Swinging and Tumbling of Fluid Vesicles in Shear Flow

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(Dated: March 23, 2022)

The dynamics of fluid vesicles in simple shear flow is studied using mesoscale simulations of dynamically-triangulated surfaces, as well as a theoretical approach based on two variables, a shape parameter and the inclination angle, which has no adjustable parameters. We show that between the well-known tank-treading and tumbling states, a new “swinging” state can appear. We predict the dynamic phase diagram as a function of the shear rate, the viscosities of the membrane and the internal fluid, and the reduced vesicle volume. Our results agree well with recent experiments.

PACS numbers: 87.16.Dg,83.50.-v,87.17.Aa

The dynamics of deformable objects such as liquid droplets \cite{1,2}, lipid vesicles \cite{3,4,5,6,7,8,9,10}, red blood cells \cite{11,12,13,14}, and elastic capsules \cite{15,16,17} in flows has received increasing attention experimentally, theoretically, and numerically in recent years. All of these objects show phenomenologically similar behaviors in shear flows — either a tank-treading rotation with a stationary shape and a finite inclination angle \(\theta > 0\) with respect to the flow direction, or an unsteady tumbling motion. However, the qualitative and quantitative behavior of the various objects can be very different, because the energies governing their shapes and thermal fluctuations are very different. In the case of fluid vesicles, which we want to investigate in this letter, the membrane deformations are determined by the curvature elasticity together with the constraints of membrane incompressibility and constant internal volume.

In simple shear flows, with flow velocity \(v = \dot{\gamma} y e_x\), a transition occurs from tank-treading to tumbling with an increasing viscosity of the internal fluid \(\eta_m\) \cite{4,8,12} or membrane viscosity \(\eta_{mb}\) \cite{9,10}. This transition is described very well by the theory of Keller and Skalak (K-S) \cite{12}, which assumes a fixed ellipsoidal vesicle shape. However, shear forces can be large enough to induce shape transformations of fluid vesicles, for example from discocyte to prolate at small membrane viscosity and small viscosity contrast between inside and outside, or from prolate to discocyte at larger membrane viscosities \cite{13,10}. In this case, it is essential to take the membrane deformability into account.

Recently, Kantsler and Steinberg \cite{4} reported the first observation of a new type of vesicle dynamics in shear flow, which is characterized by small oscillations of the inclination angle \(\theta\) and the deformation, where \(-\theta_0 \lesssim \theta(t) \lesssim \theta_0\) with \(\theta_0/\pi < 1\) and time average \(\langle \theta \rangle \approx 0\). The vesicles were found to transit from tumbling to this oscillatory motion with increasing shear rate \(\dot{\gamma}\). It is worth mentioning that such an oscillatory motion was also observed in our previous simulations (see Fig. 6 in Ref. \cite{10}), but not further analyzed. Simultaneously with the experiment, Misbah \cite{6} predicted a “vacillating breathing” mode for quasi-spherical fluid vesicles. This mode exhibits very similar dynamical behavior as seen experimentally; however, it “coexists” with the tumbling mode, and its orbit depends on the initial deformation i.e. it is not a limit cycle. Furthermore, the shear rate only enters the theory as the basic time scale, and therefore cannot induce any shape transitions. Hence it does not explain the tumbling-to-oscillatory transition seen in the experiments \cite{4}.

In this letter, we study the oscillatory dynamics of fluid vesicles, which we will refer to as the “swinging mode”, by mesoscale hydrodynamics simulations and a simplified non-linear theoretical model. The main questions we want to address are: How does the bending energy affect the dynamics? Can transitions between modes be induced by varying the shear rate? What happens beyond the quasi-spherical limit, which is the typical experimental situation? What is the effect of the membrane viscosity? Is the swinging mode stable when thermal membrane undulations are taken into account? We will show that the experiments of Ref. \cite{4} can be understood very well on the basis of our theory. Furthermore, we will present a complete phase diagram of vesicle motion as a function of shear rate and viscosity.

It is worth mentioning that elastic capsules \cite{15} and red blood cells \cite{18} can also exhibit a swinging mode; however, in this case, the angle \(\theta(t)\) is always positive during the oscillation. Very recently, this dynamics was explained by the K-S theory with an addition of an energy barrier for the tank-treading rotation caused by the membrane shear elasticity \cite{16}. Therefore, this mechanism cannot be employed to explain the swinging mode of fluid vesicles.

