Phenomenological models of kinetics of processes in the systems with continuum fluid phase for the optimization of ultrasonic cavitation energy efficiency

Roman N. Golykh
Biysk Technological Institute (branch) of Altai State Technical University named after I.I. Polzunov, 659305, Russian Federation, Altai region, Biysk city, street named after Hero of Soviet Union Trofimov, 27

E-mail: romangl90@gmail.com

Abstract. The general approach for modeling of processes in the systems with continuum fluid phase under ultrasonic cavitation influence was proposed. This approach includes studying of all stages of ultrasonic energy transformation begun from ultrasonic radiator and ended up to target change of medium structure; calculating of real energy spent for medium structure change. Models of kinetics of real processes (macromolecules mechanical destruction and dispersing of suspension particles) under ultrasonic cavitation influence were developed. They models use proposed general approach and allow to evaluate optimum modes providing maximum energy efficiency of processes and improving of final product parameters.

1. Introduction

The action by ultrasonic oscillations on the systems with fluid phase realizes cavitation and other non-linear effects (shock waves, cumulative jets, destruction of interatomic and intermolecular bonds, acoustic flows and others). These effects change the structure and the properties of the systems with the fluid phase (molecular mass and viscosity of the carrying fluid phase, fractional composition of the particles of the dispersed phase), that allows to obtain new materials or attaching unique properties to known materials (multiple increased impregnating property, contact surface area, ultimate strength after the curing, decreased content of undesirable admixtures, etc.).

Today the modes (the intensity of ultrasonic oscillations) of action allowing achieving maximum efficiency of the processes in the system with the fluid phase (for instance, chemical reaction, dispersion, coagulation, and emulsification) are mainly chosen by the experiments, which are individually for specified media [1–4]. However, such approach has some principle disadvantages, such as:

– It does not provide maximum energy efficiency of ultrasonic action with the help of determined modes. The energy efficiency is determined by ratio between energy spent for the transformation of the structure and properties of the system with the fluid phase (energy for the interatomic bonds breakage in the fluid phase, destruction or aggregation of disperse particles) and introduced acoustic energy.

– It does not guarantee that determined modes provide maximum energy efficiency during the process. It is connected with the fact, that the properties and characteristics of processed medium are changed during ultrasonic influence.
It does not allow predicting optimum modes of the action for new unknown processes or insonified medium. It is caused by the fact, that such approach does not give the possibility to determine unified regularities of the formation of structure and properties of the systems with the fluid phase.

For the solution of the problem complex interrelated model of ultrasonic oscillation energy transformation into the target change of the structure and the properties of processed media is necessary. The developed complex interrelated model is described in following sections.

2. General statements of complex interrelated model

Proposed general approach for modeling is based on consequent consideration of the following stages of ultrasonic oscillation energy transformation to the target change of the medium structure and properties (figure 1) [5].

The energy of the radiator surface oscillations generates the pressure drops in a fluid. Appearing pressure drops are dissipated in the medium with total absorption coefficient $K$ (the intensity of ultrasonic wave passed through little distance $\Delta x$ is decreased by $2K\Delta x$).

Specific power dissipated in the unit of the medium volume $2KI$ per the unit of time contains 2 components ($2KI = 2K_m I + 2K_t I$):

1) specific power spent on undesired and in some cases unallowable heating of the medium (the increase of kinetic energy of the chaotic molecule motion) – $2K_t I$;

2) specific power spent on the change of the structure (the destruction of carbon and hydrogen molecule bonds, dispersion or coagulation of the solid particles) and macroscopic properties of the medium – $2K_m I$.

According to the diagram, the macroscopic properties of the medium are changed during the influencing. Changed macroscopic properties influence on pressure drops. As follows the pressure drops being changed during influencing. For instance, due to the viscosity reducing cavitation starts running more intensively. The said factor should be taken into consideration at the optimization of the modes of the action.

According to the proposed idea the task of the optimization of the modes for the increase of energy efficiency of the ultrasonic action on the systems with the fluid phase is to maximize of total power spent on the transformation of the medium structure related to oscillation power introduced by the ultrasonic radiator.

Figure 1. Stages of ultrasonic oscillation energy transformation in the systems with the fluid phase.
trasonic radiator (the efficiency of ultrasonic cavitation action). The total power spent on the transformation of the medium structure is linearly proportional to structural component of the absorption coefficient \( K_m \).

Thus, the criterion of efficiency maximum is \( K_m(I_{PRIM}) \rightarrow \text{max} \). The criterion is used hereinafter.

To maximize the efficiency of ultrasonic cavitation action, the new definition was introduced. For any processes in systems with fluid phase, the definition is medium structure vector \( C(t) = [C_i(t), C_j(t), \ldots, C_n(t)]^T \) depending on time of medium residence in apparatus. Each \( i \)-th component of the structure vector \( C_i \) is the number concentration of the structure elements of \( i \)-th type. For instance, for the processes of destruction of macromolecules of high-molecular fluid (mechanical destruction), \( C_i \) is a number concentration of the macromolecules with the number of the monomer units \( i \), and for the dispersion of solid particles in a fluid, \( C_i \) is a number concentration of the particles with the nominal diameter \( d_i \) from the discrete set of the diameters.

