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Explosive boiling of a liquid droplet

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Abstract

A mathematical model describing growth of an internal vapor bubble produced by homogeneous nucleation within a liquid droplet during explosive boiling is presented. Existing experimental results for explosive boiling of superheated droplets confirm the predictions of the model. The difference between the present model and the classical theories of bubble growth is discussed. \bigcirc 1999 Elsevier Science Ltd. All rights reserved.

1. Introduction

Explosive boiling is a process of rapid phase transition from liquid to vapor which occurs when the liquid is highly superheated (Avedisian, 1985; Reid, 1983; Shepherd and Sturtevant, 1982). The liquid can be heated far beyond its boiling point in the absence of external nucleation sites. Homogeneous nucleation within the bulk of the liquid begins when the liquid temperature reaches the so-called superheat limit (Avedisian, 1985; Skripov, 1974), which is close to the critical temperature.

An excellent review of this phenomenon was written by Avedisian (1985). As Avedisian points out, explosive boiling has been observed during spillage of liquefied natural gases on water, preparation and burning of certain alternative fuels, melt-down of nuclear reactor fuel rods in simulated nuclear reactor accidents, mixing of water and molten metal during casting and dissolving of molten salt in water during paper pulping operations. Explosive boiling has also basic theoretical interest, being a fundamental problem in bubble dynamics and boiling heat transfer. It can be initiated experimentally also by laser heating (Chitavnis, 1987), and rapid decompression (Miller, 1985).

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There exist several experimental studies of vapor bubble growth during explosive boiling (Chitavnis, 1987; Shepherd and Sturtevant, 1982; Avedisian and Glassman, 1981; Avedisian, 1982; Frost and Sturtevant, 1986; Frost, 1988; Miller, 1985). Most of the investigators photographed droplets exploding in a bubble column apparatus to see the explosion evolving. These studies clarified many important features of the process, but not much quantitative information was obtained. Only Shepherd and Sturtevant (1982) obtained a quantitative estimation of vapor bubble growth and evaporation rate during explosive boiling.

These experiments reveal the following properties of explosive boiling at standard pressures:

- 1. Only one bubble is formed inside the droplet (Avedisian, 1982, 1985; Shepherd and Sturtevant, 1982; Avedisian and Glassman, 1981; Frost and Sturtevant, 1986; Frost, 1988).
- 2. The bubble radius grows with constant speed which is much smaller than the speed of sound (the value obtained in Shepherd and Sturtevant (1982) is 14.3 m/s).
- 3. The evaporation rate remains approximately constant during the process (Avedisian, 1985; Shepherd and Sturtevant, 1982).
- 4. The process takes 100–200 μs (Avedisian, 1982, 1985; Shepherd and Sturtevant, 1982; Avedisian and Glassman, 1981; Frost and Sturtevant, 1986; Frost, 1988).
- 5. The temperature of the vapor at the bubble surface is equal to the boiling point of the droplet liquid (Avedisian, 1985, p. 154).
- 6. The classical theory of bubble growth (Plesset and Prosperetti, 1977; Prosperetti and Plesset, 1978) does not describe explosive boiling (Avedisian, 1985; Shepherd and Sturtevant, 1982).

Little has been done to develop a theory of bubble growth during explosive boiling of a liquid droplet (see Avedisian, 1985, p. 132). Ledder (1990) considered a problem of heat transfer during bubble growth under high superheating, and Nguyen et al. (1988) modeled the bubble growth at the superheat limit by postulating that the interfacial liquid velocity is related to the degree of superheating.

Here, we present a model that reproduces internal bubble growth data in drops during explosive boiling.

2. Statement of the problem

Take a spherical liquid droplet of initial radius R_0 which is situated in another fluid. Energy added to the droplet raises its temperature. At time zero the droplet temperature reaches the superheat limit. Explosive boiling is initiated, with homogeneous nucleation forming voids which merge resulting in growth of a bubble inside the droplet as obtained in laser heating and rapid decompression. We study the bubble growth during this process.

The general physical situation is depicted schematically in Fig. 1. We choose a spherical coordinate system with its origin at the center of the droplet. Let $R_1(t)$, $R_2(t)$ be the bubble and droplet radii, respectively (see Fig. 1). Our aim is to calculate R_1 , R_2 as a function of time.

The assumptions we make are based on the experimental observation of explosive boiling of liquid droplets cited in the Introduction. They are:

- 1. Both liquids are inviscid and incompressible and the vapor is an ideal gas.
- 2. The pressure within the vapor bubble is uniform (but can change in time).



