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Methods of numerical solution of the basic cavitation equation

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Abstract. In this paper, we developed a mathematical model that allows us to study the process of homogeneous cavitation in liquids, interfacial mass transfer and the dynamics of cavitation cavities with a change in fluid pressure. A numerical simulation was performed, which made it possible to determine the dependence on time and spatial coordinates of the parameters of the liquid phase, temperature and pressure of the vapor phase, concentration and size of bubbles. A program is proposed that allows the described numerical simulation. A number of conclusions were made about the effect of the frequency of external influence on the liquid on the intensity of the formation of cavities in the liquid and calculated the amplitudes of oscillations of cavitation cavities.

Keywords: homogeneous cavitation, numerical solution, Rayleigh equation

MSC numbers: 65K05

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1. Introduction

When a liquid is heated at a constant pressure or when the pressure is lowered at a constant temperature, it is possible to achieve a state in which vapor, gas and vapor-gas bubbles (cavities) become visible and begin to grow. Such bubbles can grow at a moderate rate (if its growth is determined by the diffusion of dissolved gases into the bubble), or explosively (if the growth is due to evaporation of the surrounding liquid into the bubble). This process is called cavitation.

Thus, cavitation is the growth of a bubble (cavern), due to the dynamic pressure drop at a constant temperature. Cavitation includes a number of phenomena from the inception of the cavern to its collapse. Caverns are formed in those places where the pressure in the liquid becomes below a certain critical value. In a real fluid, the critical pressure is approximately equal to the saturated vapor pressure of this fluid at a given temperature [1, 2].

The study of the formation of bubbles and their development with a rapid change in pressure in a liquid is of great interest in the theory of non-equilibrium multiphase media [3, 4].

A convenient method for studying this problem is numerical simulation. The mathematical model should include the equations of conservation of mass, momentum and energy for the carrier phase, as well as the equations describing the process of formation of nuclei of the vapor phase and their development as a result of changes in the parameters of the surrounding liquid and interfacial mass transfer.

2. Cavitation basic equation

Significantly different spatial and temporal scales of transfers in the carrier and dispersed phases and large gradients of gas-dynamic parameters characteristic of the process under study necessitate the use of high-resolution numerical schemes for integrating fluid equations and methods for solving systems of ordinary differential equations arising in bubble dynamics models.

The purpose of the proposed scheme is a numerical study of the dynamics of bubbles at high temperatures and pressures during the propagation of a rarefaction wave. For this purpose, a mathematical model has been formulated that allows one to investigate the formation of embryos and the dynamics of bubbles. It should be noted that earlier some authors have already proposed numerical models for the development of cavitation bubbles under other conditions [5, 6, 7, 8, 9].

Creating such a model to study the dynamics of cavitation bubbles presents considerable difficulty. Firstly, this is due to the fact that the basic cavitation equation (1), which describes the dynamics of the cavitation cavity, is a nonlinear second-order differential equation and can be solved analytically only in a certain approximation. The numerical solution of the equation (1) is associated with a number of difficulties, namely: limited accuracy of the results, the need to vary the parameters in the equation over a fairly wide range (and the result depends not only on the values of these parameters, but also combination), the presence of reliable reference data on thermodynamic quantities characterizing the state of the fluid and included in the equation (1). These values, in turn, are dependent on the temperature of the liquid, its chemical composition and degree of purification.

Without taking into account vapor pressure and fluid viscosity, the basic equation of cavitation is:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 = \frac{1}{\rho} \left[\left(p_b + \frac{2\sigma}{R_o} \right) \left(\frac{R_o}{R} \right)^{3k} - \frac{2\sigma}{R} - p_0 - p(t) \right].$$
(1)

Here:

- R_0 is the initial radius of the nucleus at time t = 0;
- R is the radius of the nucleus at the next time instant t;
- ρ is the density of the fluid;
- σ is the liquid surface tension;
- k is the adiabatic index for a couple in the bud;
- p_o is the hydrostatic pressure in a liquid. It was assumed in the calculations that p_o is equal to the pressure on the binodal due to the equilibrium of the cavity and its surrounding fluid, i.e. $p_o = p_b$;
- \ddot{R} is the acceleration of the cavity wall;
- \dot{R} is the speed of movement of the cavity wall;
- $\frac{2\sigma}{B_0}$ is the Laplace pressure;
- $\frac{R_0}{R}$ is the amplitude of oscillations of the cavity;
- p(t) is the time-dependent external pressure pulse.