For any processes, by evaluation general regularities of interaction between structure elements with using statistical methods, the following equation (1) for structure vector were obtained by author. The equation was supported by initial condition (2) and bilinear (3) and differential (4) operator.

\[
\frac{dC}{dt} = B[p(r,t), C(r)] + D[p(r,t), C(r)];
\]

\[
C(0) = C_0 ;
\]

\[
B[p(r,t), C(r)] = \sum_{j,k} \sum_{i,j} \kappa(i,j,k) \beta(j,k,p(r,t))C_jC_k - C_i \sum_k \beta(i,j,p(r,t))C_j e_i ;
\]

\[
D[p(r,t), C(r)] = \sum_i \sum_j \lambda(i) \gamma(i+1,p(r,t))C_{i+1} - \gamma(i,p(r,t))C_i e_i ;
\]

where \( r \) is residence time of the allocated small volume (in comparison with the entire technological volume) of the medium in the apparatus, \( s \); \( B \) is bilinear operator that determines the effect of pairwise interaction of structural elements (dispersed particles or molecules) with each other on the medium structure vector; \( D \) is difference operator, taking into account the effect of an external field (pressure drops field) on a separate structural element; \( p(r,t) \) is field of pressure drops in the medium, depending on the microscopic coordinates \( r \) and time \( t \), Pa; \( \beta(j,k,p(r,t)) \) is the probability of the formation of a new \( i \)-th type structural element in the interaction of structural elements of types \( j \) and \( k \); \( \kappa(i,j,k) \) is the number of structural elements of the \( i \)-th type formed during an elementary act of interaction of a pair of structural elements of the \( j \)-th and \( k \)-th types; \( \gamma(i,p(r,t)) \) is the probability of destruction of an individual structural element of the \( i \)-th type by external field; \( \lambda(i) \) is the number of structural elements of the \( i \)-th type formed during the destruction of the structural element of the \( i+1 \)-th type.

The field of pressure drops \( p(r,t) \) is determined by cavitation area formation model earlier proposed by author [5]. The coefficients \( \beta(j,k,p(r,t)), \kappa(i,j,k), \gamma(i,p(r,t)), \lambda(i) \) are determined by type of process, and expressions for the coefficients were obtained by analysis of physical mechanisms of processes. The processes of macromolecules mechanical destruction and particles dispersing were considered. The physical mechanism of macromolecules mechanical destruction is pair macromolecules collision and breakage (shock wave generated by cavitation bubble increases pair macromolecules active collision probability and due to more active collisions macromolecules are broken), and mechanism of particle dispersing is high mechanical stresses caused by cavitation bubbles shock wave exceed strength of particle [5].

The structure component of the absorption coefficient is calculated according to the following expression:

\[
K_m(i) = (2I)^{-1} \frac{d\mu(r_i(C))}{dr} = (2I)^{-1} \left[ \nabla_{\mu(r_i(C))} \frac{dC}{dr} \right] = (2I)^{-1} \left[ \sum_{j,k} \kappa(i,j,k) \beta(j,k,p(r,t))C_jC_k - C_i \sum_j \beta(i,j,p(r,t))C_j e_i \right] - \left[ C_i \sum_j \beta(i,j,p(r,t))C_j + \lambda(i) \gamma(i+1,p(r,t))C_{i+1} - \gamma(i,p(r,t))C_i \right] \frac{d\mu}{dC_i} .
\]
where \( \tau \) is the duration of stay of specified volume of the medium in the apparatus, \( s \); \( u \) is the specific power of the mechanical and chemical bonds in the unit of the medium volume, \( J \cdot m^{-3} \).

In the following section the results of model analysis are presented.

3. Results of models analysis

Figure 2a shows the dependences of the structure component of the absorption coefficient on the intensity of ultrasonic action at the different viscosities of the fluid phase at the example of the macromolecules mechanical destruction process of homogeneous high-molecule fluid. Figure 2b shows the dependences of the optimum intensities providing maximum structure component of the absorption coefficient and the intensity providing maximum energy of ultrasonic oscillations transferring to the collapse of the cavitation bubbles (see [5]).

Figure 3a, b show the similar dependences for the ultrasonic dispersion of the suspensions.

The dependences shown in Figures 2a, 3a have extreme character and the maximum position determines the optimum intensity of action (Figures 2b, 3b), at which the most part of ultrasonic oscillation energy transforms into the change of insonofied medium structure (structure component of the absorption coefficient is maximum).

![Figure 3a](image1.png)  
![Figure 3b](image2.png)

**Figure 3.** Dependences of the relative structure component of the absorption coefficient due to the mechanical destruction of the molecules on the intensity of ultrasonic action at different initial viscosities (a) and the optimum intensity on the viscosity (b) (1 – optimum intensity providing maximum energy share of ultrasonic oscillations transferring to the change of the medium structure (macromolecules mechanical destruction); 2 – optimum intensity providing maximum energy part of ultrasonic oscillations leading to the collapse of the cavitation bubbles).
Figure 4. Dependences of the structure component of the absorption coefficient at the dispersion on the intensity of ultrasonic action at different initial viscosities of the fluid phase (a) and optimum intensity providing maximum energy efficiency of the dispersion on the viscosity of continuum fluid phase (b) (1 – optimum intensity providing maximum energy share of ultrasonic oscillations transferring to the change of the medium structure (dispersing); 2 – optimum intensity providing maximum energy part of ultrasonic oscillations leading to the collapse of the cavitation bubbles).

