Abstract

Objectives: This work focuses on development of the mathematical models and theoretical research of the ultrasound ablation system in respect of the calculation of High Intensity Focused Ultrasonic Fields and modeling of biological tissue heating. Methods: Theoretical calculations of acoustic fields in linear approximation were made using Rayleigh integral. For description of nonlinear High Intensity Ultrasonic Fields, finite-difference modeling of Westervelt and Khokhlov–Zabolotskaya–Kuznetsov (KZK) equations were used. Findings: Theoretical and numerical models of High Intensity Focused Ultrasound (HIFU) Transducers were developed. The results of theoretical modeling of HIFU Transducers were presented. The characteristics of High Intensity Ultrasonic Fields, including the acoustic pressure, intensity and heat sources at different excitation modes of Ultrasound Transducers were calculated. Numerical solutions of the Khokhlov–Zabolotskaya–Kuznetsov (KZK) parabolic equation were obtained for nonlinear Focused Ultrasonic Fields. The obtained results were discussed. Applications/Improvements: The obtained results can be used in the development of HIFU Transducers for Medical Ultrasound Ablation Complexes, for the treatment of socially significant diseases.

Keywords: Acoustic Pressure, HIFU, Numerical Modeling, Nonlinear Fields, Transducers, Ultrasound

1. Introduction

Ultrasound has found usage in all aspects of the medical field, including diagnostic, therapeutic, and surgical applications\(^1^4\). Traditional therapeutic applications of ultrasound are: Treatment of soft tissues and bone diseases, wound healing, hyperthermic treatment of cancer, surgical treatment of Parkinson’s disease, using focused ultrasound, treatment of glaucoma and retinal detachment, treatment and surgical treatment of benign and malignant tumor of prostate, kidneys and liver, vascular therapy and computer-assisted surgery\(^1^4\).

Recent advances in physical acoustics, imaging method and image processing, piezoelectric materials, and designs of ultrasound transducers have led to the emergence of new methods and equipment for ultrasound diagnostic, therapy and aesthetic medicine, as well as to the development of traditional and new areas of application\(^8^1^8\).

Ultrasound Transducers are the main element of all ultrasonic equipment. The therapeutic transducers are usually made of hard ferroelectric piezoceramics of PZT system and, more recently, of porous piezoelectric ceramics and piezocomposites\(^1^1^4^4\).

Development of advanced designs of High Intensity Focused Ultrasound Transducers, as well as selection of the modes of therapeutic treatment of biological tissues is impossible without theoretical analysis and ultrasonic fields modeling\(^1^5^1^8\).

This article is dedicated to development of the mathematical models and theoretical study of the
ultrasound ablation system with regards to the calculation of focused ultrasonic fields of High Intensity Focused Ultrasound Transducers and modeling of biological tissue heating.

In the process of modeling and optimization, it is assumed that the developed ultrasonic source is a focused transducer in the shape of spherical bowl with the following parameters: Operating frequency \( f \) outer diameter \( D \) there is a circular hole in the center (for the diagnostic transducer accommodation) of diameter \( d \) of about 40 mm, and the radius of curvature of the emitting surface \( F \) circa 50 mm. Full acoustic power of the source \( W \) ranges from 100 W to 300 W, to provide the density at the focal point of at least 1000 W/cm\(^2\).

Ultrasound source parameters \( f, D, d, F, N, W \) in the developed model are not fixed, i.e. if required, they can be changed in order to find the optimal variant. As a working version of the design, it is recognized that the spherical bowl is filled with the acoustic coupling medium (oil, water) and is protected by a membrane (polyethylene, polyurethane) with a flat outer surface, placed into contact with a biological tissues or water. The distance from the output surface of the source to the focus point is about 30 mm.

2. Peculiarities of the Theoretical Description of the Focused Fields with Small Amplitude

Modeling of the acoustic field of ultrasound medical devices in general is a very difficult task. Analytically, such tasks are generally not solved, i.e., the only possible approach is the numerical modeling. Therefore, the problem of theoretical description is mainly conditioned upon the practical limits of modern computers. The “straight forward” modeling on the basis of the equations of hydrodynamics is possible, but in practice it is usually unrealizable because of the limits on the necessary memory and computing speed. Even using the advanced supercomputers, only those tasks, in which certain simplifying assumptions are used, may be solved.

One of the frequently used simplifications is the assumption on small amplitude of acoustic waves. In this case, the description of the ultrasonic field can be carried out in the approximation of linear acoustics. In the case of linearity, the principle of superposition is used, which, in particular, allows narrowing the problem down to the harmonic (sinusoidal) waves research: \( p(\mathbf{r}, t) = P(\mathbf{r}) \exp\left(-i\omega t\right)/2 + P^*(\mathbf{r}) \exp\left(i\omega t\right)/2 \), where \( p \) - acoustic pressure, \( P \) - its complex amplitude, \( \omega \) - cyclic frequency. Relevant equation for the harmonic waves is the Helmholtz equation: \( \Delta P + \left(\omega^2/c_0^2\right)P = 0 \), where \( c_0 \) - speed of sound in the medium. The equation must be solved in conjunction with the boundary condition, determined by the mode of vibration of the ultrasonic source.