The vesicle dynamics is described by several dimensionless quantities. For a vesicle of volume \(V\) and surface area \(S\), the reduced volume \(V^* = (R_V/R_S)^3 = (1 + \Delta_S/4\pi)^{-3/2}\) and \(\Delta_S = S/R_S^2 - 4\pi\), where \(R_V = (3V/4\pi)^{1/3}\) and \(R_S = (S/4\pi)^{1/2}\). The relative viscosity of the inside fluid and membrane are \(\eta_m = \eta_m/\eta_0\) and \(\eta_{mb} = \eta_{mb}/\eta_0R_S\), where \(\eta_0\) is the viscosity of the outside fluid. The shape relaxation time of vesicles with bending rigidity \(\kappa\) is given by \(\tau = \eta_0 R_S^3/\kappa\) (for \(\eta_m = 1\)). This time is used to define
A reduced shear rate $\dot{\gamma}^* = \dot{\gamma}$.

The hydrodynamics of fluid vesicle can be studied very well by hybrid simulations of a dynamically-triangulated membrane model $^{19}$ and a particle-based mesoscale solvent, multi-particle collision dynamics $^{20}$. A detailed description of this method can be found in Ref. 10.

We have simulated a prolate vesicle with a viscous membrane at $V^* = 0.78$ and $\eta_{mb} = 1$. Figure 1 shows the time development of vesicle shape and $\theta$. The shape parameter is $\alpha_D = (L_1 - L_2)/(L_1 + L_2)$, where $L_1$ and $L_2$ are the maximum lengths in the direction of the eigenvectors of the gyration tensor in the vorticity ($x, y$) plane. The vesicle is found to exhibit a tumbling motion for $\dot{\gamma}^* = 0.92$, but a swinging motion for $\dot{\gamma}^* = 3.68$. As $\dot{\gamma}^*$ increases, the tumbling frequency $f_{tmb}$ decreases, see Fig. 2 while the frequency of the swinging motion increases. The shear rate $\dot{\gamma}^*$ at the tumbling-to-swinging transition is found to increase with increasing membrane viscosity $\eta_{mb}$. These results are consistent with the experiments of Ref. 2.

In order to obtain a better understanding of the vesicle dynamics, we now derive an approximate theoretical model. First, we follow Refs. 2, 3 and employ the Stokes approximation and perturbation theory for quasi-spherical vesicles. The vesicle shape is expanded in spherical harmonics $Y_{l,m}$ as $R = R_Y(1 + \sum_{l,m} u_{l,m} Y_{l,m})$. The free energy of the membrane with bending rigidity $\kappa$ and surface tension $\sigma$ is $F = \int dS \left[ \sigma + (\kappa/2)(C_1 + C_2)^2 \right]$, where $C_1$ and $C_2$ are the principal curvatures at each point of the membrane. With the harmonic approximation, it is given by $F = (\kappa/2) \sum_{l,m} E_l |u_{l,m}|^2 + O(|u_{l,m}|^4)$, where $E_l = ((l + 2)(l - 1)(l + 1) + \sigma R_Y^2/\kappa)$. The flow fields inside and outside of the vesicle are described by the Lamb solution, with no-slip boundary conditions on the membrane. The flow stress on the membrane is balanced with the elastic forces due to bending and tension. This implies that the undulation amplitudes $u_{l,m}$ are determined by

$$\frac{\partial u_{l,m}}{\partial t} = \frac{i\dot{\gamma}}{2} u_{l,m} - \frac{\kappa \Gamma_1 E_l}{2\eta_0 R_Y^2} u_{l,m} \mp i h \delta_{l,2} \delta_{m,\pm 2},$$

(1)

where $h = 60\sqrt{2\pi/15}/(32 + 2\eta_{mb}^* \sigma)$ and $\Gamma_1 = l(l+1)/(l+1)/(l+2)(l+2)$, $\delta_{l,2} = \exp(\mp 2i\theta)$, where $\theta$ corresponds to the inclination angle $\theta$. Since the curvature energy does not contribute in this case, compare Ref. 3 we have to go beyond the harmonic approximation. Therefore, we replace the force $\kappa \Gamma_1 r$ in Eq. (1) by $\partial F/\partial r$. This implies

$$\frac{\partial r}{\partial t} = -\frac{\Gamma_2}{2\eta_0 R_Y^2} \left( \frac{\partial F}{\partial r} - 2\lambda r \right) + \gamma h \sin(2\theta),$$

(2)

$$\frac{\partial \theta}{\partial t} = \frac{\dot{\gamma}}{2} (-1 + h \cos(2\theta)),$$

(3)

$$\frac{\partial u_{2,0}}{\partial t} = -\frac{\Gamma_2}{\eta_0 R_Y^2} \left( \frac{\partial F}{\partial u_{2,0}} + \lambda u_{2,0} \right).$$

