Mechanisms of cavitation fragmentation of aerosol droplets in an ultrasonic field

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Aerosol technologies often require increasing the dispersion of droplets already present in the air. We proposed a mathematical model and investigated the mechanisms of ultrasonic cavitation fragmentation of aerosol droplets. Expressions for the minimum radiation pressure required for fragmentation of droplets were obtained.

Keywords: aerosol, ultrasound, cavitation, fragmentation.

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The dispersion and concentration of particles are the main characteristics of aerosols, which determine the effectiveness of technological processes. Aerosol technologies are used in various fields of science, industry and medicine. Aerosol particles can be used for the delivery of medicinal substances [1], air purification [2], in agriculture [3], nanotechnology [4] and in other tasks. Aerosols with high dispersion are in increasing demand with the development of aerosol technologies. In this case, it is often necessary to increase the dispersion of particles already existing in the air. For example, in order to effectively remove harmful compounds from the atmosphere due to chemical and photochemical reactions on aerosol particles, it is necessary that aerosol particles remain in the air for as long as possible and have a large specific surface area [5].

It is known that ultrasonic exposure can both contribute to particle enlargement and fragmentation. For example, ultrasonic particle crushing in an aqueous medium is known and used in technologies for homogenization, powder dispersion, etc. The use of ultrasound for crushing particles in the air is complicated by the fact that power losses are high when transferring particles from the air to the substance, therefore, powerful ultrasound sources and special radiation focusing methods are needed to achieve droplet crushing rather than coagulation. Such devices are already being created [2], therefore, for practical implementation it is important to consider in more detail the mechanisms of ultrasonic crushing of aerosol droplets. A criterion was proposed in the theoretical study [6] that determines the predominant mechanism of ultrasound action on a droplet aerosol (crushing or coagulation).

The processes of ultrasonic coagulation are well studied both theoretically and experimentally. The processes of ultrasonic liquid dispersion (transformation of a solid liquid medium into an aerosol) have also been well studied. However, the secondary fragmentation of aerosol droplets already existing in the air in the ultrasonic field has not yet been sufficiently studied. The purpose of this study is to theoretically consider the mechanisms of crushing aerosol droplets suspended in air in powerful ultrasonic fields.

Let us consider a drop with a radius R_d containing a gas bubble (cavitation embryo) with a radius R_b. The model of bubble oscillation in a drop was obtained by Obreshkov et al. [7]. Modifying this approach for the case of ultrasonic exposure, we obtain the equation of pulsation of a cavitation bubble in the form

$$R_b(1-\alpha)\frac{d^2R_b}{dt^2}+\left(\frac{3}{2}-2\alpha+\frac{\alpha^4}{2}\right)\left(\frac{dR_b}{dt}\right)^2 + \frac{1}{\rho}\left[P_a-P_s-P\sin(\omega t)+\frac{2\sigma}{R_b}+\frac{4\eta}{R_b}\frac{dR_b}{dt} - \left(P_a+\frac{2\sigma}{R_0}\right)\left(\frac{R_0}{R_b}\right)^{3\gamma}\right]=0. \quad (1)$$

The bubble and drop are considered spherical, $\alpha = R_b(t)/R_d(t)$, $R_d(t) = R_d(0) + R_b(t) - R_b(0)$, P_s is the saturated vapor pressure, σ is the surface tension, η is the dynamic viscosity of a liquid, ρ is its density, P is the sound pressure amplitude, ω is the angular frequency of ultrasound ($\underline{\omega} = 2\pi f$, f is the frequency, [Hz]), R_0 is the initial radius of the bubble. For $\alpha = 0$, the equation (1) reduces to the classical equation of bubble dynamics in a continuous medium („drops" of infinite size).

