REORIENTATION OF A NON-SPHERICAL MICRO-CAPSULE IN SHEAR FLOW

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Summary Dynamics of a capsule and a biological cell is of great interest in chemical engineering and bioengineering. Although dynamics of a rigid spheroid is well understood by Jeffery's theory, that of spheroidal capsule remains unclear. In this study, motion of a spheroidal capsule or a red blood cell in creeping shear flow is investigated. The results show that the orientation of a non-spherical capsule is variant under time-reversal, though that of a rigid spheroid is invariant. Surprisingly, the alignment of a non-spherical capsule over long time duration shows transition depending on the shear rate, which can be utilized for a particle alignment technique.

INTRODUCTION

About a century ago, Jeffery analytically derived the motion of a non-spherical object in creeping linear background flow [1]. Since then, Jeffery's theory has been used to describe the alignment of rods and ellipsoids, such as carbon nanotubes, liquid crystal, bacteria and platelets. The theory states that the trajectory of a non-Brownian rigid ellipsoid in Stokes flow is invariant under time reversal and that reorientation over long time duration does not occur under simple shear flow conditions. The time reversibility can be destroyed by introducing inertia effects or visco-elastic properties of the surrounding fluid, because the motion is no longer independent of time in these cases. However, the effect of particle deformability on the time reversibility is not well clarified. This study investigates this question using a capsule as a model deformable object.

A capsule is a liquid drop enclosed by a deformable membrane, which is of great interest in the chemical engineering, bioengineering, and food industries. Many capsules in realistic situations are not perfect spheres because of the inhomogeneity of the membrane properties or folding due to unbalanced osmotic pressure. If one places a non-spherical capsule in creeping shear flow, how does the orientation change relative to the flow field over long time duration? Jeffery speculated that an ellipsoid may alter its orientation so that the viscous energy dissipation of the system becomes minimal. However, this may not be true for a capsule with large deformation. Although many former studies have examined the dynamics of a non-spherical capsule, none of them can answer this question. In this study, the motion of a non-Brownian spheroidal capsule or a red blood cell (RBC) in creeping shear flow is investigated numerically.

MODELS & NUMERICAL METHODS

A capsule is assumed to be filled with an incompressible Newtonian fluid of viscosity $\lambda\mu$ and freely suspended in another fluid with the same density but viscosity μ. When the thickness of the capsule wall is small compared to its size and radius of curvature, the membrane can be modelled as a 2D hyper-elastic surface without bending rigidity. In this study, we use two kinds of constitutive laws for the membrane: the neo-Hookean (NH) law and the Skalak (SK) law. The NH law describes isotropic volume-incompressible rubber-like material properties, whereas the Skalak law expresses the area incompressibility of a biological membrane.

To calculate capsule deformation accurately, fluid-structure interactions between the motion of the internal and external fluids and that of the capsule membrane have to be solved precisely. We assume that the flow is Stokesian, i.e., inertia free, and the flow field is solved by a boundary element method. A finite element method is employed to solve the membrane mechanics. Because the governing equations and numerical methods have already been described in detail in [2,3], they are explained only briefly here. Let the position of material points on the membrane be given at time t. The membrane deformation is calculated from the position by comparison with its reference, and the tension on the membrane can be derived from the constitutive laws. The weak-form local equilibrium equation of the membrane is solved by a finite element method to determine the viscous load on the membrane. Then, the velocity at the material point is calculated from a boundary integral equation of Stokes flow using a boundary element method. Finally, the material point is updated by a second-order Runge-Kutta time-marching method, and the process is repeated. The reference shape of the capsule is assumed to be spheroid or biconcave. The aspect ratio between the principal axes of the spheroid is represented by α. A linear triangular mesh with 5120 elements is used to discretize the membrane. The accuracy of the method was validated for small deformations by comparing with the analytical asymptotic solution, as well as for large deformations by comparing with former numerical and experimental studies.

The motion of a capsule in simple shear flow is simulated, where x is the flow direction, y is the velocity gradient direction, and z is the vorticity direction. The capillary number Ca represents the ratio of the viscous force to the elastic force and is given by $\mathrm{Ca} = \mu\gamma R/ G_s$, where G_s is the membrane shear modulus, γ is the shear rate, and R is the radius of a sphere that has the same volume as the ellipsoid or the biconcave capsule.

