Numerical simulation for homogeneous nucleation boiling

Mohammad Nasim Hasan, Masanori Monde and Yuichi Mitsutake
Department of Mechanical Engineering, Saga University, 1 Honjo, Saga, Japan 840-8502

The process of rapid liquid heating with time dependent boundary temperature condition has been simulated by using the idea of 1D semi-infinite heat conduction in conjunction with theory of homogeneous nucleation boiling. A control volume adjacent to the boundary and having the size of critical cluster is considered and the corresponding energy balance is made for two parallel competing processes taking place inside: transient external heat addition and internal vaporization heat consumption due to bubble nucleation and subsequent growth. Results obtained are presented in terms of the maximum attainable liquid temperature and the corresponding time to reach the temperature limit. For water heating with the identical initial and boundary conditions as reported in some literatures, the model results are found to be in good agreement with the experimental counterparts for lower boundary temperature rising rates. However, for higher values of boundary temperature rising rate, the model predicts earlier attainment of maximum liquid temperature and boiling explosion.

Key Words: Transient liquid heating, Homogeneous nucleation boiling, Boiling explosion

1. Introduction
The process of rapid liquid heating and the subsequent boiling explosion has become a subject of great interest due to its potential applications in the operation of bubble driven micro-electric mechanical systems (MEMS) and TJL printers. Due to some practical problems, it is not possible to predict accurately the boiling explosion condition especially at extremely high liquid heating rates. Therefore theoretical model is necessary for better understanding in these cases.

2. Heat transfer model
In the present study, we consider the case of rapid liquid heating with time dependent boundary temperature condition. As a first approximation, the liquid in brief contact with the solid boundary can be considered as one dimensional semi-infinite solid. Therefore the analytical solution of 1D heat conduction equation with initial condition, \( T = T_a \) and boundary condition, \( T = \beta T' \), becomes:

\[
T(x,t) = T_a + 4\beta T' \text{erfc}(x/\sqrt{4\alpha t})
\]  (1)

Where

\[
\text{erfc}(x/\sqrt{4\alpha t}) = \frac{1}{\sqrt{\pi}} \exp(-x^2/4\alpha t) - 2\text{erfc}(x/\sqrt{4\alpha t})
\]

In Eq. (1), \( T \) (K) denotes the temperature at any location, \( x \) (m) and at any time, \( t \) (s) while \( \alpha \) (m/s) and \( \beta \) (K/s) stand for the liquid thermal diffusivity and the rate of boundary temperature rise respectively.

In the present model, we consider a control volume of cross sectional area, \( A \) (m\(^2\)) and thickness, \( x_c \) (m), adjacent to the boundary (\( x = 0 \)) as shown in Fig. 1. Due to differential heat fluxes on both sides of the control volume i.e. \( q_{in} \) (W/m\(^2\)) and \( q_{out} \) (W/m\(^2\)) at \( x = 0 \) and \( x = x_c \) respectively, heat will be added continuously to the control volume that will cause sensible heating and any possible latent heating or boiling. At sufficiently high rate of liquid heating, we assume that boiling within the control volume will be due to homogeneous nucleation only. For small value of \( x_c \), if the average liquid temperature inside the control volume, \( T_{ave} \) (K), is considered to be spatially uniform then the temporal variation of \( T_{ave} \) is found to depend on the volumetric rate of external heat addition, \( q_e \) (W/m\(^3\)), as well as internal heat consumption due to homogeneous boiling, \( q_h \) (W/m\(^3\)), according to the following energy balance equation:

\[
\frac{\partial T_{ave}}{\partial t} = \frac{1}{\rho C_v} [q_e(t) - q_h(t)]
\]  (3)

Where \( \rho \) (kg/m\(^3\)) and \( C_v \) (J/kg.K) stand for liquid density and specific heat respectively. As revealed from Eq. (3), liquid temperature within the control volume, \( T_{ave} \), will continue to increase up to a maximum value, \( T'_* \), at time \( t = t'_* \), until the heat consumption rate due to homogeneous nucleation boiling, \( q_e \), exceeds the rate of external heat addition, \( q_e \). If \( \lambda \) (W/m.K) denotes liquid thermal conductivity then the rate of volumetric heat addition, \( q_e \), can be obtained easily in terms of the heat fluxes across the control volume as:

\[
q_e(t) = \frac{1}{x_c} [q_e(t) - q_{in}(t)] = \frac{1}{x_c} \left[ \frac{\partial T_{ave}}{\partial x} + \frac{\partial q_{in}}{\partial x} \right]
\]  (4)

