BRIEF COMMUNICATIONS

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Transitions in rotations of a nonspherical particle in a three-dimensional moderate Reynolds number Couette flow

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The rotational states of three-dimensional nonspherical particles including cylindrical and disk-shaped, as well as prolate and oblate, ellipsoidal in a Couette flow are studied by using a lattice Boltzmann simulation. We discover that rotation of a nonspherical particle exhibits several different states, depending on the ranges of the particle Reynolds numbers and the geometric shape of the particle. As the Reynolds number increases, the rotation transits from one state to another state. [DOI: 10.1063/1.1517053]

Jeffery studied a single ellipsoid in a simple shear flow by ignoring the inertial effect of the particle.[1] He concluded that the final state of a spheroid depended on its initial orientation and possesses the minimum energy dissipation. Taylor was the first to experimentally validate Jeffery's hypothesis for a prolate and oblate ellipsoid in a creeping Couette flow in a qualitative manner.[2] Later, Karnis *et al.*[3] conclusively showed by experiment with the maximum Reynolds number about 10^{-3}, in contrary to Jeffery's theory, that the inertial effect brings nonspherical particles to a final rotation orbit in which an ellipsoidal particle rotates with its long body perpendicular to the vorticity vector of flow. The theoretical work of Harper and Chang[4,5] qualitatively confirmed the experimental observation of Karnis *et al.* for a neutrally buoyant dumbbell in a linear shear flow. However, Harper and Chang's analysis is only valid for the Reynolds number less than 1, thus cannot be applied to large Reynolds number cases. Some analysis and simulations at zero Reynolds number[6,7] were reported. The most recent numerical and experimental[8–10] work for a single nonspherical particulate suspension at moderate Reynolds numbers are two-dimensional in nature, because one of the rotational axes is fixed in space. Therefore, rotational behavior in a large Reynolds number in a three-dimensional couette flow is unknown.

This Brief Communication summarizes our recent work on simulations of the dynamic rotational behavior of a nonspherical particulate suspension of various geometric shapes in a Couette flow with the Reynolds number up to 467. We use the lattice Boltzmann equation (LBE)[11–15] for the fluid part and the six-dimensional equations of motion for the particle.[16–19] The particle is allowed to rotate and translate freely without any restrains. The LBE model used in the present work is a 15-velocity lattice BGK model[12–14] in three dimensions.

We use (x,y,z) and (x',y',z') to represent the space-fixed and body-fixed coordinate system, respectively. Angle θ is the polar angle between the vorticity vector (z-axis) of the flow and the symmetric axis of revolution (z') of the particle, and ϕ is the angle between the xz plane and the $x'z$ plane if the body-fixed coordinate system is initially overlapped with the space-fixed coordinate system. The computational domain size $N_x \times N_y \times N_z$ ranges from 64^3 to 128^3 in the simulations. We only consider particles with the symmetry of revolution. The rotational motion is affected by both the confinement ratio $r_1 = N_z/c$ and the aspect ratio $r_2 = c/a$, where c and a are the length of the semi-axis and the radius of revolution, respectively. In this work, we keep the confinement ratio $r_1 = 4$ and aspect ratio $r_2 = 2$. The effects of these ratios on the rotational motion shall be reported elsewhere. Two walls are placed at $x=0$ and $x = N_x + 1$, respectively. The shear is imposed by moving the two walls with opposite velocities, $(0,U,0)$ and $(0,-U,0)$. Periodic boundary conditions are imposed in the y- and z-directions. The particle Reynolds number is defined by $R = 4Gc^2/\nu$, where the shear rate $G = 2U/N_z$ and ν is the fluid kinematic viscosity.

We conducted a number of simulations with different nonspherical particle shapes to fully investigate the rotational motion of a nonspherical suspension in the Couette flow. We discover that the rotational motion of a nonspherical particle has several different states depending on the ranges of the particle Reynolds number and the particle shape. As the Reynolds number increases, the rotational motion of a nonspherical particle sharply transits from one state to another.

