Deformability Affects Vesicle Migration and Entrapment in Vortical Flows

Gökberk Kabacaoğlu
Department of Mechanical Engineering,
Ihsan Doğramacı Bilkent University
Ankara, 06800, Turkey

Enkeleida Lushi
Department of Mathematical Sciences,
New Jersey Institute of Technology
Newark, 07102, NJ, USA

(Dated: December 6, 2022)

We use numerical simulations to systematically investigate the vesicle dynamics in two-dimensional (2D) Taylor-Green vortex flow in the absence of inertial forces. Vesicles are highly deformable membranes encapsulating an incompressible fluid and they serve as numerical and experimental proxies for biological cells such as red blood cells. Vesicle dynamics has been studied in free-space/bounded shear, Poiseuille and Taylor-Couette flows in 2D and 3D. Taylor-Green vortex flows are characterized with even more complicated properties than those flows such as non-uniform flow-line curvature, shear gradient. We study the effects of three parameters on the vesicle dynamics: the ratio of the interior fluid viscosity to that of the exterior one, the ratio of the shear forces on the vesicle to the membrane stiffness (characterized by the capillary number) and the vesicle deformation. Vesicle deformability is a nonlinear function of these three parameters. Although the study is in 2D, our findings contribute to the wide spectrum of intriguing vesicle dynamics: vesicles becomes entrapped in the vortex by migrating towards the vortex center if they are sufficiently deformable. If not so, they migrate away from the vortex center and travel across the periodic arrays of vortices. In biological cells, vortex flows are frequently observed and found to be responsible for the molecular transport. Our results show that the soft particles migrate towards the vortex center and stay trapped there in vortex flows, whereas, the stiff ones can be transported across.

I. INTRODUCTION

Phospholipid molecules containing a hydrophilic head and a hydrophobic tail come together and form a lipid bilayer which consists in biological membranes [1]. The lipid bilayer is fluid but impermeable to many molecules except water molecules. Vesicles are the bilayer sacs that show rich dynamics in their flows even at small velocity and length scales [1, 2]. Vesicles of approximately 10µm in diameter are numerical and experimental proxies for biological membranes encapsulating only a liquid such as red blood cells. There have been extensive studies on vesicles which are theoretical [3–6], experimental [7–15], and computational [16–22]. They have immense application areas in micro/nano-scale biotechnology: they are used as containers for biochemical reactions [23, 24] and molecular transport [25, 26] as vectors for targeted drug delivery [27, 28]. Vesicles show a wide variety of equilibrium shapes and complex non-equilibrium dynamics in their creeping flows (i.e., the flows where the viscous forces dominate the inertial forces). Vesicles mostly have the so-called parachute shape, which is symmetric shape [29, 30] and the asymmetric shape, called a slipper [10, 17, 30, 31]. This complicated dynamics of vesicles arise from the nonlinear interaction of the membrane deformation and the fluid flow. Designing and controlling vesicles require understanding the rich vesicle dynamics. An important application area is designing microfluidic devices and techniques [32, 33] for medical diagnoses of diseases based on the fact that vesicles show different dynamics depending on their deformability.

The dynamics of a single vesicle has been studied in several fundamental setups so far: free-space/confined shear [3, 12, 36–40] and Poiseuille flows [5, 12, 18, 41–50]. Taylor-Couette flow and confined Couette flow [51]. In those flows, vesicles are observed to show various migration and orientation dynamics stemming from the complicated interplay between the vesicle deformability and the imposed flow characteristics such as the shear rate and the flow-line curvature. Elastic fibers are also deformable objects modelled as an Euler-elasticia, i.e., they are inextensible with resistance to bending and stretching. Like vesicles, fibers are also studied in shear flow [52] and cellular flow [53]. It is shown that dynamics of flexible fibers and vesicles exhibit similar basic features especially when their equilibrium aspect ratio is the same and vesicle is stiff [17]. In a more complicated setup [54, 55] the entrapment of fibers and microswimmers is studied upon colliding with an obstacle, which has applications in filtration to oil recovery to the transport and spreading of biological agents.

