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An Euler–Lagrange method considering bubble radial dynamics for modeling sonochemical reactors

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ABSTRACT

Unsteady numerical computations are performed to investigate the flow field, wave propagation and the structure of bubbles in sonochemical reactors. The turbulent flow field is simulated using a two-equation Reynolds-Averaged Navier–Stokes (RANS) model. The distribution of the acoustic pressure is solved based on the Helmholtz equation using a finite volume method (FVM). The radial dynamics of a single bubble are considered by applying the Keller–Miksis equation to consider the compressibility of the liquid to the first order of acoustical Mach number. To investigate the structure of bubbles, a one-way coupling Euler–Lagrange approach is used to simulate the bulk medium and the bubbles as the dispersed phase. Drag, gravity, buoyancy, added mass, volume change and first Bjerknes forces are considered and their orders of magnitude are compared. To verify the implemented numerical algorithms, results for one- and two-dimensional simplified test cases are compared with analytical solutions. The results show good agreement with experimental results for the relationship between the acoustic pressure amplitude and the volume fraction of the bubbles. The two-dimensional axi-symmetric results are in good agreement with experimentally observed structure of bubbles close to sonotrode.

1. Introduction

Acoustic cavitation concerns the formation of bubbles from nuclei, their convection, oscillation and collapse [1]. These bubbles are responsible for dissipation of the acoustic energy in the liquid medium. Thus, determining the correct bubble distribution is an important goal in designing sonochemical reactors. The most important technological problem is upscaling the laboratory reactors to industrial scales ones in which the uniformity of the cavitational activity cannot be guaranteed. This uniformity, in addition, is disturbed due to external instruments such as aluminum foils and hydrophones during experimental investigations [2,3]. Furthermore, the majority of experimental investigations are on the behavior of a single bubble during a short period of time such as the work of Lauterborn et al. [4] and Dangla and Poulain [5]. These experiments are of limited value to understand the state of a bubble swarm which is the most significant factor affecting the cavitational activity. Thus, to understand the design aspects of sonochemical reactors such as the dependency of the cavitational activity on the operating parameters and their optimum values [6], theoretical models as well as experimental investigations should be utilized [7].

Computational models may help in optimizing the geometry and operating parameters of a reactor. However, formulating a comprehensive physical model is still a challenge since not all of the phenomena are completely understood [8]. Furthermore, the disparity of the length and time scales causes severe mathematical problems. A majority of models dealing with bubbles in an acoustic field focus on a Rayleigh type equation for a single bubble during one or several acoustic periods [9,10]. As a result the pressure and temperature at the bubble position during the oscillation and after its collapse are predictable. These parameters may help in estimating the optimum design parameters such as cavitational yield in a reactor [11]. Furthermore, the energy analysis of a single bubble dynamics could be helpful in determining the dissipation of power in the whole geometry of the reactor [12,13]. However, predicting the heat and mass transfer as well as the chemical consequences at a microscopic scale in these models is still of challenge. Furthermore, the swarm behavior of bubbles cannot be figured out from single bubble dynamics.

The second group of the models concerns the modeling of the cavitational activity by finding the acoustic pressure amplitude as a field quantity. In this category, the acoustic pressure is predicted without considering the effect of bubbles [14] or by estimating their effect using simplifications [15,16]. These approaches allow to determine the effect of parameters such as frequency and intensity of the ultrasound source or the boundaries, with respect to sound propagation and damping [17].

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Most of the aforementioned references do not concentrate on the bulk medium motion. This flow field may be a result of external momentum sources, such as the inlet/outlet of a continuous feed reactor. Alternatively, they may be due to a strong acoustic source (acoustic streaming). Previous studies on the fluid motion in presence of a sound field are limited to investigate the acoustic streaming and are not for a combination with other momentum sources (see Ref. [18] or Ref. [19] and references therein). Furthermore, the experimental works in this field are usually conducted by considering some chemical characteristics such as mixing time of the reactants in a sonochemical reactor [20]. Since recent sonochemical reactors may be designed for reacting flows [21], the influence of external convective sources should also be considered. Besides that, it is important to understand the mixing and hydrodynamic characteristics due to the presence of solid/gas phases in a continuous feed reactor [22]. The idea of modeling of such a flow field is that it can help in placement of the reactants in zones of maximum cavitational intensity, flow distributors and near transducers for eliminating zones with weak cavitational activity [23].

Recently, hydrodynamic cavitation phenomena including the radial dynamics of externally driven bubbles are investigated by Abdel-Maksoud et al. [24]. However, due to the large difference between time scales of the oscillations of the bubbles and the bulk liquid flow, there are no attempts toward simultaneous modeling of these events using an Euler–Lagrange method in sonochemical reactors. The works of Parlitz et al. [25] and Mettin et al. [26] are some of the first attempts to use an Euler–Lagrange approach for the motion of bubbles under the action of ultrasound. By applying a particle model, they found that the primary Bjerknes force creates filaments of bubbles (streamers) due to the motion of the bubbles towards the nodes or antinodes of the acoustic field. Nevertheless, these works also suffer from the lack of investigating the external convective sources. Therefore, the present paper seeks to find a new method to investigate the motion of bubbles with varying radii and the formation of their quasi-steady structure under the action of a strong acoustic field.

