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Modeling the motion of capsules in flow

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ABSTRACT

This review presents the mechanical behavior of a capsule under the influence of viscous deforming forces due to a flowing fluid. We focus on artificial capsules that are initially spherical with an internal liquid core and that are enclosed by a very thin hyperelastic membrane with different constitutive laws. The recent modeling strategies are outlined together with their respective advantages and limitations. We then consider the motion and deformation of a single initially spherical capsule freely suspended in a simple shear or plane hyperbolic flow and discuss the effect of the membrane constitutive law, of initial pre-stress and of membrane buckling under compression. We then consider the flow of spherical capsules in small pores and show how it can be used to evaluate the mechanical properties of the membrane.

1. Introduction

Encapsulation consists of enclosing some internal medium with a semi-permeable membrane that controls exchanges between the environment and the internal contents. Dispersion or degradation of the capsule contents are thus avoided and release of the capsule contents can be controlled.

Capsules are found in nature in the form of cells, bacteria, seeds or eggs. For instance, red blood cells can be considered as a prototypical example of passive natural capsules that perfom very complex functions. While protecting hemoglobin and maintaining a high local concentration, they allow fixation and release of oxygen and carbon dioxide through the cell membrane. In addition the membrane mechanical properties allow the red cell to withstand the hydrodynamic stresses prevalent either in the arteries or in the microcirculation, without breaking.

Artificial capsules are widely used in many industries such as pharmaceutical, cosmetic, food industries for controlled release of active principles, aromas or flavors. They are also used for bioengineering applications like drug targeting or encapsulated cell culture for artificial organs. The release can either be sudden by breaking, or continuous by diffusion to ensure a regular effect of the therapeutic active substance.

Artificial capsules can be obtained through interfacial polymerization of a liquid droplet. The process thus leads to approximately spherical particles enclosed by a thin polymerized membrane with mechanical properties that depend on the fabrication procedure. For biological applications, the typical membranes that are used are natural or synthetic polymers such as poly-L-lysine, alginate or polyacrylates [28]. Other procedures consist of encapsulating a liquid droplet with an adsorbed layer of proteins that confers visco-elastic properties to the interface [18] or with successive layers of poly-electrolytes [20]. Phospholipid vesicles are enclosed by a bi-layer membrane with constant area, negligible resistance to shearing and a small bending resistance. They can thus take different geometrical shapes at low energy cost, provided their initial shape is not spherical. Conversely, artificial capsule deformation is achieved through stretching of the membrane and costs elastic energy. Cells such as red blood cells are intermediate between capsules and vesicles: their initial shape is not spherical and their membrane is area inextensible, but also has elastic properties due to a protein cytoskeleton on the hemoglobin side.

In this review, we consider only capsules with liquid internal contents, designed to be used in suspension in another liquid. We exclude capsules with a gelled core commonly used for vectorization or cell encapsulation. We focus on initially spherical artificial capsules enclosed by a polymer membrane and leave aside the closely related topic of lipid vesicles (the interested reader is referred to the recent comprehensive review on the mechanics of an isolated vesicle and the collective effects in a suspension of such particles [60]).

Within this framework, the main intrinsic physical properties of such capsules are:

- the radius a of the capsule;
- the rheology of the internal contents, which is usually considered to be a Newtonian liquid;
- the mechanical properties of the enclosing membrane.

The size of artificial and natural capsules varies from a few microns to a few millimeters. Although essential, their physical properties are quite difficult to evaluate owing to their smallness and fragility. Geometry is

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determined through microscopy. The internal content is usually well defined and its properties can be measured independently. The main challenge is the assessment of the membrane properties. Different methods have been proposed that are all based on the measurement of the capsule deformation under a well defined stress such as, viscous shear [9,10,61,62], centrifugal spinning forces [24,44] or compression between two plates [7,20]. However, since the capsule membrane is usually very deformable, the analysis of the experimental data necessitates sophisticated continuum mechanics models that account for the large deformation of an elastic shell under a given load (when the membrane is rigid, the capsule can be treated as a solid particle, which simplifies the dynamics).

In most situations, capsules are suspended into another liquid and are thus subjected to hydrodynamic forces when the suspension is flowing. The motion of the suspending and internal liquids creates viscous tractions on the membrane and may lead to capsule break-up. The control of this process is of course essential for the design of artificial capsules or for the protection of natural capsules but is difficult to achieve unless we have models of the underlying mechanics. For example the encapsulation of hemoglobin for artificial blood has been an active research topic for many years. The experiments have shown that the artificial blood cells could be damaged in the circulation, and that this damage was directly related to the shape and deformability of particles [38]. Artificial blood is an example that illustrates the importance of the control of capsule rupture in flow. This requires understanding the mechanical behavior of the objects used for encapsulation, which is often complex. Good, accurate mechanical models are thus needed to help design and optimize capsules.

Modeling the mechanical behavior of a capsule, under the influence of viscous deforming forces due to a flowing fluid is a very difficult problem of continuum mechanics that involves strong fluid–structure interactions where the internal and external flows are dominated by viscous and pressure forces and where the interface is a thin solid shell undergoing large deformations. This complex problem has been studied for many years, starting in the early 1980s with asymptotic solutions valid for initially spherical capsules undergoing small deformation and enclosed by a hyperelastic [4] or linearly visco-elastic membrane [5]. These solutions are still used either to validate numerical models or to analyze data, when applicable. Recent years have seen the development of numerical models that allow to consider different flow situations that are not accessible to analytical solutions. The advantage of such models is that they compute quantities that cannot be measured such as the stress level in the membrane. They can also be used to perform an inverse analysis of experimental data on flowing capsules and lead to an evaluation of the membrane mechanical properties.

