Small non-sphericity of a convergent shock wave arising in a cavitation bubble in acetone during its collapse

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Abstract. A numerical study of the features of the growth of small deformations of a radially-convergent shock wave in a collapsing cavitation bubble in acetone has been performed. The liquid temperature and pressure are 273.15 K and 15 bar, respectively. At the beginning of collapse, the bubble radius is 500 μm, the bubble is filled with the saturated vapor of acetone. The initial bubble non-sphericity in the form of the second, fourth and sixth spherical harmonics are considered. The dynamics of the vapor in the bubble and the surrounding liquid are governed by the axisymmetric gas dynamics equations closed by wide-range equations of state. The bubble surface is explicitly traced. It is shown that the small non-sphericity of the shock wave during its convergence, similarly to that of the surface of a bubble during its collapse, increases with decreasing its radius in the form of oscillations with growing amplitude. Moreover, the dependence of the increase in the amplitude of those oscillations on the radius of the shock wave in the interval from its formation to its reaching the “hot” bubble nucleus with a radius \( r < 0.25 \mu m \), can be described by a power law with an index of \(-1.18\).

1. Introduction

It is known that very high densities, pressures and temperatures can be achieved inside bubbles during their collapse [1-5]. The highest degrees of compression and heating of the vapor-gas bubble content are attained when radially converging shock waves arise in a bubble during its collapse [2-5]. The convergence and focusing of the shock waves lead to the occurrence of a “hot” core with ultrahigh densities, pressures, and temperatures in a small central region of bubbles. It is shown in [6] that liquids with a higher molecular weight and a lower adiabatic exponent of their vapor are more favorable for realizing cavitation bubble content compression by radially-convergent shock waves. According to [7, 8], in this respect, acetone and tetradeacane are much more preferable than water.

It is clear that a “hot” core in a small central region of a bubble is easier to form when the shape of the radially converging shock wave entering into this region is close to spherical. However, this is usually a very difficult problem because a bubble during collapse and therefore the shock wave in the course of its convergence are always to some extent non-spherical. In particular, the bubble sphericity perturbations arise owing to the action of gravity, the non-uniformity of the liquid pressure field around the bubble, the presence of neighboring bubbles, etc. [9-11]. The energy focusing during the convergence of a non-spherical shock wave is lower than it is in the case of the convergence of a similar spherical wave [12]. Applying the spherically symmetric approximation, it is estimated in [5]...
that the radius of the “hot” core of a cavitation bubble in deuterated acetone collapsing under the experimental conditions of [4] is of the order of 100 nm.

Features of the variation of the non-sphericity of the shock waves radially convergent to some point in a fluid have been studied in [13-17]. The growth of small non-sphericity of such waves in the case of Van der Waals gas is investigated in [13] based on an approximate geometrical theory of shock wave propagation. It is found that the shock wave sphericity perturbations grow as inverse power of the shock wave radius and that the growth is fairly weak, but not as weak as it is in ideal gas. The same approach is used in [14] to show that the shape of the shock wave in an ideal gas recovers after its reflection from the point of its convergence. The growth of the non-small non-sphericity of the convergent shock waves in a gas is considered in [15], using direct numerical simulation. Strong dependence of this growth on the value of Van der Waals excluded volume in Van der Waals equation of state is revealed. An increase in the amplitude of the non-sphericity of a converging shock wave in a collapsing ellipsoidal cavitation bubble in deuterated acetone is studied in [16]. To this end, two-dimensional (axisymmetric) generalization of the model of [5] with wide-range equations of state is applied. It is shown that if the bubble non-sphericity amplitude at the beginning of collapse is about 0.0033 of the bubble radius, the shock wave becomes strongly non-spherical (i.e., its non-sphericity amplitude exceeds 0.5 of its radius) even before its entering into the “hot” core. A similar approach is applied in [17] to find that under the conditions considered in [16], the shock wave remains close to spherical (i.e., its non-sphericity amplitude does not exceed 0.1 of its radius) at its entering into the “hot” core if the amplitude of the initial non-sphericity of the bubble is less than $10^{-5}$ of its radius.

The present paper concentrates on studying the influence of the form of non-sphericity of a cavitation bubble in acetone at the beginning of its collapse on the growth of the non-sphericity of a radially converging shock wave arising inside the bubble in the final stage of its collapse. The initial bubble non-sphericities in the form of the spherical harmonics in the long-wave range are considered.

2. Problem statement

The collapse of a single slightly non-spherical cavitation bubble in acetone is considered. At the beginning of collapse (at time $t = 0$), the vapor in the bubble and the surrounding liquid are motionless, the pressure $p_e$, and temperature $T_e$ of the liquid are 15 bar and 273.15 K, respectively, the vapor in the bubble is at a saturated state with a pressure of 0.094 bar. The initial radius of the bubble is $R_0 = 500 \mu\text{m}$. Under such conditions, a radially converging shock wave arises in the bubble near its surface in the final stage of its collapse. The main attention is directed to studying the influence of the form of a small initial bubble non-sphericity on the growth of the amplitude of the small non-sphericity of this wave during its convergence until it enters into the central region of the bubble with a radius $r < 0.25 \mu\text{m}$.