This equation is also known as the Rayleigh-Plisset equation. It is important that in the equation (1) it is assumed that:

- caverns remain spherically symmetrical throughout the time,
- inside the cavity there are spatially homogeneous areas,
- the length of the sound wave is much larger than the radius of the cavity (otherwise, the spherical symmetry will be broken and the task will become insoluble),
- there are no bulk forces,
- neglected,

- fluid viscosity is not taken into account,
- liquid density is much greater than gas density,
- liquid compressibility is much less than gas compressibility,
- gas inside the cavity is stable,
- vapor pressure remains unchanged when the cavity moves.

3. Numerical solution of the cavitation equation

We have written a program for the numerical solution of the basic cavitation equation in the Compaq Visual Fortran Professional programming language. This is the main program. The equation in the form (1) is unacceptable for numerical solution due to large values of the frequency of external influence $f = (10^3 \div 10^9)$ Hz, small values of the initial size of the cavity $R = (10^{-9} \div 10^{-6})$ m and the small integration step dt. The procedure for normalizing the basic cavitation equation is described in section 4.

The main program is based on the Runge-Kutta method.

At start-up, the main program requests the input of external parameter values for which the liquid is examined (liquid temperature T, oscillation frequency f etc.) Then an array of tabular data is accessed, from which the surface tension values of corresponding to the given temperature are taken sigma, coefficient of fluid viscosity μ , of fluid pressure and vapor pressure at the saturation line and at the boundary of thermodynamic stability, etc. Note that temperature-dependent tabular data are discrete values Ranks, and, as a rule, the points in which there are tabular data do not correspond to a given temperature T. Therefore, the main program refers to the auxiliary subroutine 1, which approximates or extrapolates the tabular data to a given point.

A number of parameters included in the equation (1) are not tabular and, in addition, depend on the temperature of the liquid. This is, for example, the initial radius of a cavitation bubble R_0 , pressure p_1 , at which the first germ of homogeneous cavitation appears, the initial phase of external oscillations φ_0 . To calculate these quantities, the main program refers to subroutine 2, which is based on calculated by subroutine 1 data calculates the specified values.

Let us dwell on the explanation of the temperature dependence of φ_0 . For the case of homogeneous cavitation, the initial phase of oscillations φ_0 depends on the time point t_1 , in which the first germ appears in the defect-free volume of the fluid and which later is already affected by external pressure. The instant of time t_1 is related to the temperature of the fluid T. This connection is expressed by an integral equation, the upper limit of integration of which is the required time t_1 , and the lower one is the initial moment of time $t_0 = 0$.

We have written subroutine 3, which receives a task for calculating the time t_1 from subroutine 2, the necessary tabular data is from subroutine 1, and the result of the calculation is reported to the main program.

Having collected all the necessary data, the main program calculates the basic cavitation equation for the maximum amplitude of oscillations of the cavity, and, if necessary, other parameters (maximum pressure and maximum temperature inside the cavity, etc.)

The scheme proposed here is common to any liquid. Replacing an array of tabular data of one liquid with an array of data corresponding to another liquid, we obtain a numerical solution of the cavitation equation for any liquid. A similar technique was proposed for calculating the parameters of titanium in the liquid state [10].

4 Dynamics of cavitation bubbles under the action of sinusoidal pressure

Now we define the shape of the external pressure pulse, under the action of which cavitation occurs (p(t) in the equation (1)). Consider the case of sinusoidal pressure in the form:

$$p(t) = p_a \sin(\omega t + \varphi_0), \tag{2}$$

where p_a is amplitude of external influence,

 $\omega = 2\pi\nu = \frac{2\pi}{T}$ is the frequency of external oscillations, φ_0 - the initial phase of external oscillations at time t = 0. Substitution of the (2) in the equation (1) gives:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 = \frac{1}{\rho} \left[\left(p_b + \frac{2\sigma}{R_o} \right) \left(\frac{R_o}{R} \right)^{3k} - \frac{2\sigma}{R} - p_b - p_a \sin(\omega t + \varphi_0) \right].$$
(3)

The solution of the equation (3) is the dependence of the nucleus radius R/R_0 on t/T, where T is the period of change of external influence [11]. Knowing this dependence, we can determine the maximum radius of the nucleus R_{max} and the amplitude of oscillations of the bubble $\frac{R}{R_0}$ at any time, as well as the maximum amplitude R/R_0 . Equation (3) was solved numerically by the Runge–Kutta method which was described earlier in section 3.