Another interesting setup in which the vesicle dynamics need to be investigated is Taylor-Green (TG) flow [57]. It consists of an array of vortices and can be considered a toy model of turbulent flows although it cannot reproduce all the features in turbulent flows and also has some features that are not present in turbulent flows such as closed streamlines. Vortices are ubiquitous in biological flows as they facilitate mass and momentum transfer [58, 59]. TG flow shows characteristics similar to those
FIG. 1. (a) The streamlines and the flow-line curvature in TG cell with the color scheme showing the background flow speed (nondimensionalized by the imposed flow strength). (b) Inward migrating vesicle with no viscosity contrast $\lambda = 1$. (c) Outward migrating vesicle with high viscosity contrast value $\lambda = 10$. Both cases have the same capillary number $Ca = 17$ (the flow strength is $400U$). The gray lines show the trajectories of the vesicles. The time of a snapshot is indicated by the color filling in the vesicle (the filling color gets darker to indicate the later times). In (b) the vesicle is initialized near the edge of the cell whereas in (c) it is initialized near the vortex center. On one hand, the softer vesicle ($\lambda = 1$) aligns its main axis with the flow-lines and migrates inwards. On the other hand, the stiffer one ($\lambda = 10$) tumbles periodically while migrating outwards. The black arrows along the vesicle membranes show the force/length (Eq. 3) the vesicle applies to the fluid. (d)-(g) The effects of other parameters on the vesicle dynamics are shown. Each row shows snapshots from a simulation with the varied parameter written on the very right. The spectrum of purple colors are for vesicles migrating inwards and that of green colors are for those migrating outwards. The darker colors belong to the later times. Additionally, the position of a frame with respect to the leftmost black line qualitatively indicates the position of the vesicle with respect to the vortex center. (d)-(e) The viscosity contrast is $\lambda = 3$ and the reduced area is $\Delta = 0.6$. The capillary number is $Ca = 17$ for (d) and $Ca = 0.04$ for (e). (f)-(g) The viscosity contrast is $\lambda = 4$ and the flow strength is $8U$. The capillary number is $Ca = 0.1$ for (f) and $Ca = 0.5$ for (g).
The flow near the vortex center resembles the Taylor-Couette flow in terms of the flow-line curvature and the shear rate. The flow-lines in a unit TG cell have almost constant curvature near the vortex center. Further away from the vortex center, the streamlines have non-zero curvature only around the $x = y$ line (see Fig. 1). The tangential component of a Taylor-Couette flow is $\eta_0 \times 1/r$ and the radial component is zero, which results in curved flow-lines whose curvature increases as $r \to 0$ where is also the high shear rate region. The shear rate in TG cell reaches its maximum value near the vortex center and disappears near the edges of the cell.

In this article, we study the transport of a vesicle (a model biological cell) in cellular flows (i.e., Taylor-Green vortex) in a 2D setup in the limit of zero Reynolds number (i.e., the inertial forces are negligible). The vesicle is modeled as an Euler elastica and its flow is governed by the Stokes equations. We aim at investigating the effects of vesicle deformability and shape on the vesicle dynamics. Specifically, we vary three nondimensional parameters: the capillary number (the ratio of the flow scale to the vesicle’s relaxation time scale), the viscosity contrast (the ratio of the interior fluid viscosity to that of the exterior one) and the reduced area (the drift of the vesicle shape from a circle). We observe that the increasing deformability leads the vesicle to align itself with the flow-lines and to be trapped in the Taylor-Green cell by migrating towards the vortex center (see Fig. 1) while stiffer vesicles migrate towards the edges of a TG cell and leaves the cell eventually.

**II. METHODS**

We consider a vesicle in Taylor-Green cell (see Fig. 1). The imposed flow is two-dimensional, time-independent and periodic

$$v^\infty(x) = U(\sin(x) \cos(y), - \cos(x) \sin(y))$$

for $(x, y) \in [0, \pi]^2$ with $U$ the flow strength. The TG cell contains a vortex at the center. A 2x2 array of the TG cells have a hyperbolic stagnation point at its center. That point is connected to other stagnation points through stagnation streamlines (separatrix). We carry out the numerical simulations using a boundary integral formulation:

$$v(x) = \frac{2}{1 + \lambda} v^\infty(x) + \frac{1}{2\pi \eta_0 (1 + \lambda)} \int_G G(x - y) \cdot f(y) ds(y)$$

