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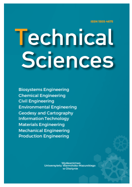

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MODELING THE PHENOMENON OF ULTRASONIC WAVE PROPAGATION IN SELECTED FLUIDS USING COMSOL – A CASE STUDY

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A b s t r a c t

The aim of this study was to model the propagation of acoustic waves with frequencies in the ultrasound range in three selected fluids. Ultrasonic wave propagation in the studied fluids was tested in a laboratory to validate the model. The laboratory tests involved simple measurements of the time of flight of an ultrasonic wave with a frequency of 5 MHz in fluids with different parameters: demineralized water, rapeseed oil, and gelatinized potato starch colloid. In the second part of the study, the COMSOL Multiphysics program was used to develop a model of ultrasonic wave propagation in the same fluids. The model was developed using the Transient analysis type in the Pressure Acoustics application mode of the Acoustics Module. The modeling results were somewhat different from those obtained in laboratory tests; therefore, they did not meet the research assumptions in this stage of research. The limitations of the presented model were discussed. The study demonstrated that medium density was a parameter that exerted the greatest influence on the modeling process.

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Introduction

An acoustic wave is a mechanical oscillation of pressure produced by particles of a medium that is transmitted from the source in all directions. The propagation of ultrasound waves is modeled for scientific purposes to improve processes and analyses involving ultrasound. The behavior and propagation of sound are researched to provide greater control over ultrasound waves and to effectively use these waves in various applications. The first attempts to model the propagation of acoustic waves were made in the 1990s (ZHU 1995, YOUZWISHEN, MARGRAVE 1999). The conducted research can be divided into studies that attempted to model audible sound and ultrasound, although the latter category has been less extensively analyzed. The present study focuses on ultrasound modeling. However, it should be noted that most of the existing models can be used to examine both audible sound and ultrasound. Moreover, models can focus on different aspects of sound propagation. Some models are focusing on acoustic geometry, some on material or medium properties and other on the source of the sound (LIU, MANOCHA 2020).

Models of the audible acoustic fields generate important information that can be used in many practical applications. Sound propagation can be modeled to improve indoor acoustics in existing and designed premises by testing various locations, parameters, and characteristics of sound sources, sound receivers, sound absorbing and insulating materials. Sound propagation models also facilitate analyses of outdoor spaces and terrain features, and they can be used to determine the optimal position of amplifying equipment during mass events or barriers that mitigate the transmission of sound in noisy locations, and to decrease the relevant costs. The latest application for sound propagation modeling, where its role is growing, seems to be also video games and virtual reality environments (LIU, MANOCHA 2020).

The acoustic properties of indoor spaces can be analyzed with the use of various methods that does not take different medium properties into consideration, including wave equations, geometric computation methods (ray tracing and image source methods), finite element method, and statistical methods (WINKLER-SKALNA 2010). The choice of the optimal method is determined by the type and size of the modeled volume and the expected results. These methods are complementary, and they are often combined.

The AFD Package for Matlab developed by YOUZWISHEN and MARGRAVE (1999) based on the finite difference method is an example of a digital tool for modeling sound propagation. This tool was designed to develop speed models or to model the trajectory of acoustic wave propagation. According to the cited authors, the main limitation of the AFD toolkit is its limited bandwidth due to the fact that is based on the finite difference algorithm.

Sound propagation in both existing and designed chambers can be modeled with the method of fundamental solutions (MFS). This approach has been used to model sound propagation in a 3D absorbing acoustic dome (ANTONIO et al. 2007), but according to the authors, the MFS, similarly to the boundary element method (BEM), is suitable for modeling only small spaces and low-frequency waves.

Indoor sound propagation and diffusion can be also modeled with the finite--difference-time-domain (FDTD) method. According to YAKOTA et al. (2002), the FDTD is an excellent approach to visualizing and analyzing the phenomenon of indoor sound propagation, and it can be used not only to solve sound propagation problems, but also to educate future sound engineers and architects.

Sound propagation can also be modeled with dBSea 2.0 software (Irwin Carr Consulting, GB) which has been used to analyze underwater transmission of sound generated by ships (KOCHANOWICZ 2020) and during the construction of offshore wind farms (OTAWSKI et al. 2021). The rapid development of virtual reality techniques also creates numerous possibilities for modeling and visualizing acoustic waves (DEINES et al. 2007, VORLÄNDER 2008).

Modeling of ultrasound waves and audible acoustic waves provides highly useful information for research and practical purposes because ultrasound has numerous applications in many areas of science and daily life, including medicine (for both therapeutic and diagnostic purposes), non-destructive technical diagnostics, echolocation, carcass meatiness assessment, cleaning and sterilization, as well as support and monitoring of production processes (such as drying, emulsification, extraction, products monitoring and product flow) (MCCLEMENTS 1995, ŚLIWIŃSKI 2001, NOWAK et al. 2017). Therefore, ultrasound waves are modeled for example to optimize and improve the efficiency of processes in which they are used.