To achieve the minimum error of the result obtained numerically, it is necessary that the dt step is minimal. However, the decrease in the interval dt leads to the fact that the ratio $\frac{dR}{dt}$ tends to infinity and this tendency is all the greater when approaching the critical point. This leads to the opposite effect, in which the error of numerical calculations, on the contrary, increases. To exit the situation, the equation (3) is normalized so that the ratio $\frac{dR}{dt}$ varies from 1 to 100. For this, a change of variables is introduced:

$$R^* = \frac{R}{R_0}, \quad \tau = 2\pi f t = \omega t, \quad z = \frac{dR}{dt}.$$

Preliminary estimated calculations show that the R^*, τ, z variables obtained by changing the variables do not exceed a few hundred, which fully meets our requirements. After changing the variables, we have:

$$z^* = \frac{dR^*}{d\tau} = \frac{d(\frac{R}{R_0})}{d(\omega t)}, \quad \frac{dz}{dt} = \frac{d^2R}{dt^2}, \quad \frac{dz^*}{d\tau} = \frac{d^2(\frac{R}{R_0})}{d(\omega t)^2}$$
$$\frac{d^2R}{dt^2} = -\frac{3}{2}\frac{1}{R}\frac{dR}{dt} + \frac{1}{\rho R}\left[\left(p_b + \frac{2\sigma}{R_o}\right)\left(\frac{R_o}{R}\right)^{3k} - \frac{2\sigma}{R} - p_b + p_a\sin(2\pi ft + \varphi_0)\right]$$

Multiplying both sides of the last equation by $\frac{1}{R_0\omega^2}$ gives:

$$\frac{d^2\left(\frac{R}{R_0}\right)}{d(\omega t)^2} = -\frac{3}{2} \frac{R_0}{R\omega R_0} \frac{d\left(\frac{R}{R_0}\right)}{d(\omega t)} + \frac{R_0}{\rho R\omega^2 R_0^2} \left[\left(P_b + \frac{2\sigma}{R_o}\right) \left(\frac{R_o}{R}\right)^{3k} - \frac{2\sigma R_0}{RR_0} - p_b + p_a \sin(\tau + \varphi_0) \right],$$

$$\frac{d^2 R^*}{d\tau^2} = -\frac{3}{2} \frac{1}{R^*} \frac{dR^*}{d\tau} \frac{1}{\omega R_0} + \frac{1}{\rho \omega^2 R_0^2} \frac{1}{R^*} \left[\left(P_b + \frac{2\sigma}{R_o} \right) \left(\frac{1}{R^*} \right)^{3k} - \frac{2\sigma}{R_0} \frac{1}{R^*} - p_b + p_a \sin(\tau + \varphi_0) \right].$$
(4)

The amplitude of the external influence p_a was considered maximum, separated by 5% from the thermodynamic stability of the fluid (spinodal) and determined from the condition:

$$p_a = 0.95(p_b - p_s),$$

where p_b is the pressure on the binodal, p_s is the pressure on the spinodals, calculated according to the theory of homogeneous nucleation.

The magnitude of the fluid pressure on the spinodals was determined by us earlier in the works [12, 13].

To calculate $\varphi_o = -\frac{p_a}{p_1}$ it is necessary to determine the pressure values p_1 , at which in the stretched liquid, one vapor nucleus appears in 1 cm³, as well as a stretching time of t_1 to a pressure of p_1 (for the entire temperature range of T). The time of stretching the fluid t_1 to the pressure p_1 is determined from the condition:

$$p_1 = p_b - p_a \sin(\omega t_1).$$

The described studies of the dynamics of nuclei of homogeneous cavitation in water under the action of sinusoidal pressure show that there are ranges of temperatures and frequencies ν of external influences in which cavitation occurs most

intensely, and the size of the bubbles increases in tens, thousands and even millions of times compared with the original size [14]. For water, such intervals are $\nu < 50MHz$ and $t < 317^{\circ}C$. This suggests that, under the conditions being considered, T and P inside the bubbles can increase by several orders of magnitude.

5. Summary

Thus, a mathematical model was constructed, which allows to investigate nonadhesion, interfacial mass transfer and the dynamics of bubbles with a change in fluid pressure. Numerical simulation made it possible to determine the dependence on time and spatial coordinates of the parameters of the carrier phase, volume content, temperature and pressure of the vapor phase, concentration and size of bubbles.

It is numerically determined that the frequency of external influences affects the rate of evaporation inside the cavitation bubble. At too high frequencies, and, consequently, short durations of the period, evaporation into the cavity does not have time to occur and the maximum amplitude of oscillations of the bubble is not high. At low frequencies, of the order of (1 - 500) kHz, intense evaporation of gas or vapor into the bubble occurs and its subsequent compression to its original size, the maximum amplitude of oscillations of the cavity in this case increases sharply, reaching values of $R/R_0 \sim 10^6$ with frequency $\nu = 250$ kHz and temperature $T = 310^{0}C$ [15]. With such significant compressions, the local temperature in the cavities increases [16] to values at which initiation of a nuclear fusion reaction is possible, as described in [17, 18, 19] and [20].

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