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Bubble collapse near a fluid-fluid interface using the spectral element marker particle method with applications in bioengineering

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ABSTRACT

The spectral element marker particle (SEMP) method is a high-order numerical scheme for modelling multiphase flow where the governing equations are discretised using the spectral element method and the (compressible) fluid phases are tracked using marker particles. Thus far, the method has been successfully applied to two-phase problems involving the collapse of a two-dimensional bubble in the vicinity of a rigid wall. In this article, the SEMP method is extended to include a third fluid phase before being applied to bubble collapse problems near a fluid-fluid interface. Two-phase bubble collapse near a rigid boundary (where a highly viscous third phase approximates the rigid boundary) is considered as validation of the method. A range of fluid parameter values and geometric configurations are studied before a bioengineering application is considered. A simplified model of (micro)bubble-cell interaction is presented, with the aim of gaining initial insights into the flow mechanisms behind sonoporation and microbubble-enhanced targeted drug delivery. Results from this model indicate that the non-local cell membrane distortion (blebbing) phenomenon often observed experimentally may result from stress propagation along the cell surface and so be hydrodynamical in origin.

1. Introduction

The dynamics of bubble collapse has received substantial attention in the literature over the past 100 years. Starting with Lord Rayleigh (1917), who considered the collapse of a spherical cavity in an infinite expanse of incompressible fluid, subsequent experimental, numerical and analytical studies have highlighted a complex physical process, where possible observed phenomena include jet formation, pressure shockwave emission and toroidal bubble formation (see, for example, Benjamin and Ellis, 1966; Lauterborn and Ohl, 1997). Research is motivated by the prevalence of bubbles in nature and industry and their fundamental role in many fluid systems. Cavitation damage due to bubble collapse is now a well-known phenomenon, and has negative consequences in a number of areas. In biomedicine, for example, ultrasound mediated drug delivery (Hernot and Klibanov, 2008; Lentacker et al., 2014; Wu and Nyborg, 2008) and shock-wave lithotripsy procedures (Freund et al., 2009; Kodama and Takayama, 1998) can generate cavitation bubbles that may cause cell death and hemorrhaging in the surrounding tissue, respectively. However, bubbles may also be used to dissolve blood clots (see e.g. Unger et al., 2002), break through the blood-brain barrier (see e.g. Ting et al., 2012) and clean and sterilise surfaces (see e.g. Chahine et al., 2016; Song et al., 2004). Numerical studies of bubble dynamics have been dominated by the boundary element method (BEM), originally used in this context by Blake et al. (1986, 1987). The method requires the assumption of irrotationality, which considerably simplifies the governing equations. While this assumption has proven effective for moderate to high Reynolds numbers (Curtiss et al., 2013; Klaseboer and Khoo, 2004a, b) and in cases of weak flow compressibility (Wang, 2014; Wang and Blake, 2010), it precludes some key physics necessary in the modelling of multiphase biomedical flows, such as strong compressibility (i.e. ultrasound) and general non-Newtonian effects.

Numerical solutions of the full Navier-Stokes equations for bubble dynamics problems have received considerably less attention in the literature than boundary elements, most likely due to the increased implementation difficulty and computational time. Shopov and Minev (1992); Shopov et al. (1990) and Shopov et al. (1992) considered a finite element approximation of the incompressible Navier-Stokes equations, where the mesh was fitted to the bubble surface and evolved in a Lagrangian manner. Fitting the computational mesh to the bubble surface could substantially increase the computational time, particularly under significant topological changes. Popinet and Zaleski (2002) produced a well-defined (unfitted) interface over a finite volume grid by

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interpolating through bubble surface marker points using cubic splines. They found good agreement with experimental results for the incompressible phase of the dynamics but concluded that compressibility and thermal effects may be required for the compressible phase (bubble rebound).

Wang and Blake (2010) developed an approximate theory for bubble dynamics in a compressible fluid using matched asymptotic expansions. The perturbation was performed to second order using the bubble-wall Mach number (assumed to be small). The bubble dynamics could then be numerically modelled using traditional boundary elements with compressibility appearing in the far-field boundary condition. Due to the assumption of a small Mach number, the method may not be able to accurately capture the bubble behaviour during the latter stages of collapse when larger degrees of compressibility may be required. However, excellent agreement was found with the Keller-Herring equation for spherical bubbles and test cases included the behaviour of a bubble under both a weak and strong acoustic wave. Wang (2014) subsequently applied the compressible BEM model to bubble collapse near a rigid wall. During the incompressible phase of the bubble dynamics, Wang (2014) achieved excellent agreement with experimental observations. During the bubble rebound, where compressibility is important, the agreement was an improvement on previous results (e.g. Popinet and Zaleski, 2002) but still differed when compared to experiments (see their Fig. 7). It is likely that the secondary collapse phase required an amount of compressibility which is beyond the scope of the BEM model. In their boundary element study, (Lee et al., 2007) took a different approach and approximated compressible effects by incorporating a loss in energy (provided by experimental data) during the bubble rebound and found very good agreement with experimental results, including the capture of the elusive counterjet. Müller et al. (2010) considered collapse of a gas filled bubble near a rigid wall using a finite volume technique for the *compressible* Euler equations. They showed that when a bubble collapses near a rigid wall (in the absence of viscosity, buoyancy and surface tension), the compressible bubble contents interact with reflected pressure shock-waves (caused by the oscillation of the bubble), producing vortices in the gaseous bubble contents. These vortices rotate in opposite directions and are directed towards the rigid wall. The vortices pull the gaseous bubble contents and bubble surface towards the rigid wall producing the well-known toroidal shape and high-speed liquid jet. Importantly, these are observations which cannot be obtained from incompressible and irrotational simulations such as BEM. The above studies, particularly that of Müller et al. (2010), illustrate the importance of compressibility, even in situations commonly assumed to be predominantly incompressible. It is evident that if compressible effects are to be included then the full compressible Navier-Stokes (or Euler) equations must be considered.