We first report the results of an prolate ellipsoid with the revolution symmetry, i.e., with two equal short semi-axes $a = b$, and $c = 2a$. We find three final rotational states corresponding to different ranges of the Reynolds numbers between 0 and 467. The first state corresponds to a low Reynolds range $0 < R < 205$. In this low Reynolds number state, the particle rotates about its short symmetric axis that is parallel to the flow vorticity vector periodically and the long axis of the particle is always perpendicular to the flow vorticity vector. We call this first state "tumbling." The prolate ellipsoid is rotating stably within a shearing plane (parallel to xy plane). The shearing plan is an orientational attractor. The word "tumbling" was first used by polymer scientists to describe the orientational states of rodlike molecules in liquid-crystalline polymers.[20] Several states such as tumbling, wagging, flow aligning, log-rolling, and kayaking were identified in the polymers and these states depend on initial orientation, shear rates, the strength of the nematic interactions as well as Brownian motions. The similar phenomena "tumbling" and "log-rolling" are found in this work and will be reported shortly although the physical origin is entirely different from that of polymeric nematics.

Figure 1(a) shows the evolution of the directional cosines $(s_1, s_2, s_3) = (\cos\beta, \cos\gamma, \cos\theta)$ at $R = 32$,[21] which is typical in the low Reynolds number range, where β, γ, and θ are the angles between z'-axis and x-, y-, and z-axis, respectively. If the initial orientation of the particle differs from the final state, it is unstable and thus quickly enters to the final state of $\theta = 90°$. In the low Reynolds range, when the ellipsoid reaches the final rotational state, ω_z is a periodic function in time.

As the Reynolds number continuously increases to the second range, approximately $205 < R < 345$, the rotational behavior of the prolate ellipsoid undergoes a sharp transition. At its final state the prolate spheroid precesses about the vorticity with a nutational motion. In other words, the end of the revolution axis of the prolate spheroid describes a spherical ellipse with its major axis at $\phi = 90°$ and minor axis at $\phi = 0°$. θ has a minimum value θ_1 at $\phi = 0°$ and $\phi = 180°$ and a maximum θ_2 at $\phi = 90°$ and $\phi = 270°$. We call this state "precessing and nutating." As the Reynolds number increases in the range, the mean value of θ monotonically decreases. Obviously, unlike the first state, the particle angular velocity vector of the second state is neither parallel nor perpendicular to z-axis. In this state, angular velocity is periodic in time.

When the Reynolds number passes beyond 345 approximately, the rotational motion of the particle undergoes another sharp transition. In the high Reynolds number range $R > 345$, the prolate ellipsoid in its final state rotates about its long symmetric axis parallel to the flow vorticity vector, i.e., $\theta = 0°$, with a constant angular velocity. We call this state "log-rolling." It looks like logs rolling on a river. Figure 1(b) shows the directional cosines at $R = 350$. The angular velocity in this "log-rolling" case is $(\omega_x, \omega_y, \omega_z) = (0, 0, 0.385)$. It appears that the vorticity direction is a stable orbit attractor.