Ultrasound and audible sound waves can also be modeled using geometric computation methods (VORLÄNDER 2008). This approach was applied by MACKIEWICZ (2019) to model the propagation of an ultrasound beam emitted by a transducer. In the cited study, the trajectory of individual rays was traced by modeling their refraction and reflection with the use of Snell's law which states that when a ray

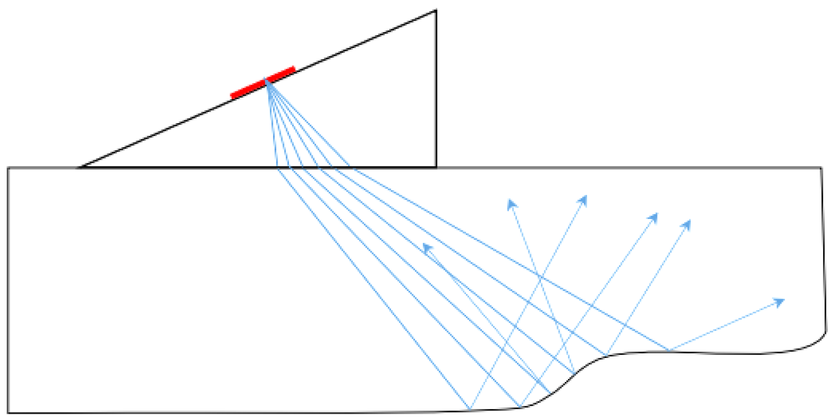

Fig. 1. Modeling an ultrasound beam with the geometric method: a beam emitted by a transducer is propagated in the examined medium
Source: based on MACKIEWICZ (2019).

of light passes the boundary of two media, it is refracted and propagated through the second medium until it encounters a boundary or an internal discontinuity. When the ray arrives at the discontinuity, it is reflected according to the laws of geometrical optics (the angle of incidence is equal to the angle of reflection), and it continues its trajectory until the next discontinuity.

The trajectory of individual rays is monitored to model the propagation of the ultrasonic beam after it is reflected from curved surfaces or defects inside the medium. The geometric trajectory of rays is depicted graphically to generate an overall image of beam propagation, where the density of rays denotes acoustic pressure in a given region. However, the geometric method is not suitable for modeling beams in the near field of a transducer (VORLÄNDER 2008). In complex 3D objects, where light is reflected multiple times, the beam's trajectory has to be simulated with dedicated software, such as the BeamTool. However, to determine the trajectory of a directional light wave based on the simple laws of geometrical optics, the surface against which light is reflected must have relatively small curvature. This condition must be met for the wave to be analyzed as a plane wave during successive reflections and refractions. If the size of discontinuities within the propagation medium is equal to or smaller than the wavelength, the ray tracing method will not produce correct results because an ultrasonic wave passing through these types of defects does not travel in a straight line in a random direction, but is scattered in all directions, making it impossible to monitor the analyzed phenomenon.

ZHU (1995) modeled the propagation of acoustic waves in ultrasound echolocation. The aim of the cited study was to improve mobile ultrasonic emitters. The author developed three models, two discrete and one continuous. The study demonstrated that models based on wave equations are most accurate, but more time-consuming (continuous modeling), whereas geometric models (discrete modeling) are less effective and less accurate because they do not provide information about wave structure or wave phenomena (excluding reflection).

One of the most advanced mathematical computing models for monitoring ultrasound attenuation in the skull was proposed by GUO et al. (2022) who considered the thickness of various bone tissues in the analysis. The results were presented for different head tissues, including scalp, skull, and brain tissue. The study revealed that the thickness of the skull exerted the greatest influence on ultrasound attenuation, and the attenuation caused by the skull was 4.7 to 7.1 times greater than that caused by the remaining tissues. Therefore, the relationships between skull thickness and the attenuation coefficient were determined using the finite element method in the COMSOL Multiphysics v 5.4. program. This method was applied to model the skull geometry and to test the response of a model composed of the skull only (single-layer model) and a model composed of the skull, scalp, and brain tissue (multilayer model). The authors concluded that the adopted mathematical model can effectively calculate ultrasound attenuation for different skull thicknesses with minimum and maximum errors of 0.11% and 6.64%, respectively. The obtained results were consistent with those of a laboratory experiment. According to the authors, the main limitation of the proposed model was that some characteristics, such as the viscoelasticity and non-uniformity of tissues, non-linear effects, and shear waves of the ultrasound field, were not considered in the simulation. They concluded that these tissues and ultrasound field characteristics should be considered in future research to construct a reliable transcranial-focused ultrasound model.

In the present study, attempts were made to model sound propagation with the use of a similar method to that described by GUO et al. (2022). The proposed system is simpler, but the characteristics of the tested media were incorporated into the model to determine their impact on modeling results in the COMSOL program.