Lind and Phillips developed a Spectral Element Marker Particle (SEMP) method for fully compressible bubble collapse problems in both Newtonian (Lind and Phillips, 2012) and viscoelastic fluids (Lind and Phillips, 2013) with small to moderate Reynolds numbers. SEMP uses the marker particle method (Rider and Kothe, 1995) to track the fluid phases. The marker particle method is Lagrangian in nature and bears semblance to both the VOF (Hirt and Nichols, 1981) and the MAC (Harlow and Welch, 1965) methods. A colour function C is determined by tracking massless marker particles. Each particle is assigned a particular colour depending upon the phase in which it resides, and because a particle of fluid will remain of that fluid type (assuming no change in phase), a particle will keep its colour indefinitely. Within fluid-fluid interface regions, where two (or more) differently coloured sets of marker particles reside, a weighted average is taken of the surrounding particles to determine an interpolated colour at a desired grid point. In this article, SEMP is extended to include a third phase, that may be used to model deformable biological matter (e.g. cells or tissue). While there have been a number of works considering bubble collapse near deformable surfaces (see e.g. Klaseboer and Khoo, 2004b; Ohl et al., 2009), few include sufficient physics to model the complex multiphase biomedical processes that motivate this work. Indeed, the eventual aim is to gain insights into the flow mechanisms behind sonoporation (e.g. Lentacker et al., 2014) and microbubble-enhanced targeted drug delivery (e.g. Hernot and Klibanov, 2008).

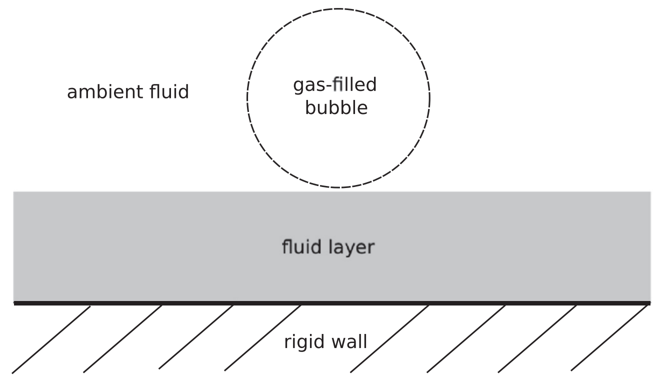

Fig. 1. Schematic of the bubble Ω_b surrounded by an ambient fluid Ω_f and placed near a fluid layer Ω_c backed by a rigid wall.

This article is structured as follows. The mathematical model and governing equations are introduced in Section 2 with their numerical approximation discussed in Section 3. The three-phase method is validated in Section 4 before a numerical investigation into the effect of viscosity and the thickness of the third phase is given in Section 5. A simplified model of (micro)bubble-cell interaction is presented in Section 6 before the article is concluded in Section 7.

2. The mathematical model and governing equations

Consider a two-dimensional (2D) domain Ω, which contains a gas-filled bubble Ω_b of initial density $\rho_{b,0}$, surrounded by fluid Ω_f of initial density $\rho_{f,0}$, placed near a fluid layer Ω_c such that $\Omega_f = \Omega \setminus (\Omega_b \cup \Omega_c)$. Note that all variables with index b will refer to those associated with the bubble, those labelled f with the ambient fluid and those labelled c with the fluid layer. A schematic is given in Fig. 1.

In general, the equations governing fluid motion are the mathematical statements of conservation of momentum

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{S}, \tag{1}$$

and conservation of mass

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \boldsymbol{u} = 0,$$

where $\boldsymbol{u}$ is the velocity, p is the pressure, $\boldsymbol{S}$ is the extra-stress tensor and ρ is the density. In the majority of bubble simulations in the literature (see e.g. Blake et al., 1986; Curtiss et al., 2013; Lee et al., 2007; Popinet and Zaleski, 2002), the fluid phases are assumed to be incompressible. However, in modelling bubble dynamics, particularly growth or collapse, one needs to account for the change in volume of the bubble, and so any fluid that may reside within must be modelled as compressible. Furthermore, and as discussed in the introduction, compressibility is known to play an important role in the final stages of bubble collapse, contributing significantly to energy dissipation (Lee et al., 2007). Also, in the context of biomedical flows, if one requires accurate descriptions of any acoustic fields applied to or emitted from the bubble, compressibility and the complete conservation of mass equation must be retained. Accordingly, a thermodynamic equation of