2. Theory

2.1. Field quantities

For small amplitude waves, the distribution of the acoustic pressure may be described by the linear wave equation. Decomposing this equation into a spatially varying amplitude and a harmonic contribution, results to a Helmholtz type equation

$$\nabla^2 p + k^2 p = 0. \tag{1}$$

Here, $k = \omega/c$ denotes the wave number in which ω is the frequency of the wave, c is the speed of sound in the medium and p is the acoustic wave amplitude.

The motion of the turbulent, Newtonian, incompressible fluid may be governed by the RANS models, i.e., the convection equations for mass and momentum together with a transport model for the turbulent kinetic energy k and the turbulent dissipation rate ϵ. Here, the standard $k-\epsilon$ model is selected for turbulence modeling. Details of the model are not presented here. In the following, $\mathbf{U_f}$ denotes the fluid velocity.

2.2. Lagrangian approach for bubble motion

The motion of each individual bubble in a Lagrangian approach is governed by Newton's second law

$$m_b \frac{d\mathbf{U_b}}{dt} = \mathbf{F_G} + \mathbf{F_{AM}} + \mathbf{F_{vol}} + \mathbf{F_D} + \mathbf{F_{Bj1}}, \tag{2}$$

in which m_b is the mass of the bubble and $\mathbf{U_b}$ is its velocity. The Right Hand Side (RHS) of Eq. (2) contains the gravitational force $\mathbf{F_G} = \left(1 - \frac{\rho}{\rho_b}\right) m_b \mathbf{g}$, the added mass force $\mathbf{F_{AM}} = \frac{m_b \rho}{2\rho_b}\left(\frac{D\mathbf{U_f}}{Dt} - \frac{d\mathbf{U_b}}{dt}\right)$, the volume variation force $\mathbf{F_{vol}} = \frac{\rho}{2\rho_b}\frac{dm_b}{dt}(\mathbf{U_f} - \mathbf{U_b})$ which represents momentum transfer due to changes in the bubble volume [27], the drag force and the primary Bjerknes force. In these equations, ρ_b is the density of the bubble that is mainly filled with gas such as air. The last two forces are explained in the following.

The drag force is a result of the relative motion between the bubble and the surrounding fluid and can be expressed as

$$\mathbf{F_D} = -m_b \frac{\mathbf{U_b} - \mathbf{U_f}}{\tau_b}, \tag{3}$$

where τ_b is the relaxation time for the bubble. The value of τ_b, which represents the time for a bubble to respond to the changes in the local fluid velocity, can be obtained as

$$\tau_b = \begin{cases} \frac{\rho_b d_b^2}{18\mu} & : Re_b < 0.1 \\ \frac{4}{3}\frac{\rho_b d_b}{\rho C_D |\mathbf{U_f} - \mathbf{U_b}|} & : Re_b > 0.1 \end{cases}$$

in which d_b is the diameter of the spherical bubble, Re_b is the bubble Reynolds number defined based on the relative velocity between bubble and the surrounding fluid and the drag coefficient, C_D, is obtained from the Schiller and Naumann relation [28].

As the acoustic pressure is oscillatory in time, the average of the primary Bjerknes force on the bubble during one acoustic cycle is calculated as follows

$$\mathbf{F_{Bj1}} = -\langle V(t)\nabla p(t)\rangle_t, \tag{4}$$

where $V(t)$ is the volume of the bubble and $\nabla p(t)$ is the pressure gradient at the bubble position. The operator $\langle . \rangle_t$ denotes averaging in time.

2.2.1. Updating the bubble position

To find the new position of a bubble as $\mathbf{x}_b^{n+1} = \mathbf{x}_b^n + \mathbf{U}_b^{n+1} dt$, the updated bubble velocity $\mathbf{U}_b^{n+1}$ is obtained by substituting Eqs. (3) and (4) and the gravitational, added mass and volume variation forces into Eq. (2). To calculate drag, added mass and volume variation forces, the updated value for the bubble velocity is applied, that means a backward (implicit) Euler method is used. After some algebraic operations, the updated bubble velocity is obtained as below

$$\mathbf{U}_b^{n+1} = \frac{\mathbf{U}_b^n + \frac{2dt}{2\rho_b + \rho}\left((\rho_b - \rho)\mathbf{g} + \left(\frac{\rho}{2V_b}\frac{dV_b}{dt} + \frac{\rho_b}{\tau}\right)\mathbf{U}_{@b} - \frac{1}{V_b}\langle V_b \nabla p(t)\rangle_t\right)}{1 + \frac{2dt}{2\rho_b + \rho}\left(\frac{\rho}{2V_b}\frac{dV_b}{dt} + \frac{\rho_b}{\tau}\right)}, \tag{5}$$

in which $\mathbf{U}_{@b}$ is a new notation for $\mathbf{U_f}$ to show the velocity vector of the liquid at the bubble position. This vector is interpolated from the solution of the flow field at each time step.

2.3. Bubble dynamics

For the sake of simplicity, it is assumed that the spherical shape of the bubbles remains unchanged and the radial dynamics of a bubble including the compressibility effects to the first order of acoustical Mach number, $\dot{R}/c$, are modeled by the Keller–Miksis equation (KME) [29]

$$\rho\left(\left(1 - \frac{\dot{R}}{c}\right)R\ddot{R} + \frac{3}{2}\dot{R}^2\left(1 - \frac{\dot{R}}{3c}\right)\right) = \left(1 + \frac{\dot{R}}{c} + \frac{R}{c}\frac{d}{dt}\right)\left(p_g - \frac{2\sigma}{R} - \frac{4\mu\dot{R}}{R} - p\right), \tag{6}$$