Fig. 1. Schematic illustration of explosive boiling of a liquid droplet.

- 3. The evaporation rate is constant and equal to its maximal possible value, which is the kinetic theory limit to the mass flux that can be attained in a phase-change process.
- 4. The flow, bubble and droplet are radially symmetric and the bubble is formed at the center of the droplet.

In the present radially symmetric configuration, the viscous shear effects vanish. However, in preparation for further non-concentric cases (see also Appendix A), we analyzed the possibility of viscous interactions arising. Experiments (Shepherd and Sturtevant, 1982), indicate that the process of explosive boiling takes less than 200 µs for droplets of 5×10^{-4} m initial radius. During this period, vorticity, which diffuses at the rate $\sqrt{(vt)}$ (Batchelor, 1967, p. 279) can penetrate to less than 5 µm, i.e. two orders of magnitude less than the initial radius. As a result, one can assume that the fluids are inviscid.

Also, the bubble growth and fluid velocity are much smaller than the speed of sound and hence both fluids can be considered incompressible. Finally, the ideal gas equation of state is a good description of vapor behavior.

Assumption 2 is based on the analysis of the dynamics of spherical bubbles (Prosperetti et al., 1988) which showed that the pressure distribution in the bubble can be considered uniform.

Assumption 3 is our main hypothesis. It allows possible non-equilibrium effects during rapid evaporation taking place at the bubble surface to be accounted for. The experimental data cited previously show that the evaporation rate is very high, and approximately constant. In principle the evaporation rate can be obtained from kinetic theory (Ytrehus and Ostmo, 1996), but because such a calculation would require a value of the accommodation coefficient, which is generally not known, we propose our model. This is the kinetic theory limitation for the mass flux through the bubble surface (Van Carey, 1992, Chap. 4). The evaporation rate is thus given by the Hertz–Knudsen formula (Van Carey, 1992, p. 114)

$$J = p_{\rm s} \sqrt{\frac{M}{2\pi \Re T_{\rm s} \acute{y}}} \tag{1}$$

Here J is the evaporation rate, T_s is the boiling temperature for the droplet liquid, p_s is the saturation pressure at this temperature, M is the molar mass of the vapor and \Re is the universal gas constant.

It should be stressed that we use the boiling temperature of the liquid in the Hertz–Knudsen formula, and not the temperature of the overheated liquid, following Avedisian (1985, p. 154).

Assumption 4 has been used in previous studies of explosive boiling (Ledder, 1990; Nguyen et al., 1988). It was shown to be a good approximation for explosive boiling of laser heated droplets (Chitavnis, 1987). One can show (see Appendix A) that this approximation is reasonable if the deviation from concentricity does not exceed 25%.

Before we proceed it is important to emphasize the difference between the present analysis and the classical theories of bubble growth. The theory of inertial growth (Rayleigh, 1917) assumes constant pressure inside the bubble. This assumption is incorrect at the first stages of explosive boiling, as we shall see later. On the other hand, the theory of Plesset and Prosperetti (Plesset and Prosperetti, 1977; Prosperetti and Plesset, 1978) stipulates that the pressure inside the bubble be equal to the saturated vapor pressure neglecting possible non-equilibrium effects.

3. Theoretical model

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For spherically symmetric flow the radial component of velocity v_r is defined by conservation of mass

$$v_{\rm r} = \frac{R_1^2}{r^2} v_{\rm r}|_{R_1 + 0} \tag{2}$$

From conservation of mass at the bubble surface one obtains

$$v_{\rm r}|_{R_1+0} = \dot{R}_1 - \frac{J}{\rho}$$
(3)

$$v_{\rm r}|_{R_1 - 0} = \dot{R}_1 - \frac{J}{\rho_{\rm G}} \tag{4}$$

while conservation of momentum results in

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$$p|_{R_2-0} - p|_{R_1+0} = p|_{R_2+0} - p_i + \frac{2\sigma_1}{R_1} + \frac{2\sigma_2}{R_2} + J^2\left(\frac{1}{\rho} - \frac{1}{\rho_G}\right)$$
(5)

Here p is the pressure in the liquid phase, p_i is the pressure inside the growing bubble, ρ is the density of the droplet, ρ_G is the density of the vapor in the bubble, σ_1 and σ_2 are surface tension coefficients at these surfaces, respectively, and dots denote time derivatives. Eq. (5) shows that momentum flux follows from pressure difference and surface tension force.

