Features of shock-wave compression of cavitation bubble content during collapse in acetone and tetrade cane

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Abstract. Strong compression of the medium in cavitation bubbles during their collapse in acetone at temperatures of 273 and 293 K and tetrade cane at a temperature of 663 K is considered. The features of the behavior of the maximum values of the thermodynamic parameters in the case of the formation of converging shock and isentropic compression waves inside the bubbles in wide ranges of the liquid pressures are studied. The influence of the shock and isentropic waves and their mutual interaction on the level of the maximum values of the thermodynamic parameters attained inside the bubbles is illustrated.

1. Introduction
The possibility of achieving high densities, pressures, and temperatures in a bubble at the final stage of its collapse is of great interest both for science and applications [1, 2]. The highest values of these thermodynamic parameters are realized when converging shock waves are formed in the bubble cavity. In this case, the reached temperatures and densities can exceed $10^7$ K and $10^8$ g/cm$^3$, respectively [1-4]. A criterion for the formation of the converging shock waves in a bubble during its collapse was presented in [5]. According to that criterion, a gas medium with a large molecular mass $M$ and a low adiabatic index $\gamma$ is more suitable for the implementation of the shock waves. Applying this criterion, the possibility of the shock waves appearance in vapor bubbles collapsing in acetone ($M = 58$ g/mol, $\gamma = 1.125$) and tetrade cane ($M = 198$ g/mol, $\gamma = 1.0265$) was investigated in [6-8]. The ranges of the liquid pressure were determined, in which the shock-wave compression of the bubble content is implemented in cold (273 K) and warm (293 K) acetone and hot (663 K) tetrade cane. In the present work, the features of the realization of the shock-wave regime of the bubble content compression in these liquids are studied. In particular, the influence of the interaction between the converging isentropic compression and shock waves arising inside collapsing bubbles on the achieved levels of the maximum values of thermodynamic parameters is considered.

2. Problem statement
The collapse of a single cavitation (vapor) bubble in an infinite volume of liquid (acetone and tetrade cane) is explored. At the beginning of the collapse, the bubble is at rest, its radius is $R_0 = 500 \mu$m. Two values of the initial temperature $T_0$ of acetone (273 and 293 K) and one value of that of tetrade cane (663 K) are considered. The liquid pressure $p_0$ far from the bubble varies over a wide range from 0.17 to 100 bar. The initial vapor pressure is equal to the saturation pressure $p_S$ at temperature $T_0$. The degree of compression of the vapor in the bubble is estimated using the maximum values of pressure, temperature, and density at the boundary of a small central region of the bubble.
with $r \leq 0.25 \text{ µm}$, where $r$ is the radial coordinate measured from the center of the bubble. Inside this small area, the results obtained are not always adequate, since the model of the present work does not take into account the influence of dissociation, ionization, and non-sphericity of the shock waves.

The dynamics of the vapor in the bubble and the dynamics of the surrounding liquid are described by the equations [4, 9]:

$$
\frac{\partial}{\partial t} (pr^2) + \frac{\partial}{\partial r} (p wr^2) = 0,
$$

$$
\frac{\partial}{\partial t} (p wr^2) + \frac{\partial}{\partial r} (p wr^2 + pr^2) = 2 pr,
$$

(1)

$$
\frac{\partial}{\partial t} (psr^2) + \frac{\partial}{\partial r} [w(r^2 + p)] = \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial T}{\partial r} \right).
$$

In Eqs. (1), $w$ is the radial velocity, $e = U + w^2/2$ is the specific total energy, $U$ is the specific internal energy, and $\kappa$ is the coefficient of thermal conductivity. The boundary conditions have the form [4, 9]

$$
r \to \infty: \quad p = p_0, \quad T = T_0;
$$

$$
r = R(t): \quad \dot{R} = \dot{w}_1 + \frac{j}{\rho_1} = \dot{w}_g + \frac{j}{\rho_g}, \quad \rho_l = \rho_g - \frac{4\mu w_1}{R} - \frac{2\sigma}{R},
$$

(2)

$$
\kappa_r \left( \frac{\partial T}{\partial r} \right)_{j_t} - \kappa_g \left( \frac{\partial T}{\partial r} \right)_{s_g} = j_l(p_j), \quad T_t = T_g.
$$

Here, $\mu$ is the dynamic viscosity of the liquid, $\sigma$ is the surface tension, $l$ is the heat of evaporation, $j$ is the rate of evaporation and condensation per unit surface area. The subscripts $l$ and $g$ indicate the reference to liquid and vapor, respectively. To determine $j$ in the processes of nonequilibrium evaporation and condensation, the Hertz-Knudsen-Langmuir formula is used [9].

