УДК 532.528

THE WAYS OF PRODUCING AN UNIFIED MATHEMATICAL MODEL FOR THE CAVITATING FLOW IN HYDRODYNAMIC CAVITATION REACTORS

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Розглянуто шляхи побудови загальної математичної моделі кавітаційних реакторів. Запропоновано універсальну математичну модель, яка адекватно описує динаміку парогазових бульбашок та кавітаційного кластера в широкому інтервалі зміни режимних параметрів. В рамках моделі проаналізовано вплив температури та газовмісту рідини на ефективність кавітаційної дії. Показано можливість модифікації моделі стосовно оптимізації роботи кавітаційних реакторів.

Рассмотрены пути построения общей математической модели кавитационных реакторов. Предлагается математическая модель, которая без использования ограничивающих допущений адекватно описывает динамику парогазовых пузырьков и кавитационного кластера в широком интервале изменения режимных параметров. В рамках модели рассмотрено влияние газосодержания и температуры жидкости на интенсивность кавитационного воздействия. Обсуждается возможность модификации модели применительно к оптимизации работы кавитационных реакторов.

Possible ways of constructing a general model of cavitation reactors are considered. A mathematical model is proposed that without using any limiting assumptions describes adequately the dynamics of vapor-gas bubbles and the behavior of a cavitation cluster in a wide range of regime parameters. In the framework of the model, the influence of gas content and liquid temperature on the cavitation intensity is considered. The possibility of modifying the model as applied to optimizing the operation of cavitation reactors is discussed.

References 17, figures 4.

Key words: hydrodynamic cavitation, mathematical model, gas-vapor bubble, cavitation cluster.. m – mass; P – pressure; T – temperature; R – bubble radius; w – velocity; μ – dynamic viscosity; ρ – density; σ – surface tension; τ – time;**Subscripts:** ac – acoustic; b – bubble; cl – cluster; g – non-condensable gas; l – liquid; lR – liquid parameter at the bubble interface; min – minimum; sat – saturated vapor.**Introduction**

In recent years there has been a trend of widespread use of hydrodynamic cavitation in various industrial technologies, such as wastewater treatment and sterilization, the creation of nano-emulsions, the synthesis of biodiesel, food processing and others [1,2]. The cavitation technique not only produces the desirable transformation but also reduces the total processing cost and is found to be more energy efficient than many other conventional techniques.

In practice, cavitation mechanisms are initiated in acoustic fields with using various ultrasonic emitters or

by creating optimal hydrodynamic conditions in the liquid flow [1-5]. To implement the hydrodynamic cavitation processes in solving scientific and applied problems various types of rotory-pulsed apparatuses [1,5], Venturi nozzles [2,3,6,7], orifice plates [3,6,8], pulsation dispersers [9,10] centrifugal pumps [11] are used. The experience in using of these devices in scientific research and in carrying out various technological operations proves that the realization of the cavitation phenomena allows to dramatically affects the heat and mass transfer, the hydrodynamic, chemical and biophysical processes in liquid at the micro- and nanoscales [2,7,10,11].

The choice and justification of the most effective method of cavitation influence on the liquid material to be handled, as well as the use of the most suitable type of cavitation device, depend on the specific technological task. Obviously, the study of cavitation phenomena with a view to their rational and efficient use in industrial technologies requires a unified approach to the analysis of cavitation mechanisms and prediction of their action on the studied object, regardless of the type of cavitation reactor.

The paper discusses some aspects of the processes and phenomena of hydrodynamic cavitation with recommendations for a rational reactor design and optimal operating parameters. The ways of constructing a mathematical model of cavitation reactors are considered, which are based on both the results of our own research on the study of hydrodynamic cavitation and the analysis of well-known publications on this topic.

