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DYNAMICS OF A SPHERICAL ENCLOSURE IN A LIQUID DURING ULTRASONIC CAVITATION

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The paper investigates the process of pulsation of a spherical cavity (bubble) in a liquid under the influence of a source of ultrasonic vibrations. The pulsation of a spherical cavity is described by the Kirkwood-Bethe equations, which are one of the most accurate mathematical models of pulsation processes at an arbitrary velocity of the cavity boundary. The Kirkwood-Bethe equations are essentially non-linear, therefore, to construct solutions and parametric analysis of the bubble collapse process under the influence of ultrasound, a numerical algorithm based on the Runge-Kutta method in the Felberg modification of the 4-5th order with an adaptive selection of the integration step in time has been developed and implemented. The proposed algorithm makes it possible to fully describe the process of cavitation pulsations, to carry out comprehensive parametric studies, and to evaluate the influence of various process parameters on the intensity of cavitation. As an example, the results of calculating the process of pulsation of the cavitation pocket in water are given and the influence of the amplitude of ultrasonic vibrations and the initial radius on the process of cavitation of a single bubble is estimated.

Key words: ultrasonic cavitation, pulsations of a cavity in liquid, Kirkwood-Bethe equations, nonlinear differential equations, numerical algorithm, cavitation intensity

INTRODUCTION

With a local decrease in pressure of the liquid to the pressure of saturated vapor, a process of formation of pockets or bubbles filled with vapor and gas occurs, which is called cavitation. When acoustic vibrations pass through the liquid, acoustic cavitation occurs, which is an effective means of concentrating the energy of a low-density sound wave into a high energy density associated with pulsations and collapse of cavitation bubbles. The general picture of a cavitation bubble formation is as follows. In the phase of rare faction of the acoustic wave in the liquid, a gap is formed in the form of a cavity, which is filled with the saturated vapor of this liquid. In the compression phase, under the action of increased pressure and surface tension forces, the cavity collapses, and the vapor condenses at the interface. A gas dissolved in the liquid diffuses into the cavity through the walls of the cavity, which is then subjected to strong adiabatic compression.

At the moment of collapse, gas pressure and temperature reach significant values. After the collapse of the cavity, a spherical shock wave propagates in the surrounding fluid, rapidly decaying in space. Ultrasonic cavitation is used in the technological processes of liquid purification and degassing, emulsification. In this case, the resonating bubbles act as a mixer, increasing the contact area between two liquids or between a liquid and its bounding surface. In this way, the processes of purification and emulsification of difficult-to-mix liquids are carried out. Ultrasonic cavitation is widely used to excite chemical reactions in an aqueous medium. Cavitation can initiate some chemical processes that do not occur at all without action. Under the influence of cavitation, many chemical reactions are greatly accelerated. For example, if high-intensity ultrasonic waves are applied to polymer solutions, then their viscosity decreases due to the destruction of chemical bonds in the chain of molecules [1-3].

Recently, ultrasonic cavitation has found more and more widespread applications in medicine. It has a damaging effect on red blood cells, yeast cells, and bacteria and is therefore often used for cell extraction. So, using cavitation, it was possible to extract enzymes with a low molecular weight. Cavitation is also used to remove viruses from infected tissue. It was found that at a low intensity of cavitation, the growth of organisms is stimulated, then with an increase in intensity, a certain limit of growth sets in, and, finally, it stops altogether [2]. The rate of death of organisms increases with increasing exposure time and temperature. It is assumed that the destruction of bacteria is due to both the action of cavitation inside the bacteria and the formation of hydrogen peroxide in water. A significant role in the destruction of viruses is played by the release of gas from the solution, as well as the change in pressure.

In the study of cavitation processes, one of the main tasks is to determine the dependence of the bubble radius on time, the bubble collapse time, and the velocity of its boundary movement. One of the most accurate models for describing the process of bubble pulsation is

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the Kirkwood-Bethe model [3-5]. It contains a nonlinear differential equation, the solution of which can only be obtained using numerical methods. Various aspects of the development and application of numerical methods to solving complex problems of mechanics are demonstrated in [6-8]. In this paper, the authors propose and implement a numerical algorithm for solving the Kirkwood-Bethe equation based on the Runge-Kutta-Felberg method of 4-5th order with an adaptive selection of the integration step. Examples of calculations and parametric analysis of the cavitation process of a single bubble in water are given.