In the case of a homogeneous medium, the solution can be written in the form of the Kirchhoff-Helmholtz integral, which is a mathematical notation of the outstanding Huygens-Fresnel principle:

\[
P(\mathbf{r}) = \gamma \int_S dS' \left[ p(\mathbf{r}') \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial n(\mathbf{r}')} - \frac{\partial P(\mathbf{r}, \mathbf{r}')}{\partial n(\mathbf{r}')}) G(\mathbf{r}, \mathbf{r}') \right],
\]

where the integration is carried out along the radiating surface of \( S \), \( P \) - the complex amplitude of the acoustic pressure at the observation point with coordinate \( \mathbf{r}, \mathbf{r}' \) - the radius vector of the surface element \( dS' \). \( G(\mathbf{r}, \mathbf{r}') \) - Green's function. If the observation point with the radius vector \( \mathbf{r} \) is located on the surface \( S \), then \( \gamma = 2 \), if not, then \( \gamma = 1 \). As the function \( G(\mathbf{r}, \mathbf{r}') \), for example, free space Green's function can be used

\[
G(\mathbf{r}, \mathbf{r}') = \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{4\pi |\mathbf{r} - \mathbf{r}'|}
\]

where \( k = \omega/c_0 \) - wave number, \( \rho_0 \) and \( c_0 \) - density and speed of sound of the medium. However, Representation (2) does not give solution of the problem, as in the initial formulation, the value of the complex amplitude of normal speed component \( V \) is given on the surface of the radiant (assume that the normal line is directed towards the medium), i.e., \( \partial P/\partial n = k \rho_0 c_0 V \), and the value of the complex pressure amplitude \( P(\mathbf{r}') \) is unknown. If we could choose such Green’s function that \( \partial G(\mathbf{r}, \mathbf{r}')/\partial n(\mathbf{r}') = 0 \) would be located on the surface \( S \), then the problem would be solved. As it is known, in most cases of practical interest (in particular, in the case of concave surfaces), the suitable Green’s function cannot be found. The appropriate exception is the case of a flat surface, when the Green’s function, the normal derivative of which vanishes on the surface, and the function, which itself vanishes on \( S \), are known. On substituting the two Green’s functions in Formula (2), the following two integral formulas are obtained:

\[
P(\mathbf{r}) = -2\gamma \int_S \frac{\partial P(\mathbf{r}')}{\partial n(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}') dS'
\]
\[ P(r) = 2\pi \int_{S} P(r') \frac{\partial G(r, r')}{\partial n(r')} \, dS', \]  
(4)

where \( G(r, r') \) – free space Green's function defined by Formula (2). Equation (3) written for points, external to the source surface, is called the Rayleigh integral. It is usually written using the complex amplitude of the normal component of the speed of the radiating element surface:\[ P(r) = -i \rho _0 c_0 \frac{k}{2\pi} \int_{S} V(r') e^{ik|r-r'|} \, dS'. \]  
(5)

Formula (4), which expresses the pressure in the observation point through the pressure on the surface of integration, can be named the 2\textsuperscript{nd} Rayleigh integral (then, it is reasonable to call the ordinary Rayleigh integral (3) as "the 1\textsuperscript{st} Rayleigh integral"). Formula (4) is not suitable for calculating the fields of piezoelectric sources, as it is usually assumed that the speed of the source is known, but not the pressure. At the same time, this formula can be useful in the calculation of fields in piecewise-homogeneous mediums with insignificant impedance jumps, such as layers of tissues. In this case, the Rayleigh integral Equation (5) can be used as the first step to calculate the pressure at the interface, and then the 2\textsuperscript{nd} Rayleigh integral can be used to calculate the pressure in the points of the subsequent medium.

Expression (5) gives an exact representation for the acoustic field in case of the flat radiating surface. In his work, in\[ P = \rho_0 c_0 \frac{k}{2\pi} \int_{S} V(r') e^{ik|r-r'|} \, dS', \]  
(6)

(apparently independently) in the mentioned work of\[ P = \rho_0 c_0 \frac{k}{2\pi} \int_{S} V(r') e^{ik|r-r'|} \, dS', \]  
(7)

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\[ P_{\text{max}} = K_F \cdot P_0, \]  
(8)

Here, the parameter \( K_F \), with the meaning of the rate of wave amplitude growth when focused, is

\[ K_F = kh = kF.(1 - \cos \alpha) \]  
(9)