The principle of operation of cavitation reactors. The principle of operation of cavitation reactors. Cavitation devices are designed to create conditions that ensure the formation of an ensemble of vapor bubbles (cavities) in a liquid (so-called “cavitation cluster”), their subsequent growth, compression, and final collapse. At the collapse instant the bubbles emit high-amplitude pressure pulses, which are converted into the resulting powerful energy pulse of the cavitation cluster. In the zone of bubble collapse a so-called “thermic” forms, which for extremely short time occupies the micron-sized liquid domain with temperature of $T_l \gg 1000$ K. These short-term dynamic and thermal effects determine the effectiveness of cavitation influence on micro-objects located in liquid inside and in the vicinity of the cluster.

According to the accepted definition [2-6,9,10], cavitation occurs, if pressure in liquid p_l becomes less than the saturated vapor pressure ($p_l < p_{sat}(T_l)$), which leads to the formation and growth of bubbles, and then increases to a higher value $p_l > p_{sat}(T_l)$, which results in compression and subsequent collapse of the bubbles. This definition applies equally to acoustic and hydrodynamic cavitation, where the pressure drop and rise are caused by periodic high-frequency tension and compression of the liquid volume, or by stretching of the liquid high-speed stream when passing through a contraction of the channel. The analysis of the operation of hydrodynamic cavitation devices is based on two independent models. One of them - the cavitation model - describes the evolution of bubbles from the moment of its formation to the final collapse, regardless of the type of cavitation reactor. Another model, which can be called a cavitating flow model, takes into account the design features

of the reactor.

Cavitation models are designed to predict the behavior of a single gas-vapor bubble (or a bubble ensemble) in liquid with temperature T_l under isothermal variation in liquid pressure in the vicinity of the bubble. The dynamics of a spherical vapor-gas bubble in viscous incompressible liquid, as a result of a sharp change in external pressure $p_l(\tau)$, is described by the well-known Rayleigh-Plesset equation

$$\frac{d^2 R}{d\tau^2} = \frac{p_{lR} - p_l - 3/2 \rho_l (dR/d\tau)^2}{\rho_l R}. \quad (1)$$

Here p_{lR} is pressure in liquid at the bubble interface, which is determined from the balance of normal forces acting on the surface of growing or contracting bubble. With account of the contribution of both capillary and viscous stresses to total stresses on the bubble interface the force balance writes as follows: $p_{lR} = p_b - 2\sigma(T_{lR})/R - 4\mu_l(dR/d\tau)/R$, where pressure inside the bubble $p_b = p_g + p_v$. Obviously, the derivative $dR/d\tau$ determines the liquid radial velocity of liquid at the bubble interface ($w_{lR}(\tau) = dR/d\tau$).

Equation (1) ought to be solved together with those, which describe the change in temperature $T_b(\tau)$ and pressure $p_b(\tau)$ of gas phase within the bubble, heat and mass transfer through the interface, the phase changes kinetics with due account of liquid temperature at the interface $T_{lR}(\tau)$, as well as the temperature dependences of liquid density $\rho_l(T_{lR})$, viscosity $\mu_l(T_{lR})$ and surface tension $\sigma(T_{lR})$.

The Rayleigh-Plesset equation is also included in the system of equations of cavitation cluster models. In a cavitation cluster model the general equation system, in addition to the ones mentioned above, should also include equations, describing the force and thermal interaction between the cluster bubbles. This allows the calculation of non-stationary fields of velocities, temperatures and pressures in liquid within the cluster, where processed micro-objects are present [9].

Adequate description of cavitation mechanisms requires a strict accounting of all the above factors. However, even in the most developed reactor models, the cavitation processes are described with a large number of simplifying assumptions. For instance, the process of bubble compression is believed to be adiabatic one, vapor pressure inside a bubble is equal to the saturation vapor pressure ($p_v = p_{sat}(T_l) = \text{const}$), the parameters ρ_l , μ_l and σ are temperature-independent, etc ([3-6,8,12,13]. In some cases, calculations are performed for a single bubble only, and in analysis of cluster behavior the interaction of bubbles is not taken into account [1,3,12]. Most models use an unjustifiably large number of empirical

or adjustable parameters. According to the majority of researchers [2-6,12,13], the theoretical basis have yet to be developed to identify key parameters of cavitation, and the problem of studying cavitation mechanisms actually comes down to testing the behavior of a “black box” [6]. An analysis of publications on the topic suggests that there is currently a lack of valid reliable of cavitation models.

