



Modeling bubble dynamics and radical kinetics in ultrasound induced microalgal cell disruption



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ABSTRACT

Microalgal cell disruption induced by acoustic cavitation was simulated through solving the bubble dynamics in an acoustical field and their radial kinetics (chemical kinetics of radical species) occurring in the bubble during its oscillation, as well as calculating the bubble wall pressure at the collapse point. Modeling results indicated that increasing ultrasonic intensity led to a substantial increase in the number of bubbles formed during acoustic cavitation, however, the pressure generated when the bubbles collapsed decreased. Therefore, cumulative collapse pressure (CCP) of bubbles was used to quantify acoustic disruption of a freshwater alga, *Scenedesmus dimorphus*, and a marine alga, *Nannochloropsis oculata* and compare with experimental results. The strong correlations between CCP and the intracellular lipid fluorescence density, chlorophyll-a fluorescence density, and cell particle/debris concentration were found, which suggests that the developed models could accurately predict acoustic cell disruption, and can be utilized in the scale up and optimization of the process.

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1. Introduction

Acoustic cavitation, as the basis of many applications of ultrasound in the high frequency range (from 20 kHz to 10 MHz), usually involves the formation, growth, oscillation, and powerful collapse of bubbles or cavities. Because the event of bubble collapse occurs in small intervals of time (milliseconds) and releases large magnitudes of energy over a very small space, a significant increase in temperature (up to several thousand degrees Kelvin) and pressure (several hundred atmospheres locally) is obtained [1–4]. The extremely high temperatures and pressures formed in collapsing bubbles in aqueous solutions are capable of decomposing water vapor into highly reactive radicals such as H[•] and [•]OH [5,6]. Redox reactions initiated by these radicals have been found to weaken the composition of microbial cell walls such as glycoproteins and polysaccharides to the point of disintegration [5,7]. In addition, intense shock waves and shear forces produced by the bubble collapse are known to break down biological cell walls and membranes, wash out cell contents, and reduce particle sizes of vegetal materials [8–10].

The vast majority applications of acoustic cavitation are in wastewater treatment [11–13], textile processing [14], crystallization [15], and biological processing [2]. Acoustic cavitation has also

been reported to effectively decrease the growth rate of algae, inhibit cell division, or cause immediate damage on photosynthetic activities of algae, as well as physically breaking the cell wall/membrane. For example, Lee et al. [16] found that under high power ultrasound, acoustic cavitation could directly rupture whole cells or gas vacuoles within the cells. TEM evidence has shown this effect on a single *Microcystis aeruginosa* cell following ultrasonic treatment at 28 kHz for 30 s (intensity of 0.12 W/cm³). In a similar study using acoustic cavitation to inhibit the growth of irradiated algal cells, *Spirulina (Arthrospira) platensis*, Tang et al. [17,18] concluded that the growth rate of algal cells was reduced to 38.9% of the control in 5-min treatment due to changes in the functionality and integrity of cellular and subcellular structures. Zhang et al. [19] found that 5 min exposure of *M. aeruginosa* to 25 kHz ultrasound (intensity of 0.32 W/cm³) caused algae sedimentation and reduced the photosynthetic activity of algae population. In addition, some researchers have used acoustic energy for microalgal cell disruption and lipid extraction. For example, solvent-free ultrasound-assisted extraction significantly improved oil recovery of *Nannochloropsis oculata* compared with conventional extraction methods (Bligh and Dyer) [20]. Wang et al. [9] found that high frequency focused ultrasound and combination of high and low frequency ultrasounds were effective in microalgal cell disruption.

Some research has been conducted to understand the bubble dynamics in acoustical field and their radical kinetics. For example, Gogate and Pandit [21] described the motion of a single bubble by

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solving the Rayleigh–Plesset equation numerically, and developed an empirical correlation for predicting the pressure generated where the cavity collapses as a function of ultrasound intensity and frequency, and the initial nuclei size. In addition, for energy balance analysis of an isolated oscillating spherical bubble in water irradiated by an ultrasonic wave, the Keller–Miksis equation as a bubble dynamics model was studied by Merouani et al. [22]. In his subsequent research, the number of active bubbles in an acoustic cavitation field was also predicted by describing the dynamics of the bubble and simulating the chemical kinetics occurring in the bubble [6]. To the best knowledge of the authors, however, ultrasound induced microalgal cell disruption has never been simulated by the model of bubble dynamics in acoustical field, or their radical kinetics.

The objective of this study was to predict acoustic cavitation induced microalgal cell disruption by simulating the dynamics of bubble oscillation in an acoustical field and the radical kinetics occurring in the bubble during its oscillation, as well as calculating the pressure pulse of the bubble collapse. The concept of cumulative collapse pressure (CCP, number of bubbles multiplied by the collapse pressure of a single bubble) was used to correlate with algal cell disruption, which was represented by the change of algal cell/debris concentration, chlorophyll-a fluorescence density (CAFD) and Nile red stained lipid fluorescence density (NRSLFD).