The equation (1) was solved numerically by the Euler method (Python code). The results of the solution showed that the following scenarios are visible in the behavior of the bubble, depending on the conditions: fluctuations of the bubble near the equilibrium position, collapse of the bubble (Fig. 1, calculation for water, $f = 22$ kHz, sound level 190 dB). In all scenarios, the destruction of a drop is possible. In the first scenario, we can consider the

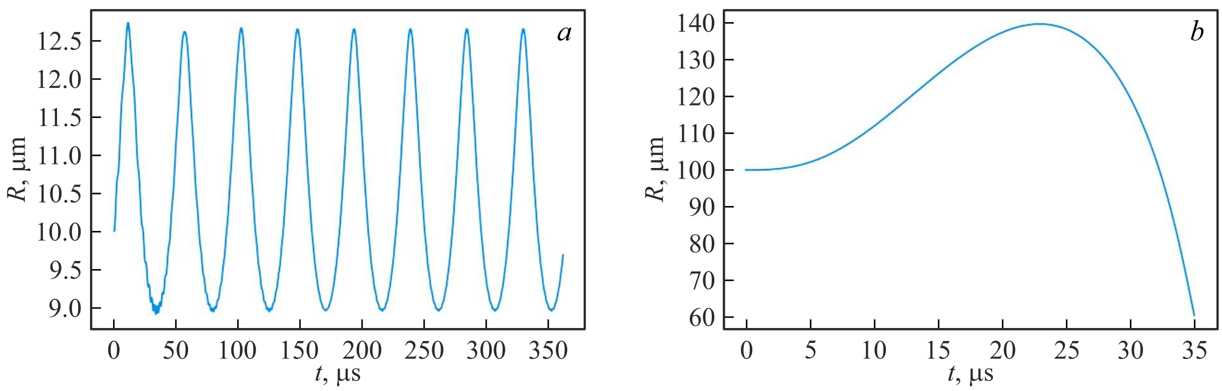

Figure 1. Dependence of the radius of the cavitation bubble on time in various scenarios: *a* — fluctuations without collapse, drop radius 0.1 mm; *b* — bubble collapse (drop radius 1 mm).

accumulation of ultrasound energy by a gas in a bubble over time, while dissipative processes can be neglected. This is the characteristic time of the droplet's interaction with the environment.,

$$t_0 = \frac{R_d}{R_b f}\sqrt{\frac{\rho_d}{\rho_g}} = \frac{\alpha}{f}\sqrt{\frac{\rho_d}{\rho g}},$$

where ρ_d and ρ_g are the densities of droplets and air, respectively. If during this time the vapors in the bubble accumulate energy exceeding the surface energy of the drop, it will collapse. The conditions for estimating the minimum sound pressure P_{cr}, which can cause droplet destruction, in this case look like this:

$$\frac{P_{\text{cr}}^2 \alpha^2 t_0}{8 \cdot c_d \rho_g \sigma} = 1, \qquad (2)$$

where c_g is the speed of sound in the air. This expression is derived from the equality condition of the ultrasound energy absorbed by the bubble, — $E_{uz} = \frac{P2}{2c_g\rho_g}\int\limits_0^{t_0} \pi R_b(t)^2 dt$ and the energy of the droplet surface $E_\sigma = 4\sigma\pi R_d^2$.

The second threshold of sound pressure, corresponding to the mechanism of destruction during bubble collapse, is found from the following relations. Absorption of ultrasonic energy by steam contained in a cavitation bubble is possible by changing its internal energy, the measure of which is temperature: $dE = \nu C_V dT$, where E is the internal energy of steam, ν is the number of moles, T is the absolute temperature, C_ν is the heat capacity at constant volume. In the ideal gas approximation for a triatomic gas, $C_\nu = 5/2R$, where R is the universal gas constant. In an isentropic process (taking into account high speeds), the temperature is related to the gas volume V by the ratio (γ is the adiabatic index): $T \cdot V^\gamma = \text{const}$. The equation (1) determines at each moment of time t the radius of the bubble and, accordingly, its volume. Then, we can determine the temperature of the gas and its internal energy at each moment of time. If at some point in time this energy exceeds the surface energy of the droplet, the droplet will collapse. Calculations show that with a slight increase in pressure above the critical pressure, the bubble collapses, or a pulse increase in temperature (internal vapor energy) occurs, while the energy will be sufficient to destroy the droplet. With a further increase in pressure, a rapid expansion of the bubble may occur with explosive destruction of the droplet.