In the given expression \( h = F \cdot (1 - \cos \alpha) \) – bowl depth. As part of the Rayleigh integral approximation, O’Neal also received the expression for the transverse pressure amplitude distribution in the focal plane in the form of a series containing the Bessel function:

\[ P/P_{\text{max}} = \frac{z}{\xi} \sum_{n=1}^{\infty} (-1)^{n+1} \left( \frac{h/\alpha}{2kF} \right)^n J_{2n+1}(\zeta), \]

where \( \zeta = (1 - i/k\xi) \cdot k \alpha \sin \Theta \). Here \( \alpha = F \sin \alpha \) – source aperture range, \( \xi \) – the distance from the observation point to the center of the radiating bowl, and \( \Theta \) – viewing angle, at which the observation point is seen from the center of the bow. If \( r' \) – transverse coordinate, i.e., the distance from the observation point to the radiant axis, then \( r = F \tan \Theta \), \( \xi = \sqrt{r^2 + F^2} \). If the focus angle \( \alpha \) is not too large, then the written out series converges very fast and the limitation by the first expansion term is quite justified. Moreover, the focal length \( F \), within the meaning, exceeds by far the diameter of the focal constriction and a
wavelength even more (otherwise the focusing will not be effective due to diffraction); therefore, the approximation \( \zeta \approx k a r / F \) is quite justified. As a result, we obtain:

\[
P / P_{\text{max}} \approx \frac{2 J_1(ka r / F)}{ka r / F} \tag{10}
\]

This expression coincides with the known in optics diffractive field distribution at the lens focus: The central part of the focal spot, the line of which is drawn along the zero of the Bessel function, is often called the “Airy disk” (about 84% of the beam energy is passed through it). Distributions described in Formulæ (6) and (10) allow to fairly easy calculate the longitudinal and transverse structure of the field in the focal area of the focused ultrasound transducer.

Note that although the above analysis concerns the sources in the form of a spherical bowl, a slight modification allows expanding it to the case of the source as a ring shaped spherical segment- this case is of interest in this project. Indeed, by virtue of the linearity of the problem, during the insertion of another bowl in a spherical bowl, which is coaxial with it (with the same curvature of the surface, but different diameter), the fluctuation can be obtained only on the ring shaped segment, if to excite the surfaces of the said bowls in the opposite phase. Accordingly, by virtue of the principle of superposition, the field of the ring will be subtraction of the fields of two bowls of various diameters.

Used in practice, the concave piezoceramic sources are, at a first glance, quite close to the said idealized source, the field of which is described by \(^2\) Formula (5). Indeed, the shape of the source surface can be made spherical with high precision. High uniformity of properties of piezoelectric ceramics allows us to hope that the occurred variations are related to the excitation of the thickness mode, for which the uniform speed distribution along the surface is typical. The latter approximation is quite popular, and in the case of flat sources it is often called as "piston type".

Over the years of the focusing radiant usage, a large number of experiments qualitatively confirmed the validity of Formulæ (6) and (10). In several studies the attempts were made to verify the results of work\(^2\) more carefully. It\(^2\) turned out that the transverse distribution of the wave amplitude in the focal plane is quite accurately described by Formula (10), particularly if the effective diameter of the source is selected appropriately.

At the same time, we cannot say this about the longitudinal structure of the field: The measured distribution of the pressure amplitude along the axis was significantly different from the predictions of Formula (6). In particular, Theory (6) predicts presence of points on the axis, where the wave amplitude is equal to zero, and in the said experiments only local minima with the final pressure amplitude were observed. Furthermore, the levels of the local maxima and the coordinates of the extreme were significantly different from the values given by Formula (6). These discrepancies cannot be explained by the low accuracy of measurements: The used hydrophones were of a pocket-size, the positioning systems were stilly accurate, the parameters of the medium and the geometric characteristics of the transducers were reliably controlled. One of the possible explanations of discrepancies between the theory and the experiment is an approximate nature of the Rayleigh integral, which was used in the derivation of Formulæ (6) and (10). In fact, the Rayleigh integral is exact only in the case of flat sources and if using the concave transducers, the solution based on it is non-strict. However, the theoretical studies, conducted by us, have shown that the inaccuracy of the Rayleigh integral cannot explain the presence of strong additional signals on the source axis. Thus\(^2\), there is no reason not to trust measurements or the way of solving the wave equation. The only one remaining ‘weak point’ is the boundary condition used in the theoretical model, which lies in the assumption of the constancy of the speed along the radiating spherical surface.

It should be noted that the assumption of a homogeneous nature of the oscillation of the surface of the piezoelectric ultrasonic vibrations sources of megahertz range is used not only in the long-published works. The\(^2\) assumption of the piston nature of the oscillation is made in a large number of theoretical works on the calculation of the ultrasonic fields of piezoelectric sources; in modern books and articles on acoustics\(^2\) this assumption is considered to be clearly justified in cases where the diameter of the source is much greater than the wavelength. Other modes of oscillations, for example flexural ones, are considered to be important only for the sources, the size of which is comparable to the wavelength (for example, in hydroacoustics).

The results of theoretical and experimental studies, in which it was shown that during the operation of the piezoceramic focusing source the uniform speed distribution
assumption is not met, are presented in works\textsuperscript{25}. The cause of this abnormal behavior was found. Moreover, the study of fields of the sources made of piezocomposite material was undertaken and it was demonstrated that their fields can be predicted with high accuracy on the basis of the piston model. Thus, when using piezoelectric ceramics, it should be noted that the oscillation of the surface can be uneven, and when using the piezocomposites, we may hope for the piston nature of the surface oscillations.

In the case of the undirected nature of the surface oscillations and at the random point in space (i.e., not only on the axis or in the focal plane), the Rayleigh integral should be calculated numerically. This approach will be used in this project.