The aim of the paper is to review the recent progress in capsule modeling under flow and to discuss the limits of the results that are thus obtained.

We focus on initially spherical artificial capsules with an internal liquid core, enclosed by a very thin hyperelastic membrane. The mechanical properties of the membrane are essential in determining the motion and deformation of the capsule. We thus first present different constitutive laws that are commonly used to describe the rheological behavior of thin membranes. The recent modeling strategies are then briefly outlined together with their respective advantages and limitations. We then consider the motion and deformation of a single initially spherical capsule freely suspended in a linear flow and discuss the effect of the membrane constitutive law and of initial pre-stress. We end with the flow of spherical capsules in small pores and show how it can be used to measure the mechanical properties of the membrane.

2. Mechanics of a flowing capsule

The equations and hypotheses for describing the flow of a capsule are now well established. For the sake of simplicity, we first consider the case where a single capsule is freely suspended in an unbounded shear flow. The effect of confinement by solid boundaries will be outlined in section 5.

2.1. Flow of the internal and external liquids

A capsule is freely suspended in an unbounded stationary shear flow with far field velocity $\mathbf{v}^\infty(\mathbf{x})$ and characteristic velocity V^∞ (Fig. 1). We use a reference frame linked to the external fluid at infinity and centred on the capsule centre of mass. It is assumed that the capsule is enclosed by an infinitely thin membrane that can be treated as an elastic surface denoted $S(t)$ at time t. The initial position of the capsule membrane points $\mathbf{X}$ and the membrane geometry are known. At time t, the displaced position of the capsule membrane points is $\mathbf{x}(\mathbf{X}, t)$ on $S(t)$. The capsule volume remains constant during flow, i.e. the time scale of mass transfer across the membrane is much larger than the convection time. The internal (superscript 1) and external (superscript 2) liquids are Newtonian and have equal density ρ, thus excluding buoyancy forces and sedimentation effects. Because the capsule is usually very small, the flow Reynolds number based on the capsule dimension is small $\rho V^\infty a/\mu^{(2)} \ll 1$, so that the motion of the internal and external liquids is inertialess and results from the instantaneous equilibrium between viscous and pressure forces. This leads to the Stokes equations:

$$-\nabla p^{(\alpha)} + \mu^{(\alpha)}\nabla^2 \mathbf{v}^{(\alpha)} = 0, \quad \nabla\cdot\mathbf{v}^{(\alpha)} = 0, \quad \alpha = 1, 2. \tag{1}$$

If the Reynolds number is not negligible, the flow inertia $\rho d\mathbf{v}^{(\alpha)}/dt$ must be added to the right-hand-side of the equation of motion, leading to the Navier–Stokes equations. The boundary conditions are:

- vanishing flow perturbation far from the capsule:

$$\mathbf{v}^{(2)}(\mathbf{x}) \to \mathbf{v}^\infty \quad \text{as} \quad |\mathbf{x}| \to \infty; \tag{2}$$

- continuity of velocity on the capsule membrane:

$$\mathbf{v}^{(1)}(\mathbf{x}, t) = \mathbf{v}^{(2)}(\mathbf{x}, t) = \mathbf{v}^{(m)}(\mathbf{x}, t) = \partial\mathbf{x}(\mathbf{X}, t)/\partial t \quad \text{as} \quad \mathbf{x} \in S(t), \tag{3}$$

where $\mathbf{v}^{(m)}(\mathbf{x}, t) = \partial\mathbf{x}(\mathbf{X}, t)/\partial t$ is the velocity of the membrane point that was at position $\mathbf{X}$ in the reference state;
- dynamic equilibrium between the viscous forces exerted by the flow of the two liquids on the interface and the elastic forces due to the deformation of the membrane:

$$[\sigma^{(2)}(\mathbf{x}) - \sigma^{(1)}(\mathbf{x})]\cdot\mathbf{n} + \mathbf{f} = 0 \quad \text{as} \quad \mathbf{x} \in S(t), \tag{4}$$

where $\mathbf{f}$ is the elastic force per unit area of deformed membrane that is exerted by the membrane on the fluids, $\sigma^{(\alpha)}$ denotes the stress tensor in liquid (α), $\mathbf{n}$ is the outward unit normal vector to $S(t)$.

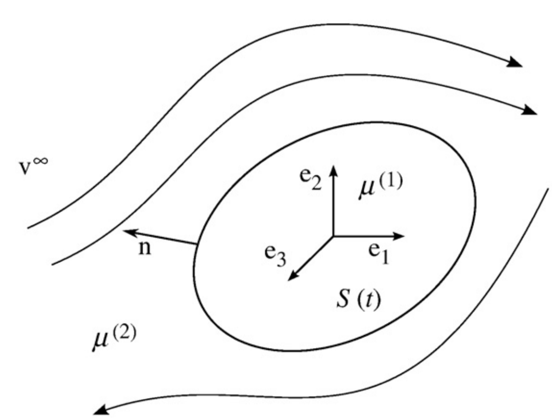

Fig. 1. Schematics of an isolated capsule freely suspended in a simple shear flow.