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RESULTS

We first investigate the motion of a spheroidal oblate capsule in simple shear flow and compare the results with those of a rigid spheroid. To examine the capsule orientation efficiently, we define the orientation vector **e** as a unit vector extending from the centre of gravity and pointing to material point P located at the revolution axis of the unstressed spheroidal capsule. θ is defined as the angle between **e** and the vorticity axis of the background shear. At time $t = 0$, the oblate capsule without pre-stress is placed at an initial angle θ_0 of π/4. The deformation at time $t > 0$ due to the background shear is calculated until the steady periodic motion is achieved.

The motions of an oblate capsule with Ca = 0.3 and 1.0 are shown in Fig.1(a) and (b), respectively (α = 0.6, λ = 1, and NH membrane). The time history of θ is also shown in Fig.1(c) for 30 periods of rotation. The results of a rigid spheroidal with the same α are also plotted in the figure for comparison. Due to the non-spherical reference shape of the capsule membrane, θ oscillates two times during one rotation. In addition to the short-time oscillation, θ tends to approach towards 0 or π/2, depending on Ca, over a long time duration. The reorientation of the capsules is also clear in observing Fig.1(a) and (b), because the material point P, which is indicated as a blue dot in the figures, moves towards $z = 0$ when Ca = 0.3, whereas it moves towards the z-axis when Ca = 1.0. We note that the final orientation is independent of the initial orientation; this was confirmed numerically by changing the initial orientation randomly. Such reorientation did not happen for a rigid spheroid, as shown in Fig.1(c). These results clearly illustrate that a deformable capsule becomes reoriented, even in simple shear flow, and the time reversibility of Jeffery's orbit can be destroyed by introducing particle deformability.

Finally, we investigate the reorientation of an RBC in shear flow. The RBC membrane is modeled by SK law, and the effect of λ is considered. When Ca is large, the material point P of the RBC again shifts to the z-axis, i.e. θ = 0. In this case, the RBC membrane have a pure tank-treading motion, and the membrane does not oscillate during the rotation. Such a pure tank-treading motion was experimentally observed under high Ca conditions.

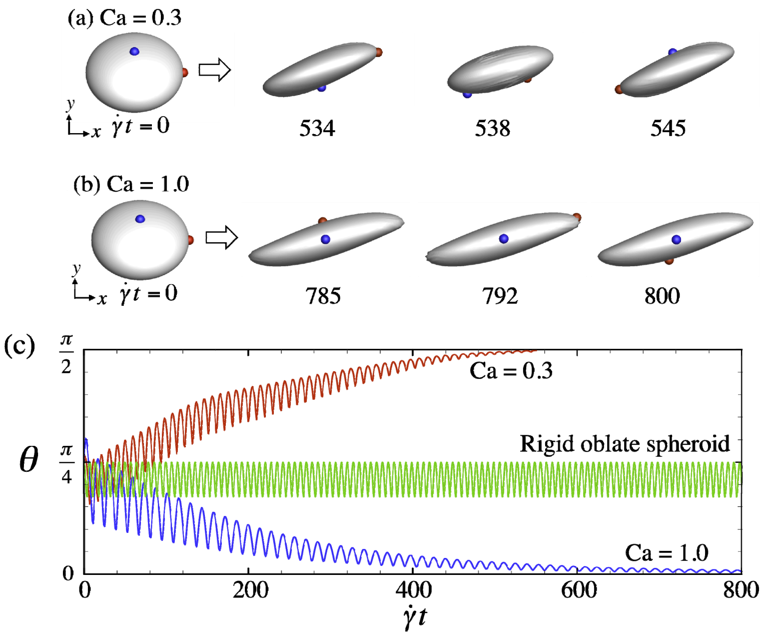

Fig.1 Oblate capsule in a simple shear flow with (a) Ca = 0.3 and (b) 1.0 (α = 0.6, λ = 1, and NH membrane). Blue and red dots are material points on the membrane, and are plotted as tracers. (c) Time change of θ, where the result of a rigid spheroid with same α is also plotted for comparison.

CONCLUSIONS

The results show that the orientation of a non-spherical capsule is variant under time reversal, although the orientation of a rigid ellipsoid is invariant. Surprisingly, the alignment of a non-spherical capsule over long time duration shows transition depending on the shear rate. The transition cannot be explained by the minimum energy dissipation, as speculated by Jeffery; the full fluid and solid mechanics are necessary to understand this phenomenon. The obtained results can be utilized for particle-alignment techniques in engineering applications and shed light on the complex dynamics of capsules and biological cells.

References

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