Materials and methods

The examined propagation media were two edible liquids – rapeseed oil and gelatinized potato starch colloid. Rapeseed oil was purchased in a local grocery store, whereas the colloid was prepared in a laboratory. A measured quantity of potato starch was dissolved in cold water and added to boiling water to obtain a gelatinized starch solution. Colloid concentration, expressed as the percentage of dry matter in the gelatinized solution, was determined by drying gel samples at a temperature of 105°C.

To determine the appropriate reference point for the studied liquids, a similar test was conducted in demineralized water as the reference liquid. The acoustic properties of demineralized water are well known and have been described in the literature, including the below empirical equation (Eq. 1) that is used to calculate the speed of sound in demineralized water, taking into consideration the temperature of the liquid medium (SIMAL et al. 2003):

$$c_w = 1403 + 5t - 0.06t^2 + 0.0003t^3 \tag{1}$$

where:

t – temperature of the medium, °C,

c_w – speed of sound in water, $m \cdot s^{-1}$.

Acoustic measurements were conducted on a measurement stand (Fig. 2) composed of a measurement cell with ultrasonic transducers mounted on opposite sides. Electroacoustic signals were emitted and received by the OPBOX 2.0 ultrasonic device (PBP Optel sp. z o.o., Poland) connected to a computer. The transducers used were narrowband and had a nominal frequency of 5 MHz and an overall diameter of 0.5 inch. Measurements were performed by passing

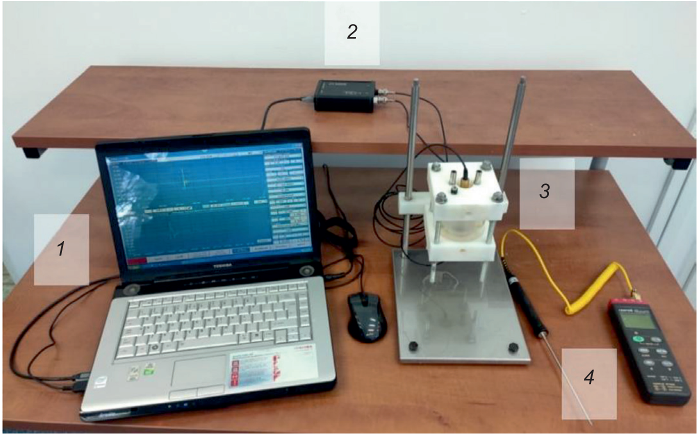

Fig. 2. Stand for acoustic measurements: *1* – computer for registering and processing the measured data, *2* – OPBOX 2.0, *3* – measurement cell, *4* – thermometer

acoustic signals through the examined medium with a temperature of 20°C. The temperature of the medium was kept constant and monitored with a temperature data logger throughout the experiment. The time taken by the ultrasonic wave to pass through the medium– from the emitter to the receiver (so called time of flight) – was determined based on the registered signal using its' positive maximum amplitude point. The speed of sound in the tested medium was calculated with a reference method based on the distance between transducers and the time of wave passage through that medium. Demineralized water with a known speed of sound was the reference liquid. The speed of sound in the tested medium was calculated with the below equation:

$$c = c_w \cdot \frac{\tau_w}{\tau} \tag{2}$$

where:

c – speed of sound,

τ – time taken by the wave to cross the examined medium.

The model was generated with the finite element method in the COMSOL Multiphysics v. 6.2 (COMSOL Inc., USA) program using the Transient analysis type in the Pressure Acoustics application mode of the Acoustics Module. The parameters of the modeled processes, the experimental and reference materials were obtained from a materials library (water), measured independently, or acquired from other sources (rapeseed oil and gelatinized starch solution).

To simplify the problem, a 2D axial-symmetrical model was generated in COMSOL. The modeled area with a radius of 30 mm and a height of 55 mm was divided into 471 elements with normal size and 268 vertices. The geometric model is presented in Figure 3.

