Acoustic pressure and temperature distribution in a novel continuous ultrasonic tank reactor: a simulation study

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Abstract. This study addresses the design of continuous ultrasonic tank reactor (CUTR) and focusing on the study of acoustic pressure and temperature distribution inside the CUTR. The total volume of inner CUTR was design to be 235 mL; a cooling water layer was also developed to achieve a well temperature control during the ultrasonic processing. A three-dimension CUTR was firstly established in Comsol Multi-physics. After combining physical models (i.e. pressure acoustics frequency domain, fluid flow and heat transfer), the acoustic pressure and temperature distribution were presented. The highest acoustic pressure was able to reach to 414 atm when the averaged processing temperature was determined to be 75.0 °C; and the core temperature was able to raise to 79.6, 86.1, 103.2, 133.3, 166.6, 268.2, 364.1 °C depending on the residence time ranging from 15 to 120 min at 15 min interval with the assistance of high-intensity ultrasound (frequency: 20 kHz, intensity: 11.90 W cm⁻²) at a temperature of 75.0 °C. Therefore, results of this study indicated two typical consequences of ultrasound processing: 1) an extremely high-pressure cycle leading to the strong agitation and turbulence, and 2) a momentary, albeit high temperature generated during ultrasonic processing.

1. Introduction
Ultrasound is defined as any sound with its frequency above 20 kHz, which is beyond the threshold of human hearing. Passing ultrasound wave through targeted media results in a continuous wave-type motion, and the motion creates two of alternative cycles, namely compression and expansion. In a liquid, cavities are generated during the expansion cycle due to a large negative pressure overcoming the liquid’s tensile strength, and the compression cycle generates positive pressure, which can push molecules together. The cavities keep growing with the absorption of acoustic energy; upon reaching a critical size, the cavities will implode, release energy and heat to the surroundings, reaching up to an extraordinarily high temperature of about 5,500 °C, followed by a flash cooling at the rate of more than a billion °C s⁻¹. Hence, cavitation generated by HIU brings a unique environment for chemical reactions [1, 2].

Different intensity and frequency of ultrasound have different applications. Low-intensity
ultrasound (less than 1 W cm\(^{-2}\)) with the frequency range of 1-10 MHz is utilized as a nondestructive detection method and has already been utilized in food process control and characterization of food properties. It is worth noting that high-intensity ultrasound (HIU) with the power from 1 to 1,000 W cm\(^{-2}\) is able to expand the cavities much faster than low-intensity ultrasound, which has drawn much attention in the food industry. Currently, HIU with the lower frequency range of 20-100 kHz has been treated as an alternative to conventional processing due to its low energy consumption as well as the reduction of processing time and thermal effects [3, 4]. As an emerging technology, HIU has some existing applications in food processing, e.g. ultrasound-assisted cutting, sterilization, extraction, drying, freezing, etc. [2]. HIU is also a potential candidate for the production of foods with modified properties, e.g. stabilization of whey protein [5]. Very recent applications on promoting Maillard reaction (MR) for generating different types of flavor compounds with the assistance of high-intensity ultrasound: more than 6 of different pyrazines were generated after introducing HIU in a MR model system of xylose-lysine and glucose-serine [6, 7]; and more than 4 different types of sulfur-containing flavor compounds were formed in a MR model system of glucose-methionine [8]. An oil-in-water MR model system was treated by HIU, and a significantly promotion of MR was observed in the MR model system of glucose-glycine; meanwhile, different types of flavor compounds were detected depending on different unsaturation level of oils [9]. Therefore, it is necessary to develop the CUTR and study the acoustic pressure and temperature distribution inside the CUTR for a better understanding on the ultrasonic processing, which is helpful on determining the processing conditions for HIU-assisted processing.

2. Materials and methods

2.1. Design of the CUTR

The design of a CUTR was presented by AutoCAD (2017, Autodesk Inc., USA) as shown in Figure 1.

![Figure 1. Design of CUTR: top view (A), 3D model of CUTR (B), front view (C) and left view (D).](image)

The building material of CUTR in this study was stainless steel with heat capacity at constant pressure (\(C_p\), 475 J kg\(^{-1}\) K\(^{-1}\)), thermal conductivity (\(K\), 44.5 W m\(^{-1}\) K\(^{-1}\)) and density (\(\rho\), 7850 kg m\(^{-3}\)). In general, there were four major parts of CUTR from outside to inside, namely a cooling water jacket, a highly thermal-conductive layer, an inner reactor, and an ultrasonic probe with front diameter of 34
mm which inserted into the inner reactor (BS2d34, Hielscher, Germany). The cooling water jacket was covered more than 80% of total surface of inner reactor, which was able to take away a number of heats generated by high intensity ultrasound during processing. The thickness of highly thermal-conductive layer was varied from 0.60 cm (bottom layer) to 0.70 cm (side and upper layers), which was able to endure pressure up to 10 bar. The shape of inner reactor was a cylinder with the total volume of 235 mL after inserting the ultrasonic probe. The pre-prepared sample solution was always pumped from bottom of the reactor and flowed out at the top. Moreover, there were 15 screw spikes in total for assembling and fastening each parts of the CUTR.