SOLUTION TO THE MOTION EQUATION OF A SPHERICAL BUBBLE BOUNDARY IN LIQUID

Let us consider the process of pulsation and collapse of a spherical cavitation pocket of radius *R(t)*, where *t* – time, due to the generation of pressure waves by an ultrasonic source of oscillations. The motion of the bubble wall in a compressible fluid is described by the Kirkwood-Bethe equation [9-11]:

$$R\left(1-\frac{\dot{R}}{c}\right)\ddot{R}+\frac{3}{2}\left(1-\frac{\dot{R}}{3c}\right)\dot{R}^2-\left(1+\frac{\dot{R}}{c}\right)H-\frac{R}{c}\left(1-\frac{\dot{R}}{c}\right)\dot{H}=0 \quad (1)$$

$$c=c(t)=\sqrt{c_0^2+(n-1)H} \quad (2)$$

$$H=H(t)=\frac{n}{n-1}\frac{A^{\frac{1}{n}}}{\rho_0}\left\{\left[\left(P_0+\frac{2\sigma}{R_0}\right)\left(\frac{R_0}{R}\right)^{3\gamma}-\frac{2\sigma}{R}+B\right]^{\frac{n-1}{n}}-(P_0-P_m\sin\omega t+B)^{\frac{n-1}{n}}\right\} \quad (3)$$

where c_0 and P_0 – the speed of sound and pressure in an unperturbed liquid, *c* – the local value of the speed of sound in the vicinity of the cavity surface, R_0 – initial radius of the cavity, *H* – free enthalpy on the cavity surface, P_m – amplitude of the ultrasonic field, $\omega=2\pi\nu$ – circular frequency (ν is the frequency ultrasonic vibrations), σ – coefficient of surface tension of the liquid (for water $\sigma=73\cdot10^{-3}$ *N/m*), *A, B, n* – determining constants of the liquid model (for water *A* = 3001 *atm*, *B* = 3000 *atm*, *n*=7), γ – a polytropic index that determines the state of the gas in the cavity (γ=1 in the case of isothermal pulsations and γ=4/3 in the case of adiabatic pulsations [12-14].

For equation (1), the initial conditions must be specified:

$$R(0)=R_0, \dot{R}(0)=V_0 \quad (4)$$

where V_0 – initial velocity of the cavity boundary.

To solve the nonlinear equation (1), we use the Runge-Kutta method in the Felberg modification of 4-5th orders [15-17]. For this, we represent (1) in the form:

$$\dot{\boldsymbol{R}}=\boldsymbol{F}(t,\boldsymbol{R}) \quad (5)$$

$$\boldsymbol{R}=(R,V)^T, \boldsymbol{F}=(F_1,F_2)^T \quad (6)$$

$$F_1=V \quad (7)$$

$$\boldsymbol{F_2}=\frac{(\boldsymbol{c}+\boldsymbol{V})\boldsymbol{H}}{\boldsymbol{R}(\boldsymbol{c}-\boldsymbol{V})}+\frac{\boldsymbol{U}}{\boldsymbol{c}}-\frac{\frac{3}{2}\left(\boldsymbol{c}-\frac{\boldsymbol{V}}{3}\right)\boldsymbol{V}^2}{\boldsymbol{R}(\boldsymbol{c}-\boldsymbol{V})} \quad (8)$$

$$U=\frac{A^{\frac{1}{n}}}{\rho_0}\left\{\left[\left(P_0+\frac{2\sigma}{R_0}\right)\left(\frac{R_0}{R}\right)^{3\gamma}-\frac{2\sigma}{R}+B\right]^{-\frac{1}{n}}\left[-\frac{3\gamma V}{R}\left(P_0+\frac{2\sigma}{R_0}\right)\left(\frac{R_0}{R}\right)^{3\gamma}+\frac{2\sigma V}{R^2}\right]+\omega P_m\cos\omega t(P_0-P_m\sin\omega t+B)^{-\frac{1}{n}}\right\} \quad (9)$$

$$c=c(t)=\sqrt{c_0^2+(n-1)H} \quad (10)$$

The scheme of the Runge-Kutta method in the modification of Felberg 4-5th orders for the system of nonlinear ordinary differential equations (5-10) has the form [18-20]:

$$\boldsymbol{R}_{n+1}=\boldsymbol{R}_n+\sum_{i=1}^{6}w_i\boldsymbol{k}_i \quad (11)$$

$$\boldsymbol{k}_1=h_n\boldsymbol{F}(t_n,\boldsymbol{R}_n) \quad (12)$$

$$\boldsymbol{k}_i=h_n\boldsymbol{F}\left(t_n+\alpha_i h_n,\boldsymbol{R}_n+\textstyle\sum_{j=1}^{i-1}\beta_{ij}\boldsymbol{k}_j\right), i=\overline{2.6} \quad (13)$$

where h_n – time step, which can be variable.