The calculation of field becomes much more difficult in the case when the medium is heterogeneous, especially when the heterogeneity is strong, and therefore during the spread the visible scattering occurs. An effective way to solve this problem, although it requires more complex algorithms and more powerful computers, is a numerical integration of the Helmholtz equation or of the original equations of hydrodynamics by the method of finite differences or the finite elements.

3. Peculiarities of the Theoretical Description of High-Power Focused Ultrasound Beams

Since the high intensity mode required for hemostasis is characterized by nonlinear propagation of acoustic waves, a theoretical description requires more complex models as compared with the case of low intensities.

For the highly focused fields, the nonlinear model of Westervelt equation type can be used, which is a generalization of the classical wave equation to the nonlinear case in the approximation of the lack of back propagating waves. In\textsuperscript{21} still more complex models are based on the solution of the full non-linear wave equation. However\textsuperscript{22}, such approaches are extremely laborious and require large computing capabilities and time-consuming calculations (up to several days) on supercomputers, i.e., are practically inapplicable to practical problems when it is required to analyze the ultrasonic field, depending on several parameters. This difficulty can be significantly reduced by using an evolutionary equation for the quasi-plane waves. Relevant equation in nonlinear acoustics is known as the Khokhlov-Zabolotskaya-Kuznetsov equation. In\textsuperscript{23} models based on non-linear equations of KZK type apply to the research of fields of the lithotripters, focused pulse emitters and HIFU-sources\textsuperscript{24}.

KZK equation is written as follows:

$$\frac{\partial}{\partial \tau} \left[ \frac{\partial p}{\partial z} - \frac{\beta}{\rho_0 c_0^2} p \frac{\partial p}{\partial \tau} - \hat{L}[p] \right] = \frac{c_0^2}{2} \Delta_{\perp} p \tag{11}$$

Here $p(x, y, z, \tau)$ – acoustic wave shape, $z$ – coordinate along the beam axis, $x$ and $y$ – transverse coordinates, $\tau = t - z / c_0$ – time in associated coordinate system, $\beta$ – acoustic nonlinearity of the medium parameter, $\rho_0$ – density, $c_0$ – sound speed, $\hat{L}[p]$ – a linear operator, characterizing the dispersion-dissipative properties of the medium\textsuperscript{25}, $\Delta_{\perp} = \partial^2 / \partial x^2 + \partial^2 / \partial y^2$ – transverse Laplacian. In the case of axial symmetry, which is assumed in studies of this project, the Laplacian is expressed through the radial coordinate $r = \sqrt{x^2 + y^2}$ as follows: $\Delta_{\perp} = \partial^2 / \partial r^2 + r^{-1} \partial / \partial r$.

The classical form of KZK equation was derived for thermo-viscous liquids, for which

$$\hat{L}[p] = \frac{b}{2 \rho_0 c_0^3} \frac{\partial^2 p}{\partial \tau^2} \tag{12}$$

where $b = \zeta + 4 \eta / 3$ – dissipative coefficient, $\zeta$ – volume viscosity, $\eta$ – shear viscosity. When using the Operator (12) in the linear approximation, the absorption coefficient is obtained, which is proportional to the square of the frequency. In the biological medium, the absorption coefficient behaves differently, depending on the frequency in almost linear fashion. Hence, the operator $\hat{L}[p]$ has to be modified accordingly. Selection of the right operator for different biological tissues can be made on the basis of the frequency dependence of the absorption coefficient. In\textsuperscript{21} generally, the operator $\hat{L}[p]$ can be expressed in terms of the frequency dependence of the absorption coefficient $a(\omega)$ and the speed of sound $c(\omega)$ as follows:\textsuperscript{24}:

$$\hat{L}[p] = \int_{-\infty}^{\infty} K(\tau - \tau') p(x, y, z, \tau') d\tau', \tag{13}$$

$$K(\tau) = \frac{2}{\pi} \int_{0}^{\infty} \left[ \frac{\omega}{c(\omega)} - \frac{\omega}{c(x)} \right] \sin \omega \tau - \tau - a(\omega) \cos \omega \tau \right] d\omega \tag{14}$$

Here $\omega = 2\pi f$, where $f$ – frequency. Finding an exact expression for the kernel $K(\tau)$ is not possible.
in most practical cases, because the behavior of the absorption coefficient \(a(\omega)\) and the speed of sound \(c(\omega)\) are usually known only in a certain frequency range, and certainly unknown at very high frequencies included in the Integral (14). At the same time, if the law \(a(\omega)\) is known in the frequency range, over which the spectrum of the involved ultrasonic wave is extended, it is possible to write a kernel with the datum of the wave, necessary for the calculation.