$$+ \frac{2(1 - \lambda)}{\pi (1 + \lambda)} \int_G v(y) \cdot T(x - y) \cdot n(y) ds(y),$$

where $\gamma$ is the vesicle membrane, $v$ is the membrane velocity, $G$ and $T$ are the Green’s functions of the Stokes flow $[60]$, $x$ and $y$ are points on the membrane, $f$ is the membrane force/length, $n$ is the outward normal to the membrane, $\eta_0$ and $\eta_1$ denote the viscosity of the suspending fluid and the fluid inside the vesicle, respectively, and $\lambda = \eta_1 / \eta_0$ is the viscosity contrast between the internal and the external fluids. The membrane applies force due to its resistance to bending and its inextensibility. The form of the force/length is obtained by taking the functional derivative of the Helfrich bending energy $E = \frac{c}{2} \int c^2 ds + \int \xi ds$ that includes the tension $\xi$ to enforce the membrane inextensibility:

$$f(x) = -\kappa \left[ \frac{d^2 c}{ds^2} + \frac{1}{2} c^3 \right] n + \xi c n + \frac{d\xi}{ds} t,$$

where $\kappa$ is the membrane’s bending modulus, $c$ is the membrane curvature, $\xi$ is the tension that acts like a local Lagrange multiplier enforcing membrane inextensibility, and $t$ is the tangent to the membrane. The membrane force Eq. 3 balances the jump in the traction across the vesicle membrane. The details of the numerical scheme to solve the integral equation formulation can be found in $[60]$.

**III. RESULTS**

**Description of the numerical experiments.** Let $A$ and $L$ denote the area enclosed by a vesicle and its arclength, respectively. Then, the vesicle’s reduced area (deflation) is defined as the ratio of the enclosed area to the area of a circle having the same perimeter $L$: $\Delta = \sqrt{A/[\pi (L/2\pi)]^2}$ $(0 < \Delta \leq 1, \Delta = 1$ for a circle). In addition to the reduced area, the dimensionless numbers that enter the problem of free-space vesicle flows are (1) the viscosity contrast value $\lambda$, and (2) the capillary number $Ca = \eta_0 U R^3 / \kappa$ where $\kappa$ is the membrane bending stiffness and the vesicle’s characteristic size $R$ is defined as the radius of a circle that has the same perimeter as the vesicle, i.e., $R = L/2\pi$. We have experimented numerically by varying those dimensionless parameters. We have considered the vesicles with the reduced area values $\Delta = (0.4, 0.6, 0.9)$. We have kept the size of Taylor-Green cell and the area $A$ of the vesicle the same while changing the reduced area. That has led the ratio of the cell size to the vesicle size $R$ to change with the reduced area. The ratio is approximately 12, 15 and 20 for the reduced area values $\Delta = (0.4, 0.6, 0.9)$, respectively. The range of the capillary number we have covered is $Ca \in [10^{-2}, 10]$ and the range of the viscosity contrast values is $\lambda \in [1, 100]$. These are physically meaningful ranges for red blood cells in microcirculation $[61]$.

**Tank-treading vesicles migrate inwards.** As observed in several other flows (e.g., Taylor-Couette, Couette, Poiseuille) vesicles in TG flow tank-tread for low viscosity contrast values with almost a fixed orientation with respect to the imposed flow direction at the vesicle’s center. Like in Taylor-Couette flow, tank-treading vesicles migrate towards the vortex center (inwards). In Fig. 1, we superimpose the snapshots from the simulation of a
Inward migrating vesicle (Fig. 1b)

Outward migrating vesicle (Fig. 1c)

FIG. 2. Dynamics of a vesicle in Taylor-Green cell for low viscosity contrast value \( \lambda = 1 \), the top row and for high viscosity contrast value \( \lambda = 10 \), the bottom row. What is plotted is the dispersion, i.e., \( L^2 \)-norm of the distance vector from the vesicle’s center of mass to the vortex center (the first column), the orientation angle between the vesicle’s main axis and the imposed velocity vector at the vesicle’s center of mass (the second column), and the phase angle of a point on the membrane (i.e., the tank-treading angle) on the same figures. The background colors in the plots correspond to the flow-line curvature where the vesicles are at the corresponding instants. The color scale for the curvature is given in Fig. 1b (the yellow is zero curvature and the blue is the maximum curvature). On the one hand (the first row), the inward migrating vesicle has nearly constant orientation angle and its membrane is tank-treading. On the other hand (the second row), the outward migrating vesicle is tumbling with a very slowly tank-treading membrane. The tank-treading vs. tumbling dynamics of a vesicle aligns with its migration direction.