The realistic equations of state for the liquids and vapors [10, 11] are used, constructed on the basis of experimental data and having the form of the sums of the potential $p^{(p)}$, $U^{(p)}$ and thermal $p^{(T)}$, $U^{(T)}$ components of the pressure $p$ and internal energy $U$ and constant $U^{(ch)}$ (for $U$)

$$
p(p,T) = p^{(p)}(p) + p^{(T)}(p,T), \quad U(p,T) = U^{(p)}(p) + U^{(T)}(T) + U^{(ch)}.
$$

(3)

For $p^{(p)}$, $U^{(p)}$, the generalized Born-Meier potential is used, and $p^{(T)}$, $U^{(T)}$ are defined by the expressions $p^{(T)}(p,T) = p \Gamma(p) U^{(T)}, U^{(T)}(T) = c_v T$, where $\Gamma$ is the Grüneisen coefficient. The heat capacities $c_v$ of liquid and vapor are assumed constant. The parameters of the equations of state for acetone and tetradecane are taken from [10] and [11], respectively.

The cavitation bubble collapses due to the initial pressure drop between $p_0$ (in liquid) and $p_g$ (in the bubble). The greater difference causes the faster and stronger collapse. As a consequence, depending on the liquid pressures $p_0$, three scenarios of the bubble content compression can be distinguished: nearly uniform compression, compression by radially converging isentropic (non-shock) waves and compression by radially converging shock waves [2, 12]. The strongest compression is achieved in the latter scenario [2]. As the liquid pressure $p_0$ increases, the degree of the bubble content compression increases.

Figure 1 shows the influence of the liquid pressure $p_0$ on the maximum values of the thermodynamic parameters (calculated at the boundary of a small central region of the bubble with $r \leq 0.25 \text{ µm}$) attained inside the bubble during its collapse in cold ($T_0 = 273$ K) and warm ($T_0 = 293$ K) acetone and hot ($T_0 = 663$ K) tetradecane. These results were presented in [6-8] (except for those corresponding to the bubble collapse in cold acetone at $p_0 = 40$ and 50 bar).
Figure 1. Dependences of the maximum pressure $p_{\text{max}}$ (a), density $\rho_{\text{max}}$ (b), and temperature $T_{\text{max}}$ (c) at the boundary of a small central region of the bubble with $r \leq 0.25 \mu m$ on the liquid pressure $p_0$ during the collapse of cavitation bubbles in cold ($T_0 = 273$ K, curves 1) and warm ($T_0 = 293$ K, curves 2) acetone and hot tetradecane ($T_0 = 663$ K, curves 3). The symbols indicate the computed values obtained during vapor compression without (small crosses) and with (other symbols) the formation of the convergent shock waves.

It was found earlier [8] that in cold acetone in the entire range of $p_0$ considered, only the scenario of the bubble content compression with the formation of converging shock waves in the bubbles is realized. In contrast, all three scenarios described above are implemented in warm acetone and hot tetradecane. The first scenario (nearly uniform compression) takes place at $p_0 \leq 1$ bar in acetone and at $p_0 \leq 13$ bar in tetradecane. The second scenario (compression by the convergent isentropic waves) is realized if $1 < p_0 \leq 2$ bar in acetone and if $13 < p_0 \leq 18$ bar in tetradecane. The results corresponding to these two scenarios are indicated in figure 1 by small crosses. The third scenario (compression by the convergent shock waves) is implemented at $p_0 > 2$ bar in acetone and at $p_0 > 18$ bar in tetradecane. The scenario of compression by the shock waves in warm acetone is realized in two variants. At pressures $2 < p_0 \leq 3$ bar, the strongest vapor compression is achieved at the second focusing of the convergent shock wave, while at pressures $p_0 > 3$ bar it is attained at its first focusing. In the cases of cold acetone and hot tetradecane, the maximum values of the thermodynamic parameters are achieved only in the second variants of the shock-wave scenario. As is known, the ratio $\rho_+ / \rho_-$ of the densities on the shock wave ($\rho_-, \rho_+$ are the values ahead and behind the shock front, respectively) is limited. In the case of $p_0$ less than a certain value, the ratio $\rho_+ / \rho_-$ does not reach its maximum due to the low intensity of the shock wave, and only when $p_0$ is sufficiently large, the ratio takes its maximum value. In figure 1, the results corresponding to the first case (at $p_0 = 0.17$ and 0.3 bar in cold acetone and at $p_0 = 2.5$ and 3 bar in warm acetone, at $p_0 = 19, 20,$ and 21 bar in tetradecane) are shown by full symbols, and those corresponding to the second case are presented by the same but open symbols. The influence of changing the compression scenarios on the attained maximum values of thermodynamic parameters in the bubble is described in [6, 7].