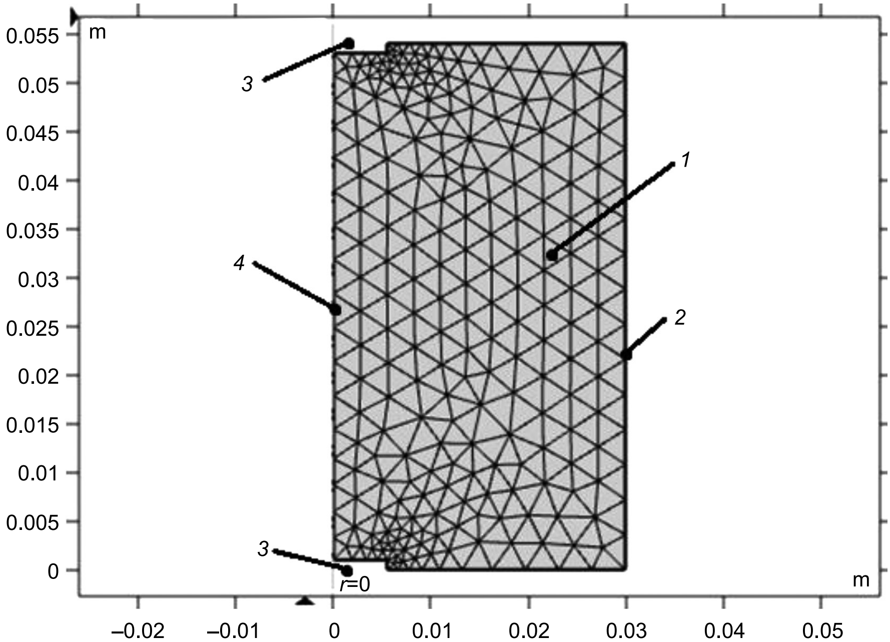

Fig. 3. A 2D axial-symmetrical geometric model with a triangular mesh:
1 – domain (modeled liquid), *2* – internal surface of the cell wall,
3 – location of transducers, *4* – axis of symmetry

The model developed in COMSOL was validated with three types of media in the virtual measurement cell: water, oil, and colloid. The media were previously analyzed on the measurement stand presented in Figure 2. For the needs of the model, water and oil properties were obtained from the COMSOL database. Information about the speed of sound in rapeseed oil was not available in the materials library. Therefore, the value of this parameter was determined at c_o = 1,454.89 m·s^{-1} based on the results of empirical measurements conducted with the use of laboratory equipment. When the starch colloid was used as the medium, a new material was generated in the model, and its key parameters (speed of sound – c_k and density – ρ_k) were also determined empirically at c_k = 1486.5 m·s^{-1} and ρ_k = 1,007.7 kg·m^{-3}. To validate colloid density measurements, this parameter was also calculated with the use of an equation proposed by NOWAK and MARKOWSKI (2020) (Eq. 3):

$$\rho = -0.000126 \cdot t^2 \cdot c + 0.0223 \cdot t \cdot c + 0.833 \cdot c \cdot t^2 - 37.5 \cdot t - 148 \quad (3)$$

where:

t – temperature of the medium, °C.

The calculated colloid density was 1,008.3 kg·m^{-3}, and it was similar to the measured value.

The main parameters of the examined media are presented in Table 1.

Table 1

The main parameters of the modeled media

Medium	Speed of sound [m·s^{-1}]	Density [kg·m^{-3}]
Water	1,480.0	998.2
Oil	1,454.9	917.0
Coloid	1,486.5	1,007.7

As part of the Pressure Acoustics physics implemented in COMSOL, the Transient method was used to solve the following equations:

Acoustic model of the medium (domain):

$$\nabla \cdot \left(-\frac{1}{\rho_c}(\nabla p_t - q_d\right) - \frac{k_{eq}^2 p_t}{\rho_c} = Q_m \tag{4}$$

where:

ρ_c – medium density, kg·m^{-3},
p_t – acoustic pressure, Pa,
k – wave number, 1·m^{-1},
q_d – dipole domain source, N·m^{-3},
Q_m – monopole domain source, 1·s^{-2}.

$$p_t = p + p_b \tag{5}$$

where:

p – locally calculated pressure, Pa,
p_b – barometric pressure, Pa.

$$k_{eq}^2 = \left(\frac{\omega}{c_c}\right)^2 - k_m^2 \tag{6}$$

where:

ω – angular velocity (frequency), rad/s.

Acoustic model of medium boundaries was used as a *Sound Hard Boundary (Wall)* which adds a boundary condition typical for a hard wall which was used in the experiment cell (polymethyl methacrylate for the cylindrical wall, and polyamide for the bottom and lid). For such a boundary condition the normal component of the acceleration (and thus the velocity) is zero:

$$-n \cdot \left(-\frac{1}{\rho_c} (\nabla p_t - q_d) \right) = 0 \tag{7}$$

Source model:

$$-n \cdot \left(-\frac{1}{\rho_c} (\nabla p_t - q_d) \right) + i \, \frac{k_{eq}}{\rho_c} p + \frac{i}{2k_{eq}\rho_c} \Delta || p = Q_i \tag{8}$$

Numerical calculations were performed with a viscous model (where water was the medium in the measurement cell) using the Transient analysis in the Pressure Acoustics application mode of the Acoustics Module in COMSOL. An elastic model was applied to oil and starch colloid because the bulk viscosity of these media was unknown (only dynamic viscosity was known). Bulk viscosity and dynamic viscosity are the required parameters in a viscous model. The model was calculated for the following frequencies: 50 kHz, 100 kHz, 500 kHz, 1,000 kHz, and 5,000 kHz. The model had 444 degrees of freedom.