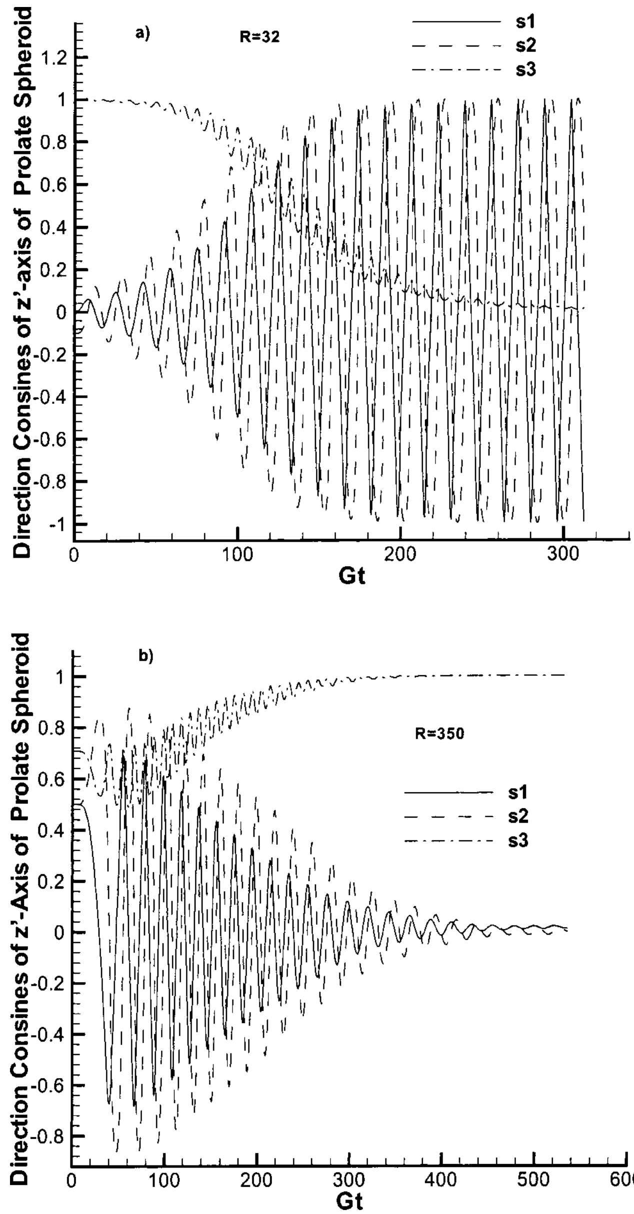

FIG. 1. The directional cosines $(s1, s2, s3)$ of the z'-axis of the prolate spheroid against time (a) at $R = 32$, (b) $R = 350$.

Aidun, Lu, and Ding (1998) and Ding and Aidun (2000) reported that when the Reynolds number increased to a critical value, the ellipsoid rotation was stopped at a critical Reynolds number R_c due to the effects of streamline separation that generated a negative torque on the nonspherical particles. The critical Reynolds number in Ding and Aidun's work (2000) was $R_c = 81$ for a 3D oblate ellipsoid and $R_c = 29$ for 2D elliptical particle. Their numerical results are in good agreement with Zettner and Yoda's experimental results in a two-dimension space. However, our simulations show that as the Reynolds number increases rotation may transit from one state to other but is never stopped. The difference lays on that our simulations are in a 3D space while the simulations of Aidun *et al.* were in a 2D space due to a

