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Citation: [AIP Conference Proceedings](#) **1685**, 040020 (2015); doi: 10.1063/1.4934415

View online: <http://dx.doi.org/10.1063/1.4934415>

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Nonlinear Dynamics of a Vapor Bubble Expanding in a Superheated Region of Finite Size

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Abstract. Growth of a vapor bubble in a superheated liquid is studied theoretically. Contrary to the typical situation of boiling, when bubbles grow in a uniformly heated liquid, here the superheated region is considered in the form of a millimeter-sized spherical hot spot. An initial micron-sized bubble is positioned at the hot spot center and a theoretical model is developed that is capable of studying bubble growth caused by vapor pressure inside the bubble and corresponding hydrodynamic and thermal processes in the surrounding liquid. Such a situation is relevant to the dynamics of vapor cavities that are created in soft biological tissue in the focal region of a high-intensity focused ultrasound beam with a shocked pressure waveform. Such beams are used in the recently proposed treatment called boiling histotripsy. Knowing the typical behavior of vapor cavities during boiling histotripsy could help to optimize the therapeutic procedure.

INTRODUCTION

A high-intensity focused ultrasound (HIFU) beam can superheat the propagation medium and initiate boiling. Such conditions occur in certain regimes of HIFU therapy such as thermal ablation and histotripsy [1]. Heat deposition from the focused beam results in a localized hot spot of about a millimeter that coincides with the focal region of the beam. If the medium is superheated, *i.e.*, its temperature exceeds boiling temperature, a vapor bubble can grow from an existing nucleus, reaching a millimeter in size within several milliseconds or even faster. Such rapid growth creates significant stresses around the bubble and may result in the radiation of audible sound sometimes called ‘popcorn noise’. If characterized, these sounds may be useful in monitoring some treatments; moreover, millimeter-sized boiling bubbles may also provide useful targets for monitoring treatments with ultrasound imaging. The current paper is devoted to a theoretical study of vapor bubble dynamics under conditions of spherical symmetry.

BASIC EQUATIONS

Following the approach discussed in the thesis [2], the theory is built from first principles, based on the conservation of mass, momentum and energy; the equation of state; and the laws of heat and mass transfer [3, 4]. Liquid that is pushed by the expanding bubble is supposed to behave as an incompressible medium. Although the hot spots created by a HIFU beam have a somewhat ellipsoidal shape, it is reasonable to simplify the problem by considering a spherically symmetric heated region. Under such simplification and with the assumption that an initial nucleus is positioned at the center of the hot region, the entire problem becomes spherically symmetric. Then the equation of motion of liquid around the bubble is reduced to a Rayleigh-Plesset type equation for the radial dynamics [5, 6]. Both the liquid and the gaseous phases have to be taken into account in modeling the heat transfer. Acoustic pressure generated by the growing bubble, as well as other parameters characterizing the growth, can be calculated afterwards from the system of equations that relate these parameters with each other.

Evolution Equations for the Main Parameters

Consider a system of first-order ordinary differential equations for six independent variables that depend only on time: bubble radius R , bubble wall velocity $V = \dot{R}$, liquid pressure at the bubble wall p_w , pressure inside the bubble p_i , amount of vapor inside the bubble (number of moles) n_v , and the liquid temperature at the bubble wall T_w [2]:

$$\dot{n}_v = 4\pi R^2 \frac{\hat{\sigma}}{\sqrt{2\pi M \mathcal{R} T_w}} (p_{sat} - p_v) \quad (1)$$

$$\dot{p}_i = \gamma p_i \left(\frac{\dot{n}_v}{n_v} - \frac{3V}{R} \right) + (\gamma - 1) \frac{3k_g}{R} \frac{T_w - \theta}{\delta_\theta} \quad (2)$$

$$\dot{R} = V \quad (3)$$

$$\dot{V} = k_{2V} \left\{ \frac{k_{1V}}{C} \left(\dot{p}_i + \frac{2\sigma}{R^2} V + \frac{4\mu}{R^2} V^2 \right) + \frac{1}{R(1-V/C)} \left[\left(1 + \frac{V}{C} \right) H - \frac{3}{2} \left(1 - \frac{V}{3C} \right) V^2 \right] \right\} \quad (4)$$

$$\dot{p}_w = \dot{p}_i + \frac{2\sigma}{R^2} V + \frac{4\mu}{R^2} (V^2 - R\dot{V}) \quad (5)$$