The rate of volumetric heat consumption due to homogeneous boiling, \( q_h \), can be determined by multiplying the latent heat of vaporization, \( L \) (J/kg), with the rate of vapor generation per unit volume, \( T_G \) (kg/m\(^3\).s) as:

\[
q_h = \frac{1}{x_c} \left[ \frac{\partial T_{ave}}{\partial x} + \frac{\partial q_{in}}{\partial x} \right]
\]
\[ q_\text{v}(t) = L \Gamma_c(t) \]  

(5)

The vapor mass generation rate per unit mixture volume due to homogeneous nucleation boiling, \( \Gamma_c(t) \), can be expressed in terms of the homogeneous nucleation rate, \( J \) (m\(^3\)s\(^{-1}\)), bubble radius, \( r \) (m) and vapor density, \( \rho_v \) (kg/m\(^3\)), as:

\[ \Gamma_c(t) = 4 \pi \int_0^t \left( \rho_v r^2 \frac{\partial r(t', r)}{\partial t} \right) dt' \]

(6)

Among different models of nucleation rate, \( J \), and bubble radius transient, \( r(t, t') \), we follow Carey [1] and Skripov [2] for \( J \) and \( r(t, t') \) respectively. It is noteworthy that the thickness of the control volume, \( x_v \), is considered to be equal to the size of equilibrium critical cluster or vapor embryo, \( 2r_c \) (m) at maximum liquid temperature, \( T' \). For instance Carey [1] proposed the following relation for \( r_c \) as:

\[ r_c = \frac{2 \sigma}{\rho_v (T')} \exp \left\{ \frac{\left( \rho_l (T') - \rho_v (T') \right) R}{\rho_l (T')} \right\} - \rho_l \]  

(6)

Where \( \rho_l \), \( \rho_v \), \( \sigma \) and \( R \) denote bulk liquid pressure, saturation pressure, liquid density and universal gas constant respectively.

3. Results and discussion

Equation (3) is solved together with Eq. (6) for water heating at atmospheric pressure with the identical initial and boundary conditions as reported in Ref. [3-5]. Figure 2 depicts the time history of transient external volumetric heat addition, \( q_\text{v}(t) \), boiling heat consumption, \( q_\text{L}(t) \) and the resultant temperature escalation for boundary temperature rising rate, \( \beta = 3.73 \times 10^7 \text{ K/s} \). As shown in Fig. 2, liquid temperature reaches the maximum value, \( T' \) at \( t = t' \), when the rate of boiling heat consumption, \( q_\text{v} \) just exceeds the rate of external heat addition, \( q_\text{L} \). Figure 3 illustrates the temperature vs. time curves for different boundary temperature rising rates. At higher boundary temperature rising rates, average liquid temperature attains the maximum value, \( T' \) earlier and the magnitude of the maxima increases for higher values of \( \beta \). Figure 4 also makes this fact clear where the effect of heating rate on \( T' \) and \( t' \) is shown quantitatively. A comparative study of the present simulation results with earlier experimental observations as in Ref. [3-5] indicates that for lower values of \( \beta \) simulation results are close to the experimental counterparts but for higher values of \( \beta \) simulation results predicts earlier attainment of maximum liquid temperature, \( T' \), or in other words, earlier occurrence of boiling explosion. This may be partly due to measurement problems involved in case of higher boundary temperature rising rates and the thermal capacitance of the heater materials as reported in [5].

It is important to mention that for all values of \( \beta \) under consideration, critical vapor embryo contains more than 100 molecules at \( t = t' \) that corresponds to a Knudsen number of about 4. Therefore vapor embryo may be considered as continuum for the application of Eq. (6). The input heat flux to the control volume i.e. \( q_w \) is found to vary from 186.69 MW/m\(^2\) to 1328.8 MW/m\(^2\) at \( t = t' \) for boundary temperature rising rate, \( \beta \), ranging from 3.73E07 K/s to 1.80E09 K/s.

4. Conclusion

From the present model, it is quite evident that the semi-infinite 1D heat conduction concept in conjunction with homogeneous nucleation theory can be applied for the prediction of boiling explosion during rapid liquid heating.

![Temporal variation of T<sub>avg</sub>, q<sub>v</sub>(t) and q<sub>L</sub>(t) for β = 3.73E07 K/s](image1)

![Temperature vs. time curve for different boundary temperature rising rates](image2)

![Maximum liquid temperature (T') and time to attain (t') curve for different boundary temperature rising rates](image3)