In this case R_0 corresponds to the initial radius of the cavity, and V_0 – to the initial velocity of the cavity boundary movement. The coefficients w_i and β_{ij} are shown in Fig. 1. This scheme has the fifth order of accuracy h_n. If

i	α_i	β_{ij}					w_i	w_i^*
1	0	0	0	0	0	0	$\frac{16}{135}$	$\frac{25}{216}$
2	$\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0	0	0
3	$\frac{3}{8}$	$\frac{3}{32}$	$\frac{9}{32}$	0	0	0	$\frac{6656}{12825}$	$\frac{1408}{2565}$
4	$\frac{12}{13}$	$\frac{1932}{2197}$	$-\frac{7200}{2197}$	$\frac{7296}{2197}$	0	0	$\frac{28561}{56430}$	$\frac{2197}{4104}$
5	1	$\frac{439}{216}$	-8	$\frac{3680}{513}$	$-\frac{845}{4104}$	0	$-\frac{9}{50}$	$-\frac{1}{5}$
6	$\frac{1}{2}$	$-\frac{8}{27}$	2	$-\frac{3544}{2565}$	$\frac{1859}{4104}$	$-\frac{11}{40}$	$\frac{2}{55}$	0

Figure 1: Coefficients of the Runge-Kutta method in Felberg modification of 4-5th orders

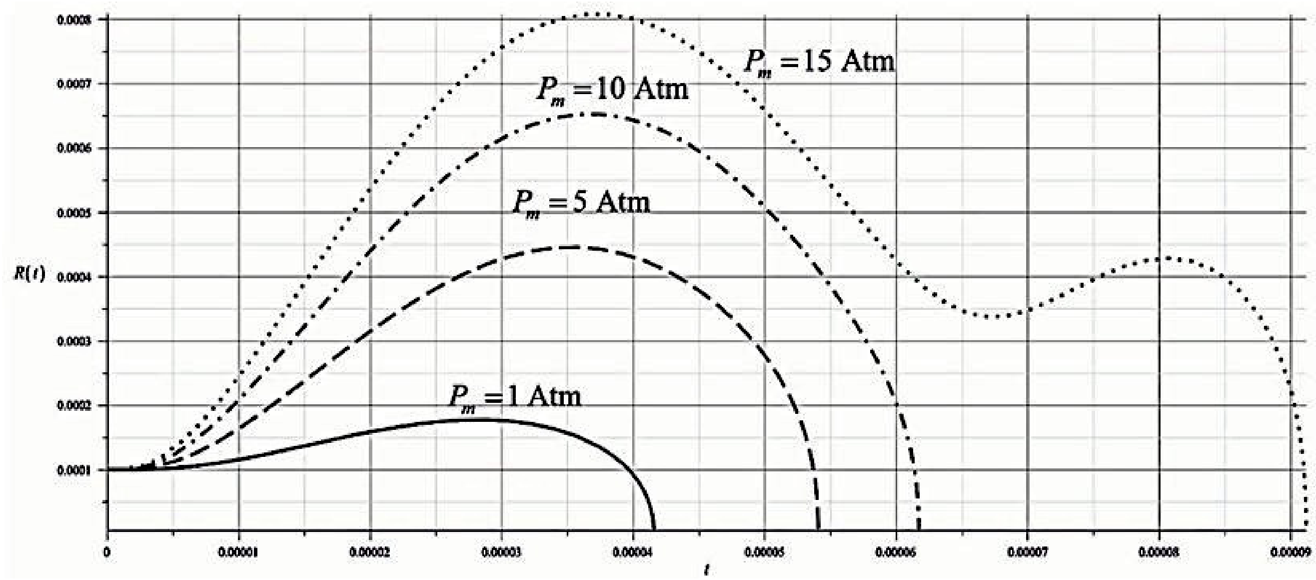

Figure 2: Time dependence of bubble radius with varying P_m

in (11-13) we use the coefficients w_i* (Fig. 1) instead of w_i, then the resulting circuit will have the fourth-order. At each step, the error is estimated [21-23]:

$$\|\boldsymbol{\Delta}_{n+1}\| < \varepsilon, \boldsymbol{\Delta}_{n+1} = \sum_{i=1}^{6}(w_i - w_i^*)\boldsymbol{k}_i \qquad (14)$$

where ε – the required accuracy, and the norm is understood as the maximum modulus element of the vector: $\|a\| = max(|a_1|,|a_2|)$, $a=(a_1,a_2)^T$.