Cavitating flow models describe the pressure variation $p_l = f(\tau)$ in a fixed elementary liquid volume during its movement in a channel of variable geometry. The calculated values $p_l(\tau)$ are included then in equation (1), which enables determination the cavitation cluster behavior in a particular reactor with a given channel geometry. For the flow of liquid through a Venturi tube or an orifice plate the dependence $p_l = f(\tau)$ is calculated using the Bernoulli equation [4,5] or the Reynolds averaged Navier-Stokes equation [3-6, 13]. In solving the problems of optimizing the structural-operational parameters of cavitation reactors of this type, ready-made software products of the ANSYS type are used [3,14]. Of particular difficulty is the theoretical description of unsteady hydrodynamic processes in rotary pulsation apparatuses (rotary disintegrators), which are used in various technologies as effective cavitation reactors. This is due to the complexity of the design of such devices and the need to take into account the diverse factors of influence on the processed medium [1,2]. It is also worth noting that mass-flow rate of a two-phase boiling flow through any cavitation reactor varies periodically with time, which determines the specific feature of the cavitation flow modeling.

Analysis of cavitation mechanisms. One of the most detailed cavitation models is the unified mathematical model of the bubble ensemble dynamics (BED model) [9,15]. Unlike other known models, it takes into account the force and thermal interaction of bubbles in the ensemble,

which enables accurate calculation of the pressure change in liquid inside the cluster ($p_{cl} = f(\tau)$) and precise definition of the cavitation inception. A feature of this model is the description of interphase heat and mass transfer in the framework of molecular kinetic theory. Using the same general system of equations, the model adequately describes the bubble cluster dynamics in boiling processes, as well as in the processes of hydrodynamic and acoustic cavitation over the entire temperature range of liquid phase existence up to the thermodynamic critical point [9]. The model uses the generally accepted assumption that a bubble ensemble is monodisperse one at all stages of its evolution. The BED model has been successfully used to calculate cavitation reactors of various types in solving specific technological problems [7,9-11].

This paper presents the results of numerical investigations on effect of various factors on the cavitation intensity, performed using the BED model

As noted above, to initiate the cavitation process it is necessary that liquid pressure $p_l(\tau)$ should be sharply decreased to a value $p_{\min}$, lower than saturated vapor pressure ($p_{\min} < p_{\text{sat}}(T_l)$), and then rapidly increased to value $p_l > p_{\text{sat}}(T_l)$. These conditions, schematically presented in Fig. 1a, are applied equally to acoustic and hydrodynamic cavitation. It is fundamentally important that before the formation of cavitation bubbles (cavitation inception) the values $p_{\min}$ should be in the region of negative pressures ($p_{\min} \leq 0$) when liquid is in a state of tension. In the theory of acoustic cavitation this is obvious, but when analyzing the processes of hydrodynamic cavitation in almost all known works on cavitation it is assumed a priori that $0 < p_{\min} < p_{\text{sat}}(T_l)$ [2,6,8,12,13]. This approach excludes the possibility of describing the reactor operation, since the question of directional control of the concentration and

Fig.1. Schematic representation of the conditions for creating cavitation (a), and typical curves of pressure change over time in fixed volume of water flow in different hydrodynamic cavitation reactors: - in the Venturi nozzle (b), in the channels of a rotary-impulse apparatus (b), in the tube of a pulsating disperser. (d).

initial size of bubbles is no longer considered. The necessity of fulfilling the condition $p_{\min} \leq 0$ is considered in detail in [3,9]. The calculated data presented in Fig. 1b,c,d indicate that the condition $p_{\min} \leq 0$ is satisfied for any types of hydrodynamic cavitation reactors. These calculated results are in good agreement with experimental data [3-5, 9-11,].

