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# Parametric study of acoustically-driven microbubble cavitations in a sonochemical reactor

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ABSTRACT

The bubble cavitation along a solid wall is investigated with a three-dimensional model based on the indirect boundary element method. Kinetic energy and Kelvin impulse are calculated in order to quantify the strength of cavitation. The influences of acoustic wave amplitude and frequency and liquid properties on the strength of cavitation are investigated. This study was carried out in order to better understand the relation between microscale processes and macroscale parameters in a sonochemical reactor used for impregnation of fabrics with nanoparticles.



## 1. Introduction

The initial interest in studying bubble cavitation was linked to observations of structural damage of propeller blades for fast steamships [1]. One of the pioneering works refers to investigation of the collapse of a spherical void in a liquid by Lord Rayleigh [2]. In fact, cavitation is a general design consideration for many machinery and hydraulic applications [3]. For example, water flow over a dam spillway with abrupt geometric change of surface may lead to separation, allowing air influx resulting in cavitation which can cause structural damage to the spillway tunnel or chute. Due to significant drop of water pressure in the presence of a control valve, the collapse of produced bubbles may tear the materials (both the valve itself and the adjacent pipeline) [4].

Since the discovery of jet formation under certain circumstances during the bubble collapse by Naude and Ellis [5] and Benjamin and Ellis [6], a series of experimental and theoretical work have been carried out in order to better understand this process. By employing high-speed Cine photography, Gibson [7] successfully recorded liquid jets adjacent to solid boundaries during bubble collapse, suggesting that the jet formation is responsible for the cavitation damage. Kimoto [8] observed stress pulse on boundary surface, which resulted from both micro-jet impingement and the remnant cloud collapse shock. Numerical techniques have been implemented to simulate the geometric change of a cavitation bubble along a solid wall. Blake et al. [9] employed the boundary element method (BEM) to develop an axisymmetric model, simulating bubble expansion and subsequent collapse. It was pointed out that a set of particular conditions existed to reach a maximum degree of cavitation damage. Blake et al. [10] also tried some simple analysis of a bubble nearby a rough boundary of concave or convex shape. Results showed development of a jet towards the wall when it was concave. By contrast, the convex shape brought about different types of nonsphericity. In case of a slightly convex wall, jets were generated on both ends of the bubbles. However, a needle-like roughness of the wall yielded a high-speed jet away from the wall. Furthermore, Wang [11] developed a fully three-dimensional model with the same numerical technique (BEM) and investigated the bubble along an inclined wall in combination with the effects of buoyancy force. Meanwhile, lots of efforts have been made to overcome the instability of the numerical approaches by using strategies such as smoothing schemes [12] and the elastic mesh technique [13].

Cavitations in liquids can be useful in certain applications. The extracorporeal shock wave lithotripsy (ESWL) is well employed as non-invasive treatment of kidney stones. The collapse of cavitation bubbles is identified to play a significant role in the ultimate stone fragmentation [14]. Some extreme conditions (e.g. high temperature) accompanied with cavitation help degrade pollutants and organic substances, and also purify waste water. For a review of applications of cavitation in biochemical engineering the reader is referred to [15]. With regard to chemical industry, the high energy densities and heat concentration achieved during bubble

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collapse can increase the rate of or can initiate chemical reactions [16]. This is mainly because of generation of highly reactive free radicals.

In respect to lifetime, a bubble in general can be described as ‘stable’ or ‘transient’ [16]. A stable bubble experiences relatively gentle oscillation without significant energy concentration and last longer, whilst a transient one collapses usually within one or several cycles, accompanied with highly localized energy, high pressures and temperatures at the bubble interior. Transient bubble cavitation provides effective conditions for the process of sonochemical reactions.

The current work involves a sonochemical coating system, which is employed to produce antimicrobial textiles. The schematic of the sonochemical reactor is presented in Fig. 1 [17]. The reactor is filled with liquid that could be ethanol ($C_2H_5O$), water or mixture of these two. Textiles are fed into the reactor through a roller system between two ultrasonic transducers which generate cavitation bubbles. The collapse of bubbles with jet formation around the surface of the textile propels suspended metal oxide (MO) nanoparticles (e.g. MgO and ZnO) in the liquid onto the textile; hence the process of impregnation of the fabric with the nanoparticles occurs. The process itself is somewhat more complicated and is explained in more detail in [17]. However, for the purpose of this study we focus on the bubble dynamics during the collapse in order to define the more optimal reactor-scale parameters which would lead to higher temperature/pressure and jet velocities yielding faster reaction and more durable impregnation of the fabric with MO nanoparticles.

In the next section the choice of the numerical technique and related theories are elaborated and parameters which describe the characteristics of the evolving bubble are introduced. Based on the developed model, the results of a parametric study of the dynamics of the cavitation bubble are presented in Section 4, followed by conclusions on the optimization of reactor parameters for achieving more optimal bubble cavitation for the coating process.