The approximation of obtained dependences allows determining, that the optimum intensity $I_{\text{OPT}}$, at which it is achieved maximum of the structure component of the oscillation absorption coefficient for the processes realized in the cavitation mode (macromolecules mechanical destruction and dispersion), is linearly proportional to the intensity providing maximum part of ultrasonic oscillation energy leading to the collapse of the cavitation bubbles $I_{\text{OPT,CAV}}$:  

$$ I_{\text{OPT}} = \mu I_{\text{OPT,CAV}}; $$  

where $\mu$ is the correction coefficient depending on the presence/absence of the interphase surface in the insonified system with a liquid phase ($\mu=0.63$ for the mechanical destruction of macromolecules and $\mu=1.75$ for the dispersion).

The obtained result can be practically used to modify of automatic system of continuous maintenance of optimum influence intensity. Existing system provides optimum intensity at which the maximum part of ultrasonic oscillation energy leading to the collapse of the cavitation bubbles [6]. The modification is multiplication measured $I_{\text{OPT,CAV}}$ to coefficient $\mu$ depending on process type. The operation will take into account kinetics of real process and increase ultrasonic cavitation energy efficiency for process realization up to 1.3÷1.8 times (see figures 3, 4).

The parameters of medium (after ultrasonic processing) on intensities $I_{\text{OPT}}$ and $I_{\text{OPT,CAV}}$ (the total energy is constant, $It = \text{const}$, $t$ is influence time) is presented on figures 5, 6.

Figure 5. Dependences of the final viscosity of the oligomer (process of macromolecules mechanical destruction) on its initial viscosity when exposed to...
ultrasonic vibrations with various optimal intensities $I$, which provide maximum $K (I_{OPT \text{ CAV}})$ and $K_m (I_{OPT})$ (for each intensity, the exposure time $t=\varepsilon I^{1}, \varepsilon=2000 \text{ J/cm}^2$).

![Graphs showing weight part and diameter range for different fraction compositions and intensities: (a) initial fraction composition, (b) $I_{OPT \text{ CAV}}$, (c) $I_{OPT}$](image)

Figure 6. Fraction compositions of brown coal after ultrasonic dispersing with various optimal intensities $I$, which provide maximum $K (I_{OPT \text{ CAV}})$ and $K_m (I_{OPT})$ (for each intensity, the exposure time $t=\varepsilon I^{1}, \varepsilon=28800 \text{ J/cm}^2$).

The data presented in figures 5, 6 follows, that using $I_{OPT}$ instead of $I_{OPT \text{ CAV}}$ improves final product parameter at same total introduced ultrasonic energy. For example, for macromolecules mechanical destruction the oligomer viscosity at $I_{OPT}$ is less than at $I_{OPT \text{ CAV}}$ (up to 1.3 times), for particles dispersing the mass fraction of small particles (less than 20 µm for brown coal) at $I_{OPT}$ is more than at $I_{OPT \text{ CAV}}$ (up to 1.5 times).

The obtained results were confirmed by experiments and may be used for making of control program for ultrasonic devices, which are necessary for processes realization.

4. Conclusion
Thus, it is proposed general approach to the modeling of the processes of the formation of the structure and properties of the systems with a fluid phase in the ultrasonic fields. The models developed on the base of the approach allowed determining optimum modes (the oscillation intensity) providing maximum efficiency of the ultrasonic action and improving of final product parameters.

Acknowledgement
The reported study was supported by Russian Science Foundation (Project No. 18-79-00094) and Russian Foundation for Basic Research (Project No. 19-48-220014). The calculating of the final product parameters at optimum and non-optimum intensities was performed under supporting by RFBR.

References
[1] Feng L, Liu S, Zheng H, Liang J, Sun Y, Zhang S and Chen X 2018 Ultrason. Sonochem. 44 53–63
[2] Zhang Y, Ma L, Cai L, Liu Y and Li J 2017 Ultrason. Sonochem. 36 88–94
[3] Sato K, Li J-G, Kamiya H and Ishigaki T 2008 J. Am. Ceram. Soc. 91 2481–87
[4] Hielscher T 2005 ENS’2005 (Paris: France) p 138
[5] Golykh R N 2018 IOP Conf. Ser.: Earth Environ. Sci. 193 012012
[6] Khmelev V N, Barsukov R V, Genne D V, Shalunov A V, Abramenko D S and Ilchenko E V 2011 Practical investigations of the method of indirect parameter checkout of the acoustic load parameters International Conference and Seminar on Micro/Nanotechnologies and Electron Devices. EDM’2011: Conference Proceedings pp 241–4