Practice shows [2-5,10,11] that the level of cavitation intensity is highly dependent on the gas content of liquid, or on the relative proportion of neutral gas in the initial micronuclei. This is in good agreement with the results of the calculation according to the model [9], which are presented in Fig. 2. Even relatively small gas content in an micronucleus in the stage of bubble formation dramatically reduces the degree of dynamic impact in the final stage of the bubble collapse. This is explained by the fact that the presence of a neutral gas prevents the bubble from being compressed to its minimum size, which excludes the possibility of its collapse with subsequent emission of a high-amplitude pressure pulse [4,5,9,15]. For the reactor

to operate efficiently, it is necessary to ensure an extremely high rate of lowering liquid pressure to negative values, and thus initiate the growth of micro- and nanoscale vapor nuclei with relatively low content of neutral gases. In acoustic cavitation this is achieved by increasing the frequency and intensity of the sound field.

Another important factor determining the level of dynamic and thermal effects on an object as a result of the collapse of a cavitation cluster is the value of liquid temperature T_l . When a single bubble collapses, the amplitude of the pressure pulse rapidly and monotonously decreases with increasing temperature [5,9]. However, experiments show [7,16], when a cavitation cluster collapses, a maximum is recorded in the temperature dependence of the pressure pulse amplitude ($p_{\text{imp}} = f(T_l)$) in the temperature range $T_l = 45 \div 55^\circ\text{C}$. This is characteristic of both hydrodynamic and acoustic cavitation.

Figure 3 shows the temperature dependences of the pressure pulse amplitude $p_{\text{imp}} = f(T_{l\infty})$ calculated

Fig.2. The pressure (1) and temperature (2) of the medium inside the extremely compressed cavitation bubble, depending on the relative gas content in the initial micro-bubble.

Fig.3. Influence of liquid temperature on the intensity of cavitation action: 1 - loss of mass of an aluminum sample due to cavitation erosion in acoustic field at various values of liquid temperature (experimental data [16]); 2 - change in pressure amplitude during collapse of a bubble cluster in an acoustic field depending on liquid temperature (calculation with the BED model).

The frequency of the ultrasonic field $f_{ac} = 20 \text{ kHz}$, the field intensity $p_{ac} = 0.12 \text{ MPa}$.

with the model [9] during the collapse of a cavitation cluster in pure water in an acoustic field with a frequency $f_{ac} = 20$ kHz at field intensity value $P_{ac} = 0,12$ MPa (solid line). The curves show a pronounced maximum at liquid temperature of $T_l = 55^\circ\text{C}$ (solid line). The dotted line shows the experimental data [16] on erosive mass loss of an aluminum sample in water over a certain period of time during cavitation ultrasonic exposure, depending on liquid temperature. It is seen that the maximum erosion is recorded at the same temperature. The reason for the appearance of the maximum in the curves $P_{ac} = f(T_l)$ in the temperature range $T_l = 45\text{--}55^\circ\text{C}$ is still the subject of discussion. Nevertheless, this nature of the dependence of cavitation effects on liquid temperature should be taken into account when using cavitation, for example, in technological operations of extraction or sterilization, where the temperature of the liquid is an important factor in the intensity of the process.

Using the BED model a large amount of useful information can be obtained, including the specifics of the processes occurring in the most interesting and important stage of the bubble collapse. It is at this extremely short stage that intense energy transformations take place.