## 2. Formulation of the bubble dynamics problem

The bubble is assumed to be inside an ideal liquid medium, which is homogeneous, incompressible, irrotational and inviscid; therefore, the following governing equation applies:

$$\Delta\phi = 0, \tag{1}$$

where $\phi$ denotes the velocity potential and $\Delta$ is the Laplacian.

The Bernoulli equation is introduced in order to describe the change of velocity potential at the bubble surface:

$$\frac{d\phi}{dt} = -\frac{1}{2}|\nabla\phi|^2 + \frac{1}{\rho L}(p_b - p_a - p_\infty - k_s S), \tag{2}$$

where $\rho_L$ is the liquid density. $p_b$, $p_a$ and $p_\infty$ are the pressure at the bubble interior, the standard atmospheric pressure and the acoustic pressure, respectively. $\kappa_s$ represents the sum of the principal curvatures on the bubble surface and $S$ denotes surface tension of the liquid. The introduced wave pressure is given by the following expression:

$$P_\infty = \bar{p} + p_{\mathrm{amp}} \sin(\omega t - \mathbf{k} \cdot \Delta\mathbf{x} + \theta), \tag{3}$$

where $\bar{p}$ is constant and $p_{\mathrm{amp}}$ represents the pressure amplitude of the wave. The regular wave is characterized with wave frequency $f$ ($\omega = 2\pi f$) and wave length $\lambda$ ($\mathbf{k} = 2\pi/\lambda$), which has a phase $\theta$. $\Delta x$ is the relative coordinate at any location from the wave source point, i.e. $x_s$.

The evolving bubble is accompanied with variations in physical quantities such as bubble volume $V_b$, the pressure and the temperature at the bubble interior, i.e. $p_b$ and $T_b$. In the numerical model developed, $V_b$ is computed at each time step together with the equivalent bubble radius $\bar{R}$ ($V_b = 4\pi\bar{R}^3/3$) which describes variation in the bubble size.

To evaluate $T_b$ and $p_b$, the thermal processes inside the bubble must be accounted for. Heat and mass transfer occur at the interface between the ambient liquid and the bubble interior during bubble evolution. Szeri et al. [18] introduced the slow and the rapid dynamics in order to classify the mechanism of the thermal process. When a bubble evolves slowly, sufficient time exists for heat and mass transfer to take place at the interface. Hence, the temperature inside the bubble remains close to the ambient temperature. The slow process can be considered to be an isothermal process. On the other hand, a rapid dynamics implies that the time required for heat and mass transfer far exceeds the time of the bubble evolution, thereby resulting in an adiabatic process inside the bubble. In the current work, we employ the criterion for differentiating the abovementioned isothermal and adiabatic processes, according to [19]: “...the collapse of the cavity becomes adiabatic when partial pressure of the gas inside the cavity equals the

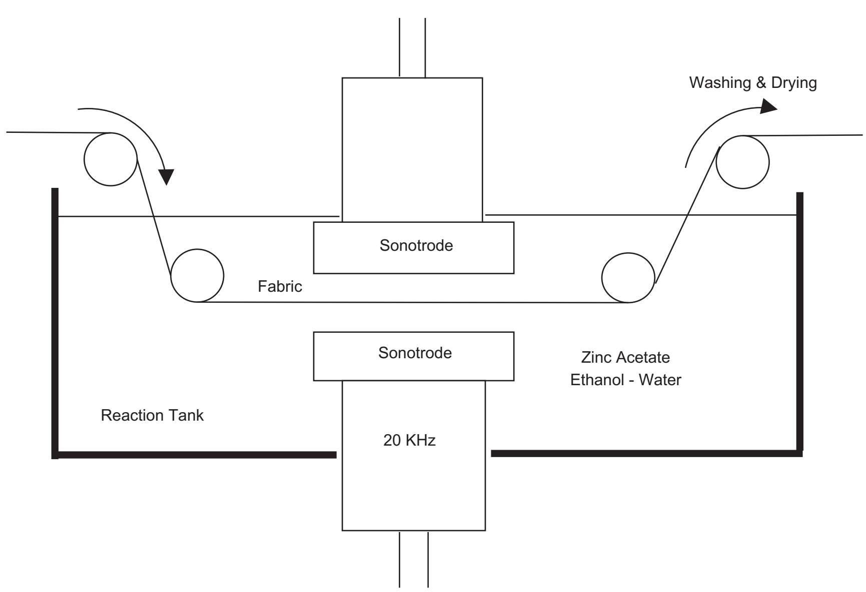


**Fig. 1.** Sketch of the sonochemical reactor for impregnation of fabric with antibacterial and antifungal nanoparticles [17].