Experimental and numerical study of acoustic pressure distribution in a sonochemical reactor

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Abstract. In this work, it is shown numerically in COMSOL Multiphysics and experimentally that a change in the NaCl concentration in water significantly affects the distribution of acoustic pressure in a laboratory sonochemical reactor. Thus, in distilled water under the action of ultrasound, two areas of increased pressure were observed, one of which was located directly above the ultrasound source, and the second was near the surface of the liquid, this effect is associated with the reflection of sound waves from the surface of the liquid. With the increase in the salt content, the maximum value of the acoustic pressure in the liquid decreases, which is associated with the dependence of the acoustic impedance of the liquid on the salt concentration and the peculiarities of the dynamics of vapor-gas bubbles in such solutions.

1. Introduction

At this stage of industrial development, ultrasonic exposure has found application in such areas as: materials science, chemical synthesis [1, 2], water treatment [3, 4], biotechnology [5], electrochemical processes [6], food industry [7], reprocessing of spent nuclear fuel [8], also ultrasound is used in mineral processing by flotation methods [9]. The versatility of using ultrasound allows you to combine it with other technologies, proving the huge potential of its use in various fields. Despite extensive research on ultrasound on a laboratory scale, only a few developments have found their application in industry, mainly for the following reasons:

1. lack of experience in ultrasound applications in areas such as ultrasound or sonochemical engineering;
2. the influence of many parameters on the processes in sonochemical reactors, most of which cannot be fixed in the industrial use of ultrasound;
3. complexity of multiphysical calculations in the design of sonochemical reactors.

Numerical modeling of the spatial distribution of acoustic pressure inside sonochemical reactors is of interest to many scientists around the world. In particular, researchers are interested in predicting cavitation events inside the reactor [10].

Numerical modeling in systems where the liquid under study contains various inclusions, such as gas and vaporgas bubbles, solid particles, and salt ions present in solutions, has been poorly studied [11, 12] and...
therefore is of particular interest, but requires experimental verification due to the lack of generally accepted calculation methods.

In this paper, the acoustic pressure distribution is experimentally investigated and, in addition, the possibility of using a numerical model with a minimum number of parameters for a qualitative description of the structure of the acoustic pressure distribution occurring in a sonochemical reactor is demonstrated.

2. Description of the numerical model, experimental setup and measurement method

The numerical calculation was performed in an axisymmetric formulation in the COMSOL Multiphysics package. The model does not take into account the movement of the liquid and the occurrence of cavitation bubbles. In calculations, the liquid is assumed to be stationary and has the same properties throughout the volume.

The calculated area consisted of a cylinder with a round base with a radius of 55 mm (Fig. 1) and a height of 140 mm, in contrast to the experiment, which used a cuvette in the form of a parallelepiped. This assumption was made to speed up calculations. On the walls of the cuvette, the reflection conditions were set. At the bottom of the cuvette was a cylindrical piezoelectric element with a radius of 40 mm and a height of 10 mm, which served as an ultrasound source. To recreate the operation of the ULTRASONIC source, the equation of deformation of the piezoelectric element under the action of a flowing current was calculated.

![Figure 1. Numerical results and computational grid: 1-air; 2-water; 3-piezoelectric element; 4-plexiglass](image)

In areas filled with water and air 1 and 2 (Fig. 1), the acoustic wave propagation equation was calculated:

$$\Delta p - \frac{\omega^2}{c^2} = 0,$$

where $p$ is the fluid pressure, $\omega$ is the cyclic frequency of the acoustic wave, and $c$ is the speed of sound.

The speed of sound in a liquid is $c$, its density is $\rho$ were linearized by salt concentration and temperature:

$$c = 1449.2 + 4.623s + 0.0546t^2 + 1.39(s - 35),$$

$$\rho = 998.186 + 0.761s,$$

where $c$ is the speed of sound; $\rho$ - density; $s$ - salt concentration, $\sigma$; $t$ - temperature, °C.

To conduct a full-scale experiment and verify the model, an experimental cuvette with dimensions of 110×116×160 mm³ was made of plexiglass with a thickness of 3 mm (Fig. 2). The ultrasound source was located flush with the bottom of the experimental setup (Fig. 2, No. 4).

To measure the intensity of the acoustic field generated from a 28 KHz ultrasound source in a liquid, a ks0272 piezoceramic sensor was used (Fig. 2, №3). The sensor diameter was 2 cm. The readings of this sensor were processed using an Arduino UNO microcontroller (Fig. 2, №2) and a personal computer (Fig.
Nine measurement points were selected for verification. One of them was located in the Central area of the ditch, four in the middle of the sides, and four more were located in the corners. The height from the bottom was varied and amounted to 20, 75, 130 mm. The results were averaged over three experiments. In addition, the method of tracer visualization (PIV) and fluorescence visualization (Fig. 3) was used for results comparison of experimental and numerical results.

To use the PIV method, reflective polyamide particles with neutral buoyancy were introduced into the liquid, with an average size of 65 microns. The motion of the particles was recorded on a high-speed video camera (Fig. 3, №2). A solid-state permanent laser with a wavelength of $\lambda = 532$ nm was used as the light source (Fig. 3, №1). The laser beam was opened by a cylindrical lens. The data obtained were processed using the DaVis-LaVision software package. Also, the fluorescent dye Rhodamine B was used to visualize the acoustic flow. In this case, the propagation dynamics of the fluorescent substance was recorded on a high-speed Basler a504kc camera.