Proceeding in the accepted manner in the theory of bubble growth (Avedisian, 1985; Prosperetti and Plesset, 1978) we obtain the following equation for the bubble radius R_1 :

$$\left(R_1 \ddot{R}_1 + 2\dot{R}_1^2 - 2\dot{R}_1 \frac{J}{\rho} \right) \left[1 - \frac{R_1}{R_2} \left(1 - \frac{\rho_1}{\rho} \right) \right] + \frac{1}{2} \left(\dot{R}_1^2 - 2\dot{R}_1 \frac{J}{\rho} + \frac{J^2}{\rho^2} \right)$$

$$\left[\frac{R_1^4}{R_2^4} \left(1 - \frac{\rho_1}{\rho} \right) - 1 \right] - \frac{J^2}{\rho_G \rho} + \frac{J^2}{\rho^2} = \frac{1}{\rho} \left[p_i - p_\infty - \frac{2\sigma_1}{R_1} - \frac{2\sigma_2}{R_2} \right]$$

$$(6)$$

Here ρ_1 is the density of the continuous (external) medium and p_{∞} is the pressure far from the droplet.

Substituting Eq. (3) in Eq. (2) and calculating the liquid velocity at the droplet surface we obtain, for the droplet radius

$$\dot{R}_2 = \left(\dot{R}_1 - \frac{J}{\rho}\right) \frac{R_1^2}{R_2^2}$$
(7)

From Eq. (4) the vapor density inside the bubble is

$$\rho_{\rm G} = \frac{J}{\dot{R}_1 - v_{\rm r}|_{R_1 - 0}} \tag{8}$$

Utilizing the model of Prosperetti et al. (1988) one can write

$$\rho_{\rm G} = \frac{J}{\dot{R}_1 + \frac{1}{3} \frac{R_1}{\gamma} \frac{\dot{p}_{\rm i}}{p_{\rm i}}}$$
(9)

where γ is the ratio of specific heats for the vapor.

For the experiment of Shepherd and Sturtevant (1982) we obtain $\dot{R}_1 \approx 15$ m/s. On the other hand, the second term in the denominator does not exceed 0.6–0.7 m/s and therefore can be neglected. Then

$$\rho_{\rm G} = \frac{J}{\dot{R}_1} \tag{10}$$

Finally the pressure inside the bubble is

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$$p_{\rm i} = \rho_{\rm G} \frac{R}{M} T_{\rm s} \tag{11}$$

and the evaporation rate J is given by Eq. (1).

4. Results

For verification of the model we made calculations for explosive boiling of a butane droplet immersed in ethylene glycol comparing them with experiments by Shepherd and Sturtevant (1982).

These results were the only full and accurate data we could find in the literature. The internal bubble is not centered in these runs but, as shown in Appendix A, this does not qualitatively change the analysis.

Fig. 2 shows the bubble radius R_1 as a function of time for our model (1), in comparison with the experiment (Shepherd and Sturtevant, 1982) (crosses) and the calculations based on the classical theory of bubble growth (Plesset and Prosperetti, 1977; Prosperetti and Plesset, 1978) (2), and Rayleigh's theory of inertial bubble growth (Rayleigh, 1917) (3). Both of the latter calculations were taken from Shepherd and Sturtevant (1982). The linear regression of the experimental data is also shown (4).

We see from Fig. 2 that during the first one-third of the process there is full agreement between the experiment and the predictions of our model and that even at the late stages, the difference between the theory and the experiment is always less than 10%. This is far better than predictions of previous theories.

To estimate the influence of material properties on explosive boiling we made calculations for a few qualitative experiments although it is not possible to make direct comparisons between the bubble sizes in the calculation and the experiment due to insufficient experimental data. The experiments that were chosen are the boiling of a water droplet in decane (Avedisian and Glassman, 1981), of a pentane droplet in glycerol (Frost, 1988; Frost and Sturtevant, 1986) and of a diethyl ether droplet in glycerol (Frost, 1988; Frost and Sturtevant, 1986).

Fig. 3 shows the calculated bubble radius versus time dependence for these three cases with the calculation for the experiment of Shepherd and Sturtevant (1982). One sees that the dependence is approximately linear in all the cases and the boiling of water is the fastest. The bubble growth rate obtained in the calculation is 16.3 m/s for butane, 23.2 m/s for water, 17.5 m/s for pentane and 17.2 m/s for diethyl ether.

The dimensionless pressure inside the bubble p_i/p_{∞} is shown in Fig. 4. One sees that at the beginning the pressure increases because the bubble can not expand sufficiently fast to respond to such a high evaporation rate while during the second part of the process the pressure remains approximately constant. We can show that the behavior of the pressure depends on the ratio of the densities of the droplet liquid and the host liquid.

