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Energy analysis during acoustic bubble oscillations: Relationship between bubble energy and sonochemical parameters

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ABSTRACT

In this work, energy analysis of an oscillating isolated spherical bubble in water irradiated by an ultrasonic wave has been theoretically studied for various conditions of acoustic amplitude, ultrasound frequency, static pressure and liquid temperature in order to explain the effects of these key parameters on both sonochemistry and sonoluminescence. The Keller–Miksis equation for the temporal variation of the bubble radius in compressible and viscous medium has been employed as a dynamics model. The numerical calculations showed that the rate of energy accumulation, *dE/dt*, increased linearly with increasing acoustic amplitude in the range of 1.5–3.0 atm and decreased sharply with increasing frequency in the range 200–1000 kHz. There exists an optimal static pressure at which the power *w* is highest. This optimum shifts toward a higher value as the acoustic amplitude increases. The energy of the bubble slightly increases with the increase in liquid temperature from 10 to 60 °C. The results of this study should be a helpful means to explain a variety of experimental observations conducted in the field of sonochemistry and sonoluminescence concerning the effects of operational parameters.

1. Introduction

A direct consequence of ultrasound transmission through a liquid is the growth of adventitious bubble nuclei, which may collapse violently, generating localized hot-spots of extreme pressure and temperature (~1000 atm and ~5000 K respectively [1,2]). This phenomenon, termed acoustic cavitation, is responsible for the vast majority of applications involving ultrasound (e.g. materials synthesis, environmental remediation, food technology, etc.) and also for the emission of broad wavelength light: sonoluminescence [3,4].

Cavitation systems (multibubble) are extremely complex in nature with numerous interdependent parameters that influence the bubble dynamics and thus the overall efficiency (chemical and/or physical) of the system. From an engineering point of view, cavitation systems would be ideally studied with a single cavitation bubble with known size pulsating in known acoustic pressure field. Such studies of single bubble cavitation provide the means to understand the dependence of operational parameters (such as ultrasonic frequency, acoustic amplitude, static pressure, liquid temperature,...) on the bubble dynamics and thus, to explain the efficiency of sonochemical processes utilizing cavitation phenomena. A lot of research studies in the literature have addressed the matter with this approach. Gogate et al. [5,6] have correlated the iodine liberation rate to the extremes of temperature and pressure obtained at the transient collapse using a bubble dynamics model. Sivasankar et al. [7] also took a similar approach and explained some trend in sonochemistry of KI oxidation. Prasad Naidu et al. [8] explain the trend in the rate of iodine liberation with the sonication of aqueous KI solution of various concentrations and different gas atmospheres using the Rayleigh–Plesset equation for the radial motion with Flynn's criterion [9] that suggests the adiabatic collapse phase of the cavity on the basis of the assumption of partial pressure of gas in the bubble equals the vapor pressure of the cavitating media at the operating parameters. The used form of the Rayleigh–Plesset equation in Prasad Naidu's study does not take into account the compressibility of the liquid medium, and hence, Prasad Naidu et al. terminated their simulations at the instance when the bubble wall velocity reaches the velocity of sound in water. Gogate and Pandit [10] added the liquid compressibility to Prasad Naidu's assumptions and developed an empirical correlation that predicts the collapse pressure as function of intensity, ultrasound frequency and initial nuclei size. Kanthale et al. [11] used simulation results provided by a single bubble dynamics model to discuss their results on the effect of ultrasound frequency and acoustic power on both sonochemistry (H_2O_2 yield) and sonoluminescence.

However, most reported studies (including those cited above) correlated their experimental results to the maximum temperature or pressure reached in the bubble at the end of the collapse. In this

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study, we related the efficiency of both sonochemical reactions and sonoluminescence to the energy of the cavity which includes simultaneously the temperature and pressure inside a bubble, the collapse duration and other dynamic factors. The energy of the collapsing bubble has been theoretically estimated for various operating conditions of ultrasonic frequency, acoustic amplitude, static pressure and liquid temperature.

2. Model

Before describing the model, we would like to mention that the phenomenon of bubble collapse and subsequent fragmentation depends on many factors such as the surface instability, local flow conditions and the bubble population in the vicinity of the bubble [7]. We assume that in sonochemistry applications, the cavitation is transient and the bubble breaks apart (fragments) at the first collapse after an initial expansion. Therefore, we are only interested in the first expansion and subsequent violent collapse.

The bubble dynamics model used in the present study and the assumptions therein have been fully described in our previous works [12,13]. The following is a brief description of the model. A gas and vapor filled spherical bubble isolated in water oscillates under the action of a sinusoidal sound wave. The radial dynamics of the bubble is described by the Keller–Miksis equation that includes first order terms in the Mach number $M = \dot{R}/c$ [14–16]:

$$\left(1-\frac{\dot{R}}{c}\right)R\ddot{R}+\frac{3}{2}\left(1-\frac{\dot{R}}{3c}\right)\dot{R}^2=\frac{1}{\rho_L}\left(1+\frac{\dot{R}}{c}+\frac{R}{c}\frac{d}{dt}\right)\left[p-p_\infty-\frac{2\sigma}{R}-4\mu\frac{\dot{R}}{R}+P_A\sin(2\pi ft)\right] \quad (1)$$

in this equation dots denote time derivatives (d/dt), R is the radius of the bubble, c is speed of sound in the liquid, ρ_L is density of the liquid, σ is surface tension, μ is liquid viscosity, p is pressure inside the bubble, p_∞ is ambient static pressure, P_A is acoustic amplitude and f is the sound frequency. The acoustic amplitude P_A is correlated with the acoustic intensity I_a, or power per unit area, as $P_A = (2I_a\rho_L c)^{1/2}$ [3,10].

