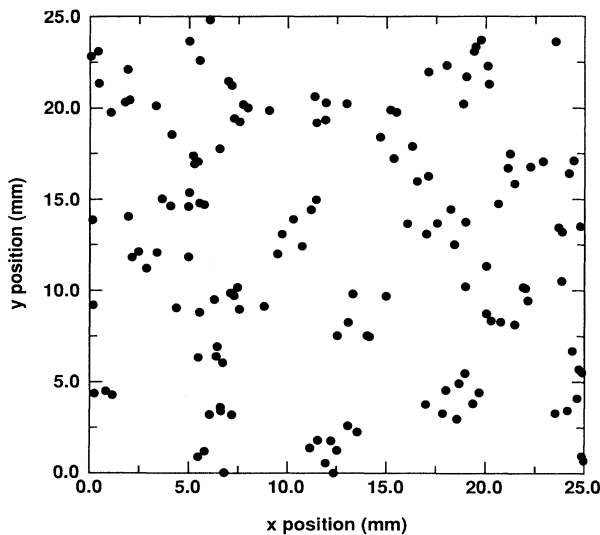


FIG. 1. Locations of active sites on a surface (600 sites on the surface, $D_b=1.4$ mm, $t_D=0.03$ s, $K=4$, $K_R=1.8$, $\tau_w=0.02$ s, 10^6 sites/m 2 , $x_0=0.6$).

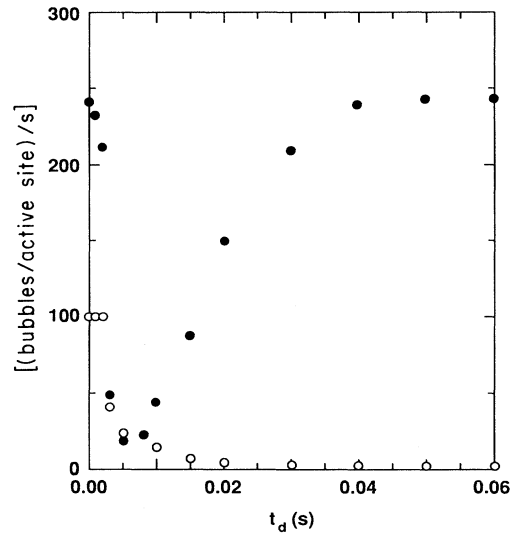


FIG. 2. Effect of t_D on the percentage of active sites and on the average bubble emission rate per active site (600 sites on the surface, $D_b=1.4$ mm, $t_D=0.03$ s, $K=4$, $K_R=1.8$, $\tau_w=0.02$ s, 10^6 sites/m 2 , $x_0=0.6$). \circ , active sites (%); \bullet , bubble emission rate.

conditions but with constant $D_b = 1.4$ mm, only 11% of the sites were active, but an average 31 bubbles/s active site were emitted. Thus, the effect of increasing the variance of D_b was the same as while decreasing t_D , i.e., to increase the number of active sites. The reason is that the range of thermal interference increases with D_b , hence bubbles emitted with $D_b < \bar{D}_b$ cause less interference, whereas the effect of bubbles emitted with $D_b > \bar{D}_b$ is smaller, since the delay effect tends to approach an asymptotic value rather than increase indefinitely (see Fig. 2).

V. CONCLUSIONS

This work has aimed to predict qualitatively site interaction effects, and it appears that the experimentally obtained variations in active-site density and the form of active-site spatial distribution are indeed in agreement with the simulation results.

The simulation results, as well as the experimental findings, concur with the derived kinetic equations in the possibility of attaining a stable steady-state solution and in the formation of active-site clusters. The latter conclusion is also confirmed by the dynamic percolation theory analysis, whereby the steady-state nucleate boiling process may be described as directed percolation on a lattice of nucleation sites.

To improve the precision of the proposed models, better established values for t_D and τ_w seem necessary. Also, improved models for single-site behavior as a function of the heat flux are required; such models are as yet unavailable.