Due to the adiabaticity of processes at the final stage of the bubble compression, temperature inside the extremely compressed bubble significantly exceeds the critical temperature, so that the bubble and its immediate environment pass into the state of supercritical fluid (SCF), where there is no difference between the gaseous and liquid phases. Any substance in the SCF state is able, like gases, to seep through solid materials and dissolve substances like liquids. It is known, for example, that almost all both organic and inorganic substances dissolve in supercritical

water. In the supercritical state, water mixes unlimitedly with oxygen, hydrogen and hydrocarbons, facilitating their interaction with each other - all oxidation reactions occur in it extremely quickly [17]. The most indicative characteristics of an extremely compressed bubble in the SCF state are shown in Fig. 4a.

Figure 4b,c shows the change in pressure (b) and liquid temperature (c) calculated with the BED model at the bubble interface over a nanosecond period of its stay in the SCF state. These results prove that when analyzing the cavitation effect on supramolecular and microbiological objects, as well as on the kinetics of chemical reactions, it is necessary to take into account the transition of the liquid in the vicinity of the bubble, as well as the vapor-gas mixture in the bubble itself, to the state of supercritical fluid.

Conclusions

The study of cavitation phenomena with a view to their rational and efficient use in industrial technologies requires a unified approach to the description of cavitation mechanisms, regardless of the type of cavitation device. Within the framework of this concept, a mathematical model is developed and improved, which, taking into account the determining factors and an adequate representation of thermophysical system parameters, will provide an opportunity to evaluate and control the level of impact on liquid disperse systems, depending on the design and operating parameters of cavitation reactors. These optimization strategies developed through the theoretical analysis of many experimental studies may help in the design, optimization, and scale-up of hydrodynamic cavitation on an industrial scale for conducting various

Fig.4. Schematic representation of an extremely compressed cavitation bubble in the state of supercritical fluid (a), and typical nature of the change in time of pressure (b) and temperature (c) in water at the bubble interface at final stage of the bubble collapse.

chemical and physical processes.

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ШЛЯХИ ПОБУДОВИ УНІФІКОВАНОЇ МАТЕМАТИЧНОЇ МОДЕЛІ КАВІТАЦІЙНОЇ ТЕЧІЇ В ГІДРОДИНАМІЧНИХ КАВІТАЦІЙНИХ РЕАКТОРАХ

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Застосування потужних кавітаційних механізмів є одним з найбільш дієвих способів досягнення високих енергетичних показників в технологіях пов'язаних з обробкою рідинних дисперсних середовищ з мінімальними непродуктивними енерговитратами. Вивчення явищ кавітації з метою їх раціонального та ефективного використання в промислових технологіях вимагає єдиного підходу до аналізу кавітаційних ефектів і прогнозування їх впливу на досліджуваний об'єкт незалежно від типу кавітаційного реактора. На сьогодні відсутня чітка теоретична база для обґрунтування можливості або обмежень використання кавітаційних пристроїв при вирішенні конкретних технологічних завдань.

У роботі обговорюються шляхи побудови загальної математичної моделі кавітаційних реакторів, в основі якої лежать як результати наших власних комплексних досліджень по кавітації, так і аналіз публікацій інших авторів по вивченню механізмів кавітаційних механізмів. Пропонується уніфікована математична модель, яка в рамках загальних термодинамічних положень з максимальним урахуванням визначальних чинників адекватно описує динаміку одиничних бульбашок і кавітаційних кластерів в широкому діапазоні зміни режимних параметрів з мінімальною кількістю обмежуючих припущень.

В рамках моделі проаналізовано ряд факторів, таких як температура і газовміст рідини, які суттєво впливають на інтенсивність кавітаційної дії. Стосовно до задачі оптимізації роботи кавітаційних реакторів обговорюються шляхи подальшої модифікації цих моделей відповідно до їх застосування при вирішенні задач оптимізації роботи кавітаційних реакторів.

Бібл.17, Рис. 4.

Ключові слова: гідродинамічна кавітація, математична модель, парогазова бульбашка, кавітаційний кластер.

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Отримано 25.02.2020

Received 25.02.2020