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Numerical simulations on the dynamics of a spheroid in a viscoelastic liquid in a wide-slit microchannel

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Abstract

The translational and orientational dynamics of a spheroid suspended in a viscoelastic liquid flowing in a wide-slit microchannel is studied by 3D finite element simulations. An Arbitrary Lagrangian-Eulerian formulation is adopted to handle particle motion. The particle dynamics, with specific interest on the migration phenomenon and on the long-time orientation, is studied by computing the trajectories of the spheroid and the orbits described by its orientation vector. The effects of the initial distance from the channel centerplane and of the initial orientation on the particle motion is investigated, for low and moderate Weissenberg numbers. A ‘migration state diagram’ giving the long-time equilibrium positions of the particle for all possible initial configurations is derived: in most cases, the particle goes to the centerplane, but there are circumstances where also the wall is an attractor.

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1. Introduction

Microfluidics, i.e., the manipulation of fluids in channels with dimensions ranging from tens to hundreds of micrometres, has received a growing interest over the last decades [1, 2]. Microfluidic devices offer, indeed, a number of advantages as compared to macroscopic systems, e.g., a precise control of the flow rates due to the laminar flow conditions, high surface to volume ratios, the need for very small amount of samples, the possibility to run multiple analyses simultaneously, and the handling of small particles [1, 2].

Indeed, one of the most relevant use of microfluidic devices is in the synthesis, functionalization, and analysis of particles with characteristic dimensions comparable to those of the channels in which they flow. In this regard, particle manipulation, i.e., the control and positioning of particle trajectories, is mandatory. Hence, it is not surprising that several techniques aiming at the manipulation of particle trajectories have been proposed, based on external fields, auxiliary streams, or inertial effects [3, 4].

Recently, a technique able to precisely control particle trajectories in simple straight microchannels by employing viscoelastic fluids has been developed [5, 6, 7]. Fluid elasticity generates some dynamical action on the suspended particles, leading to motions across the streamline of the flow field (migration). Many important studies have appeared in the last five/ten years, aimed at clarifying the effects of channel geometries, flow conditions, and fluid rheological properties on the direction of particle migration [6, 7].

The increasing popularity of this viscoelasticity-based particle manipulation technique is essentially due to the need for extremely simple, low-cost and easy-to-use devices (basically, a syringe pump and a straight microchannel). Several applications have been, in fact, developed, including flow-focusers, separators, fractionators, microrheometers [6, 7].

Viscoelasticity-induced migration phenomenon in microchannels has been mainly studied for spherical particle suspensions. However, non-spherical particles are encountered in a variety of microfluidic systems. For instance, particles of interest in biology and medicine, e.g., viruses, bacteria, marine organisms, and red blood cells (RBCs), usually have complex shapes. In addition, man-made particles with micro- and nanometric size and non-spherical shape are used in applications such as barcoding techniques and drug delivery [8, 9, 10]. Unlike spheres, non-spherical particles suspended in a fluid medium subjected to an external flow field undergo complex three-dimensional motions by varying their orientations. In microfluidic systems involving viscoelastic suspending fluids, the presence of confinement (i.e., particle size of the same order of channel characteristic dimension) and fluid elasticity further complicates the particle dynamics, as recently demonstrated on a viscoelastic suspension of peanut-shaped particles in a rectangular microchannel [11, 12]. The experiments show that elasto-inertial lift drives spherical and non-spherical particles at different trajectories, allowing separation by shape. The orientational motion of peanuts particles in a viscoelastic fluid has been also tracked, showing that the particle orients along the flow direction, in contrast with the Newtonian case, where it experiences a never-ending ‘tumbling motion’. A systematic investigation of the migration phenomenon and the

orientational dynamics of dilute viscoelastic suspensions of non-spherical particles in microchannels is, however, missing.

Aim of this work is to study, by 3D Direct Numerical Simulations, the translational and orientational dynamics of a spheroidal particle suspended in a viscoelastic fluid flowing in a slit microchannel. The macroscopic governing equations are solved by the finite element method. The Arbitrary Lagrangian-Eulerian (ALE) technique is used to handle the particle motion. Remeshing and projection of the already calculated fields on the new grid are employed to deal with mesh distortion. The effect of the initial particle position and orientation on particle motion, with specific interest on the migration phenomenon, is investigated.

2. Mathematical model

2.1. Governing equations

Figure [1](#) displays a scheme of the system investigated in this work. A rigid, non-Brownian, spheroidal particle is immersed in a viscoelastic liquid flowing between two parallel plates (wide-slit channel) under a pressure-driven flow. A Cartesian reference frame is selected with origin at the center of the domain. We denote with x the flow direction, y the gradient direction (orthogonal to the plates), and z the ‘neutral’ direction. The particle has major and minor axes a and b , respectively, and we define the aspect ratio as $AR = a/b$. The particle orientation vector (a unit vector) is denoted by $\mathbf{p}$.