For biological tissues in the range of medical ultrasound frequency, the absorption coefficient can be approximated by the power law of the form

\[
a(\omega) = a_0 \left(\frac{\omega}{\omega_0}\right)^n,
\]

where \(a_0 = a(\omega_0)\) and \(\omega_0\) – certain characteristic frequency; e.g. \(\omega_0/(2\pi) = 1\) MHz. The index of power \(n\) depends on the type of tissue, and for most soft biological tissues it is close to 1 \(n = 1\). The frequency dependence of the speed of sound can be calculated from the Relation (15) by means of local dispersion relations:

\[
c(\omega) - c_0 = \frac{2c_0 a_0}{\pi \omega_0} \left(\frac{\omega_0}{\omega}\right)^{\eta - 1}, \quad \eta \neq 1
\]

Here \(c_0 = c(\omega_0)\) – the speed of sound at frequency \(\omega_0\). Although the dispersion of the speed of sound, expressed by the Formula (16), in biological tissues is relatively weak, it should be considered for the retention of the principle of causality.

The absorption law in the Formula (15) does not consider a quadratic growth at high frequencies caused by the viscosity of water. The role of this part of the absorption is insignificant in the megahertz range, but can be important at high frequencies, in particular for higher harmonics, typical for the waves with shock front. Therefore, in numerical calculations the absorption should be modified as follows:

\[
a(\omega) = a_0 \left(\frac{\omega}{\omega_0}\right)^n + \frac{b}{2\rho_0 c_0^3} \omega^2,
\]

High-frequency supplement \(\Delta a = b\omega^2/(2\rho_0 c_0^3)\) describes the classic absorption law, quadratic as to frequency.

4. The Dimensionless Notation of KZK Equation. Typical Dimensionless Parameters of the Problem

Equation (11) should be solved for the specific boundary condition defined by the considered therapeutic source. Let \(z = 0\) be the plane on which the acoustic pressure at the source is set. The corresponding distribution \(p(x, y, z, t)\) may vary depending on the radiant used. Nevertheless, many of the distinctive features can be learned by examining an idealized circular focusing piston radiant. In the parabolic approximation of diffraction theory, in which the KZK equation is written down, such source can be set by the following distribution of acoustic pressure where \(z = 0\):

\[
p(x, y, z = 0, t) = \begin{cases} p_0 \cos \left(\frac{\omega_0}{2c_0} r^2 \right), & r \leq a_0 \\ 0, & r > a_0 \end{cases}
\]

Here \(p_0\) – wave amplitude in the center of the source, \(\omega_0 = 2\pi f_0\), \(f_0\) – operating frequency, \(F\) – focal length, \(a_0\) – the radius of the piston source, \(r = \sqrt{x^2 + y^2}\) – radial coordinate. Since the source is axially symmetric, the transverse Laplacian has the form of \(\Delta_T = 1/r \partial^2/\partial r^2 (r \partial^2/\partial r)\).

We rewrite the equation in dimensionless form. We proceed from the record of the operator \(\hat{L}[p]\) in the form (12). We obtain the following:

\[
\frac{\partial}{\partial \sigma} - \frac{\partial P}{\partial \sigma} - NP - A \frac{\partial^2 P}{\partial \theta^2} = 1 \frac{\partial^2 P}{R \partial R^2} + \delta \frac{\partial^2 P}{\partial R^2}.
\]

Here \(P = p/p_0\) – acoustic pressure normalized to the amplitude of the waves at source \(p_0\), \(\sigma = \omega_0\tau\) – dimensionless time, \(\sigma = z/F\) – distribution coordinate normalized to the focal length, \(R = r/a_0\) – transverse coordinate normalized to the radius of the source aperture. As is evident from the dimensionless Notation (19), instead of the 8 parameters \(\omega_0, p_0, c_0, \rho_0, a_0, F, \beta, b\) there are only three independent dimensionless numbers: \(N, A, G\). They are expressed through the initial parameters as follows:

\[
N = \frac{\beta_0 a_0 p_0 F}{c_0^3 \rho_0},
\]

\[
\frac{A}{} = \frac{c_0^3 \rho_0 p_0 F}{\beta_0},
\]

\[
\frac{G}{} = \frac{c_0^3 \rho_0 p_0 F}{\omega_0^3},
\]

\[
\frac{\Delta}{} = \frac{c_0^3 \rho_0 p_0 F}{\omega_0^3}
\]

\[
\frac{\beta}{} = \frac{c_0^3 \rho_0 p_0 F}{\omega_0^3},
\]

\[
\frac{b}{} = \frac{c_0^3 \rho_0 p_0 F}{\omega_0^3}
\]
Absorption of Nonlinear Waves

Parameter \( N = F / x_d \) describes the acoustic nonlinearity, which mainly depends on the amplitude of the wave at the source. Parameter \( G = x_d / F \) describes the diffraction and is quantitatively identical to the value of the linear coefficient of the gain of the field at the focus. And finally, parameter \( A = F / x_d \) describes the absorption on a frequency of radiation. Note that in the mediums as water ones, this parameter is usually very small, and so in many cases it cannot be taken into account. That is why only two parameters, \( N \) and \( G \) are really important. Two typical scales were used herein above: \( x_d = k a_0^2 / 2 \) – the diffraction length for the linear beam, \( x_i = \rho_0 c_0^3 / (\beta \rho_o a_0) \) – nonlinear length equal to the length of the formation of the shock front in a plane harmonic wave, \( x_d = 2 \rho_0 c_0^3 / (\beta \rho_o a_0) \) – the length of absorption of the plane linear wave at the initial frequency.

