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Numerical simulation of the coalescence of two bubbles in an ultrasound field

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ARTICLE INFO	A B S T R A C T
<i>Keywords:</i> Ultrasound irradiation Bubbles coalescence Bjerknes force Drainage time	The coalescence of two bubbles under ultrasound irradiation is numerically investigated. The results indicate that ultrasound may accelerate the coalescence process, depending on the initial phase. The time-averaged nonzero Bjerknes force promotes bubble coalescence by dragging bubbles to nodes or antinodes, depending on their size. At the beginning of the coalescence process, a film forms between the two bubbles. The film drainage time first increases then decreases as a function of initial distance. This study contributes to an understanding of

the effects of ultrasound on bubble coalescence.

1. Introduction

Sonochemical reactions have various industrial applications because of the unique conditions generated through acoustic cavitation, which are in many cases favorable to those of conventional reactions [1–7]. For example, compared with other methods, ultrasound instruments are easy to operate and generate no or relatively few harmful byproducts. In addition, the application of ultrasound can considerably enhance or promote chemical reactions via acoustic cavitation.

In the last two decades, the sonoluminescence and dynamics of single bubbles under irradiation of ultrasound have been widely investigated [8–13]. However, in almost all sonochemical reactors, countless bubbles aggregate into clusters or 'bubble clouds' [8]; hence, the results of single-bubble studies cannot be accurately extrapolated to industrial systems. Therefore, investigation of multibubble systems is necessary; however, this is often hampered by the complex interactions between numerous cavitation bubbles. Servant et al. [9] calculated the sound pressure field taking into account the emergence of bubbles. However, in their study, the bubble radius was homogeneous and the average effect of bubbles was considered. In another study, Yasui et al. [10] calculated the influence of bubble–bubble interactions. They described a destruction mechanism of microbubbles, which was in good accordance with experiment results.

Bubble coalescence has attracted scientific interest for many years. Tabor and co-authors measured and analyzed the forces in bubble and droplet systems using atomic force microscopy [14]. They further found electrostatic interactions between bubbles have an impact on bubble coalescence [15]. Vakarelski et al found the liquid film drainage rate between two bubbles is affected by pH value of the liquid and gas type of the bubble [16]. Ultrasonic standing waves can concentrate homogeneously dispersed bubbles at acoustic pressure nodes or antinodes, and subsequent coalescence of bubbles takes place owing to Bjerknes forces, which are the radiation forces induced by the ultrasound pressure gradient [17]. Excluding buoyancy, the most potent driving forces for bubble translations in a liquid is the Bjerknes forces [18].

Ashokkumar and co-authors systematically investigated the bubble coalescence process induced by ultrasound [19–23]. In particular, they studied the influence of acoustic frequency, power and water-soluble additives on bubble coalescence [19,20] and captured coalescence using a high-speed camera [21]. In 2015, they investigated the influence of acoustic pressure and bubble size on the coalescence of two contacting bubbles [22]. In that study, they found that under the influence of an acoustic field, the coalescence time was probabilistic in nature, exhibiting upper and lower limits. Furthermore, they reported that bubbles with larger average size and bubble pairs with larger size difference exhibited longer coalescence times. Despite substantial experimental investigation, the exact mechanism of coalescence of two bubbles in an ultrasound field is still unclear, since it is almost impossible to control the ambient ultrasound pressure around bubbles, the initial bubble velocity and the collision position of bubbles. For these reasons, we are restricted to statistical conclusions.

In this paper, as a first step to understanding the mechanism of the bubble coalescence in an ultrasound field, I present a numerical model to calculate the coalescence of two bubbles, which includes the effect of bubble radius, ultrasound pressure amplitude, and initial distance between bubbles.

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2. Theoretical and numerical methods

2.1. Bubble dynamics

For a bubble in an ultrasound field, the pressure changes with time and therefore bubble volume oscillate. The bubble radius, R(t), varies as [24]:

$$R\ddot{R} + \frac{3}{2}\dot{R}^{2} = \frac{1}{\rho} \left[\left(P_{0} + \frac{2\sigma}{R_{0}} - P_{\nu} \right) \left(\frac{R_{0}}{R} \right)^{3\kappa} - \frac{2\sigma}{R} - \frac{4\mu\dot{R}}{R} - P_{0} - P(t) \right]$$
(1)

where R_0 is the equilibrium bubble radius, P_0 (=1.013 × 10⁵ Pa) is the hydrostatic pressure of the liquid, P_v (=2338 Pa) is the vapor pressure, ρ (=998 kg·m⁻³) is the liquid density, η (=1 × 10⁻³ Pa·s) is the viscosity, σ (=0.072 N·m⁻²) is the surface tension between liquid and air, and κ (=1.4) is the polytropic index of the gas within the bubble. The time-varying ultrasound pressure is P(t), By solving Eq. (1), the relationship between bubble radius and time can be obtained.

The spatial distribution of the standing-wave field is written as

$$P(z, t) = P_0 - 2P_A \cos(kz) \cos(\omega t + \varphi_0)$$
⁽²⁾

where P_A is the amplitude and ω (= $2\pi f$) is the circular frequency of the ultrasound wave (here, *f* indicates the ultrasound frequency), *k* is the wave number of the ultrasound wave, *z* is the space axis, and φ_0 indicates the initial phase of the incident waves.