Results and discussion

The results produced by the model are presented in Figures 4-6 as axial-symmetric diagrams and 3D domains which represent the media in the measurement cell (water, oil, and colloid), where the acoustic wave is transmitted from the emitter (top transducer) to the receiver (bottom transducer). Acoustic wave propagation in each medium was modeled in sound pressure units [Pa]. The frequency of the emitted wave influenced the distribution of acoustic pressure disturbances, which supported the determination of ultrasound transmission.

In the above figure drawings, the length of the propagated wave is clearly visible at frequencies of 50 kHz and 100 kHz, which is a positive modeling result indicating that wavelength decreases with an increase in frequency. These results are consistent with the physics of the studied phenomenon. The length of the ultrasonic wave was estimated at 30 mm at 50 kHz, 15 mm at 100 kHz, and 3 mm at 500 kHz. At a frequency of 1,000 kHz, according to the model, the wave seems to be completely absorbed by each tested medium (Figs. 4*g*, 4*h*, 5*g*, 5*h*, 6*g*, 6*h*) (disappearance of acoustic pressure) before it reached the receiver, which contradicts the results of acoustic measurements, where the signal was clearly registered by the receiver even at a frequency of 5,000 kHz. This discrepancy could be attributed to the fact that the applicability of digital acoustic models is limited to low frequencies (DEINES et al. 2007) or the mesh used was to coarse, and to check it we should use finer mesh in the next study.

The models for all tested media were compared at a frequency of 100 kHz (Fig. 7). This frequency was selected because it best depicts the differences in the results noted in each tested medium.

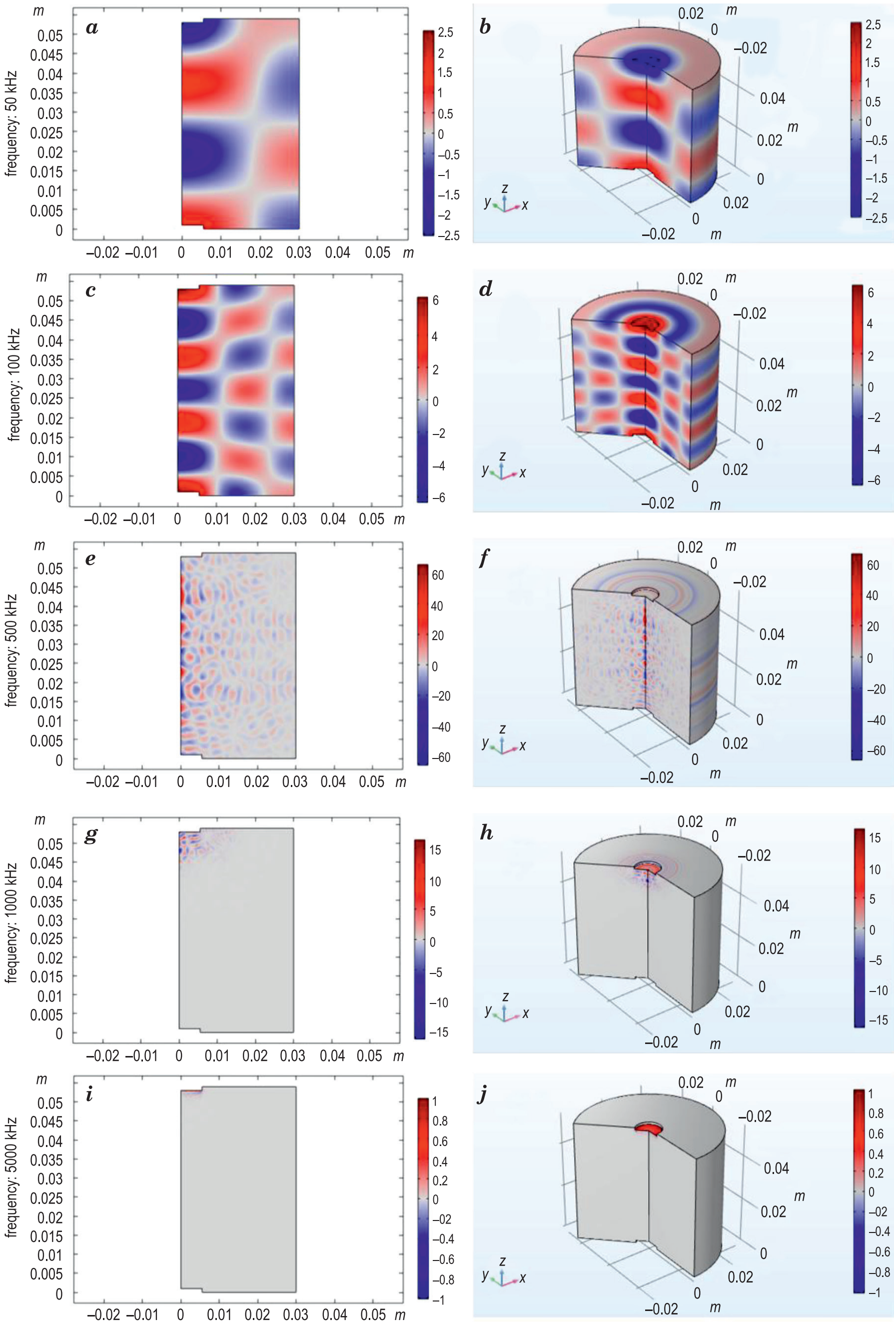

Fig. 4. Viscous model of acoustic pressure distribution [Pa] for water:
a, *c*, *e*, *g*, *i* – 2D symmetry, *b*, *d*, *f*, *h*, *j* – 3D view