5. Heat Release during the Absorption of Nonlinear Waves

In the ultrasound ablation problem to be solved in this work, it is important to be able to calculate the heat release during the absorption of the ultrasound beam. We first consider the arbitrary case, without limitation of the type of the parabolic approximation, but for classical thermoviscous liquid. The literature often uses the formula for the amount of heat released per unit time per unit volume (volumetric density of heat sources power) in the form of \( Q = 2 a I \), where \( a \) – absorption coefficient, \( I \) – wave intensity. However, this expression is valid only for a plane linear harmonic wave. If the wave is not plane (as in the case of a focused beam) or, for example, standing, then the above simple expression does not apply. We derive the required expression based on the Navier-Stokes equation. Note that since the energy characteristics are quadratic in the acoustic disturbances, it is sufficient to consider the Navier-Stokes equation in the linearized form:

\[
G = \frac{\omega_0 a_0^2}{2c_0 F}, \quad (22)
\]

\[
A = \frac{b \omega_0^2 F}{2c_0 \rho_0}. \quad (23)
\]

Here \( v \) – oscillating speed, \( P \) – acoustic pressure, \( \eta \) and \( \zeta \) – coefficients of shear and of volume viscosity. We use effective viscosity coefficient. The

\[
\rho_0 \frac{\partial v}{\partial t} = -\nabla p + \left( \zeta + \frac{\eta}{3} \right) \nabla(\nabla \cdot v) + \eta \nabla(\nabla \cdot v) \cdot v. \quad (24)
\]

Note that Expression (32) is suitable for any kind of waves including flat and the harmonic wave, when it goes into
the above-mentioned formula $Q = 2aI$. The attention shall be paid to the presence of the derivative of pressure with respect to time in the formula. This means that the absorption is determined not so much by the intensity of the waves as the steepness of the profile: In case of the nonlinear steepening of the wave of the profile and formation of shock fronts, the heat power of sources is markedly increased as compared with the linear case.

Next, we consider the parabolic approximation, in which the KZK equation is written down. If we average the energy flow energy according to the conservation Law (28) over the period of the wave and apply the intensity $I = \langle S \rangle$ , then for the quasi plane wave the supplement can be neglected due to the viscous stress and $I = \langle p\nu \rangle$ can be written down. Further averaging the energy conservation Law (28) over the time period, we write out the relation between the power of heat sources and the intensity:

$$Q = -\nabla \cdot I,$$

(33)

According to the equation of motion, we can write in first approximation:

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0} \nabla p,$$

(34)

We now proceed to the “running” time $t' = t - z/c_0$. Then, the following equations for the longitudinal $v_\perp$ and transverse $v_z$ components of speed imply from the equation (34):

$$\frac{\partial v_\perp}{\partial t'} = -\frac{1}{\rho_0} \nabla_\perp p,$$

(35)

$$\frac{\partial v_z}{\partial t'} = -\frac{1}{\rho_0} \frac{\partial p}{\partial z} + \frac{1}{\rho_0 c_0} \frac{\partial p}{\partial t'}.$$  

(36)

From these expressions in the first nonvanishing approximation, we can write:

$$v_\perp = -\frac{1}{\rho_0} \nabla_\perp \int p' \tau'$$

(37)

$$v_z = \frac{p}{\rho_0 c_0}.$$  

(38)

Hence follows the expression for the heat sources:

$$Q = -\nabla \cdot I = -\frac{1}{\rho_0 c_0} \frac{\partial}{\partial z} (p') + \frac{1}{\rho_0} \nabla_\perp \cdot \left\langle p\nu \int p' \tau' \right\rangle.$$  

(39)

Note that in the parabolic approximation $\nabla^2 \perp \sim \partial^2 / \partial z^2$, i.e., in Expression (13), both terms have the same order of smallness; the second term cannot be neglected. The first term corresponds to the approximation of plane waves, and the second term takes into account the diffraction, in particular, additional energy flows due to the convergence and divergence of the beam.

We decompose the described wave into Fourier series:

$$p(r_\perp, z, \tau) = \frac{1}{2} \sum_{n = -\infty}^{\infty} C_n (r_\perp, z) \exp(-i \omega_0 \tau),$$

(40)

where $C_n$ – harmonic amplitudes, $\omega_0$ – frequency of the source. Then

$$\left\langle p^2 \right\rangle = \frac{1}{2} \sum_{n = -\infty}^{\infty} |C_n|^2.$$

(41)

The primitive of the pressure has the following expression:

$$\int p' = \frac{1}{2} \sum_{n = -\infty}^{\infty} \left\langle C_n \nu [\exp(-i \omega_0 \tau + n)] \right\rangle.$$  

(41)

Hence it follows:

$$\left\langle p\nu \int p' \tau' \right\rangle = \frac{1}{2} \sum_{n = -\infty}^{\infty} \left\langle C_n \nu [C_n^* - C_n^* C_n] \right\rangle.$$  

(42)

Given that $C_{-n} = C_n^*$ (this follows from the actuality of the acoustic pressure value), we obtain:

$$\left\langle p\nu \int p' \tau' \right\rangle = \frac{1}{4} \sum_{n = 0}^{\infty} \frac{1}{\omega_0 c_0} \left\langle C_n \nu [C_n^* - C_n^* C_n] \right\rangle.$$  

Hence it follows

$$Q = \frac{1}{2 \rho_0 c_0} \sum_{n = 1}^{\infty} \left\langle C_n \Delta_{\perp} C_n^* - C_n^* \Delta_{\perp} C_n - \frac{\partial |C_n|^2}{\partial z} \right\rangle.$$  

(43)

This is the desired expression for the heat sources.

