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A new pressure formulation for gas-compressibility dampening in bubble dynamics models

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ABSTRACT

We formulated a pressure equation for bubbles performing nonlinear radial oscillations under ultrasonic high pressure amplitudes. The proposed equation corrects the gas pressure at the gas–liquid interface on inertial bubbles. This pressure formulation, expressed in terms of gas-Mach number, accounts for dampening due to gas compressibility during the violent collapse of cavitation bubbles and during subsequent rebounds. We refer to this as inhomogeneous pressure, where the gas pressure at the gas–liquid interface can differ to the pressure at the centre of the bubble, in contrast to homogenous pressure formulations that consider that pressure inside the bubble is spatially uniform from the wall to the centre. The pressure correction was applied to two bubble dynamic models: the incompressible Rayleigh–Plesset equation and the compressible Keller and Miksis equation. This improved the predictions of the nonlinear radial motion of the bubble vs time obtained with both models. Those simulations were also compared with other bubble dynamics models that account for liquid and gas compressibility effects. It was found that our corrected models are in closer agreement with experimental data than alternative models. It was concluded that the Rayleigh–Plesset family of equations improve accuracy by using our proposed pressure correction.

1. Introduction

The behaviour of strongly collapsing bubbles under the effect of ultrasonic waves, as well as the spectacular effects that arise from acoustic cavitation such as sonoluminescence, sonochemistry and extremely high and localised temperature and pressures, has been analysed by simplified bubble dynamic models such as the Rayleigh–Plesset family of equations. The traditional Rayleigh–Plesset equation (RPE) is a second order ordinary differential equation that represents the oscillation of gas bubbles in a liquid under the action of ultrasonic fields. For small to moderate pressure amplitudes the bubble radius will increase and decrease concomitantly with the decrease and increase of the acoustic pressure. However, for high intensity fields, where the amplitude of the acoustic wave is higher or equal than the Blake threshold, inertial bubbles will exhibit a manyfold volume increase followed by a dramatically sharp compression usually referred as bubble collapse. During the expansion stage the bubble stores potential energy that is subsequently transformed into kinetic energy during the compression stage. Depending on the pressure amplitude of the acoustic wave the conversion from potential to kinetic energy can induce a drastic velocity increase approaching or even exceeding the speed of sound in the liquid. The term bubble collapse comes from experimental observations showing bubble destruction and fragmentation at the end of the compression stage. However, single bubble sonoluminescence has shown that inertial bubbles do not necessarily undergo fragmentation but they can also exhibit subsequent dampened rebounds that die off before the end of a single acoustic period. When bubbles collapse the volume reduces drastically approaching the van der Waals core size. This happens so rapidly that the compression can be considered adiabatic because the time scale of heat diffusion is longer than the time scale of the radial movement of the bubble wall [1]. Consequently, the bubble temperature rises to thousands of kelvin degrees emitting picosecond flashes of light [2]. The conversion of compressed acoustic energy into light is known as sonoluminescence (SL).

The RPE assumes spherical symmetry, and thus shape stability, a uniform pressure inside the bubble [3], liquid incompressibility and a speed of the bubble wall well below the speed of sound in the liquid and gas phases [4]. The RPE, even though is remarkably simple, captures important features exhibited during cavitation such as the initial explosive expansion an subsequent violent collapse where the bubble compresses at a speed approaching or surpassing the speed of sound in the liquid, contradicting one of the

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theoretical assumptions of the model [5] but nevertheless predicting that behaviour correctly. It however fails to accurately simulate the dampened rebounds [2,6] that have been observed from single bubble sonoluminescence (SBSL) experiments.

The aim of simplified models is to predict not only the expansion, collapse and rebounds of single bubbles but also the extreme temperature and pressure reached during bubble collapse, as well as the diffusion and trapping of solvent (water) because at those conditions sonochemistry occurs. The thermal behaviour can be predicted with a coupled energy conservation equation, while the diffusion and trapping of water vapour can be modelled via a coupled vapour mass transfer equation. Water vapour evapora tion–condensation inside the bubble is a crucial factor to predict peak temperatures exhibited at collapse. This is because the water vapour that diffuses inside the bubble during the initial bubble expansion is trapped during the compression stage due to the slow diffusion compared to the rapid inertial collapse. This results in an increased heat capacity of the mixture of gases and vapours inside the bubble [7] that reduces peak temperatures at collapse. Neglecting water transport results in unrealistically high peak temperatures. Furthermore, the endothermic chemical reactions occurring inside the bubble reduce peak temperature further due to the endothermic dissociation of water vapour [8]. Hence, understanding the behaviour of inertial bubbles, sonoluminescence and sonochemistry requires not only an accurate coupling of bubble dynamics, energy balance, vapour diffusion and sonochemical reactions but also a correct representation of the physical properties as a function of thermal and compositional changes [9]. Recent numerical studies conducted by Cogné et al. [10] and Shen et al. [11] show that accounting for variations on the wall temperature influence rebounds slightly and may have implications for sonochemistry but this effect will not be considered in our work.