In the present work the features of the scenario of the bubble content compression by the convergent shock-waves in the cold and warm acetone and hot tetradecane are considered in more detail.

3. Results

3.1. Cold acetone

As can be seen in figure 1, during the bubble collapse in cold acetone, the values of $p_{\text{max}}$ and $T_{\text{max}}$ grow very rapidly, starting from the smallest value equal to $p_0 = 0.17$ bar. The growth of these parameters is explained by an increase in the intensity of the convergent shock wave. The value of $\rho_{\text{max}}$ first
experiences a sharp rise in the range $0.17 \leq p_0 \leq 0.3$ bar, after that it changes much more slowly. As noted above, the ratio $\rho_*/\rho_*$ (of the densities on the shock wave during its convergence) does not reach its maximum at $p_0 < 0.3$ bar and reaches it at $p_0 \geq 0.3$ [8]. The value of $\rho_{\text{max}}$ changes very little in the range from $p_0 = 0.3$ bar to $p_0 \approx 3$ bar (figure 1b), after that (to $p_0 \approx 15$ bar) it noticeably increases. The growth rate of $\rho_{\text{max}}$ slightly decreases in the interval $15 \leq p_0 \leq 30$ bar. At $p_0 = 40$ bar, the value of $\rho_{\text{max}}$ even drops, but at $p_0 = 50$ bar it again turns out to be noticeably higher.

The features of the change in the maximum values of the thermodynamic parameters observed in figure 1 in the scenario of the vapor compression by the shock-waves in the case of cold acetone (as well as in the cases of warm acetone and hot tetradecane) are explained by figures 2 and 3. These figures illustrate the density distributions for a number of values of $p_0$ at which the shock-wave scenario is realized.

![Figure 2. Radial density distributions at $p_0 = 3$ (a), 20 (b), and 50 (c) bar during the collapse of a cavitation bubble in cold ($T_0 = 273$ K) acetone (the circles indicate the density values at the bubble surface, the vertical dashed line shows the boundary of a small central region of the bubble with $r \leq 0.25$ μm).](image-url)

At $p_0 \leq 10$ bar, only one converging shock wave is formed in the collapsing bubble, at $p_0$ in the range 15-30 bar and at $p_0 \geq 30$ bar there appears two and three such waves, respectively. The corresponding variants of the scenario of the bubble content compression by the convergent shock-waves are illustrated in figure 2 for three values of the liquid pressure $p_0 = 3, 20$ and 50 bar. In particular, one shock wave is formed during bubble collapse at $p_0 = 3$ bar (figure 2a). Its intensity increases so much that the ratio $\rho_*/\rho_*$ of the densities reaches its maximum (curves 5 and 6). At $p_0 = 20$ bar (figure 2b), the bubble collapses with the formation of two converging shock waves in its cavity, the second of which overtakes the first. At $p_0 = 50$ bar (figure 2c), three converging shock waves are formed in the bubble. The formation of the third shock wave is illustrated by curve 6. This wave does not have time to catch up with the convergent shock wave resulted from the interaction of the first two shock waves. The latter shock wave causes the formation of a diverging shock wave at the center of the bubble at the time of its focusing. The third converging shock wave and the diverging one interact. After the interaction, the diverging wave continues its outward propagation, while the converging one is soon focused at the center of the bubble, leading to a maximum increase in thermodynamic parameters in the central region of the bubble (curve 7 in figure 2c). As a result of the interaction of the first two shock waves, the spatial density distribution becomes significantly more complicated (curve 4 in figure 2b and curve 3 in figure 2c), which also results in a complication of the density distributions at the instant of the extreme vapor compression (curves 7 in figure 2b,c).