Let us consider, for example, the linear acoustic beam. Then the KZK equation gives the following parabolic equation for the amplitudes of harmonics:

$$\frac{\partial C_n}{\partial z} = \frac{1}{-2i \omega_0 c_0} \Delta_{\perp} C_n - a \left(\frac{\nu \omega_0}{c_0}\right) C_n.$$  

(44)

Hence it follows: $\Delta_{\perp} C_n / (\nu \omega_0 / c_0) = -2 \left\{ \frac{\partial C_n}{\partial z} + a \left(\frac{\nu \omega_0}{c_0}\right) C_n \right\}$, which gives:
\[ Q = \frac{1}{2\rho c_0^2} \sum_{n=1}^{\infty} \left\{ C_n \left[ \frac{\partial C_n}{\partial z} + a (\omega_o) C_n \right] + C_n \left[ \frac{\partial C_n}{\partial \omega} + a (\omega_o) C_n \right] - \frac{\partial C_n^2}{\partial z^2} \right\} \]

\[ = \frac{1}{2\rho c_0^2} \sum_{n=1}^{\infty} 2a_n (\omega_o) C_n \]

As we can see, the obtained result has easy-to-understand form:

\[ Q = \sum_{n=1}^{\infty} 2a_n I_n, \quad (45) \]

where \( a_n = a (\omega_o) \) – the absorption coefficient of the \( n \)-th harmonic, and \( I_n = \left| C_n \right|^2 / (2\rho c_0^2) \) - the intensity of this harmonic. According to the Equation (19), the total heat source in a non-harmonic (in particular, in a nonlinear) wave is the sum of the heat sources of individual harmonics, where the absorption for each harmonic can be considered to be in the plane wave approximation. Note that during the numerical solution of the KZK equation, the method of splitting into physical factors is commonly used, in which the account nonlinear operator (responsible for the exchange of energy between the harmonics) is applied at each stage to the calculated wave function independently of the linear operator (responsible for the diffraction and absorption). Given that the harmonic interaction itself leads only to the exchange of energy between them without loss of total energy (i.e., there is no dissipation), it can be concluded that the formula for the heat sources in Equation (45) remains applicable for the non-linear calculation.

During the modeling of the ultrasonic field in respect of the task of this project, Equation (11) is solved by the method of finite differences in the frequency representation. The result of the calculations is represented by complex amplitudes of the harmonics \( C_n(r, z) \). The form of the wave is calculated on the basis of it. Harmonic intensity \( I_n(r, z) = \left| C_n \right|^2 / (2\rho c_0^2) \), the total intensity of the wave \( I(r, z) = \sum_{n} I_n(r, z) \) and the power of heat sources \( Q(r, z) = \sum_{n} 2a_n I_n \) are also calculated.

**6. Discussion**

Let us consider some examples of numerical calculations of nonlinear fields and heat sources during the focusing of ultrasound in oil.

We assume that the radiant is placed into the absorbing medium with the parameters of castor oil and the parameter of nonlinearity as in the water, \( \varepsilon = 3.5 \). The calculations were performed for two frequencies of 1.6 MHz and 2 MHz with the initial intensity of 5, 10 and 20 W/cm². Let us analyze how nonlinear effects for these two frequencies will show themselves with the increase of the intensity on the radiant.

Figure 1 shows the dependencies of the intensity, normalized to the initial intensity at the source, along the axis of the radiant. It is evident that the increase of the initial intensity results in the increase of the concentration of the intensity at the focus point. However, this effect is not very strong (<25%) and occurs only in the maximum area of the field at a distance of ± 1 mm from the focus point.

Similarly, Figure 2 illustrates the normalized intensity distributions in the focal plane. It is evident that the transverse structure of the intensity distribution changes only near the maximum \( r < 0.1 \) mm, where the increase in intensity of concentration is observed. In general, the transverse structure of the beam at large distances from the axis is the same, as in the situation with the linear focusing.

Figures 3 and 4 show the two-dimensional spatial distribution of the intensity on the plane of the axis of the radiant. The levels of the intensity are presented in absolute units, kW/cm². The figures in the left series correspond to the initial intensity of 5 W/cm², when the non-linearity effects are minor. The coefficient of gain of the linear field at the focus point, if there were no absorption, for the frequency of 2 MHz is greater than for the frequency of 1.6 MHz which is proportional to the frequency value, but the absorption towards the focus point for the frequency of 2 MHz is stronger. As we can see from the Figure, the integrated effect of a stronger absorption of higher frequency dominates, and the intensity value at the focus point is bigger for 1.6 MHz radiant. The degree of manifestation of nonlinear effects at the focus point is also determined by the competing effects: Nonlinear effects are strengthened with

![Figure 1](image-url)
the increase of frequency, but are less expressed at lower intensity and the length of the focal area. As a result, non-linear effects, expressed in the nonlinear strengthening of the intensity coefficient at the focus point, also turned to be stronger than for lower frequency of 1.6 MHz. In general, the size of the focal spot for the intensity changes slightly with an increase of the initial intensity of the radiant from 5 W/cm$^2$ to 20 W/cm$^2$.