The expansion of the bubble is assumed as isothermal and its total compression is considered as adiabatic [17–19]. We also assume that the vapor pressure in the bubble remains constant during the bubble expansion phase and there is no gas diffusion during expansion and no mass and heat transfer of any kind during collapse.

On the basis of the above assumptions, the pressure and temperature inside the bubble at any instant during adiabatic phase can be calculated from the bubble size, using the adiabatic law:

$$p=\left[P_v+P_{g0}\left(\frac{R_0}{R_{max}}\right)^3\right]\left(\frac{R_{max}}{R}\right)^{3\gamma} \quad (2)$$

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

where P_v is the saturated vapor pressure, $P_{g0} = p_\infty + (2\sigma/R_0) - P_v$ is the gas pressure in the bubble at its ambient state ($R = R_0$), R_0 is the ambient bubble radius, T_∞ is the bulk liquid temperature, R_{max} is the maximum radius of the bubble and γ is the ratio of specific heats capacities (c_p/c_v) of the vapor/gas mixture. The maximum internal temperature (T_{max}) and pressure (p_{max}) reached in the bubble at the end of the bubble collapse are approximated by:

$$T_{max}=T_\infty\left(\frac{R_{max}}{R_{min}}\right)^{3(\gamma-1)} \quad (4)$$

$$p_{max}=\left[P_v+P_{g0}\left(\frac{R_0}{R_{max}}\right)^3\right]\left(\frac{R_{max}}{R_{min}}\right)^{3\gamma} \quad (5)$$

where R_{min} is the minimum radius of the bubble at the collapse.

The Keller–Miksis equation (Eq. (1)) that describes the dynamic of the cavitation bubble is a second-order nonlinear differential equation. This equation has been numerically integrated using the fourth-order Runge-Kutta method. All the physical properties (saturated vapor pressure, density, surface tension, viscosity and sound velocity) in the above equations are calculated for water as function of liquid temperature T_∞ and static pressure p_∞. The equations for the physical properties have been described in our previous work [13].

In the present study, energy analysis is carried out on the basis of internal energy (ΔE). The variation in the internal energy of the bubble ΔE during its lifetime is given as the sum of internal energies of the two parts, isothermal (noted ΔE_{iso}) and adiabatic (noted ΔE_{ad}), and as $\Delta E_{iso} = 0$, the internal energy of the bubble resumed to (ΔE_{ad}), which is given as:

$$\Delta E=\Delta E_{ad}=\Delta W+\Delta Q \quad (6)$$

where ΔQ is the heat exchanged with the liquid during adiabatic phase ($\Delta Q = 0$) and ΔW is the work done to the system (the bubble). ΔW is given for an instant t of the adiabatic phase by:

$$\Delta W=\frac{p(t)V(t)-p_{min}V_{max}}{\gamma-1} \quad (7)$$

here $p(t)$ and $V(t)$ are the internal pressure and temperature at any instant t during adiabatic phase and p_{min} and V_{max} are, respectively, the maximum volume of the bubble and the minimum internal pressure achieved in the bubble, (both p_{min} and V_{max} are corresponding to R_{max}).

The time scale in which the energy is accumulated in the cavity is of primary importance in order to compare the efficiency of the cavities oscillating with different operating parameters. So, we describe the power w as ΔE divided by the duration of bubble collapse τ_c:

$$w=\frac{\Delta E}{\tau_c} \quad (8)$$

3. Results and discussion

It is well established that the ambient bubble radius R_0 for an active bubble depends on experimentally controllable parameters, particularly on the ultrasonic frequency and acoustic amplitude [20–23]. The active bubbles are those collapsing violently and which are capable of producing sonochemistry and sonoluminescence. Recently, Brotchie et al. [23] demonstrated that the ambient radius for an active bubble increased with increasing acoustic amplitude and decreased with increasing ultrasound frequency. In our previous work [12], we have studied in detail the influence of ultrasound frequency in the range of 200–1000 kHz and acoustic amplitude (up to 3 atm) on the ambient radius R_0 for an active bubble in sonochemical reaction using the same dynamics model adopted in this investigation. The obtained theoretical results agree well with the experimental results. Thus, in the present study, the ambient bubble radius R_0 for the numerical simulations of the bubble dynamics were selected as function of frequency and acoustic amplitude according to our previous study. The selected values are presented in Table 1.

3.1. Bubble dynamics and energy analysis

In Fig. 1a and b, the calculated results during the collapse of the bubble are shown as function of time for an ultrasonic frequency of 300 kHz and acoustic amplitude of 2.5 atm. In Fig. 1a, the reduced bubble radius and internal energy ΔE are shown. During the