Numerical investigation of strong compression of vapor inside spherical cavitation bubbles

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Abstract. Numerical investigation of possibility of realizing shock waves in cavitation bubbles during their collapse in water, acetone, and tetradecane is performed. The radius of the bubble is 500 μm, the liquid pressure and temperature are in the ranges of 1-100 bar and 293-313 K, respectively. A numerical technique is used in which the movement of the interphase boundary is governed by the Rayleigh-Plesset equation. The thermodynamic parameters of the vapor are assumed uniform, the state of the vapor being described by the modified Van der Waals equation. The shock waves inside a bubble in tetradecane are found to arise in all the conditions under consideration. By contrast, inside the bubble in acetone they do not appear at relatively low pressures, while inside the bubble in water they never arise. At equal initial data the shock wave is formed much closer to the interface in the case of tetradecane.

1. Introduction
Dynamics of gas bubbles in liquids is of large scientific and practical significance. Of particular interest is energy accumulation during high-speed cavitation bubble collapse taking place near solids at both small and great distances from their surfaces. Such accumulation can lead to cavitation erosion (solid surface destruction), chemical transformations, bubble glowing, etc. For example, if a bubble at collapse remains close to spherical, very high pressures, densities, and temperatures can be achieved inside its cavity during the final stage of compression of its content.

The compression of the bubble content can be with [1] or without [2] formation of converging shock waves. Most important case is that with the shock waves since they result in the highest pressures and temperatures. Moreover, at their focusing in the central region of the bubble the reflected shock waves occur, propagating in the surrounding liquid. Such diverging shock waves can act on the nearby solid surface as localized short-run pulses of high pressure to result in the surface damages. Therefore, knowledge on the bubble collapse scenarios (with or without the shock waves) is of interest for applications.

The implementation of a shock or shockless scenario of bubble collapse depends on a number of factors. A criterion of formation of converging shock waves in a bubble during its high-speed collapse is proposed [3]. That criterion allows one to estimate the effect of some of the most important physical factors. It is shown in [3] that the shock bubble content compression scenario depends on the vapor properties (molecular weight, specific heat ratio) as well as the conditions of the bubble collapse (liquid pressure and temperature, the initial radius of the bubble). It should be noted that the criterion of [3] implies the use of some results of full hydrodynamic simulation with realistic wide-range equations of state which usually are rather complex.
In this paper, a comparison of water, acetone, and tetradecane is conducted about possibility of formation of shock waves inside cavitation bubbles collapsing in these liquids. A similar comparison of acetone and water was made in [3] at a pressure 15 bar and a temperature 293 K. It was found in [3] that for implementing shock waves in those conditions acetone is much more favorable. The present paper essentially differs from [3] in that much larger liquid pressure and temperature ranges are considered here, namely, those from 1 through 100 bar and from 293 through 313 K, respectively. Another difference is that not only acetone and water but also tetradecane are studied here. Tetradecane is taken following the recommendations in [3], according to which a liquid with the higher molecular weight and the lower specific heats ratio is more preferable for the shock waves. The formation of shock waves in a bubble is stated by a criterion based on results of applying a simple mathematical model in which the movement of the interface is governed by the Rayleigh-Plesset equation, the vapor in the bubble is assumed uniform, the vapor state is described by a modified Van der Waals equation [4].

2. Problem statement
Collapse of a single spherical cavitation bubble in liquid (water, acetone and tetradecane) due to the difference between the initial pressure in the bubble and the pressure in the surrounding liquid is considered. At the beginning of the collapse the temperature $T$ of the liquid and vapor is $T_0$ everywhere, the liquid pressure far from the bubble is $p_0$, the vapor pressure $p_b$ is equal to the saturation pressure $p_S(T_0)$ throughout the bubble. At the initial time moment $t=0$ the bubble radius $R$ is 500 μm, the velocity of the vapor in the bubble, the surrounding liquid, and their interface is zero.

The possibility of forming a shock wave in the cavitation bubble during its high-speed collapse in water, acetone and tetradecane is studied at various liquid pressure $p_0$ and temperature $T_0$ ranging from 1 through 100 bar and from 293 through 313 K, respectively.

3. Technique of estimating formation of shock waves
The appearance of a shock wave in a bubble during its collapse is estimated by using a quite simple numerical technique, in which the bubble radius $R$ is governed by the Rayleigh-Plesset equation

$$
\left(1 - \frac{\dot{R}}{c_l}\right)R\dot{R} + \frac{3}{2}\left(1 - \frac{\dot{R}}{3c_l}\right)\dot{R}^2 = \left(1 + \frac{\dot{R}}{c_l}\right)p_b - p_0 + \frac{R}{c_l} \left(\frac{\dot{p}_b - \dot{p}_0}{\rho_l} \right)
$$

where $c_l$ is the speed of sound in liquid, $p_0$ is the liquid density, the overdot means time derivative.