If inequality (14) is not fulfilled, then on the current cycle the time step decreases by a factor of 2 and the values of the bubble radius and the velocity of its boundary are recalculated. The step value then returns to the selected initial value [24-26]. Thus, the algorithm makes it easy to implement an adaptive selection of the step h_n on each cycle in time.

ANALYSIS OF THE RESULTS OF EQUATIONS

Using the proposed algorithm, the dynamics of bubble pulsations in water under the influence of ultrasonic vibrations with a frequency of v=20 *kHz* was calculated. The influence of the amplitude of ultrasonic oscillations P_m on the mode of bubble pulsations is analysed. In the calculations, the following values of the remaining parameters of the problem were used: c_0=1500 *M/s*; ρ_0=1000 *kg/m*^{3}; *A*=3001 *atm*; *B*=3000 *atm*; *n*=7; σ=73·10^{-3} *N/m*; P_0= 1 *atm*; γ=1; R_0=10^{-4} *m*; V_0=0.

Figure 2 shows the dependences of the bubble radius on time for various values of the amplitude of ultrasonic vibrations P_m. Figure 3 shows the time dependences of the velocity of the bubble boundary for different values of the amplitude of ultrasonic vibrations P_m. It can be seen that at P_m≥5 *atm*, the collapse rate of the bubble begins