The fluid flows in the slit with an imposed flow rate Q . The inflow and outflow sections are denoted by S_{IN} and S_{OUT} (see legend of Fig. [1](#)). The lower and upper walls are reported in yellow in Fig. [1](#) and are denoted by

Figure 1: Schematic representation of the system investigated in this work. The legend on the right indicates the labels of the domain surfaces where boundary conditions are applied.

S_{W1} and S_{W2} , respectively. To simulate a wide-slit and infinitely long channel, both the domain width W and length L must be chosen sufficiently larger than the gap H . In these conditions, we can impose symmetry on the lateral boundaries S_{SYM1} and S_{SYM2} .

Assuming incompressibility and neglecting inertia of the fluid, its governing equations are:

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta_s\mathbf{D} + \boldsymbol{\tau} \quad (3)$$

Equations (1)-(3) are the momentum balance, the mass balance (continuity) and the expression for the fluid stress tensor, respectively. In these equations $\boldsymbol{\sigma}$, $\mathbf{u}$, p , $\mathbf{I}$, η_s , $\mathbf{D}$ are the stress tensor, the velocity vector, the pressure, the unity tensor, the viscosity of a Newtonian ‘solvent’, and the rate-of-

deformation tensor, respectively. The viscoelastic stress tensor $\boldsymbol{\tau}$ needs to be specified by choosing a constitutive equation. In this work, we select the Giesekus model:

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} + \frac{\alpha\lambda}{\eta_p} \boldsymbol{\tau} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} = 2\eta_p \mathbf{D} \quad (4)$$

where η_p is another viscosity, λ is a relaxation time, the symbol $(\overset{\nabla}{\boldsymbol{\tau}})$ denotes the upper-convected time derivative:

$$\overset{\nabla}{\boldsymbol{\tau}} \equiv \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\tau} - (\nabla \mathbf{u})^T \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \nabla \mathbf{u} \quad (5)$$

and α is a (dimensionless) constitutive parameter. We recall that the Giesekus model predicts shear-thinning for α greater than zero; the limiting case $\alpha = 0$ corresponds to the Oldroyd-B model. Finally, the zero-shear viscosity is defined as $\eta_0 = \eta_s + \eta_p$.

By assuming also that particle inertia is negligible, force- and torque-free conditions hold:

$$\mathbf{F} = \int_{S_p(t)} \boldsymbol{\sigma} \cdot \mathbf{n} dS = \mathbf{0} \quad (6)$$

$$\mathbf{T} = \int_{S_p(t)} (\mathbf{x} - \mathbf{x}_p) \times (\boldsymbol{\sigma} \cdot \mathbf{n}) dS = \mathbf{0} \quad (7)$$

where $\mathbf{F}$ and $\mathbf{T}$ are the total force and torque acting on the particle due to the fluid motion, $\mathbf{n}$ is the outwardly directed unit normal vector on the particle surface S_p , $\mathbf{x}$ is a point of the spheroidal surface, and $\mathbf{x}_p$ is the particle centroid.

Regarding the boundary conditions, no-slip is imposed at the channel walls:

$$\mathbf{u} = \mathbf{0} \quad \text{on } S_{W1} \text{ and } S_{W2} \quad (8)$$

and symmetry is applied on the lateral surfaces:

$$\mathbf{u} \cdot \mathbf{k} = 0 \quad \text{on } S_{SYM1} \text{ and } S_{SYM2} \quad (9)$$

$$(\boldsymbol{\sigma} \cdot \mathbf{k})|_x = (\boldsymbol{\sigma} \cdot \mathbf{k})|_y = 0 \quad \text{on } S_{\text{SYM1}} \text{ and } S_{\text{SYM2}} \quad (10)$$

where $\mathbf{k}$ is the unit vector along the z -direction. To simulate an infinitely long channel, periodicity is prescribed between the inflow and outflow sections, together with a flow rate in inflow:

$$\mathbf{u}|_{S_{\text{IN}}} = \mathbf{u}|_{S_{\text{OUT}}} \quad (11)$$

$$(\boldsymbol{\sigma} \cdot \mathbf{i})|_{S_{\text{IN}}} = (\boldsymbol{\sigma} \cdot \mathbf{i})|_{S_{\text{OUT}}} - \Delta p \mathbf{i} \quad (12)$$

$$\int_{S_{\text{IN}}} \mathbf{u} \cdot \mathbf{i} dS = Q \quad (13)$$

where $\mathbf{i}$ is the unit vector along the x -direction and Δp is the pressure drop along the channel (in between S_{IN} and S_{OUT}). The flow rate in Eq. (13) is imposed through a constraint where the associated Lagrange multiplier is identified as the unknown pressure difference Δp [13].