At an arbitrary instant of time $t$, the surface of the bubble in the spherical coordinates $r$, $\theta$, $\varphi$ with the origin in the center of the bubble can be presented as

$$r = R(t) \left[ 1 + \sum_{n=2}^{\infty} e_{b,n} (t) P_n (\cos \theta) \right],$$

where $R$ is the bubble radius, $e_{b,n}$ is the non-dimensional amplitude of the bubble shape deflection from the spherical one in the form of $P_n (\cos \theta)$, $P_n$ is the Legendre polynomial of degree $n$.

At the beginning of collapse, the surface of the bubble (1) is taken in the form

$$r = R_0 \left[ 1 + e_{b,0} P_0 (\cos \theta) \right],$$

where $e_{b,0}$ is the initial value of $e_{b,n}$.

The influence of the form of the initial small bubble non-sphericity on the increase in the amplitude of the small non-sphericity of the shock wave during its convergence is investigated for the initial perturbations of the spherical shape of the bubble in the form of even spherical harmonics $n = 2, 4, 6$ at $e_{b,n,0} \leq 0.0001$. The long-wavelength range of the initial perturbations is chosen because such
perturbations more easily arise in practice. It is also important that with an increase in the harmonic number, the amount of computation costs grows rather rapidly.

3. Mathematical model and numerical technique

A mathematical model is used [18], in which the vapor and liquid dynamics is governed by the following equations (more precisely, by their axisymmetric version)

\[
\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{u} = 0, \quad \frac{d\mathbf{u}}{dt} + \nabla p = 0, \quad \frac{dE}{dt} + \nabla \cdot (p\mathbf{u} - \kappa \nabla T) = 0, \tag{3}
\]

where \(\rho\) is the density, \(\mathbf{u}\) is the velocity, \(p\) is the pressure, \(E = e + u^2/2\), \(e\) is the specific internal energy, \(T\) is the temperature, and \(\kappa\) is the heat conductivity. Equations (3) are closed by wide-range equations of state for liquid and vaporous acetone, \(p = p(\rho, T), e = e(\rho, T)\), in the form of Mie-Grüneisen [19]. The boundary conditions on the bubble surface are as follows

\[
\rho^+ (\mathbf{D} - \mathbf{u}^+) \cdot \mathbf{n} = \rho^- (\mathbf{D} - \mathbf{u}^-) \cdot \mathbf{n} = j, \quad p^+ = p^- , \tag{4}
\]

\[
T^+ = T^-, \quad (\kappa \nabla T \cdot \mathbf{n})^+ - (\kappa \nabla T \cdot \mathbf{n})^- = jl , \tag{5}
\]

where \(\mathbf{D} = D \cdot \mathbf{n}\) is the velocity of displacement of a bubble surface element, \(\mathbf{n}\) is the outward unit normal, \(l\) is the latent heat of evaporation, \(j\) is the rate of the phase transformations. The upper sign + (−) indicates that the parameter corresponds to the liquid (vapor). Far away from the bubble, \(p = p_\infty, T = T_\infty\). The initial distribution of parameters in the vapor is assumed uniform, and in the liquid it is determined based on the fact that the influence of the liquid compressibility at the beginning of collapse is not significant. Note that this model is a generalization of the one-dimensional model of [5] to the axisymmetric case.

To analyze the non-sphericity of the shock wave, an expansion of its front similar to (1) is used

\[
r = R_\theta (t) \left[ 1 + \sum_{n=2}^{\infty} e_\theta,n (t) P_n (\cos \theta) \right],
\]

where \(R_\theta\) is the radius of the shock wave, \(e_\theta,n\) is the dimensionless amplitude of its non-sphericity.

Equations (3)-(5) are solved numerically using a technique of [18]. In that technique, the initial stage of bubble collapse is simulated with replacing partial differential equations (3)-(5) by ordinary ones of the second order in the radius of the bubble and the amplitude of small perturbation of its sphericity, whereas equations (3)-(5) are used in the final stage. Equations (3)-(5) are solved numerically by applying a modification of the Godunov method of the second order of accuracy in space and time along with moving grids with explicitly tracing the bubble surface. For moderate non-sphericity of the shock wave, a stationary spherical reference system is utilized together with computational grids radially-divergent from the bubble center. After the shock wave becomes strongly non-spherical, cylindrical coordinates are used as a fixed reference system. At the same time, in the central region of bubble, a transition is made from a curved radially-divergent grid to a rectilinear oblique grid, close to uniform Cartesian one.