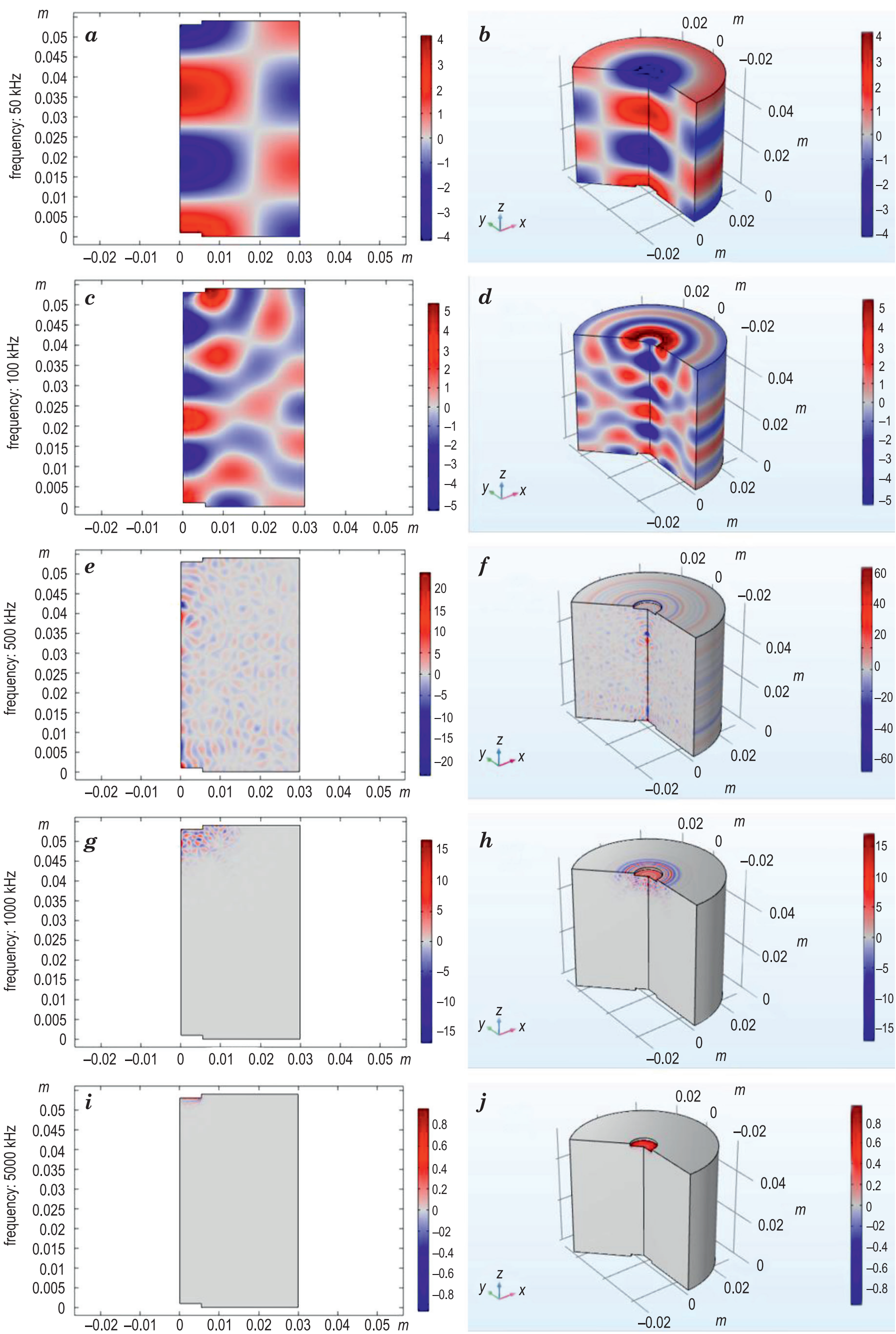

Fig. 5. Elastic model of acoustic pressure [Pa] for oil:
a, *c*, *e*, *g*, *i* – 2D symmetry, *b*, *d*, *f*, *h*, *j* – 3D view