By neglecting the surface tension and the evaporation terms and taking into account that the bubble growth is approximately linear in time, i.e. $\ddot{R}_1 \approx 0$. One can obtain from Eq. (6) an approximate formula for the bubble pressure



Fig. 2. Bubble radius as a function of time: (+) experiment (Shepherd and Sturtevant (1982)); (1) present theory; (2) classical theory (Shepherd and Sturtevant, 1982); (3) classical inertial growth rate (Shepherd and Sturtevant, 1982); (4) linear regression of the experimental data.

$$\frac{p_{\rm i}}{\rho} = \frac{p_{\infty}}{\rho} + \frac{3}{2}\dot{R}_1^2 + \dot{R}_1^2 \left(1 - \frac{\rho_1}{\rho}\right) y \left(\frac{y^3}{2} - 2\right)$$
(12)

where $y = R_1/R_2$.



Fig. 3. Bubble radius as a function of time during explosive boiling: (1) butane droplet in ethylene glycol; (2) water droplet in decane; (3) pentane droplet on glycerol; (4) diethyl ether droplet in glycerol.

Differentiating with respect to y one obtains that

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{p_{\mathrm{i}}}{\rho}\right) > 0 \quad \text{if} \quad \rho_{1} > \rho$$



Fig. 4. Bubble pressure as a function of time during explosive boiling: (1) butane droplet in ethylene glycol; (2) water droplet in decane; (3) pentane droplet in glycerol; (4) diethyl ether droplet in glycerol.

and vice versa, i.e. the pressure cannot fall if the host liquid has greater density than the droplet liquid.

One can adopt a similar approach to develop semi-analytical formulae for the bubble growth rate \dot{R}_1 and the final value of the bubble pressure p_f . Neglecting the above-mentioned terms and assuming $R_1 \approx R_2$ and $p_i \approx p_f$ we obtain an approximate form of Eq. (6) at the final stage

of the process

$$\frac{3}{2}\dot{R}_{1}^{2}\rho_{1} = p_{\rm f} - p_{\infty} \tag{13}$$

or

$$\frac{2}{3}\frac{p_{\rm f} - p_{\infty}}{R_1^2 \rho_1} = 1$$
(14)

The exact calculation from the full Eq. (6) shows that the value for the ratio (14) is 0.92 for butane, 0.95 for pentane, 0.94 for diethyl ether and 1.29 for water. All these values are close to one, so that Eq. (13) is a reasonable approximation.

Using Eqs. (10)–(11) and neglecting p_{∞} in Eq. (14) we can write:

$$\dot{R}_{1} = b_{0} \left(\frac{2}{3} \frac{J}{\rho_{1}} \frac{\mathscr{R}}{M} T_{s}\right)^{1/3}$$
(15)

where b_0 is an empirical coefficient, independent of material properties.

One sees that the bubble growth rate depends on evaporation rate, the molar mass and the boiling temperature of the liquid and the density of the host liquid. According to the exact calculation (Eq. (6)) the value of b_0 is 0.96 for butane, 0.87 for water, 0.94 for pentane and 0.93 for diethyl ether. Eq. (15) with $b_0 = 1$ can therefore be considered a good approximation for the bubble growth rate, for such, and similar cases.

One may conclude by mentioning that the good agreement between predictions of the model and the few existing experimental results indicate that the process of explosive boiling is characterized by bubble formation by homogeneous nucleation and evaporation rate that is equal to its kinetic theory limit. On the other hand, more data is needed to verify the assumptions of the model. Therefore further quantitative experimental investigations of explosive boiling, such as Shepherd and Sturtevant (1982), would be highly desirable.

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Appendix A

The influence of the deviation from concentricity

Explosive boiling etc.

When the bubble is not situated at the center of the droplet, it will not remain spherical because otherwise the pressure could not be constant on its surface. Moreover, when the

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bubble has grown and reaches the droplet surface the evaporation will be different in different directions.

To estimate the influence of the deviation from concentricity we assume radial flow and calculate the error this assumption causes. First we calculate the pressure change on the bubble surface. Then we shall estimate the time for the bubble to reach the droplet surface.