2.2. Bjerknes force on air bubbles

A body of volume V(t) in a pressure gradient $\nabla P(z, t)$ experiences a force $-V(t)\nabla P(z, t)$. It is written as [18]:

$$F = -V(t)\nabla P(z, t)$$
(3)

The primary Bjerknes force indicate the direct part of Eq. (3), it has been deduced by Leighton [18]:

$$F_p = [3P_A k \xi_0 V_0 \sin(2kz)]/(2R_0)$$
(4)

for bubbles smaller than resonance and

$$F_p = -[3P_A k \xi_0 V_0 \sin(2kz)]/(2R_0)$$
(5)

for bubbles larger than resonance. The magnitude of F_p is determined by the volume change, which varies depending on phase of the ultrasound. In Eqs. (4) and (5), ξ_0 and V_0 are the amplitude of the radial oscillation and the equilibrium volume of the bubble. ξ_0 is calculated from the bubble dynamics (Eq. (1)).

The resonance radius (*a*) is calculated using the Minnaert equation [25]:

$$a = \frac{1}{2\pi f} \left(\frac{3\kappa P_0}{\rho} \right)^{\frac{1}{2}}$$
(6)

For an ultrasound frequency of 20 kHz, the resonance radius (*a*) is about 0.16 mm. Thus, a bubble of radius of $R_0 < a$ will move to the pressure antinode and a bubble of radius of $R_0 > a$ will move to the node.

The alternating part of the force on the bubble is $\tilde{F} = -V_0 \nabla P(z, t)$. Here, the bubble radius is assumed to be constant. Thus, the force on the bubble is written as the sum of the direct and alternating terms:

$$F = \bar{F} + \tilde{F} \tag{7}$$

where $\vec{F} = F_p$ indicates the direct part of the *F*. The secondary Bjerknes force can be written as [26]:

$$F_S = \langle F_{12} \rangle = -\frac{\rho}{4\pi d^2} \langle \dot{V}_1 \dot{V}_2 \rangle \tag{8}$$

where < > denotes the time average and *d* is the separation distance between the two bubbles (taken from the center of the bubbles), and *V*₁ and *V*₂ are the volumes of the two bubbles.

Ultrasonics - Sonochemistry xxx (xxxx) xxx-xxx

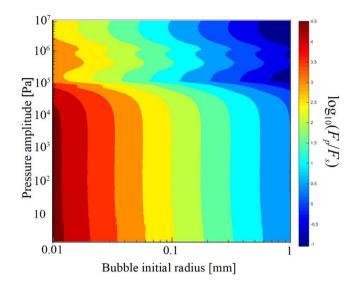


Fig. 1. Ratio of the primary to the secondary Bjerknes force. For the sub-millimeter to millimeter air bubbles, the primary Bjerknes force is two orders of magnitude greater than the secondary Bjerknes force. The ratio increases by the increase of the pressure amplitude and the decrease of the initial bubble radius.

We first compared the primary and secondary Bjerknes forces for bubbles of different initial radius. It should be noted that the size of the bubbles used to study bubble coalescence is in millimeter scale [23] which is greater than the acoustic bubbles (a few micrometers in diameter [27]). Fig. 1 shows the ratio of the primary to secondary Bjerknes force on a logarithmical scale. In the range studied, the primary Bjerknes force is greater than the secondary Bjerknes force in most of the cases. However, the secondary Bjerknes force becomes greater than the primary Bierknes force by the increase of the pressure amplitude and the increase of the initial bubble radius. Since the secondary Bjerknes force is caused by the oscillation of the bubbles, it disappears after two bubbles are in contact. For the simulation of the two separated bubbles approaching process, we selected the pressure amplitude and bubble initial radius value to ensure the primary Bjerknes force is far greater than the secondary Bjerknes force. Therefore, the secondary Bjerknes force is neglected in the simulation.

2.3. Simulation details

To simulate the bubble coalescence process, the laminar flow coupled with the phase field is solved using commercial simulation software COMSOL Multiphysics (COMSOL AB, Stockholm, Sweden). The geometry with boundary and domain conditions for the simulation of bubble coalescence is shown in Fig. 2. Because we only simulate part of the reactor, open boundary conditions were used at all outside boundaries. The volume force was used on both the bubble and the liquid. The volume force includes the primary Bjerknes force, \widetilde{F} (calculated from Eq. (7)) and the buoyancy. To solve the interfacial problem between the two phases, the phase-field model was used. This substitutes boundary conditions at the interface by a partial differential equation for the evolution of an auxiliary field that takes the role of an order parameter. The liquid and gas in the bubble were water and air, respectively. Chen et al. [28] demonstrated that as long as the horizontal width of the tank is four times larger than the initial bubble diameter, the effect due to a finite domain size can be neglected in simulations of bubble-bubble interactions. As a result, the horizontal width of the tank was set as five times that of the bubble radius in our simulation. The maximum of the mesh was limited to the 1/12 of the bubble radius in this simulation to ensure a low time cost and high computing accuracy.

For an ultrasonic frequency of 20 kHz, the ultrasound wavelength in

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