To analytically estimate the threshold of destruction by the collapse mechanism, we use the Mendeleev–Clapeyron equation, considering the pressure in the bubble at the moment of collapse proportional to the amplitude of the sound wave $P_{\max} \sim aP_{\text{cr}} : aP_{\text{cr}}V_{\text{cr}} = \nu RT_{\text{cr}}$, where a is the coefficient of proportionality. There is an empirical expression for the pressure in a bubble at the moment of collapse, characterized by a gas content of α^3: $P_{\max} \sim P_a/(81\alpha^3)$. Then the proportionality coefficient a in the problem of bubble collapse in a drop can be estimated as $a \sim P_a/(81\alpha^3)$. The following system of equations determines the critical sound pressure for the destruction of a drop according to the second scenario:

$$E_{drop} = \nu C_V (T_{\text{cr}} - T_0),$$

$$P_{\text{cr}} = \nu RT_{\text{cr}}/aV_{\text{cr}},$$

$$T_{\text{cr}} \cdot V_{\text{cr}}^\gamma = T_0 \cdot V_0^\gamma. \qquad (3)$$

Fig. 2 shows the values of the adiabatic time (Figure 2, *a*) and the values of the critical sound energy level (Figure 2, *b*). The larger the α (the relative size of the bubbles relative to the size of the droplet), the lower the required level of external pressure to destroy the droplet.

As calculations using equation (1) show, taking into account changes in temperature and steam energy over time, both „cumulative" and „catastrophic", pulsed scenarios of droplet destruction can be realized. In this case, the threshold values of the sound pressure for the destruction of a drop depend on the size of the drop and on some other parameters included in equation (1). For relatively large droplets and relatively large bubbles, the collapse mode is implemented rather than energy accumulation (the critical pressure level is lower for the collapse mode). For smaller

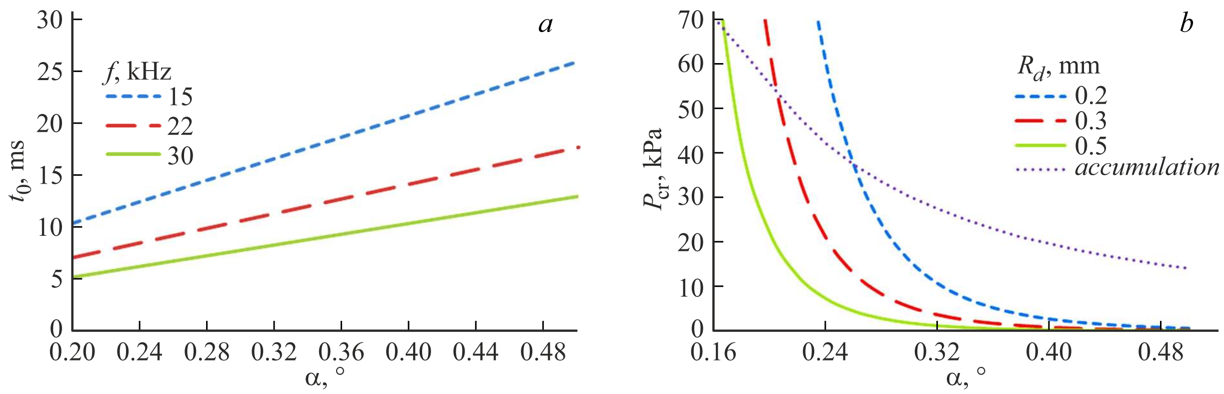

Figure 2. Critical conditions for droplet destruction: *a* — adiabatic time; *b* — critical sound pressure level — droplet destruction during this time in accumulation mode and in collapse mode.

droplets and/or relatively small bubbles, the critical mode will be determined by energy accumulation.

Thus, for the first time, a mathematical model of ultrasonic cavitation crushing of aerosol droplets was proposed and investigated. Calculations show the existence of two scenarios of droplet destruction — energy accumulation during cavitation bubble oscillations or collapse. The implementation of a specific scenario depends on the physico-chemical properties of the droplets, their size, the gas content of the liquid, and the intensity of the ultrasonic field. Critical conditions of cavitation failure are found in accordance with various scenarios.

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Conflict of interest

The authors declare that they have no conflict of interest.

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