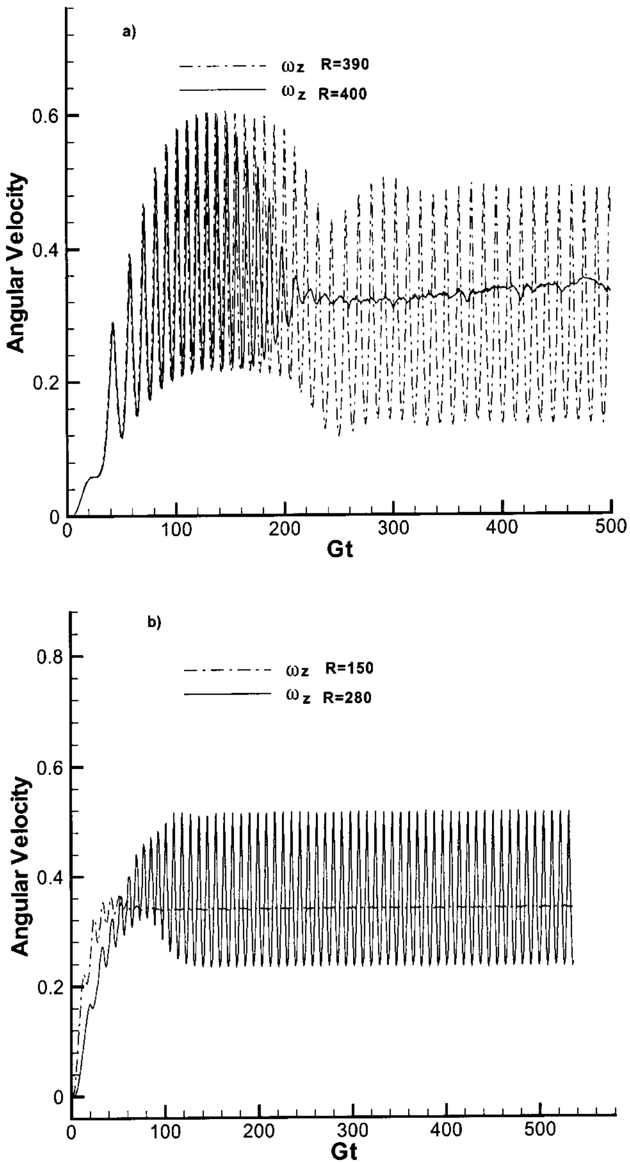

FIG. 2. ω_z against time (Gt) (a) for a cylinder at $R=390$ and $R=400$ and (b) for a disk-shaped particle at $R=150$ and $R=280$.

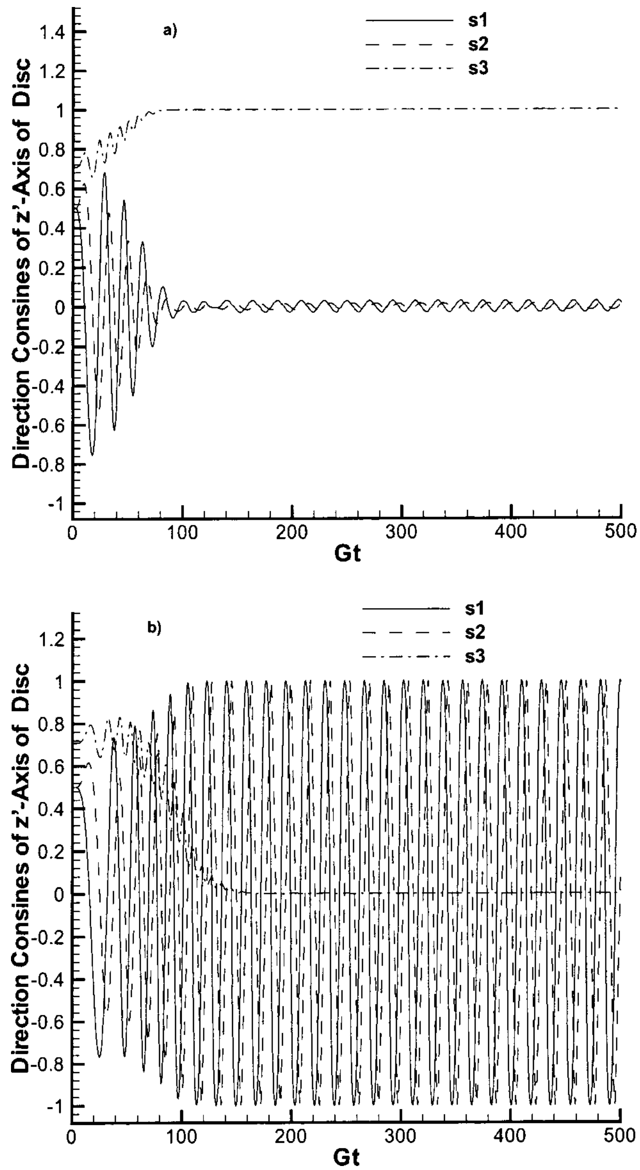

FIG. 3. The directional cosines $(s1,s2,s3)$ of the z'-axis of the disk-shaped particle as a function of time at (a) $R=150$ and (b) $R=280$.

particle's axis fixed in an unstable orbit direction.