vesicle with \( \lambda = 1 \) initialized near the edge of Taylor-Green cell. The vesicle’s reduced area is \( \Delta = 0.6 \) and the capillary number is \( Ca = 17 \). The black arrows show the hydrodynamic force/length distribution along the membrane. The vesicle becomes aligned with the imposed flow lines and migrates inwards while its membrane tank-treads (see Fig. 2b and the discussion below).

Tumbling vesicles migrate outwards. Under the same flow conditions but increasing the viscosity contrast to \( \lambda = 10 \), the vesicle starts migrating outwards while tumbling. In Fig. 2c, we show the snapshots from the simulation of the outward migrating vesicle initialized near
the vortex center. The membrane still tank-treads but much slower than it does for low viscosity contrast values (see Fig. 2). For the viscosity contrast values equal to and greater than 5, vesicle always tumbles and migrates outwards for different reduced area values and capillary numbers (see Fig. 3).

**Flow-line curvature impacts vesicle dynamics.** To illustrate that, in Fig. 2, we plot the dispersion, the angular orientation of a vesicle with respect to the flow and its membrane motion (i.e., the tank-treading angle). Time is in the x-axes and nondimensionalized with the time scale (i.e., the vortex size / flow strength). The first column in Fig. 2 shows the dispersion nondimensionalized with the vortex size. We have opted for the $L^2$-norm to measure dispersion. The plots in Fig. 2 are obtained for the inward and outward migrating vesicles in Fig. 1d and Fig. 1e, respectively. The striped background in the plots indicates the curvature of the flow-line the vesicle resides at a particular time. The color scale is given in Fig. 1d. The dispersion rate for the inward migrating vesicle increases when the vesicle is on a high curvature where the vesicle’s main axis aligns with the flow direction at its center and its membrane does not rotate or rotates much slowly. When the inward migrating vesicle is on a flow line of a lower curvature, its main axis drifts away from the flow direction and its membrane tank-treads. That is similar to the fact that vesicle with low viscosity contrast value tilts to a certain angle and tank-treads in a shear flow. Although the flow-line curvature does not have a significant impact on the dispersion and the membrane rotation of the outward migrating vesicle, its effects on the vesicle orientation are visible. High flow-line curvature pushes the vesicle to align with the flow direction but the vesicle continues tumbling on the low curvature flow-lines.

Large Ca value leads to inward migration. The capillary number measures the vesicle deformability: its higher values correspond to more deformable vesicles. Since a vesicle is more deformable for lower viscosity contrast values and we observe that vesicles migrate inwards for low viscosity contrast values, one would expect inward migration for large capillary number values. Our simulations verify that hypothesis (see Fig. 1d for $Ca = 17$ and Fig. 1e for $Ca = 0.04$). The more deformable vesicle aligns itself with the flow direction and migrates inwards whereas the stiffer one migrates outwards with tumbling. As the capillary number increases, the critical viscosity contrast value for the transition from inward migration to outward migration increases (Fig. 3). The same figure also shows that the tank-treading vs. tumbling dynamics coincides with the migration dynamics for different capillary number values.

Slender vesicles behave like slender filaments. As the reduced area increases, vesicle becomes more rounded and hence its dynamics becomes less complex. As Fig. 3 shows, for the reduced area $\Delta = 0.9$ the transition from the inward migration (also tank-treading) to outward migration (tumbling) happens at the same viscosity contrast value ($\lambda = 5$) for a wide range of capillary number values. For more deflated vesicles (i.e., $\Delta \leq 0.4$), we observe dynamics similar to elastic filaments such as stretch-coil instability [33]. This buckling instability drives the meandering dynamics of elastic filaments. Figure 3 shows that the vesicle of $\Delta = 0.4$ migrates outwards for a wide range of viscosity contrast values compared to the $\Delta = 0.6$ case. We speculate the reason to be the fact that the instability promotes the outward migration. Increasing the capillary number for a fixed viscosity contrast values less than 5 and for $\Delta = 0.4$ leads the vesicle to align with the flow streamlines and migrate inwards.