APPENDIX A: ANALYSIS OF THE STABILITY OF THE STATIONARY SOLUTION OF KINETIC EQUATIONS FOR THE PROBABILITY DENSITY FUNCTION OF ACTIVE NUCLEATION SITES

In order to analyze the stability of the solution given by Eq. (31), we employ a linear perturbation analysis, i.e., consider the solution of Eqs. (21) and (24) in the form

$$f_A(\mathbf{r}, t) = f_A^s(\mathbf{r}) + \xi_A e^{-i\omega t}, \quad (\text{A1})$$

$$f_S(\mathbf{r}, t) = f_S^s(\mathbf{r}) + \xi_S e^{-i\omega t}, \quad (\text{A2})$$

$$f_D(\mathbf{r}, t) = f_D^s(\mathbf{r}) + \xi_D e^{-i\omega t}, \quad (\text{A3})$$

where $\xi_A e^{-i\omega t}$ is a perturbation, and by virtue of expression (30), $\xi_A + \xi_S + \xi_D = 0$. Substituting (A1)–(A3) into Eqs. (21) and (24), assuming that the disturbance is uniform in space and neglecting terms of high orders in ξ , the following set of linear homogeneous equations for ξ_A and ξ_S is obtained:

$$\begin{aligned} \omega i \xi_A - \xi_A r_B x_0 - r_D (\xi_A + \xi_S) \\ - \pi (KD_b)^2 r_B \xi_A [\eta_A^s + f_A^s(\mathbf{r})] = 0, \end{aligned} \quad (\text{A4})$$

$$\omega i \xi_S + \xi_A r_B x_0 - \pi D_b^2 r_B (1 - x_0) [f_S^s(\mathbf{r}) \xi_A + \xi_A^s \xi_S] / 4 = 0. \quad (\text{A5})$$

The above set of equations has a nontrivial solution for ξ_A and ξ_S if its determinant equals zero; in this case, a quadratic equation for ω is obtained, having the following solutions:

$$\omega_+ = -iB/2 + i(B^2 + 4C)^{1/2}/2, \quad (\text{A6})$$

$$\omega_- = -iB/2 - i(B^2 + 4C)^{1/2}/2, \quad (\text{A7})$$

where

$$\begin{aligned} B = r_B x_0 + r_D + \pi (KD_b)^2 r_B [\eta_A^s + f_A^s(\mathbf{r})] \\ + \pi D_b^2 r_B (1 - x_0) \xi_A^s / 4, \end{aligned} \quad (\text{A8})$$

$$\begin{aligned} C = -[\pi D_b^2 r_B (1 - x_0) \xi_A^s / 4] \{ r_B x_0 + r_D \\ + \pi (KD_b)^2 r_B [\eta_A^s + f_A^s(\mathbf{r})] \\ - r_D [f_A^s(\mathbf{r}) x_0 r_B / \xi_A^s - r_B x_0] \}. \end{aligned} \quad (\text{A9})$$

When $C > 0$, $\text{Im}\omega_+ > 0$ and the perturbation grows exponentially with time, i.e., the stationary solution is not stable. When $C < 0$, $\text{Im}\omega_+$ and $\text{Im}\omega_- < 0$, so that the perturbation decays exponentially with time and the stationary solution is stable. From expressions (A6)–(A9) it is evident that the stability condition is satisfied if $f_A^s(\mathbf{r}) > \xi_A^s(\mathbf{r})$, i.e., if the active-site density at r is higher than its mean value calculated by averaging over the surrounding seeding sites, or otherwise if

$$f_A^s(\mathbf{r}) > \frac{\{-[\pi D_b^2 r_B (1 - x_0) \xi_A^s / 4] [r_B x_0 + r_D + \pi (KD_b)^2 r_B \eta_A^s] + r_D r_B x_0\}}{\{[\pi D_b^2 r_B (1 - x_0) \xi_A^s / 4] \pi (KD_b)^2 r_B + r_D r_B x_0 / \xi_A^s\}}. \quad (\text{A10})$$

APPENDIX B: THE STOCHASTIC NUCLEATION MODEL IN NOTIONS OF DYNAMIC PERCOLATION THEORY

The stochastic model considered above, without independent vapor seed regeneration, may be reformulated in the notions of dynamic percolation theory [14]. Consider the finite-difference approximation of Eq. (21) for a spatially homogeneous system. Let $n\tau$ ($n = 1, 2, \dots$) be the discrete time variable and $m_{i,n}$ the fraction of sites of

type i ($i = A, D, S$, or t) at time $n\tau$. Then,

$$m_{A,n} = m_{A,n-1} (1 - P_1 - Sk_1 m_{A,n-1}) + P_2 m_{D,n-1}, \quad (\text{B1})$$

where the coefficients are defined as

$$P_1 = \tau r_B x_0, \quad (\text{B2})$$

$$S = \tau r_B, \quad (\text{B3})$$

$$P_2 = \tau r_D. \quad (\text{B4})$$

In the equation (B1), k_1 is the number of neighboring sites capable of thermally interfering with any given site. The equations for m_S and m_D may be similarly obtained from (24) and (25):