The greatest interest is attracted by the analysis of the absolute values and spatial distributions of the power of heat sources in the medium due to the absorption of ultrasound energy. In case of substantially linear focus (5 W/cm$^2$), the absorption is proportional to the intensity, and these distributions are equal. With an increase in the initial intensity, nonlinear effects result in generation of higher harmonics, which are absorbed much stronger. When the gap is formed at the focus point in the wave profile, the absorption can be strengthened ten times in comparison with the harmonic wave of the same intensity. Therefore, during the nonlinear focusing, the results for the intensity cannot be used to assess the heating of the medium. Everything depends on how the time profile of the wave at the focus point is deformed, whether the gap was formed. During its formation, the efficiency and locality of the heating are changed radically.

These effects are illustrated in Figure 5, which shows dependence of the power of heat sources in the oil, normalized to the initial heating power near the radiant, along the beam axis for two frequencies and three initial intensities. If the non-linearity effects were not showed, all three curves in each Figure would coincide.

An increase of the initial intensity leads to an increase of nonlinear effects in the focal area and a strong change in the efficiency of heating in the local area around the maximum of the field at a distance of ±1 mm from the focus point. These effects are much more represented for a frequency of 1.6 MHz: heating efficiency is increased by 20 times to 20 W/cm$^2$; for a frequency of 2 MHz it is increased by 7 times compared with the values predicted in the approximation of the linear focusing.

Two-dimensional distribution of the heat sources, already denominated in absolute units kW/cm$^3$, are shown in Figures 6-7. As we can see, even when the initial intensity is 5 W/cm$^2$, the maximum value of the heat release at the focus point is somewhat higher than the calculated one for the linear beam. The increase of the initial intensity
intensity by 4 times leads to a sharp localization of the heat and its increase not by 4, but by 50 times for 1.6 MHz and by 20 times for 2 MHz.

The dramatic improvement in the localization of the heating in space and the enhancement of its effectiveness with the initial intensity of 20 W/cm$^2$ indicates that the gap is formed at the focus point in the time profile of the wave. What is more, the gap amplitude is larger for the source with a frequency of 1.6 MHz, compared with a frequency of 2 MHz. This is shown by Figures 8-11, which provide pressure wave profiles in the focal diffraction maximum along the beam axis and in the focal plane transverse to the beam axis. The profiles are normalized to the initial pressure amplitude. If the nonlinear effects did not occur, then the figures would not differ with the change in the intensity at the source, the profile would remain harmonic, i.e., it would be presented as a single period of a harmonic wave, a maximum at the focus point for the 1.6 MHz would be equal 55, and for 2 MHz it would be equal to 51.7.

It is evident that even at 5 W/cm$^2$ the nonlinear effects lead to asymmetry of the profile, the peak positive pressure at the focus point is greater than the amplitude of the linear wave, the peak negative pressure is, on the contrary, less. Distortions increase with the increase of the initial intensity, the profile contains steep section – the shock front at 20 W/cm$^2$ at the focus point (green curves) and near the focus point (blue and yellow curves). Exactly the presence of the front determines a dramatic increase in the heat release in the medium.

The discontinuous front is present only in a very local spatial area around the focus point, both along the axis and perpendicular to the axis in the focal plane. The super-fast heating occurs precisely in this area.
7. Conclusions

The main result of this work is the development of the mathematical models and effective numerical algorithm for the solution of the axially symmetric Khokhlov - Zabolotskaya - Kuznetsov (KZK) equations for nonlinear focused ultrasonic fields. It can be used for selection of the parameters of the focusing ultrasonic transducers and for calculation of the HIFU field and corresponding heat sources in the biological tissue for subsequent evaluation of heat effects.

The characteristics of high intensity ultrasonic fields, including the acoustic pressure, intensity and heat sources at different excitation modes of ultrasound transducers were calculated using developed approach. It was shown that the linear acoustic field of a spherical transducer, especially near the focus point, can be approximated with good accuracy by the acoustic field of the equivalent piston source calculated in the parabolic approximation of diffraction theory.

The undertaken studies have shown the distinctive features of focused ultrasound transducers in a wide range of parameters. It was shown that at even at low acoustic intensity less than 5 W/cm² the nonlinear effects lead to asymmetry of the profile, the peak positive pressure at the focal point is greater than the amplitude of the linear wave. Distortions increase with the increase of the initial intensity, and at the intensity 20 W/cm² the shock front is formed near the focal point that leads to dramatic increase in the heat release in the medium.

The obtained results can be useful in development of high intensity ultrasound transducers for medical complexes of ultrasound ablation applied for the treatment of socially significant diseases.

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9. References