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Large deformation of liquid capsules enclosed by thin shells immersed in the fluid

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The deformation of a liquid capsule enclosed by a thin shell in a simple shear flow is studied numerically using an implicit immersed boundary method. We present a thin-shell model for computing the forces acting on the shell middle surface during the deformation within the framework of the Kirchhoff–Love theory of thin shells. This thin-shell model takes full account of finite-deformation kinematics which allows thickness stretching as well as large deflections and bending strains. For hyperelastic materials, the plane-stress assumption is used to compute the hydrostatic pressure and the incompressibility condition yields the thickness strain component and the corresponding change in the thickness. The stresses developing over the cross-section of the shell are integrated over the thickness to yield the stress and moment resultants which are then used to compute the forces acting on the shell middle surface. The immersed boundary method is employed for calculating the hydrodynamics and fluid–structure interaction effects. The location of the thin shell is updated implicitly using the Newton–Krylov method. The present numerical technique has been validated by several examples including an inflation of a spherical shell and deformations of spherical and oblate spheroidal capsules in the shear flow.

1. Introduction

Many problems in which a viscous fluid interacts with a deformable boundary are of considerable interest in the study of fluid mechanics such as blood flow, suspension of liquid droplets in fluid. Understanding the mechanics of the interaction between the fluid and suspended particles is important in many applications such as chemical engineering, cellular biology and drug delivery. Much effort has been devoted to study the behavior of liquid capsules enclosed by elastic membrane such as red-blood cells and synthetic capsules with polymerized interfaces. Experimental and theoretical studies have revealed complex interaction of different physical properties of the capsule such as capsule shape, internal fluid viscosity and membrane material that affect the deformations of the suspended capsule in the flow.

Several experimental studies have been performed for synthetic capsules in simple shear flow [6,47,48]. Laboratory observations of red-blood cells (RBC) in the shear flow were also reported [1,15,35]. Depending on the shear rate and the stiffness of the membrane, the capsules or RBCs undergo different types of motion such as tank-treading, tumbling or transition from tumbling to tank-treading.

Theoretical study of the deformation of spherical capsules suspended in a shear flow was presented in [3,4] for small capsule deformation. For large deformation, asymptotic theories are not applicable and numerical simulations have been

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employed by a number of authors with different membrane models. In [10,13,24,43], the forces generated in the capsule membrane during the deformation are obtained using a finite element model [7,37]. Subsequently, a zero-thickness elastic shell model has been developed in [33] for computing the elastic tensions at the nodes of an unstructured quadratic triangular mesh describing the capsule membrane. This model was later used in [23,32] for studying capsule membrane with bending rigidity. Bending moments developed in [32] were expressed in terms of mean and Gaussian curvature multiplied by a corresponding bending modulus that is generally distinct from the modulus of elasticity. This constitutive law describes the mechanism that biological membranes consisting of lipid bilayers exhibit the bending moments due to a preferred three-dimensional unstressed configuration. These membrane models have been considered with different membrane constitutive laws. In most cases, the capsule membrane are considered as hyperelastic materials with neo-Hookean or Skalak strain energy functions [13,24,33,43]. The effect of the membrane constitutive laws on the deformation of capsules has been studied in [21]. Other forms of constitutive law have also been used such as the Yeoh form in [23] and the Hooke's law with 2d-Lamé coefficients in [18].

To handle the fluid–structure interaction, several methods have been employed to solve for the viscous incompressible fluid flow in conjunction with the membrane models. The boundary-element method (BEM) has been applied intensively to study the deformation of liquid capsules in Stokes flow [21,32,33]. A quadratic triangular mesh is used in [33] to discretize the membrane and the force is averaged over an element in the boundary integral. This method was plagued by numerical instabilities for high and low dimensionless shear rates due to the degradation of the grid. In [21], the boundary-element method is used in conjunction with surface interpolation by means of bi-cubic B-splines which allows accurate evaluation of high-order derivatives of the geometric quantities of the surface such as curvature. Recently, Kessler et al. [18] proposed a global spectral method in which the shape of the capsule is expanded into a set of smooth basis functions for Stokes flow. This method has the advantages that the resulting capsule shape is globally smooth and the derivatives of the basis functions are analytically known, which reduces the discretization error, especially in high-order derivatives such as the curvature. As an alternative to the boundary-element method, the immersed boundary (IB) method [30] has been employed to solve for the deformation of the elastic capsules in shear flow [13,24]. In addition, the immersed boundary method was also used with the lattice Boltzmann method (LBM) [43] to improve the efficiency by using multi-block-strategy. Recently, an implicit immersed boundary method has been proposed in [23] to improve the time step in advancing the location of the membrane with large elastic modulus. The implicit method has proven to be an efficient method in dealing with multiple liquid capsules in the flow.

In the present paper, we extent our implicit immersed boundary method [23] for simulating the deformation of liquid capsules immersed in the fluid. In [23], the zero-thickness shell model [33] was used for computing the forces generated on the membrane surface during deformation. As in [33], the implicit IB method also suffers from numerical instabilities for high and low deformations due to the grid degradation which leads to limit the extent of the simulation. In order to improve the simulation time, we employ the thin-shell model presented in [8,9] for computing stress and moment resultants. We note that in the present work, the liquid capsule is enclosed by a thin shell with finite thickness that exhibits bending resistance and the mechanism for generating the bending moments is different from that in [32]. Here, stresses developing over the cross-section of shells are integrated over the thickness to yield the stress resultants and tangential bending moments. In [8,9], the thin-shell model was proposed to compute the displacements of the shell nodal points on a subdivision surface with given loads. Here, we employed this thin-shell model to compute the stress and moment resultants with the known displacements on a quadratic triangular mesh. We also suggest a way to compute the total forces generated on each element and at each node of the mesh during the deformation.

Our goal in this work is twofold. First, we proposed a method for calculating the forces generated on the capsule surface by employing the thin-shell model [8,9] for studying non-linear deformation of liquid capsule enclosed by thin shell. Second, we investigate large deformations of capsules with various unstressed shapes. We also study different motions of non-spherical capsules such as tank-treading, tumbling and transition from tank-treading to tumbling under a broad range of dimensionless shear rate and viscosity ratio.

The remainder of this paper is organized as follow. In Section 2, we describe the governing equations for the fluid flow and introduce the shell kinematics relevant to large deformations. We begin with constitutive models and the weak form of static equilibrium equations for Kirchhoff–Love shell theory. In Section 3, we briefly summarize the immersed boundary algorithm, the spatial discretization of the thin shell and the method for advancing the membrane evolution in time. In Section 4, some numerical examples are presented to demonstrate the performance of the method and finally, some conclusions are given in Section 5.

2. Formulation

2.1. Governing equations

In a three-dimensional bounded fluid domain Ω_F that contains an enclosed thin shell $\Omega_S(t)$, we consider the incompressible Navier–Stokes equations formulated in primitive variables, written as

$$\rho(\boldsymbol{u}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}) = -\nabla p + \nabla\cdot(\mu[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T]) + \boldsymbol{f}, \tag{1}$$

$$\nabla\cdot\boldsymbol{u} = 0, \tag{2}$$