Finally, adherence is assumed on the spheroidal surface resulting in the rigid-body motion equation:

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_p) \quad \text{on } S_p \quad (14)$$

where $\mathbf{U}$ and $\boldsymbol{\omega}$ are the particle translational and angular velocities, respectively.

As inertia is neglected, no initial condition for the velocity field needs to be specified. On the other hand, since the time-derivative of the viscoelastic stress tensor appears in the constitutive equation, an initial condition for $\boldsymbol{\tau}$ is required. We assume a stress-free condition, i.e., that the extra stress is zero everywhere in the fluid at the initial time:

$$\boldsymbol{\tau}|_{t=0} = \mathbf{0} \quad (15)$$

Once the fluid velocity, pressure and stress fields are calculated along with the particle kinematic quantities, the particle position and rotation are updated by integrating the following equations:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{U} \quad (16)$$

$$\frac{d\Theta}{dt} = \omega \quad (17)$$

with initial conditions $\mathbf{x}_p|_{t=0} = \mathbf{x}_{p,0}$ and $\Theta|_{t=0} = \Theta_0$. To track and update the particle orientation, quaternions are used [14, 15, 16]. Hence, instead of solving Eq. (17), the particle orientation is computed by: i) updating the quaternions through the computed angular velocity, ii) calculating the rotation matrix from the quaternions, iii) applying the rotation matrix to the initial orientation vector $\mathbf{p}_0$ [15, 16].

The governing equations are made dimensionless by choosing the gap H as characteristic length, the average velocity $\bar{u} = Q/(WH)$ as characteristic velocity, and $\eta_0\bar{u}/H$ as characteristic stress. Then, the following dimensionless parameters appear: the Weissenberg number $Wi = \lambda\bar{u}/H$, the confinement ratio $\beta = a/H$, the particle aspect ratio $AR = a/b$, the viscosity ratio $\eta_r = \eta_s/\eta_0$, the constitutive parameter α , the initial particle position $\mathbf{x}_p/H$ and orientation $\mathbf{p}_0$. In what follows, all the symbols will refer to dimensionless quantities.

2.2. Numerical method

The governing equations are solved through the finite element method with the SUPG formulation [17] and the log-representation for the conformation tensor [18, 19] to stabilize the constitutive equation. The particle translational

and angular velocities are treated as additional unknowns and are included in the weak form of momentum equation. The force- and the torque-free condition are imposed through Lagrange multipliers in each node of the spheroidal surface.

During a simulation, the particle changes its position and orientation. The particle motion is handled by using the Arbitrary Lagrangian-Eulerian (ALE) technique [20]. A boundary-fitted, tetrahedral mesh describes the particle surface and the surface mesh nodes are moved in order to follow the particle motion. The mesh nodes in the fluid need to be moved as well, in order to reduce the mesh distortion. The mesh displacement is computed by solving a Laplace equation assuring smooth variation [20]. Since the position of the particle along the flow and neutral directions does not alter the particle dynamics, the mesh moves in x - and z -direction with the particle center and the corresponding translational velocity mesh components are subtracted from the convective term of the constitutive equation [21]. During the particle motion, the mesh elements progressively deform. The quality of the evolving mesh is evaluated in terms of changes of element volume and aspect ratio compared to the values of the undeformed mesh [20]. Once one of these two indicators overcomes a threshold, mesh is regenerated, and the calculated fields are projected from the old mesh to the new one. The constitutive equation is discretized through a semi-implicit Gear scheme. The resulting linear systems are solved by the the sparse direct solver PARDISO [22]. For further details on the implementation, the reader is referred to Ref. [21].

Spatial and temporal convergence as well as the choices of the domain width W and length L in order to assure unperturbed flow far from the particle

are checked for all the calculations presented in this work. Regarding the domain size, we found that (in dimensionless terms) $W = L = 5$ is sufficient. Depending on the parameters, spatial convergence is obtained with a number of mesh elements ranging from 40000 to 85000, whereas time convergence requires a (dimensionless) time step from 0.005 to 0.01. In general, finer meshes and lower time steps are needed at larger Weissenberg numbers and for particles initially starting close to the wall.

We would like to conclude this section by giving some information about the computational times. As compared to our previous work on spherical particles in a wide-slit channel [21], the present simulations are much more time-consuming, for two reasons: i) since the orientational dynamics for spheres is irrelevant, a master curve ‘migration velocity vs position’ could be identified, which required short simulations (just the time to extinguish the initial transient due to the viscoelastic stress development), ii) no remeshing and projection were needed, as the sphere only slightly translates along the migration direction during the whole (short) simulation. In contrast, the orientational changes of a non-spherical particle do not allow us to study the migration phenomenon by a simple master curve, as particles at the same position with different orientation will have, of course, different migration velocities. Hence, the whole particle dynamics must be computed (with several steps of remeshing and projection), hugely increasing the simulation time. Furthermore, as detailed below, the orientational dynamics for particles initially oriented out of the flow-gradient plane is much slower than the translational one, requiring quite long simulations to identify a final orientation. A typical simulation for a spheroid initially oriented on the flow-gradient

plane takes about 2-3 weeks. The computational time increases to 9-10 weeks for simulating spheroids with their major axis out of the flow-gradient plane.