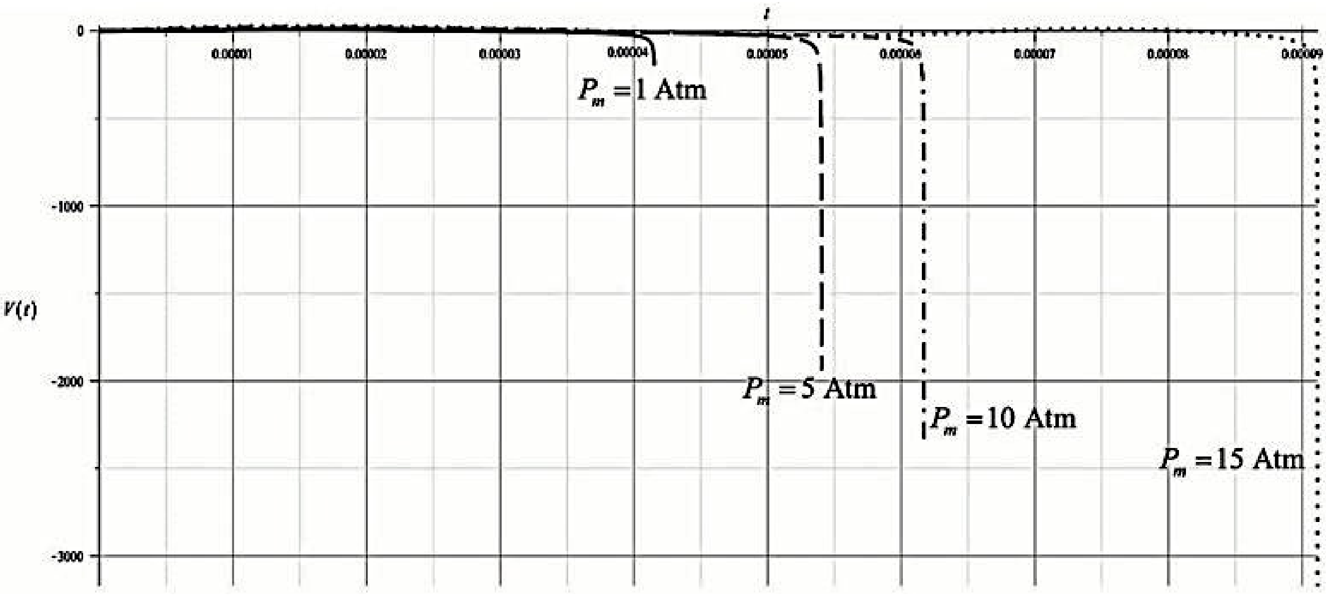

Figure 3: Time dependence of the velocity of the bubble boundary

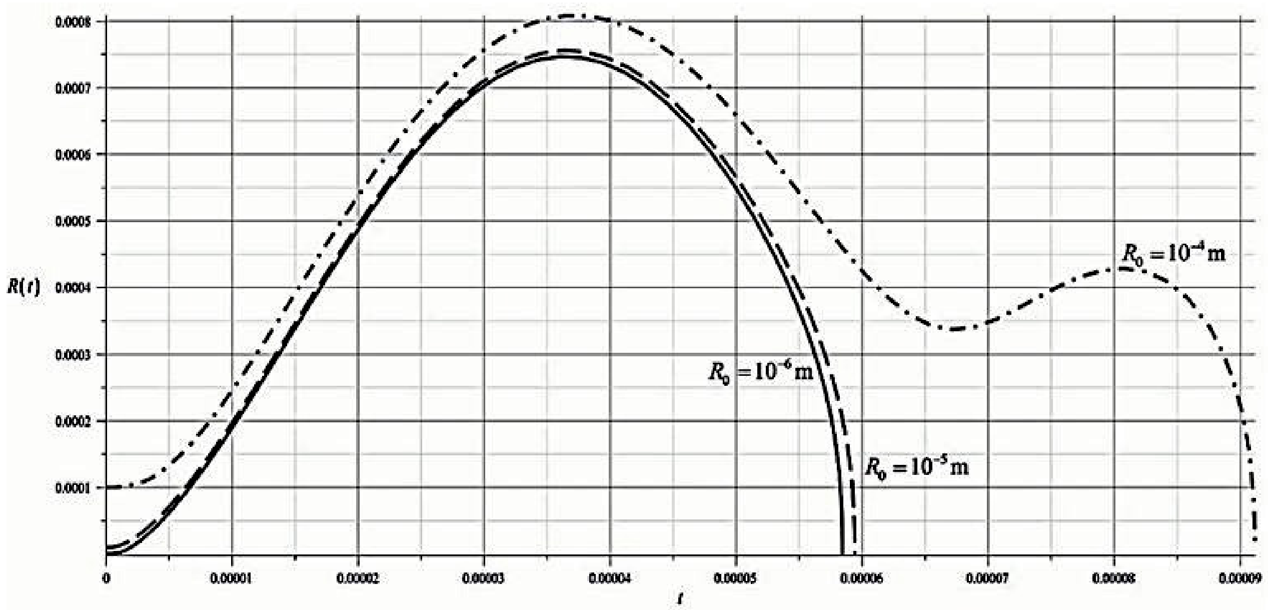

Figure 4: Time dependence of bubble radius with varying R_0

to exceed the speed of sound in the liquid, which justifies the application of the Kirkwood-Bethe model to the description of the pulsation process [27-29].

The curves in Figure 4 correspond to the dependence of the bubble radius on time at P_m= 15 *atm* and different values of the initial radius R_0. The findings reveal that for R_0>10^{-5} m, the bubble manages to perform two pulsations before the moment of collapse.

CONCLUSIONS

The process of pulsation of a cavitation pocket in the liquid is investigated. The Kirkwood-Bethe model was used to describe the motion. A numerical solution algorithm based on the Runge-Kutta-Felberg method of 4-5th order with an adaptive selection of the integration step has been developed and implemented. At each step of the algorithm in time, the error is estimated in terms of the norm of the difference of the vectors of the solution increments, calculated by schemes of the fourth and fifth order of accuracy. If this norm of the difference exceeds the desired accuracy, then on the current cycle the step is reduced by 2 times in time and the values of the bubble radius and the velocity of its boundary are recalculated. The step value then returns to the selected initial value. Examples of calculating the pulsation of a bubble in the water when exposed to ultrasound are given. The influence of atmospheric pressure, the amplitude of ultrasonic vibrations, and the initial radius of the bubble on the process of collapse of the cavitation pocket were investigated.

It is shown that if the atmospheric pressure exceeds a certain threshold value, then the bubble collapse rate begins to exceed the speed of sound in the liquid, which justifies the application of the Kirkwood-Bethe model to the description of the pulsation process. It was revealed that if the initial bubble radius exceeds a certain value, then the bubble will perform several pulsations until the moment of collapse. The same applies to the case of exceeding the amplitude of ultrasonic vibrations of a certain value. The proposed solution method makes it possible to carry out comprehensive parametric studies of the process of pulsations of cavitation pockets in a liquid under the influence of ultrasonic vibrations, to obtain estimates of the influence of various process parameters on the cavitation intensity, to create and apply technologies for the numerical simulation of cavitation phenomena. In practical terms, the results obtained can be used in the design of new and modernisation of existing experimental cavitation installations.

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