4. Results

Figures 1, 2 characterize the main features of the bubble collapse (changes in its radius, formation and convergence of a shock wave in the bubble, etc.) under the considered conditions in the case of a very small initial bubble non-sphericity. In particular, Figure 1 shows that a shock wave is formed in the bubble at \(t \approx t_2\), when the bubble radius decreases more than 10 times its initial value.
**Figure 1.** Nearly-spherical collapse of a cavitation bubble in acetone: (a) evolution of the radii of the bubble (solid line) and the shock wave (dashed line), (b) the radial distributions of the pressure (the bubble surface is indicated by open circles) at four time-moments $t_1 - t_4$ in the final stage of collapse.

The inset in (a) shows the end of collapse in more detail.

The process of the bubble content compression by the radially converging shock wave can be divided into three stages. The first stage is the time interval $t_2 \leq t \leq t_3$ between the moment $t \approx t_2$ of the appearance of the shock wave (with the radius $R_s(t_2) \approx 38 \mu m$) and the moment $t \approx t_3$ of its transformation into a strong one (with radius $R_s(t_3) \approx 22 \mu m$). Then the second stage follows, lasting until the shock wave radius takes on the value $R_s(t) \approx 1 \mu m$ (at $t \approx t_4$). At $t \approx t_4$, the shock wave interacts with the compression wave, arising earlier and catching up with the shock wave. This interaction is illustrated in Figure 2. After that the third stage, $t_4 < t \leq t_f$, follows, where $t_f$ is the moment of the shock wave focusing in the bubble center.

**Figure 2.** The pressure profiles at moment $t_4$ and the moments somewhat before and after it.

Figure 3 shows an increase in the non-sphericity of the pressure and temperature fields and the non-sphericity of the shock wave in the final stage of its convergence to the bubble center in the case of the initial bubble non-sphericity with $\varepsilon_{b,n,0} = 0.0001$ where $n = 6$. At the presented time moments, the shock wave radius $R_s$ is equal to 5.5, 2.5 and 0.65 $\mu m$, respectively. At the first of the given moments the shape of the shock wave is close to spherical. At the second moment, both the shock wave and the pressure and temperature fields behind it become clearly non-spherical, with non-sphericity in the form of a harmonic with $n = 6$ (which corresponds to the initial non-sphericity of the bubble). At the
Figure 3. The change in the pressure (left) and temperature (right) fields in the central region $r < 6 \mu m$ of the bubble in the final stage of the shock wave convergence for $\varepsilon_{b,n,0} = 0.0001$, $n = 6$.

last of the presented time moments, the amplitude of the non-sphericity of the shock wave and the pressure and temperature fields behind it increases to quite large values. As a result, the non-sphericity here is determined by not only the harmonic with $n = 6$, but also those with other numbers, which manifests itself in the formation of dents and peaks (and their subsequent alternation) in the pressure and temperature contours in the vicinity of the shock wave.

It follows from Figure 4 that small perturbations of the spherical shape of the shock wave during its convergence, similar to that of the bubble surface during its collapse, increases with decreasing its radius in the form of oscillations with growing amplitude. The difference between these oscillations
for the non-sphericities in the form of harmonics with different $n$ mainly manifests itself in their frequency, which increases with rising $n$. An analysis of the results presented in Figure 4 shows that the amplitude of the oscillations of the small non-sphericity of the bubble (in the form of any harmonic) grows with decreasing its radius according to a power law with an exponent of about $-1.23$. Similarly, at the second and third stages of the convergence of the shock wave, the amplitude of oscillations of its non-sphericity (also in the form of any harmonic) increases with decreasing its radius according to a power law, but with an index of about $-1.18$. In a small interval between the second and third stages, where the interaction of the shock wave with the compression wave catching up with it is realized (Figure 3), the increase turns out to be more rapid. Figure 4b indicates that at the first stage of the shock wave convergence, the amplitude of oscillations of its non-sphericity in the form of a harmonic with $n = 4$ increases with decreasing its radius according to a power law with an exponent close to $-1.18$. Based on the relative short duration of the first stage in terms of the $r/R_0$ coordinate, one can assume that the same growth-law is also valid at this stage for the shock wave non-sphericities in the form of harmonics with $n = 2$ and 6. This makes it possible to conclude that the dependence of the growth in the amplitude of oscillations of the small non-sphericity of the shock wave on its radius in the interval from the moment of its formation ($t \approx t_2 \approx 11.11 \mu s$) to that ($t \approx 11.13 \mu s$) of its entering into the “hot” core $r < 0.25 \mu m$ of the bubble can be described by a power law with an exponent of $-1.18$.

Computations with different values of the small initial bubble non-sphericity amplitude $\varepsilon_{b,n,0}$ reveal that as long as the shock wave non-sphericity amplitude $\varepsilon_{s,n}$ remains small (does not exceed 0.1), the dependence of $\varepsilon_{s,n}$ on $\varepsilon_{b,n,0}$ is linear. An analysis of the results in Figure 4 shows that the shock wave remains close to spherical with $\varepsilon_{s,n} < 0.1$ upon its entering into the small central region $r < 0.25 \mu m$ of the bubble if the initial bubble non-sphericity in terms of $\varepsilon_{b,n,0}$ is not higher than 0.00001.

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