2.2. Multi-physics modeling
The multi-physics modeling was established through Comsol Multi-physics (V 5.1, Sweden). A three-dimension of the reactor was firstly built up, and three physics models were subsequently introduced into the reactor, including pressure acoustics frequency domain, fluid flow (laminar flow and turbulent flow) and heat transfer.

Three-dimension CUTR model developed for the symmetric flow cell is established as follow. The model representation is based on computer-aided design (CAD) import module kernel. The physical model, i.e. pressure acoustics in frequency domain (ACPR) model, was firstly built up based on the Helmholtz equation Eq. (1). The second model was non-isothermal flow, turbulent flow, k-ε (NITF) physical model, which was based on Reynolds-averaged Navier-stokes (RANS) equations: k (turbulent kinetic energy)-ε (dissipation) model. The third model was heat transfer model including solid and liquid heat transfers Eq. (2). These models were conjugated through frequency (acoustic pressure) and stationary (temperature distribution) studies. The RANS: k-ε equation was conjugated to Eq. (1) through pressure distribution and Eq. (2) through flow rate distributions (u). Moreover, heat source (Q) was calculated based on acoustic pressure (P), efficiency of ultrasound transducer (η, 85-90%, provided by the manufacture of HIU instrument) as well as ultrasound absorption coefficient in the sample (αabs) through Eq. (3), which in turn were conjugated through the heat transfer equation.

\[
\nabla \cdot \left( \frac{1}{\rho} \left( \nabla P \right) \right) - \frac{\omega^2}{\rho c_p} = 0 \quad (1)
\]

\[
\rho c_p \left( \frac{\partial T}{\partial t} + u \cdot \nabla T \right) + \nabla \cdot \left( -k \nabla T \right) = Q \quad (2)
\]

\[
Q = \frac{\rho c_p}{\rho c_p \cdot \eta \cdot \alpha_{abs}} \quad (3)
\]

Initial conditions adopted for the simulation included: an amplitude of ultrasound output (25 μm), a frequency of ultrasound output (20 kHz), an ultrasound absorbance coefficient of prepared sample (0.025 Np m⁻¹), an initial temperature of prepared sample (25 °C), an environmental temperature (24 °C) and an initial velocity of cooling water (3.89 m s⁻¹). Initial velocities of the prepared sample were based on various residence times.

3. Results and discussion

3.1. Acoustic pressure distribution in the CUTR
Results of the frequency study (acoustic pressure distribution) and the stationary study (average temperature distribution when processing temperature was 75 °C) were presented in Figure 3.
The maximum acoustic pressure distribution during compression cycle and expansion cycle are shown in Figure 2A and 2B, respectively. The core acoustic pressure could reach 414 atm during compression and expansion cycle. The influences of acoustic pressure distribution include physical properties of media and parameters of HIU. Therefore, the established model of acoustic pressure distribution is a powerful tool to simulate the theoretical values as long as inputting different parameters based on the processing conditions.

3.2 Temperature profile of sample stream and cooling water in the CUTR

The average temperature distributions when the processing temperature was set to 75 °C at various residence times (from 15 to 120 min, respectively) are shown in Figs. 3A to 3G. According to a previous modeling prediction on ultrasound induced heating, bubbles implosion caused by alternating of expansion cycle and compression cycle could heat surrounding contents to around 5,550 °C (Suslick, 1989). It is necessary to understand that the model simulation in the study only produced an approximate average temperature distribution within the chamber based on ultrasound heat effect but not a flash temperature distribution in the chamber. Therefore, based on the simulation, the highest average core temperature reached to 364.1 °C when the residence time was set to 120 min with a flow rate of sample stream at 1.96 mL min⁻¹. The average core temperature was decreased to 79.6 °C when the flow rate of sample stream increased to 15.67 mL min⁻¹ with the residence time of 15 min. Both the average core temperature and acoustic pressure distributions indicated two typical consequences of ultrasound processing: the extremely high-pressure cycle leading to agitation and turbulence and momentary high core temperature.
4. Conclusions
In this study, the CUTR was firstly design that achieved an excellent temperature control and minimized the loss of volatile products during ultrasonic processing. The simulation of acoustic pressure distribution in the CUTR was presented to reach up to 414 atm with the assistant of HIU (frequency of 20 kHz and intensity of 11.90 W cm\(^{-2}\)); the results of temperature distribution were highly based on the designed residence time: the core temperature during ultrasonic processing was reached to 364.1 °C with the longest residence time (120 min). The results of this simulation again prove that the HIU is able to generate a high, albeit momentary, temperature and pressure environment. Furthermore, such an environment is favored by a number of chemical reactions, e.g. MR, etc., that provides a potential application to produce food flavors with the assistant of HIU by using the CUTR.

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