We have repeated simulations for a cylindrical particle with the aspect ratio $r_2=l/d=2$, l and d being the length and the diameter of the cylinder, respectively. For this cylindrical particle, we only find one transition point in the Reynolds number, approximately equal to 395, in the interval of $0<R<467$, as opposed to two transition points for the prolate ellipsoid with the same aspect ratio r_2. The two states below and above the transition Reynolds number correspond to "tumbling" ($\theta=90°$) and "log-rolling" ($\theta=0°$), respectively. That is, there exists no intermediate state of "precessing and nutating" ($0°<\theta<90°$). Figure 2(a) shows the angular velocity component ω_z ($\omega_x=\omega_y=0$) as a function of time at $R=390$ and 400, corresponding to two states before and after the transition, respectively.

A cylinder has two flat ends of circles sharply connected by a cylindrical surface while the prolate spheroid has one smoothly curved surface. The different shapes cause the different flow patterns and, in turn, lead to that a cylinder lacks "precessing and nutating" state.

We have also had simulations for a disk-shaped particle, with $r_2=l/d=1/2$. There is only one transition point at $R\approx230$. When $R<230$ the disk-shaped particle is "rolling" about the short symmetric axis (which happens to be z'-axis) parallel to the flow vorticity ($\theta=0°$) vector. When $R>230$, it is "tumbling" about the diameter of the disk (i.e., $\theta=90°$) periodically. The results for the disk-shaped particle at $R=150$ and $R=280$ are shown in Fig. 2(b) for the angular velocity and in Fig. 3 for the orientation. Unlike the cylinder, the disk-shaped particle transfers from a "rolling" to a "tumbling" state at $R=230$.

The transition mechanism in the rotational motion is due to the changes in flow pattern. At the low Reynolds numbers, the particle is rotating about its short symmetric axis parallel to the flow vorticity and the long body is perpendicular to the vorticity vector. Torques exerted on the particle by shearing would bring the long body tumbling along flow direction.

This rotating orbit is stable and the shearing plane is an attractor. However, when the Reynolds number increases, the recirculating flow[8] near the particle in the channel center increases dramatically and the instability of flow turbulence due to the stream line separation would repel the particle in the shearing plane to align particle's long axis with the flow vorticity direction. Therefore vorticity axis becomes a stable orbit attractor at the higher Reynolds number.

We have also tested an oblate ellipsoid with $r_2 = c/a = 1/2$. The oblate ellipsoid is ''rolling'' about its short symmetric axis parallel to the flow vorticity vector at the low Reynolds number range and ''inclined rolling'' in an intermediate Reynolds number range. The only difference between ''rolling'' and ''inclined rolling'' is that $\theta = 0°$ for ''rolling'' while $\theta > 0°$ for ''inclined rolling.'' The ''tumbling'' state is not observed for the reason that the Reynolds number is not high enough.

In conclusions, we have discovered some common characteristics describing the final states of the rotational motion for a nonspherical particle suspension in the Couette flow. There are several rotational states depending on the range of the Reynolds numbers and particle shapes. The rotational state undergoes sharp transitions as the Reynolds number changes. When the Reynolds number is small before any transition can take place, the particle at final state always rotates about its shortest symmetric axis parallel to the flow vorticity vector and with its long body perpendicular to the vorticity vector. In this case the shearing plane is a stable rotational orbit attractor. When the Reynolds number is sufficiently large, the particle always rotates about its longest symmetric axis which is parallel to the flow vorticity vector. The vorticity direction is a table orbit attractor. In fact, a cylinder transfers from a ''tumbling'' to ''log-rolling'' state while a disk-shaped particle transfers from a ''rolling'' to a ''tumbling'' state as the Reynolds number increases. For the smooth nonspherical particle such as a prolate ellipsoid, there exists an intermediate state (''precessing and nutating'') between the above two states. In this intermediate state, the prolate ellipsoid rotates periodically with the end of long axis tracing a spherical ellipse. The particle with sharp edges such as cylinder does not have the intermediate state.

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