![Figure 2. Experimental setup diagram](image1)

![Figure 3. Experimental setup diagram for visualization](image2)

### 3. Results

The results obtained during the experiment were marked in the fields of absolute pressure values obtained using a numerical model. Thus, the figure 4, a) shows the results obtained for distilled water, b) - distilled
water with a NaCl content of 2%, c) - distilled water with a NaCl content of 15%, d) - distilled water with a NaCl content of 30%.

The red font shows numbers obtained from experiments whose results do not agree with the results of numerical modeling. Since the sensor used was not a point sensor, but a plate with a diameter of 2 cm, the illustrations highlight the areas where the sensor was located.

The results shown in Figure 4, (b, c) show that the calculated data do not match the experimental data. However, the Central points obtained during the experiment in the case of distilled water (Fig.4, a) coincide with the numerical results. While the points located near the wall do not match the calculation. For a 30% salt solution (Fig.4, d), the opposite situation is observed, that is, the experimental values do not coincide over the ultrasound source, while the results at the wall are consistent with the calculated ones, which is due to the use of a simplified calculation model, which does not take into account: wall vibrations, cavitation bubble formation, convective motion, as well as features of the geometry of the experimental cell. According to experimental data, it is noticeable that an increase in the salt content in water significantly affects the intensity of the flow, as was shown earlier.

Figure 4. The results obtained using the numerical model, with experimental data plotted.
4. Discussion
This behavior is due to a small gradient of acoustic pressure between different areas of the cuvette, as shown in figure 4, (a) as well as a sharp change in the acoustic impedance when the salt content in the water increases (Fig.4). Since ultrasonic radiation is reflected from the boundaries with different values of acoustic impedance, the reflection also occurs from the surface of bubbles that arise in the liquid under the action of ultrasound from the cell walls and from the upper boundary.

In figure 5, a qualitative match is observed for the rhodamine visualization of the time-averaged particle velocity field obtained by the PIV method. When ultrasound propagates in water, the particle velocity is 30% higher than in 15% salt solution (Fig. 5). Considering the time-averaged flows for water and two salt solutions, we can notice a decrease in the average particle velocity with an increase in the salt content in water. This behavior of PIV particles in the liquid is obviously related to the distribution of acoustic pressure inside the cuvette, which was observed in the present experiments.

5. Conclusion
The experiments were performed to study the distribution of acoustic pressure arising in a sonochemical reactor with characteristic dimensions of 110x116x160 mm$^3$ for water and salt solutions. A numerical analysis of the acoustic pressure distribution occurring in a sonochemical reactor in a Comsol package is performed.
Thus, in pure water, the results of numerical simulation coincide in the Central region with the results of experiments. There is no overlap at the periphery, which may be due to the discrepancy between the geometry of the experimental cell and the calculated area. As the salt concentration in the liquid increases, the acoustic flow intensity decreases. This is due to a sharp change in the physical and chemical parameters of the liquid and an increase in the acoustic impedance for such media.

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References
[1] Cravotto G and Cintas P 2006 Power ultrasound in organic synthesis: moving cavitation chemistry from academia to innovative and large-scale applications Chemical Society Reviews 35 180–196
[2] Cintas P, Palmisano G and Cravotto G 2011 Power ultrasound in metal-assisted synthesis: From classical barbier-like reactions to click chemistry Ultrasonics sonochemistry 18 836–841
[3] Ince N, Tezcanli G, Belen R and Apikyan I G 2001 Ultrasound as a catalyst of aqueous reaction systems: the state of the art and environmental applications Applied Catalysis B: Environmental 29 167–176
[4] González-Garcia J, Sáez V, Tudela I, Díez-Garcia M I, Deseada Esclapez M and Louisnard O, 2010 Sonochemical treatment of water polluted by chlorinated organocompounds. a review Water 2 28–74
[5] Rokhina E V, Lens P and Virkutyte J 2009 Low-frequency ultrasound in biotechnology: state of the art Trends in biotechnology 27 298–306
[6] González-Garcia J, Esclapez M D, Bonete P, Hernández Y V, Garretón L G and Sáez V 2010 Current topics on sonoelectrochemistry Ultrasonics 50 318–322
[7] Chemat F, Khan M K et al. 2011 Applications of ultrasound in food technology: processing, preservation and extraction Ultrasonics sonochemistry 18 813–835
[8] Nikitenko S, Venault L, Pflieger R, Chave T, Bisel I and Moisy P 2010 Potential applications of sonochemistry in spent nuclear fuel reprocessing: a short review Ultrasonics sonochemistry 17 1033–1040
[9] Ozkan S G 2012 Effects of simultaneous ultrasonic treatment on flotation of hard coal slimes Fuel 93 576–580
[10] Dubus B and Campos-Pozuelo C 2000 Numerical modeling of high-power ultrasonic systems: current status and future trends Ultrasonics 38 337–344
[11] Higgs P W 1964 Broken symmetries and the masses of gauge bosons Physical Review Letters 13 508
[12] Laborde J-L, Bouyer C, Caltagirone J-P and Gérard A 1998 Acoustic cavitation field prediction at low and high frequency ultrasonic Ultraso nics 36 581–587