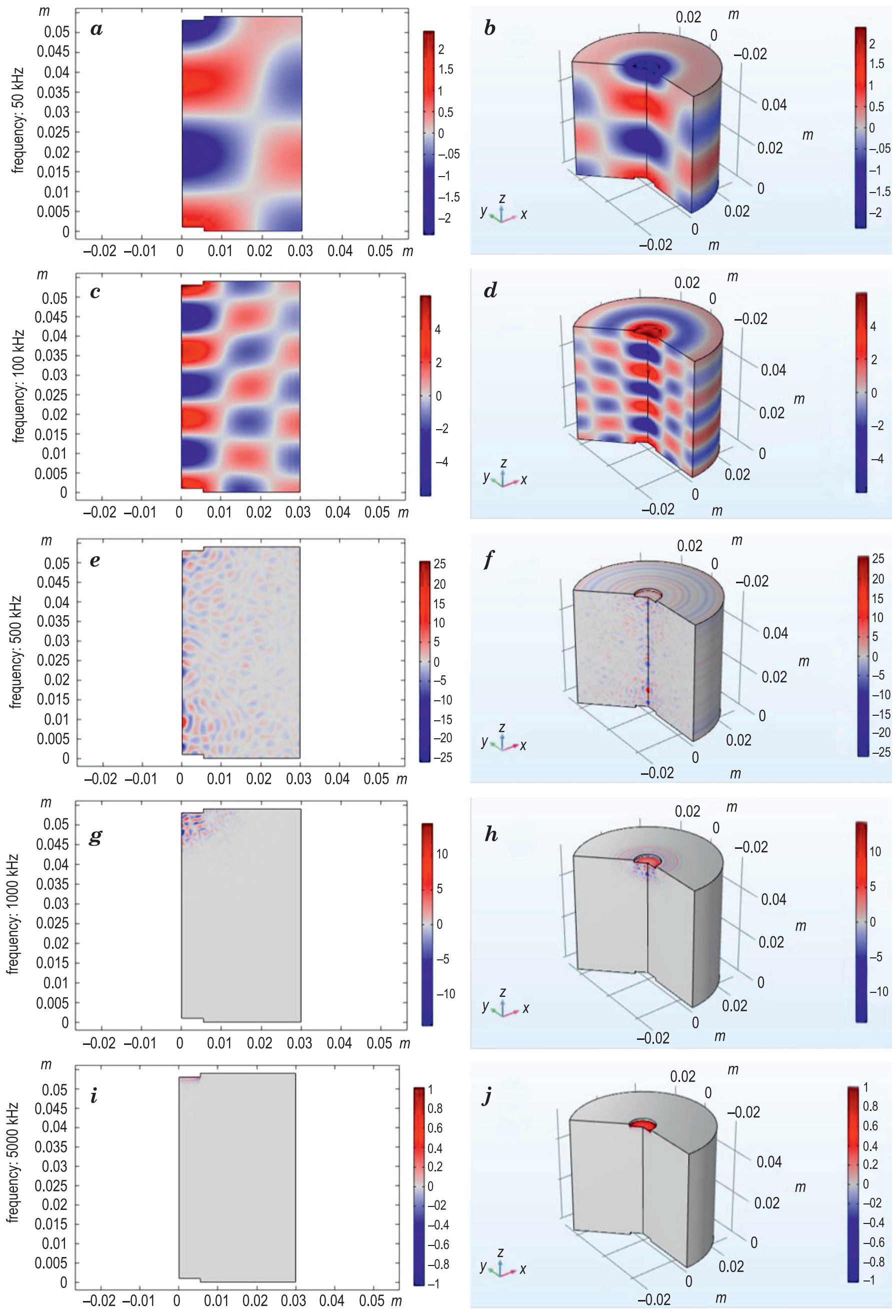

Fig. 6. Elastic model of acoustic pressure [Pa] for the starch colloid:
a, *c*, *e*, *g*, *i* – 2D symmetry, *b*, *d*, *f*, *h*, *j* – 3D view