**IV. DISCUSSION**

In a 2D flow, due to the flow-induced deformation vesicle membrane develops tension so as to keep the arclength constant (due to the inextensibility). The tension along the membrane, then, dictates the vesicle dynamics in the flow. Vesicle evolves in such a way that minimizes the non-uniformity in the tension distribution and at equilibrium the tension becomes uniform [51, 62]. To discuss the underlying mechanisms of the vesicle migration in Taylor-Green flows, we revisit the vesicle dynamics observed in some fundamental flows studied earlier in terms of the vesicle’s tension, equilibrium shape, orientation and migration.

**Tank-treading (TT) vs. tumbling (TB) behavior.** In free-space shear flow vesicles have been observed to (1) tank-tread with a stationary inclination angle, and (2) tumble, i.e., go through a periodic flipping motion. Which dynamics vesicle shows depends on three parameters: the reduced area, the viscosity contrast and the capillary number (see [12, 63] for the experimental and numerical studies). For low viscosity contrast values, vesicle tank-treads. For intermediate viscosity contrast values, vesicle shows vacillating breathing in 3D and constantly tumbles at high viscosity contrast values. The critical viscosity contrast value between tank-treading and tumbling increases with the increasing capillary number and reduced area values. The appearance of tank-treading vs. tumbling depends on the viscosity contrast, the reduced area and the capillary number qualitatively similarly in bounded/free Taylor-Couette flow, Poiseuille flow. The tank-treading motion induces an inner circulation which results in higher dissipation. However, it is shown in 2D free-space Poiseuille flow that tank-treading is a favorable dynamics under specific conditions as it helps vesicle reduces the lag between the vesicle velocity and the imposed flow [18]. As the viscosity contrast value increases, tank-treading leads to more dissipation and eventually the vesicle transitions to tumbling which reduces the dissipation and also alters the rheological properties of the vesicle solution [38].

**Migration.** Cross-stream migration in low Reynolds number flows may occur if the symmetry in the suspended particle is lost by deformation or in the presence
FIG. 3. Phase diagram. The purple area shows inward migration and the green area shows outward migration. The markers show the parameter values for which we have performed simulations. The filled circles and squares represent the tumbling and the tank-treading vesicles, respectively. For the reduced area of 0.9, the transition from inward to outward migration shifts upwards and happens at the same viscosity contrast for all values of the capillary number greater than $5 \times 10^{-2}$. Additionally, there is a small region (in yellow) where the vesicle does not show any significant migration.

of the wall [62]. Particle deformation is due to a shear gradient (as in free Poiseuille flow [48]) and/or flow-line curvature (as in Taylor-Couette flow [51]). No matter what the source for the deformation is, vesicles are observed to migrate for low viscosity contrast values for which they also tank-tread [48, 51]. The migration velocity depends on the values of the viscosity contrast and the reduced area. It increases as the reduced area decreases and as the imposed flow becomes stronger [62]. The velocity decreases as the viscosity contrast increases. Above a critical viscosity contrast value, vesicle starts tumbling and the migration is suppressed in the free Poiseuille and Taylor-Couette flows. Unlike those free-space flows, in bounded shear flow vesicles are observed to migrate for all viscosity contrast values but their ultimate position is the center-line (zero velocity) between two parallel plates for low viscosity contrast values and they migrate towards the walls depending on their initial conditions for high viscosity contrast values [65]. When the viscosity contrast is low, vesicle tilts to a certain angle and maintains it. If the vesicle is initialized below the center-line, then it tilts in the counterclockwise direction resulting in an asymmetry. For the high viscosity contrast values though, once the vesicle has started lifting, also tumbling and tumbling leads the lift-off angle to decrease and reverse its direction. At that moment, vesicle experiences pushing towards the wall. However, since the tumbling cycle results in asymmetric shapes during the two-halves of the tumbling period, the vesicle experiences net migration towards the wall. For very high viscosity contrast values, the vesicle does not even lift off the wall and aligns with the flow near the wall.