An equation for the temperature T_w will be discussed later. In Eqs. (1)-(5) the following notations are used: $k_{1V} = [p^*/(p^* + p_w - p_0)]^{\Gamma} / \rho_0$, $k_{2V} = [1 + 4\mu k_{1V}/(CR)]^{-1}$. Also, the following parameters of the liquid are introduced: $p^* = \rho_0 c_0^2 / \Gamma$ is characteristic internal pressure, c_0 is ambient sound speed, $C = \sqrt{c_0^2 + (\Gamma - 1)H}$ is sound speed at the bubble wall, Γ is an empirical constant ($\Gamma = 6.5$ for water), ρ_0 is density; p_0 is pressure far from the bubble, μ is viscosity, and σ is the surface tension between air and water. The gas content of the bubble is described by the following parameters: $\gamma = c_p / c_v$ is the adiabatic index; k_g is thermal conductivity in the gas; θ is temperature; δ_θ is the thermal boundary layer thickness; M is the molecular weight of vapor; \mathcal{R} is the universal gas constant; p_{sat} is the saturated vapor pressure; and p_v is the partial pressure of vapor. The liquid enthalpy at the bubble wall is expressed as follows:

$$H = \frac{\Gamma}{\Gamma - 1} \frac{p^*}{\rho_0} \left[\left(1 + \frac{p_w - p_0}{p^*} \right)^{(\Gamma-1)/\Gamma} - 1 \right]. \quad (6)$$

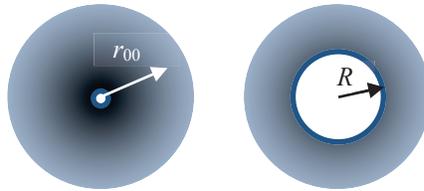


FIGURE 1. Geometry of the problem

Equations for the Bubble Wall Temperature

In addition to Eqs. (1)-(5), a similar equation for the liquid temperature at the bubble wall T_w is needed. It can be derived from the solution of the heat conduction equation and an energy balance at the liquid-gas interface. The latter can be written as follows:

$$4\pi R^2 \left(k_g \frac{T_w - \theta}{\delta_\theta} - k_L \frac{\partial T}{\partial r} \Big|_{r=R} \right) + \dot{n}_v L = 0, \quad (7)$$

where L is the heat of vaporization. The solution of the thermal conductivity problem in liquid can be reduced to two simpler solutions: one is the initial problem solution and the other is the boundary problem solution. The

temperature is divided in two corresponding parts: $T = T_1 + T_2$. If we consider the initial temperature distribution in the heated region in Gaussian form, then $T|_{t=0} = T_{00} \exp(-r^2/r_{00}^2)$, where r is the radial coordinate, r_{00} is the heated region radius, T_{00} is the temperature at the center (Fig. 1). Given the approximations used in [5, 6], the following analytical expressions are then valid:

$$T_1 = \frac{T_{00}}{\sqrt{4\pi D\tau}} \int_0^\infty dh' e^{-\frac{(3h'+R_0^2)^2}{r_{00}^2}} \left[e^{-\frac{(h-h')^2}{4D\tau}} - e^{-\frac{(h+h')^2}{4D\tau}} \right], \quad (8)$$

$$T_2 = \frac{h}{2\sqrt{\pi}} \int_0^\infty d\tau' \frac{T_w(\tau')}{[D(\tau-\tau')]^{3/2}} e^{-\frac{h^2}{4D(\tau-\tau')}}. \quad (9)$$

Here new variables were introduced: $h = (r^3 - R^3)/3$, $\tau = \int_0^t R^4(t') dt'$. Also $R_0 = R(0)$ is the initial bubble radius, $D = k_L/(\rho_0 c_p)$ is the thermal diffusivity, k_L is the thermal conductivity in the liquid, and c_p is the constant-pressure heat capacity. The solutions to Eqs. (8) and (9) make it possible to calculate the spatial derivative of the liquid temperature at the bubble wall $\partial T/\partial r|_{r=R}$. Because the same quantity is defined by Eq. (7), an expression for \dot{T}_w can be calculated numerically.