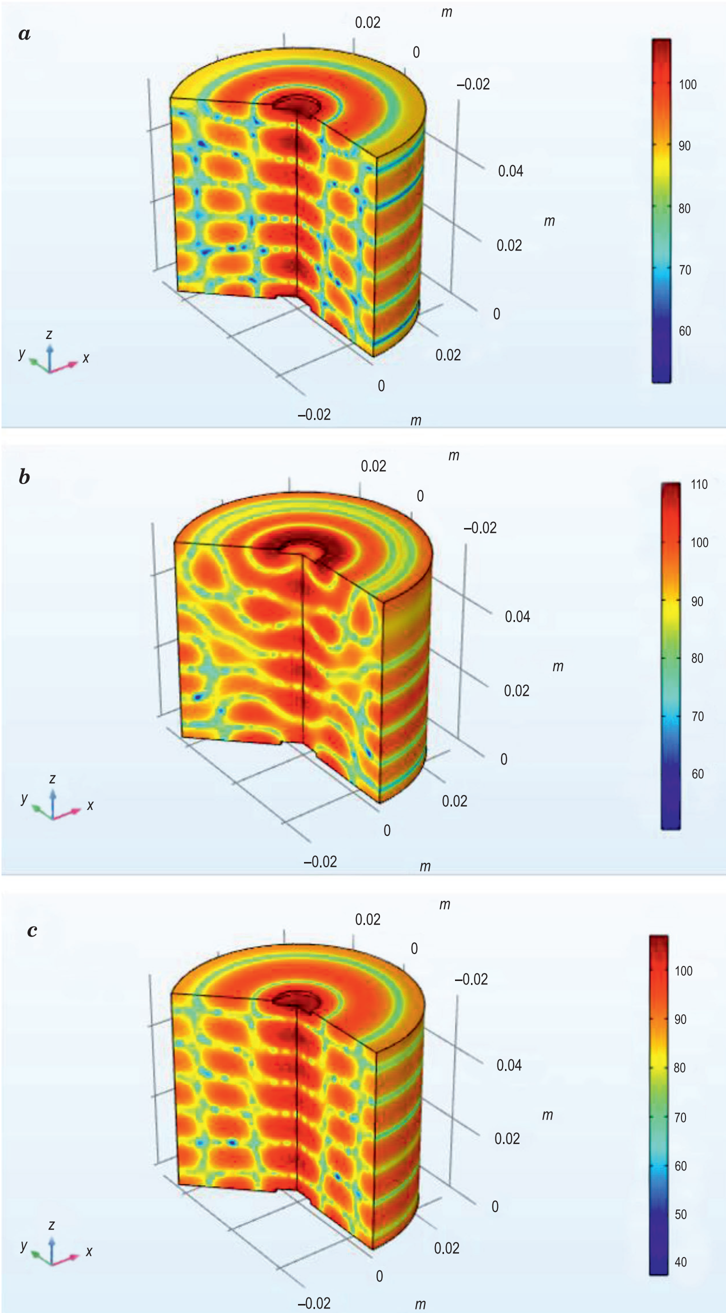

Fig. 7. The results of 3D models of acoustic pressure (dB values are presented on a color scale) for three media: *a* – water, *b* – rapeseed oil, and *c* – starch colloid, at the same wave frequency of 100 kHz

The differences between the oil model and the models for water and the starch colloid, which are highly similar in density, are apparent in Figure 7. The modeled wave was propagated differently in oil, which is characterized by lower density and lower sound speed, than in media where these parameters were similar (water and potato starch colloid). Despite the fact that wavelength was identical in water and the colloid, water was characterized by higher pressure along the axis of symmetry and in the remaining regions, including along internal cell walls.

To validate the influence of viscosity on the modeled results, water parameters were also simulated with the use of an elastic model. The results did not differ from those generated by the viscous model. These observations undermine the rationale for using the viscous model, but they could also be attributed to the relatively low viscosity of water.

Summary and conclusions

In order to meet the research objective, the propagation of an ultrasonic wave was tested in a laboratory in three media: water, oil, and gelatinized potato starch colloid. The experiment produced satisfactory results and parameters that can be used to formulate models and validate modeling outcomes. The ultrasonic wave was also modeled in the COMSOL program, but the results were only partly satisfactory.

The study demonstrated that at high frequencies, which are characteristic mainly of low-power ultrasound, waves with frequencies higher than 1,000 kHz were completely absorbed by all tested media long before they reached the receiver or the coarse mesh was inappropriate for such frequencies, what should be checked in the next studies. In such case mesh elements no larger than 0.06 mm could be used to verify this assumption. If the finer mesh would not help then the model implemented in COMSOL would turn out imperfect and should be further elaborated for the needs of modeling high-frequency ultrasound waves. The above could also be attributed to the lack of an ultrasound modeling option in the existing version of COMSOL. It can be assumed that the used model is more useful for simulating waves with a frequency below 500 kHz, such as high-power ultrasonic waves within a frequency range of 20-100 kHz. This frequency range was not tested in the present experiment. Further research is needed to validate the model geometry for high-power ultrasound for selected processing operations and for finer mesh in case of the higher frequencies.

The study revealed that the propagation of the modeled wave is determined mainly by the density of the medium (Fig. 7). Similar results were obtained for media with similar density (water and colloid), whereas the model of wave propagation in oil, a medium with considerably lower density, produced completely different results.

No differences were noted between the viscous and elastic model of wave propagation in water, which confirms that the tested COMSOL module is imperfect because it does not place sufficient emphasis on the interactions between medium particles characterized by parameters such as viscosity.

In addition to the previously mentioned directions for future research, further studies are also needed to evaluate the influence of the sound attenuation coefficient on modeling results (in particular for high-frequency waves). If the model were well developed, it could be used in the future to simulate the behaviour of an ultrasonic wave when encountering obstacles such as a media discontinuity or a foreign body.

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