(4)
A Lagrange multiplier \( \lambda \equiv \sigma R_0^2 \) is employed to satisfy the area constraint \([21]\); it is determined by \( d\Delta_S/dt = 0 \), which implies \( \Delta_S = 2u_{2,0} + 4r^2 \). Thus, Eq. (2) becomes

\[
\frac{dr}{dt} = \left\{ 1 - \frac{4r^2}{\Delta_S} \right\} \left\{ -\frac{\Gamma_2}{2\eta_0 R_0^4} \frac{\partial F}{\partial r} \right\} + \gamma h \sin(2\theta),
\]

where \( \partial F/\partial r|_{\Delta_S} = \partial F/\partial r - (2r/u_{2,0}) \partial F/\partial u_{2,0}. \) In the harmonic approximation of \( F \), the first term in Eq. (5) disappears because of \( \partial F/\partial r|_{\Delta_S} = 0 \), so that we recover the description of Ref. [8]. The prolate shape appears as an energy minimum, when higher-order terms in the free energy \( F \) are taken into account [21].

Since an expansion of the vesicle shape in spherical harmonics is difficult experimentally, more easily accessible measures of the deformation are desirable. Furthermore, a description is needed which goes beyond the quasi-spherical limit. Thus, instead of \( r \), we employ the shape parameter \( \alpha_D = (L_1 - L_2)/(L_1 + L_2) \), which is easily measurable by microscopy. Since \( \alpha_D = (\sqrt{15}/2\pi/2)r + O(r^2) \), Eq. (5) implies

\[
\frac{d\alpha_D}{dt} = \left\{ 1 - \left( \frac{\alpha_D}{\alpha_D^{\text{max}}} \right)^2 \right\} \left\{ -\frac{A_0}{\tau K V^*} \frac{\partial F}{\partial \alpha_D} + \gamma A_1 \sin(2\theta) \right\},
\]

where \( A_0 = 15\Gamma_2/16\pi = 45/8\pi(32 + 23\eta_0^m) \) and \( A_1 = h\sqrt{15}/2\pi/2 = 30/(32 + 23\eta_0^m) \). Since an accurate evaluation of the free energy \( F \) is very important, we calculate it numerically for ellipsoidal vesicles with \( (x_1/a_1)^2 + (x_2/a_2)^2 + (x_3/a_3)^2 = 1 \), see the inset in Fig. 3. The prolates \( (a_1 > a_2 > a_3) \) and oblates \( (a_1 = a_2 > a_3) \) shapes are energy minima and maxima, respectively, and \( \partial F/\partial \alpha_D \) diverges in the limit of maximum extension, \( \alpha_D \to \alpha_D^{\text{max}}(V^*) \). Eq. (6) has the same form as the simplified model studied previously [9, 10], but now has no adjustable parameters.

In a final step, in order to obtain a reliable description also for large excess areas, we replace Eq. (6) by the equation of K-S theory [12, 13], which reads

\[
\frac{d\theta}{dt} = \frac{\gamma}{2} \left\{ -1 + B \cos(2\theta) \right\},
\]

where the factors \( f_0, f_1, f_2, \) and \( f_3 \) are the functions of the ellipsoidal shape \( (\alpha_D/a_1, a_3/a_1) \), and are given in Appendix B of Ref. [10]. The K-S theory in general shows very good agreement with simulation results [2, 10]. When thermal fluctuations are taken into account, Gaussian white noises \( g_a(t) \) and \( g_\theta(t) \) are added to Eqs. (6) and (7), respectively, which obey the fluctuation-dissipation theorem, so that \( \langle g_i(t) \rangle = 0, \langle g_i(t) g_j(t') \rangle = 2k_B T/\zeta_i \delta_{ij} \delta(t-t') \), where \( i, j \in \{ \alpha_D, \theta \} \). The friction coefficients are \( \zeta_\alpha = \tau K V^*/A_0 (1 - (\alpha_D^{\text{max}})^2) \) and the rotational friction coefficient of a sphere, \( \zeta = 8\pi \eta_0 R_0^3 \). We numerically integrate Eqs. (6) and (7) with or without thermal noise using the second or fourth-order Runge-Kutta method, respectively. When \( \alpha_D(t) \) becomes zero, we set \( (\alpha_D, \theta) = (0, \pi/4) \), since \( \theta = \pi/4 \) is the inclination angle in the spherical limit.

Eqs. (6) and (7) reproduce the simulation results semi-quantitatively (see Figs. 1 and 2). This is a very good agreement, given the fact that our model certainly does not systematically take into account all higher order terms, and furthermore has no adjustable parameters. At small \( \gamma^* \), in the tumbling phase, \( \theta \) rotates with \( \alpha_D \)-oscillation of small amplitude. This \( \alpha_D \) amplitude becomes larger at larger \( \gamma^* \), see Fig. 3. Then, when \( \alpha_D(t) \) reaches zero, \( \theta \) jumps to \( \pi/4 \), see Fig. 11. This type of \( \theta \) oscillations with a jump is reminiscent of the behavior predicted for very viscous liquid drops within perturbation theory [2]. Finally, at even larger \( \gamma^* \), \( \alpha_D \) and \( \theta \) exhibit oscillations without jumps.