2. Models and computational methods

2.1. Bubble dynamics

The differential equation for the motion of the pulsating bubble is expressed as:

$$R \left(\frac{d^2 R}{dt^2} \right) + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 = \frac{1}{\rho_l} \left[\left(P_0 + \frac{2\sigma}{R_0} \right) \left(\frac{R_0}{R} \right)^{3\gamma} - \frac{2\sigma}{R} - \frac{4\mu}{R} \frac{dR}{dt} + P_v - P_\infty \right] \quad (1)$$

where water is considered as the cavitation medium, R is the radius of the bubble (μm), R_0 is the initial radius of the bubble ($10 \mu\text{m}$), ρ_l is the density of the liquid (998 kg/m^3), σ is the surface tension (0.0725 N/m), μ is the viscosity of the liquid (0.001 Pa s), P_0 is the ambient static pressure ($1.01325 \times 10^5 \text{ Pa}$), P_∞ is the variation in bulk pressure (Pa) as function of time which is given by $P_\infty = P_0 - P_A \sin(2\pi ft)$, in which f is the sound frequency (kHz), P_A is the driving pressure (Pa) that is correlated with the acoustic intensity I_a (W/m^2) as $P_A = \sqrt{2I_a \rho_l c}$, where c is the speed of sound in the liquid (1500 m/s).

The above model given by Eatock [23] is called the modified RPNNP equation. It describes a radially symmetric free bubble in an acoustic field P_∞ [24]. The modified RPNNP equation (Eq. (1)) describing the dynamics of the bubble is a non-linear second-order differential equation and can be numerically solved using the Runge–Kutta fourth-order method by Matlab (version 2014a). For the numerical simulation, growth of the bubble is considered isothermal and the collapse of the bubble becomes adiabatic when partial pressure of the gas (P_g) inside the bubble equals to the liquid-medium vapor pressure (P_v) with the consideration of Flynn's assumption [25]. When adiabatic collapse starts ($P_g = P_v$), the radius of the bubble corresponding to this point is called the critical radius, R_{crit} [26]. The temperature inside the bubble at any instant during the adiabatic phase can be calculated from the bubble size, using the adiabatic law [6]:

$$T = T_\infty \left(\frac{R_{\text{max}}}{R} \right)^{3(\gamma-1)} \quad (2)$$

where T_∞ is the bulk liquid temperature and γ is the ratio of specific heat capacities (c_p/c_v) of the vapor/gas mixture. Pressure inside the bubble during the adiabatic phase is thus given by [26]:

$$P_B = 2P_v \left(\frac{R_{\text{crit}}}{R} \right)^{3\gamma} \quad (3)$$

where $R_{\text{crit}} = R_0 \left(\frac{P_{g0}}{2P_v} \right)^{1/3}$, $P_{g0} = P_0 + (2\sigma/R_0) - P_v$, which is the gas pressure in the bubble at its ambient state ($R = R_0$).

2.2. Radical kinetics

For a bubble initially composed of oxygen and water vapor, series of reversible chemical reactions take place inside the bubble owing to the extreme conditions of temperature and pressure developed during the strong collapse phase [6,22]. A kinetic mechanism consisting of a series reversible chemical reactions (Table 1) is taken into account involving O_2 , H_2O , $\cdot\text{OH}$, $\text{H}\cdot$, O , $\text{HO}_2\cdot$, H_2 and H_2O_2 radicals. Rate expressions for the reactions involving K radicals can be represented in the general form as [27]:



in which v_{ki} is the stoichiometric coefficients of the i th reaction and X_k is the radical symbol for the k th species. K is the number of species. The superscript ' indicates forward stoichiometric coefficients, while '' indicates reverse stoichiometric coefficients. The rate r_i for the i th reaction is given by the difference of the forward and reverse rates as [27]:

$$r_i = k_{fi} \prod_{k=1}^K [X_k]^{v'_{ki}} - k_{ri} \prod_{k=1}^K [X_k]^{v''_{ki}} \quad (5)$$

where $[X_k]$ is the molar concentration of the k th species and k_{fi} and k_{ri} are the forward and reverse rate constants of the i th reaction, respectively. The forward and reverse rate constants for the i th reaction are assumed to have the following Arrhenius temperature dependence [27]:

$$K_{fi} = A_{fi} T^{b_{fi}} \exp\left(-\frac{E_{a_{fi}}}{R_g T}\right) \quad (6)$$

$$K_{ri} = A_{ri} T^{b_{ri}} \exp\left(-\frac{E_{a_{ri}}}{R_g T}\right) \quad (7)$$

where R_g is the universal gas constant, A_{fi} (A_{ri}) is the pre-exponential factor, b_{fi} (b_{ri}) is the temperature exponent and E_{fi} (E_{ri}) is the activation energy. The rate constants of the important reactions are listed in Table 1.

The simulation of the reactions started at the beginning of the adiabatic phase. The amount of water vapor and oxygen, and the temperature and pressure profiles in the bubble during adiabatic phase were obtained by solving the dynamics equation (Eq. (1)). The amount of all species (O_2 , H_2O , $\cdot\text{OH}$, $\text{H}\cdot$, O , $\text{HO}_2\cdot$, H_2 and H_2O_2) inside the bubble was calculated at any temperature by the chemical dynamic simulation through solving the reactions shown in Table 1 via Matlab. The amount of each species was defined as that of the end of the bubble collapse [22,28]. The criterion of bubble collapse was when the bubble volume reduces to the material volume of molecules present in the bubble [29].

Assuming that the bubble contents mix directly with the liquid surrounding the bubble at the end of the collapse, the number of collapsing bubbles per unit time per volume (N_{bubbles}) is determined using material balances for $\cdot\text{OH}$, $\text{HO}_2\cdot$ and H_2O_2 in the liquid phase, which is given as [22]:

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