$$m_{S,n} = m_{S,n-1} + P_1 m_{A,n-1} - k_2 (S - P_1) m_{A,n-1} m_{S,n-1}, \quad (\text{B5})$$

$$m_D = 1 - m_S - m_A, \quad (\text{B6})$$

where k_2 is the number of sites which the departing bubble may overlap. Then, the steady-state solution can be found as a fixed point of the nonlinear transformations (B1) and (B5):

$$m_S^s = P_1 / [k_2 (S - P_1)], \quad (\text{B7})$$

$$m_A^s = -(P_1 + P_2) + \{(P_1 + P_2)^2 + 4P_2 S k_1 [1 - P_1 / k_2 (S - P_1)]\}^{1/2} / (2S k_1). \quad (\text{B8})$$

Thus, a nontrivial fixed point exists only if

$$k_2 (S - P_1) > P_1. \quad (\text{B9})$$

The above solution is analogous to expression (32) above. The stability of the steady-state solution (B8) may be analyzed as above, the result being that the steady state is stable. Condition (B9) may be viewed as a percolation condition, i.e., a condition under which nucleation spreads over the whole surface. Yet another analogy to percolation processes may be pursued by analyzing the above model. Let the boiling process occur in a spatially homogeneous array of discrete nucleation sites and the time be discretized such that sites may emit bubbles only at discrete times $i\tau$ ($i=1,2,\dots$). Further suppose that the waiting time t_w is always equal to its mean τ_w and define τ such that

$$\tau = t_G + \max(\tau_w, t_D). \quad (\text{B10})$$

Also, define the delay time t_D as

$$t_D = j\tau, \quad (\text{B11})$$

where j is a non-negative integer, $j < 1$ corresponding to absence of thermal interference. Assume that the seeding interaction may be neglected. Defining q_n as the fraction of all sites which emit bubbles at time $n\tau$ and n_D as the number of sites which may interact thermally with any given site, the following difference equation may be formulated for q_n . In words, the probability that a bubble has been emitted at time $n\tau$ equals the probability that a bubble has been emitted at time $(n-1)\tau$ times the probability that no bubble emissions occur among n_D sites at time $(n-1)\tau$ plus the probability that a bubble has been

TABLE III. Solutions to q in Eq. (B13).

n_D	1	2	3	4
1	1.0	1.0	1.0	1.0
2	0.5	0.38	0.32	0.27
3	0.38	0.29	0.25	0.21
4	0.33	0.25	0.21	0.17
5	0.27	0.21	0.17	0.16

emitted at time $(n-j)\tau$ times the probability that no bubbles have been emitted from the same site during the subsequent discrete times $(n-j+1)\tau, \dots, (n-1)\tau$:

$$q_n = q_{n-1} (1 - q_{n-1})^{n_D} + q_{n-j} \prod_{k=1}^{j-1} (1 - q_{n-k}). \quad (\text{B12})$$

The above equation may also describe the boiling process with seeding interaction when there is independent seed regeneration such that $\tau_R \ll \tau$. The equation for the steady-state solution may be found from (B12) by substituting $q = q_n = q_{n-1} = q_{n-2} = \dots = q_{n-j+1}$:

$$q = q(1-q)^{n_D} + q(1-q)^{j-1}. \quad (\text{B13})$$

In Table III, nontrivial solutions of Eq. (B13) are presented. As can be seen from Table III the boiling rate decreases when the thermal interference effect increases (i.e., n_D or t_D increase), although this decrease is most noticeable for relatively low values of t_D and n_D .

Notably, Eqs. (B12) and (B13) are similar in form to the equations obtained from percolation analysis of stochastic models of galactic evolution [17]. In the latter system, it has been suggested that stars which end their lives as supernovas cause new stars to be nucleated. The stochastic model for star growth is thus similar to that employed in the present work for the boiling process, only in the absence of nucleation delay interactions. In the star growth model, as in the present boiling model, the formation of clusters is obtained, in accordance with experimental observations [17]. It has been shown that when a delay mechanism in star interaction is introduced into the stochastic model [18], oscillations are predicted in the vicinity of the steady-state solution, in accordance with experimental observations. Similar oscillations may be predicted from the stochastic nucleation model presented above. The oscillations in the number of active sites or bubble emission rate may be caused by the difference in characteristic times for seeding and delay interactions in nucleation which constitute a feedback mechanism for the nonlinear oscillations. Probably rapid surface temperature fluctuations during nucleate boiling reported by Moore and Mesler [19] can be accounted for by these nonlinear oscillations.

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