The physical mechanism of swinging can be understood on the basis of Eqs. (6), (7) as follows. At finite \( \kappa \), the shear force elongates the vesicle \( (\alpha_D \) increases) for \( 0 < \theta < \pi/2 \), but compresses it \( (\alpha_D \) decreases) for \( -\pi/2 < \theta < 0 \), since the \( \sin(2\theta) \)-term in Eq. (6) changes sign. Thus, the swinging motion is caused by a shape deformation, where \( B \) in Eq. (7) crosses the tank-treading-to-tumbling threshold periodically. First, a prolate vesicle starts tumbling because \( B < 1 \), \( \alpha_D \) decreases when \( \theta < 0 \), which implies that \( B \) increases; then \( \theta \) starts to increase again because \( B > 1 \) at small \( \alpha_D \); finally \( \alpha_D \) increases when \( \theta > 0 \). In the swinging phase, the amplitudes of \( \alpha_D \) and \( \theta \) decrease and saturate to finite values with increasing \( \gamma^* \), see Fig. 3.

A linear stability analysis of the fixed points of Eqs. (6), (7) shows that the tank-treading-to-tumbling transition always occurs as a saddle-node bifurcation at \( \theta \approx 0 \). The tank-treading-to-swinging transition is a saddle-node bifurcation for small \( \gamma^* \), but becomes a Hopf bifurcation at
increasing reduced volume

tions of the internal and the membrane viscosities. With
direction are taken into account.

θ < 0 will likely disap-

lish at which swinging can be observed, decreases, since the
dependence of the energy F on D becomes more shallow,
compare Fig. 3. Also, the region of stability of swinging
shifts to higher viscosity (ηm, or mb) with increasing V*.
On the other hand, for fixed V*, γ* is a monotonically
increasing function of ηm, or mb. This increase is found
to be much less pronounced for mb. The reason is that in
our derivation of Eq. (1), we have neglect the
ηm dependence.

In the experiments of Ref. 4, the swinging (tumbling) motion was observed for γ* ≃ 17 (4.5), ηm = 6 (8.4), and
V* ≃ 0.9, and a very small membrane viscosity ηm ∼ 0.1
(calculated from ηm ∼ 10−9 Ns/m of Ref. 22). It is men-
tioned that the swinging motion is seen in particular in
the close vicinity to the tank-treading-to-tumbling transi-
tion. Thus, the experimental data confirm our predicted
phase diagram, Fig. 3 very well. Furthermore, the oscil-
lation amplitudes also show good agreement, see Fig. 3.

In summary, we have studied the oscillatory motion of
fluid vesicles in simple shear flow. We have developed a
simplified model for the ellipsoidal fluid vesicle, which
explains the simulation and experimental results very well.
This model could be extended in the future to study the
coupling of different types of oscillation mechanisms, like
membrane shear elasticity and viscosity, in elastic cap-

FIG. 4: (Color online) Dynamical phase diagrams as a func-
tion of (a) ηmb for ηin = 1, and (b) ηin for ηmb = 0, for vari-
rable reduced volumes V*, obtained from Eqs. (5), (7) without
thermal noise. The tank-treading phase is located on the left-
hand-side of the dashed lines. The solid lines represent the
tumbling-to-swinging transitions.

θ < 0 for larger γ*. Near the boundary of these two bi-
furcations, a second range of stable fixed points appears
between the saddle and unstable fixed points at θ < 0.

How the phase diagrams of Fig. 4 shows the full phase diagrams, both for variations
of the internal and the membrane viscosities. With
increasing reduced volume V* the smallest shear rate γos*,
at which swinging can be observed, decreases, since the
dependence of the energy F on D becomes more shallow,
compare Fig. 3. Also, the region of stability of swinging
shifts to higher viscosity (ηos, or mb) with increasing V*.
On the other hand, for fixed V*, γ* is a monotonically
increasing function of ηos, or mb. This increase is found
to be much less pronounced for mb. The reason is that in
our derivation of Eq. (1), we have neglect the ηmb depen-
dence. In analogy with Eq. (7), it is plausible to expect
that in a more detailed calculation, a linear combination of
ηos and mb will appear in the both h and Γγ. If this
ηmb dependence were taken into account, the γ* lines in
Fig. 4(a) will curve upwards more strongly; this is consis-
tent with the larger ηmb dependence observed in the
simulations in Fig. 3.

In the experiments of Ref. 4, the swinging (tumbling)
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sules or red blood cells.

We thank R. Finken (Stuttgart) for his help to rederive
Eq. (1). GG acknowledges support of this work through
the DFG priority program “Nano- and Microfluidics”.

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