Vortical flow. Taylor-Green flow has nonzero shear rate and gradient, and also flow-line curvature varying with the radial position with respect to the vortex center and also along a streamline (Fig. 1). In that sense, it pretty much resembles the Taylor-Couette flow with a fundamental difference of non-uniform curvature along a streamline. So to understand why vesicles migrate in different directions, we consider two cases: (1) $\lambda = 1$ and (2) $\lambda = 10$. The trajectories of those cases are shown in Figs. 1(b) and (c); also in Fig. 2 we show the evolution of (1) the vesicle’s distance to the vortex center (dispersion), (2) the vesicle orientation with respect to the imposed flow direction and, (3) vesicle’s tank-treading angle.

Inward migration. For $\lambda = 1$, the vesicle steadily migrates inwards (Fig. 2a). The inward migration towards the high curvature and high shear rate region is also observed for the low viscosity contrast values in Taylor-Couette flows. The inward migration is accompanied by slight oscillations of the vesicle’s orientation around the imposed flow direction (Fig. 2b). The magnitude of the oscillations decreases as the vesicle approaches to the vortex center. In the high curvature regions, the vesicle’s main axis moves away from the imposed flow direction but the angle decreases in the low curvature regions. At the same time, the vesicle shows tank-treading (Fig. 2b), i.e., there is flow circulation inside the vesicle, which reduces the lag between the vesicle and the imposed flow in the expense of high dissipation. The tank-treading becomes faster in the high curvature regions. We have performed simulations by initializing the vesicle closer to the edge of the cell (only 5% of the vortex size away from the edge) for the same viscosity contrast value. We have observed persistent inward migration regardless of the initial position and orientation of the vesicle.

Outward migration. For $\lambda = 10$, the vesicle migrates outwards (Fig. 2c). As in the low viscosity contrast value case, the vesicle’s main axis moves away from the im-
posed flow direction in the high curvature regions but the vesicle cannot recover to the angle it had in the low curvature region (Fig. 2d). That is due to the slower tank-treading than in the case of \( \lambda = 1 \) (Fig. 2d). Due to the higher interior fluid viscosity, the dissipation due to tank-treading is much larger. Hence, the vesicle does not tank-tread for \( \lambda = 10 \) as fast as it does for \( \lambda = 1 \). Eventually, the vesicle constantly tumbles while it migrates. On the contrary, tumbling in Taylor-Couette flow leads to negligible migration of the vesicle. Although there are similarities between Taylor-Couette flow and Taylor-Green flow such as higher flow-line curvature and shear rate near the center, there is a fundamental difference between them: oscillating flow-line curvature along a streamline in Taylor-Green flow (vs. uniform in Taylor-Couette). The non-uniformity in the flow-line curvature inhibits symmetric tumbling as in Taylor-Couette flow and hence leads to non-negligible outward migration. Does a tumbling vesicle always migrate outwards in Taylor-Green vortex? Even when the vesicle is initialized only 5% of the vortex size away from the vortex center, it still migrates outwards for the same viscosity contrast value.

V. CONCLUSION

The significance of the present study is two-fold: (i) it systematically uncovers the complex dynamics of vesicles in a complicated flow (e.g., showing oscillatory flow-line curvatures); (ii) it sheds light on the transport of deformable particles in a biologically relevant flow as vortex- induced flows are seen in large cells. What is new to the vesicle dynamics in free-space flows is the outward migration of tumbling vesicles for high viscosity contrast values for which vesicles do not significantly migrate in free-space shear and Poiseuille flows. The nonuniformity of the flow-line curvature causes symmetry-breaking in the flow of tumbling vesicles, which leads them to migrate away from the vortex center and eventually to escape from the Taylor-Green cell. From the biological point of view, we have found that the deformable particles travel across the vortex flow towards the vortex center whereas the stiff particles stay at the edges of the vortex cell. Taylor-Green vortex is a three-dimensional phenomenon and we expect even more complicated vesicle dynamics in 3D TG flows as similar extensions of shear/Poiseuille flows to 3D have discovered rich dynamics. 

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