Take a spherical liquid droplet of initial radius R_0 . The center of the droplet is on the z-axis at the distance *a* from the origin so in spherical coordinates the droplet surface is given by

$$R_2(\theta,0) = a\cos\theta + \sqrt{R_0^2 - a^2\sin^2\theta}$$
(A1)

At t = 0 a spherical bubble begins to grow at the origin. Assuming a radial flow-field, we obtain, from Eqs. (2) and (3)

$$v_{\rm r} = \frac{R_1^2}{r^2} \left(\dot{R}_1 - \frac{J}{\rho} \right) \tag{A2}$$

we can write an equation for the trajectory of a fluid particle that at t = 0 was at $r = r_0$ as

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{R_1^2}{r^2} \left(\dot{R}_1 - \frac{J}{\rho} \right) \tag{A3}$$

or

$$r^{3} = r_{0}^{3} + R_{1}^{3} - \frac{3J}{\rho} \int_{0}^{t} R_{1}^{2} dt'$$
(A4)

Utilizing the fact that the bubble growth is approximately linear in time

$$R_1 \approx R_1 t \tag{A5}$$

one obtains the fact that the form of the droplet during the bubble growth is

$$R_2(\theta;t) = \left[R_1^3 \left(1 - \frac{J}{\rho \dot{R}_1} \right) + (a \cos \theta + \sqrt{R_0^2 - a^2 \sin^2 \theta}) \right]^{1/3}$$
(A6)

Using the unsteady Bernoulli equation and neglecting $\ddot{R_1}$ we calculate the pressure p_b at the bubble surface

$$p_{\rm b} - p_{\infty} = \frac{3}{2}\rho\dot{R}_1^2 + (\rho - \rho_1)\left(\frac{R_1^4\dot{R}_1^2}{2R_2^4} - \frac{2\dot{R}_1^2R_1}{R_2}\right) = \text{const} + (\rho - \rho_1)\dot{R}_1^2f(x)$$
(A7)

where

$$x = \frac{R_2}{R_1}; \quad f(x) = \frac{1}{2x^4} - \frac{2}{x} \tag{A8}$$

From Eqs. (A6) and (A7) one can see that the pressure change at the bubble surface will be

relatively small because at the beginning R_2/R_1 is large and hence f(x)' is small. Later R_0/R_1 is small and therefore the θ -dependent term will be small.

To obtain the upper limit for this pressure difference we shall calculate it when dp_b/dR_2 is maximal, i.e.

$$\Delta p = \left[\frac{\mathrm{d}p_{\mathrm{b}}}{\mathrm{d}R_{2}}\right] (R_{2}^{\mathrm{max}} - R_{2}^{\mathrm{min}}) \tag{A9}$$

where

$$R_2^{\max} = R_2(0;t); \quad R_2^{\min} = R_2(\pi;t)$$
 (A10)

are the maximal and minimal values of the radial coordinate at the droplet surface

$$\frac{dp_{b}}{dR_{2}} = (\rho - \rho_{1})\frac{\dot{R}_{1}^{2}}{R_{1}}\frac{df}{dx}$$
(A11)

and therefore dp_b/dR_2 is maximal when

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = 0 \tag{A12}$$

i.e. when $x = \sqrt[3]{2.5}$.

Taking $\theta = \pi/2$ as a mean value and neglecting the $J/\rho \dot{R_1}$ term, which is small, one can write Eq. (A6) as

$$R_2^3 = R_1^3 + (R_0^2 - a^2)^{3/2}$$
(A13)

and then approximately when $x = \sqrt[3]{2.5}$

$$R_1 \approx 0.87 R_0 \tag{A14}$$

Assuming $a \ll R_0$ we obtain in the linear approximation when $x = \sqrt[3]{2.5}$

$$R_2^{\max} - R_2^{\min} \approx 1.1a \tag{A15}$$

and therefore

$$\Delta p = (\rho - \rho_1) \dot{R}_1^2 \frac{0.62a}{R_0}$$
(A16)

The pressure on the bubble surface $(p_b - p_\infty)$ changes from $\frac{3}{2}\rho \dot{R}_1^2$ at the outset to $\frac{3}{2}\rho_1 \dot{R}_1^2$ at the end. Assuming that ρ , ρ_1 and $(\rho - \rho_1)$ are of the same order one sees that

$$\frac{\Delta P}{p_{\rm b} - p_{\infty}} = \frac{0.41a}{R_0} \tag{A17}$$

Therefore the error in pressure will be within a 10% range if

$$\frac{a}{R_0} \le 0.25 \tag{A18}$$

Our analysis remains correct as long as the bubble is wholly inside the droplet. To estimate the range of its validity one should calculate the time $t_{\rm f}$ when the bubble reaches the droplet surface.

One can conclude that the assumption of radial flow is reasonable when the deviation from concentricity does not exceed 25%, as given by Eq. (A18).

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