A major issue of the traditional RPE, even though it describes the initial growth and subsequent collapse, is that it does not account for the energy loss that causes dampened oscillations as observed experimentally. The foremost improvement to the RPE is to account for the compressibility of the surrounded liquid. Liquid compressibility attenuates bubble oscillations by producing sound waves in the liquid phase during the violent collapse and rebounds. This has been addressed by several authors since the work of Herring [12]. The most common corrections that account for liquid compressibility are the models derived by Keller, Miksis and Kolodner [13,14], and Prosperetti and Lezzi [15]. However, none of those models represent correctly the dampened rebounds without using unphysical values of viscosity and surface tensions that are used as fitting parameters to adjust predictions to experimental data [2,6].

A basic assumption in deriving simplified models is assuming a spatially uniform pressure inside the bubble. This is a good approximation during expansion but is not the case during a violent collapse [16]. A further refinement of the theory is to consider that if acoustic waves are launched into the liquid, similar waves should also be launched into the gas bubbles, which is the most compressible phase of the system [17]. This was addressed by Moss et al. [6] and Geers and Hunter [18] who also included dilatation of bubble surface. According to Moss et al. [6] even though wave motion in liquid provides compressible correction to the radial equation of motion, accounting for gas compressibility can result in a substantial correction to the bubble dynamics. This is because when the bubble wall velocity approaches the speed of sound of the gas, pressure differences (or pressure inhomogeneity) between the wall and the core are formed. This is in agreement with the full thermo-mechanical bubble dynamics simulation of Vuong and Szeri [19,20] showing that the gas pressure at the gas–liquid interface exceeds the homogenous pressure on collapse. This indicates wavy disturbances on the bubbles or the formation of shock waves that focus its energy towards/outwards the bubble centre.

The limitation of considering a homogenous pressure in gas-bubbles has been addressed by Prosperetti and coworkers [16,21], while the launching of shock waves inside the bubbles has been studied by Greenspan and Nadim [22], Vuong et al. [20] and Chu [23]. Lin et al. [3] developed a semi empirical hydrodynamic correction, based on a dimensionless acceleration quantity, to account for the departure from homogenous pressure. Besides the work of Moss et al. [6] and Lin et al. [3], a third approach that considers the wave generation on the liquid and gas phases was developed by Geers and Hunter [18] who formulated a hyper acoustic relationship relating bubble volume acceleration to far-field pressure profile during the formation of shock-waves. In this study we will extend the pressure correction proposed by Moss et al. [6] which was developed under the assumption of a polytropic expansion and neglecting vapour diffusion and heat transfer. Our correction is not limited to polytropic expansion as it accounts for the effect of temperature and compositional changes due to heat transfer and water vapour diffusion to and from the bubble. The proposed pressure correction was applied to two simplified bubble dynamic models: a traditional Rayleigh–Plesset equation (RPE), which does not account for liquid compressibility, and the Keller and Miksis equation (KME) [14], which is one of the most popular equations accounting for liquid compressibility.

Simplified models based on ordinary differential equations (ODE) are preferred because are simpler and it has been proven to give similar results compared to more complex bubble dynamics models. For instance, the full compressible Navier–Stokes simulation (DNS) coupled with heat and mass transfer developed by Storey and Szeri [8,24] are in almost complete agreement with the simplified numerical simulations (ODEs) developed by Toegel et al. [7], Storey and Szeri [1] and Yasui [25]. We solved the bubble dynamics together with coupled non-linear ODE's for temperature and the rate of change of water vapour but neglecting chemical reactions at bubble collapse. We followed the approach of Toegel et al. [7] who solved three coupled ODEs: the first one accounts for bubble dynamics; the second, which is an energy balance, accounts for the bubble temperature; and the last, which is a mass balance, accounts for water vapour composition inside the bubble. The mass and heat fluxes between the interior and exterior of the bubble was calculated using a characteristic thermal and vapour diffusion length that changes depending on the characteristic time scale of the bubble motion. Physical properties such as heat capacity and speed of sound of gas inside the bubble were estimated as a function of temperature and composition. The pressure corrected models were compared to the uncorrected models and to previous models that consider the effect of gas compressibility namely, Moss et al. [6], Geers et al. [17] and Lin et al. [3]. Simulated data was compared with experimental data of radius vs time from SBSL experiments. Temperature and water vapour profiles were also simulated and predictions obtained with different models were compared.

2. Mathematical model

2.1. Inhomogeneous pressure correction

The initial bubble expansion is considered isothermal where the bubble temperature is equal to the temperature of the liquid T_0. At some point during the subsequent bubble contraction, the velocity of the bubble changes very rapidly so the collapse behaves like an adiabatic compression resulting in a dramatic increase of the bubble temperature T. The RPE family of equations assume that the pressure inside the bubble is homogenously distributed and the pressure of the gas p_g is calculated with an equation of state. However, as discussed by Moss et al. [6], if the bubble radius changes