VAPOR BUBBLE GROWTH IN A UNIFORMLY OVERHEATED LIQUID

To evaluate characteristic behavior of the vapor bubble, a simplified problem was considered for the case when the liquid temperature is constant in time and uniform in space. Suppose also that the liquid is inviscid. Then only two equations remain for the bubble radius and bubble wall velocity:

$$\dot{R} = V \quad (10)$$

$$\dot{V} = \frac{1}{R(1-V/C)} \left[\left(1 + \frac{V}{C}\right) H - \frac{3}{2} \left(1 - \frac{V}{3C}\right) V^2 \right] \quad (11)$$

Numerical simulation results are shown in Fig. 2. In this calculation the initial bubble radius was $R_0 = 10 \mu\text{m}$. Other radii were also tried, but the resulting curves $R(t)$ for the stage when $R \gg R_0$ appeared to be almost insensitive to the choice of R_0 . The bubble radius grows approximately linearly and, as it may be expected, the growth rate increases with the liquid temperature.

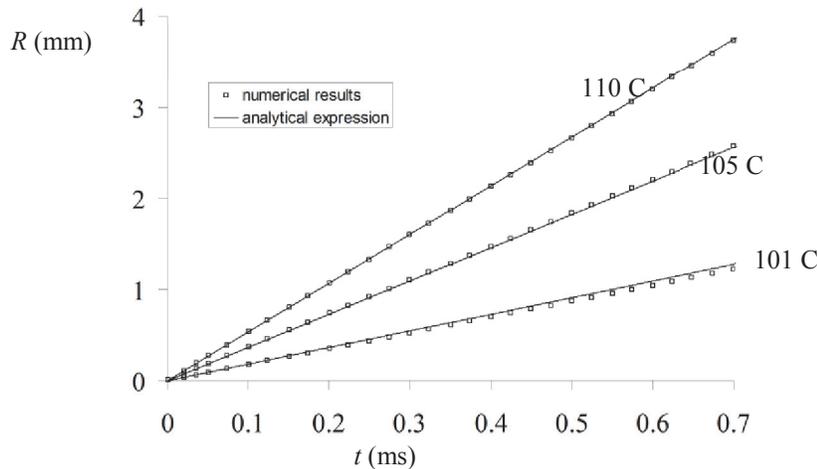


FIGURE 2. Bubble radius versus time for different temperatures of the liquid (indicated near the curves)

This numerical result can be verified analytically, if the liquid is considered incompressible. Then the enthalpy Eq. (6) can be approximated as $H = (p_w - p_0)/\rho_0$, and the bubble dynamics equation takes the Rayleigh equation form:

$$R\ddot{R} + 3\dot{R}^2/2 = (p_v - p_0)/\rho_0, \quad (12)$$

where the right-hand side is constant. In such a situation the solution can be found similarly to the Rayleigh solution of a collapsing cavity [7], but in the considered case the cavity is growing:

$$\alpha t = \int_1^{R/R_0} \frac{z^{3/2} dz}{\sqrt{z^3 - 1}} \quad (13)$$

where $\alpha = \sqrt{2(p_v - p_0)/(3\rho_0 R_0^2)}$. From here, initial growth (when $R \approx R_0$) happens quadratically with time, following the expression $R \approx R_0 \cdot [1 + \sqrt{3}(\alpha t)^2/2]$, and at the stage when $R \gg R_0$ the solution is linear in time and independent of the initial radius [6]: $R \approx \sqrt{2(p_v - p_0)/(3\rho_0)} \cdot t$. For instance, if water temperature is 110°C then $p_v \approx 1.43 \cdot 10^5$ Pa, and a microbubble grows to the radius of 1 mm within approximately 0.2 ms. The curves shown in Fig. 2 are in very good agreement with this analytical expression.

DISCUSSION

The set of equations presented in this paper is a basis for modeling the growth of superheated vapor bubbles under conditions of spherical symmetry. The preliminary results shown in Fig. 2 indicate that even at weak superheating of 101 °C a cavity of 10 micron size can grow to a millimeter-sized vapor bubble in less than a millisecond. If the liquid temperature is 110 °C, the corresponding time is even shorter, around 0.2 ms. This estimate does not account for the finite size of the heated region, which will somewhat decrease the bubble growth rate. Note that in boiling histotripsy experiments with HIFU beams, boiling temperature is reached in several milliseconds, and the vapor cavity is observed by high-speed photography almost immediately [1]. Such observations are in accord with the numerical results from this effort.

ACKNOWLEDGMENTS

We acknowledge funding from RNF №14-15-00665 and NIH EB007643.

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