The vapor pressure $p_b$ in the bubble is governed by a modified Van der Waals equation of state [4]

$$
p_b = \left(p_{b,0} + A\rho_{b,0}^{\beta_1} \left(\frac{p_{b,0} - B}{\rho_{b,0} - B}\right)^\gamma - A\rho_b^{\beta_1} \right)
$$

where $\rho_{b,0}, p_0$ are the initial and current vapor densities in the bubble, $\gamma$ is the adiabatic exponent, $A, B, \alpha$ are constants defined by the following expressions

$$
A = \frac{V_{cr}^{\alpha\beta_1} R_{cr} T_{cr}}{\alpha(V_{cr} - B)}, \quad B = V_{cr} - \frac{2V_{cr}}{\alpha + 1}, \quad \alpha = \frac{1}{2} \left(4V_{cr} \rho_{cr} + \frac{4V_{cr} \rho_{cr}}{R_g T_{cr}} \right)^2, \quad V_{cr} = \frac{1}{\rho_{cr}}, \quad R_g = \frac{R_{ug}}{M}
$$

in which $T_{cr}, p_{cr}, \rho_{cr}$ are the critical values of the temperature, pressure and density, $R_{ug}, R_g$ are the universal and specific gas constants, $M$ is the molecular weight of the vapor. The parameters used in (1)-(3) are given in Table 1.
Equations (1)-(3) are solved numerically by the Runge-Kutta method of high-order accuracy with a variable time step [5].

In the present paper as in [3] it is assumed that the shock wave arises inside a bubble in the course of its collapse if the following inequality is satisfied

\[
\min \frac{\Delta R_{sh}^*}{R} < 1
\]

where \( \Delta R_{sh}^* \) is the distance from the bubble surface (at the time moment \( t \)) to the point of possible occurrence of the shock wave.

The value of \( \Delta R_{sh}^* \) is determined by the expression

\[
\Delta R_{sh}^* \approx -\left(1 - \frac{\dot{R}}{c}\right) k \frac{c^2}{KR}, \quad k = 1 + \frac{\rho c'(\rho)}{c}
\]

where \( \rho, c \) are the vapor density and sound speed (the prime means the derivative with respect to density at constant entropy).

### 4. Validity of the shock wave formation estimate technique

The validation of the shock wave formation estimate technique based on bubble dynamics model (1)-(3) is performed by comparing its results for the water and acetone with those obtained, like in [3], by the full hydrodynamic simulation with the wide-range equations of state (but with dropping the effects of the thermal conductivity and condensation on the interface to eliminate the influence of the thin thermal layer on the boundary vapor density).

**Table 1.**

| Fluid      | \( p_{cr} \) (bar) | \( T_{cr} \) (K) | \( \rho_{cr} \) (kg/m\(^3\)) | \( M \) (g/mol) | \( \gamma \) | \( \rho_i \) (kg/m\(^3\)) | \( c_i \) (m/s) |
|------------|---------------------|------------------|-------------------------------|----------------|-------------|-----------------------------|--------------|
| Water      | 221.2               | 374.12           | 317.8                         | 18             | 1.325       | 998.2                       | 1483         |
| Acetone    | 46.6                | 508.2            | 280                           | 58             | 1.125       | 810                         | 1189         |
| Tetradecane| 16.2                | 693              | 240                           | 198.38         | 1.0265      | 763                         | 1331         |

**Figure 1.** Radial distributions of the vapor and liquid pressure at four moments (curves 1-4) of the final stage of bubble collapse in water (\( a \)) and acetone (\( b \)). Curves 4 correspond to the extreme compression of the vapor in the bubble. Circles show the interface values (the vapor is on their left).
Fig. 1 shows the change of the pressure inside the bubble and its surroundings in the end of the cavitation bubble collapse in water and acetone at \( p_0 = 15 \) bar and \( T_0 = 293 \) K. These results were obtained by the full hydrodynamic model of [3]. Fig. 1a corresponds to the bubble in water, fig. 1b to the bubble in acetone. In the former case the bubble content is compressed without a shock wave while in the latter one a converging shock wave is seen to arise in the bubble at some distance from its surface. The intensity of the shock wave rapidly increases due to the spherical convergence. Owing to the shock wave, the maximum values of the thermodynamic parameters in a small central area of the bubble in acetone are many times higher than those in the bubble in water.