Figure 3 shows the radial density distributions for a number of values of $p_0$, which are realized shortly before the moment of the first focusing of the shock waves at the center of the bubble (figure 3a), and at the moment of the extreme compression of the vapor (figure 3b). The radial density distributions in figure 3a illustrate the value of $\rho_*/\rho_*$ on the shock waves and the density change in the
following compression wave. It should be noted that for each presented value of $p_0$, the value of $\rho_0/\rho_\infty$ is retained until the moment of the shock wave focusing, as is seen in figure 2. Comparison of the cases of different $p_0$ shows an interesting feature that with rising $p_0$ the value of $\rho_0/\rho_\infty$ on the shock wave increases (from 3.6 at $p_0 = 0.6$ bar to 12.5 at $p_0 = 50$ bar), while the density ahead the shock wave $\rho_\infty$ decreases. Along with this, the density growth increases on the compression wave following the shock wave. An increase in the value of $\rho_0/\rho_\infty$ (the maximum of which in perfect gas is equal to $(\gamma + 1)/(\gamma - 1)$) with increasing $p_0$ is apparently caused by a decrease in the values of thermodynamic parameters ahead the shock wave.

It follows from figure 3b (curves I-3) that the vapor density in the central region with $r \leq 0.25 \, \mu m$ at the moment of the extreme compression takes nearly the same values in $0.6 \leq p_0 \leq 3$ bar. As a consequence, the values of $\rho_{\text{max}}$ corresponding to the boundary of this region also turn out to be close to one another. It can also be seen that with growing $r$ in $0.6 \leq p_0 \leq 3$ bar, the vapor density decreases nearly linearly, both in the region with $r \leq 0.25 \, \mu m$ (except for $r \leq 0.1 \, \mu m$) and in its vicinity. As $p_0$ increases in this range, the density gradient in the region $r > 0.25 \, \mu m$ is gradually reduced. With rising $p_0$ in the interval $3 \leq p_0 \leq 10$ bar, the density value increases almost uniformly in the entire bubble region shown in figure 3b (curves 3 and 4). At $p_0 \geq 15$ bar, as it has already been illustrated, the interaction of the converging shock waves results in much more complicated density distribution and in appearance of a density "spike" in curves 5-8 near the bubble center. It can also be seen in figure 3b that such a density spike can occur both at $r \approx 0.25 \, \mu m$ and at a lower or higher value of $r$. This explains the more complicated behavior of the $\rho_{\text{max}}$ and $T_{\text{max}}$ curves (remember that the values of $\rho_{\text{max}}$, $T_{\text{max}}$, and $p_{\text{max}}$ are determined at $r = 0.25 \, \mu m$) in figure 1. The lower values of $\rho_{\text{max}}$ are realized at the higher values of $T_{\text{max}}$.

3.2. Warm acetone

At the cavitation bubble collapse in warm acetone ($T_0 = 293$ K), the radial distributions of the vapor density at the moment of the shock wave focusing change with increasing $p_0$ similar to their alteration in the case of cold acetone (figure 3). In particular, their changes in the case of warm acetone in the ranges $5 \leq p_0 \leq 15$ bar and $15 \leq p_0 \leq 40$ bar correspond to their alteration in the case of cold acetone in the intervals $0.6 \leq p_0 \leq 3$ bar and $3 \leq p_0 \leq 10$ bar, respectively. In the case of warm acetone, the second shock wave, overtaking the first one, is formed in the bubble only at $p_0 \geq 50$ bar. The dependences of
\( \rho_{\text{max}} \) and \( T_{\text{max}} \) on \( p_0 \) in the case of warm acetone are more uniform. It is noteworthy that when (at \( p_0 = 20 \) bar) the growth rate of \( \rho_{\text{max}} \) noticeably increases, the rate of rise in \( T_{\text{max}} \) is a little reduced.