Dependences of ratio \( \Delta R_{sh}^*/R \) on the bubble radius \( R \) are presented in fig. 2 for the bubbles collapsing in water and acetone. The minimum value of such a function is used in criterion (4) to draw a conclusion about shock wave appearance in the bubble. The curves shown in fig. 2 were obtained by model (1)-(3) and by the much more complex full hydrodynamic simulation with the model of [3]. It follows from fig. 2 that the minimum values of \( \Delta R_{sh}^*/R \) for these two models are very close to each other in the case of the bubble in water, and the minimum of \( \Delta R_{sh}^*/R \) obtained by (1)-(3) is 2.3 times less than that obtained by model of [3] in the case of the bubble in acetone. Both models lead to the similar conclusions that the shock wave arises in the bubble in acetone and it does not appear in the bubble in water. This comparison indicates that model (1)-(3) can be used for estimating the minimum value of \( \Delta R_{sh}^*/R \) during bubble collapse.

![Figure 2](image)

Figure 2. Evolution of ratio \( \Delta R_{sh}^*/R \) during cavitation bubble collapse in water (curves 1) and acetone (curves 2) determined by the model of [3] (solid curves) and model (1)-(3) (dotted curves). The horizontal dash-dotted line corresponds to the critical value \( \Delta R_{sh}^*/R = 1 \) in criterion (4) (below this value the shock waves are assumed to arise in the bubble).

5. Results

Fig. 3 shows time-dependences of the bubble radius \( R \) during bubble collapse in water, acetone and tetradecane at the liquid pressure \( p_0 = 15 \) bar for the liquid temperatures \( T_0 = 293 \) and 313 K (the initial bubble radius is 500 μm). Under these conditions the mass of the vapor in the bubble in the case of tetradecane is considerably less than that in the cases of water (by more than 300 times) and acetone (by more than \( 10^4 \) times). As a result, the bubble in tetradecane collapses deeper (its minimum radius \( R_{min} \) is 1.89 μm against 41.48 μm in water and 15.27 μm in acetone). Increasing the initial liquid temperature leads to the growth of the mass of the vapor in a bubble resulting in an increase of \( R_{min} \). A bubble in tetradecane with the vapor mass equal to that in the bubble in acetone at \( T_0 = 293 \) K can be obtained by increasing the liquid temperature by more than 100 degrees.

Fig. 4 shows the dependences of the minimum values of \( \Delta R_{sh}^*/R \) achieved during the cavitation bubble collapse in water, acetone, and tetradecane on the liquid pressure \( p_0 \). Using criterion (4), it can be concluded that under the conditions considered (\( 1 \leq p_0 \leq 100 \) bar and \( 293 \leq T_0 \leq 313 \) K) the shock wave in the bubble in water does not occur. By contrast, the shockless collapse of the bubble in acetone takes place only if \( p_0 \leq 5 \) bar for \( T_0 = 293 \) K and \( p_0 < 10 \) bar for \( T_0 = 313 \) K, whereas in the bubble in tetradecane the shock waves always form.
Figure 3. Evolution of the bubble radius $R$ during bubble collapse in water (a), acetone (b), and tetradecane (c). The liquid temperature $T_0 = 293$ K (curves 1) and $313$ K (curves 2). Circles indicate $R_{\text{min}}$.

Figure 4. The minimum values of $\Delta R_{\text{sh}}^*/R$ achieved during cavitation bubble collapse in water (dotted curves), acetone (solid curves) and tetradecane (dashed curves), as functions of the liquid pressure $p_0$ for the liquid temperature $T_0 = 293$ (curves 1) and $313$ K (curves 2). The horizontal dash-dotted line corresponds to the critical value $\Delta R_{\text{sh}}^*/R = 1$ in criterion (4).

6. Conclusion
Investigation of shock wave formation in a cavitation bubble during its collapse in water, acetone, and tetradecane has been performed for the bubble with the initial radius $500 \, \mu$m at the liquid pressure $p_0$ from 1 through 100 bar and the liquid temperature $T_0$ from 293 through 313 K. A simple mathematical model is used, in which the movement of the interphase boundary is governed by the Rayleigh-Plesset equation, the vapor in the bubble is assumed uniform, being described by the modified Van der Waals equation of state. It has been shown that in all the conditions under consideration the shock waves do not appear inside the bubble in the case of bubble in water. In the case of bubble in acetone at $T_0 = 293$ K and $313$ K the shock waves occur at $p_0 > 5$ bar and 10 bar, respectively. In the case of bubble in tetradecane the shock waves always arise.

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