3.3. Hot tetradecane

The scenario of the bubble content compression by the shock waves in hot tetradecane occurs at pressures \( p_0 \geq 19 \) bar. The ratio \( \rho_0/\rho_\infty \) of the densities on the shock wave during its convergence does not reach its maximum in \( 19 \leq p_0 < 22 \) bar, and does it at \( p_0 \geq 22 \) bar. Due to the growth of \( \rho_0/\rho_\infty \) in \( 19 \leq p_0 \leq 22 \) bar, there is a noticeable rise in \( \rho_{\text{max}} \), as in the cases of cold and warm acetone in the corresponding intervals of \( p_0 \). The value of \( \rho_{\text{max}} \) grows much more slowly at \( p_0 \geq 22 \) bar (figure 1b).

A feature of the shock-wave compression scenario of the bubble content in tetradecane is that a converging isentropic compression wave is formed in the bubble at the initial stage of its collapse (figure 4a). Its focusing at the center of the bubble and the subsequent divergence of the wave appeared at the bubble center at the moment of the focusing lead to a density increase in the vicinity of the bubble center, where the convergent shock wave is then formed and converges. This diverging isentropic compression wave contributes to increasing the maximum density \( \rho_{\text{max}} \).

![Figure 4](image-url)

**Figure 4.** Radial density distributions at \( p_0 = 22 \) (a) and 30 (b) bar during the collapse of a cavitation bubble in hot (\( T_0 = 663 \) K) tetradecane (circles indicate the density values at the bubble boundary).

At the tetradecane pressure in \( 25 \leq p_0 \leq 40 \) bar, the convergent isentropic compression wave becomes so strong that the diverging isentropic wave produced by the convergent one at the moment of its focusing not only increases the density but also has a noticeable influence on the converging shock wave, which is formed before the interaction (figure 4b). And this influence suppresses the growth of the value of \( \rho_{\text{max}} \).

With rising \( p_0 \) from 40 to 50 bar, the value of \( \rho_{\text{max}} \) experiences a noticeable growth (figure 1b), and then, at \( p_0 \geq 50 \) bar, becomes nearly constant. The explanation for the mentioned growth in \( \rho_{\text{max}} \) is the following. In contrast to the \( p_0 \) range 25-40 bar, the converging shock wave at \( p_0 \geq 50 \) bar catches up with the first isentropic compression wave in the stage of their convergence. Therefore, the interaction between the converging shock and diverging isentropic waves is not realized. As a result, the growth of \( \rho_{\text{max}} \) is no longer suppressed. It can be seen in figure 1a,c that the dependences of \( \rho_{\text{max}} \) and \( T_{\text{max}} \) on \( p_0 \) have the sharpest rise with increasing \( p_0 \) in the range 40-50 bar. Note that with growing \( p_0 \) in \( p_0 \geq 50 \) bar, the maximum of the ratio \( \rho_0/\rho_\infty \) of the densities on the shock wave does not change (its value increases in acetone), which can be explained by equal (nearly unperturbed) values of thermodynamic parameters ahead the shock wave.

When the bubble collapses in tetradecane at \( 50 \leq p_0 \leq 100 \) bar, a second convergent shock wave appears in the bubble cavity, catching up with the first. The density distributions at the moment of the extreme vapor compression in tetradecane (figure 5) are in qualitative agreement with those in the case of the bubble collapse in cold acetone at \( p_0 \geq 15 \) bar (figure 3b). A “spike” of density is observed near
the center of the bubble. For all the presented values of $p_0$, the spike occurs outside the central region of the bubble with $r \leq 0.25 \ \mu m$. As a result the dependence of $\rho_{\text{max}}$ on $p_0$ is close to a constant value.

Figure 5. Radial density distributions in the central region of the bubble at the moment of the extreme compression of the vapor at $p_0 = 50$ (1), 60 (2), 70 (3), 80 (4), 90 (5), and 100 (6) bar during the cavitation bubble collapse in hot ($T_0 = 663$ K) tetradecane (the vertical dashed line shows the boundary of the small central region of the bubble with $r \leq 0.25 \ \mu m$).

4. Conclusion
The features of the change in the maximum values of the thermodynamic parameters in a cavitation bubble during collapse in acetone at temperatures of 273 and 293 K and tetradecane at a temperature of 663 K have been considered, depending on the liquid pressure. The main attention has been paid to the alteration in the maximum density value in the scenario of the bubble content compression by the convergent shock waves. The influence of the interaction between the shock and isentropic waves on the complexity of the density distribution in the central region of the bubble and on the level of the maximum values of the thermodynamic parameters has been illustrated.

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