3. Results

In this section, the simulation results will be presented. We fix the geometrical and rheological parameters to the following values: $\beta = 0.4$, $AR = 2$, $\eta_r = 0.091$, and $\alpha = 0.2$. We consider low and moderate Weissenberg numbers and vary the initial particle position and orientation. Due to the selected geometry (flow between two infinite parallel plates), the x and z coordinates of the particle centroid have no influence on the migration dynamics. Then, in what follows, we only report the time evolution of y_p that is related to the migration phenomenon. The orientational particle dynamics will be presented in terms of orientation vector $\mathbf{p}$. Because of symmetry, particle dynamics can be studied in only one-half of the channel, and it is sufficient to limit the initial orientation vector $\mathbf{p}_0$ in one quadrant (we select the one identified by the positive x - and z -axis).

We first investigate the translational and orientational dynamics of a spheroid with its major axis initially lying on the xy -plane (flow-gradient plane). Because of the symmetry, the spheroid orientation vector will remain on such a plane during the whole dynamics. Hence, two orientation vector components, p_x and p_y , are sufficient to describe the orientational dynamics. Figure 2 shows the position and orientation of the particle at different times, in the case with the spheroid initially oriented along the y -axis, i.e., with $\mathbf{p}_0 = (0, 1, 0)$, and at a distance $y_{p,0} = 0.25$ from the centerplane. The red curve is the trajectory of the barycenter. The green curve describes the motion

Figure 2: Snapshots of the dynamics of a spheroid initially orientated with the major axis along the y -axis and at a distance $y_{p,0} = 0.25$ from the centerplane. The Weissenberg number is $Wi = 0.5$. The red line denotes the trajectory of the particle barycenter. The green line is the orbit described by the tip of the orientation vector represented by the black line. For the sake of clarity, the x -axis has been shrunk.

of the tip of the orientation vector. The results clearly show a migration dynamics towards the centerplane. In addition, the spheroid rotates in a counterclockwise sense (seen from the positive z -axis), as expected, due to the velocity profile induced by the pressure-driven flow in the upper half of the channel. Since the spheroid barycenter moves ‘down’ towards the centerplane, the local shear rate (in the unperturbed Poiseuille flow) decreases, and the spheroid orientational dynamics accordingly slows down as time goes on. At long times, the particle slowly aligns along the flow direction x , with its barycenter on the channel centerplane.

The temporal trends of the particle barycenter position y_p and orientation vector components p_x and p_y are shown in Fig. 3 for different initial particle

Figure 3: (a) Trajectories of the spheroid barycenter for different initial positions. The inset shows a closer look at initial times. The particle major axis is initially aligned along the y -axis. The Weissenberg number is $Wi = 0.5$. The green shaded area is the channel region not accessible by the particle relative to its initial configuration. (b)-(c) Evolution of the orientation vector components p_x and p_y for an initial position $y_{p,0} = 0.15$ (b) and $y_{p,0} = 0.25$ (c).

positions $y_{p,0}$. In all these simulations, the orientation vector is initially aligned to the y -axis. For all initial positions, the spheroid migrates towards the channel centerplane. This is also the case for a spheroid initially located very close to the channel upper wall, as shown by the orange curve of the inset of Fig. 3a, corresponding to $y_{p,0} = 0.294$. (For a spheroid initially aligned along the y -axis and for the chosen aspect ratio, the maximum allowed value of $y_{p,0}$ is 0.3.) Notice that this behavior is at variance with the spherical particle case where, for the same flow field and fluid rheological properties, a separatrix between migration towards the centerplane and towards the wall is always found [21].

Regarding the orientational dynamics, Figs. 3b and 3c, corresponding to $y_{p,0} = 0.15$ and $y_{p,0} = 0.25$, respectively, confirm that the particle rotates around the vorticity axis with a rotation rate that progressively decreases as the particle approaches the centerplane. Since the (unperturbed) velocity gradient decreases from the wall to the centerplane, the number of rotations experienced by the spheroid decreases as well as the initial particle position moves to the centerplane. For both initial positions, at about 100 dimensionless time units, the particle aligns with the major axis along the flow direction.

In Fig. 4, the distribution of the first normal stress difference $N_1 = T_{xx} - T_{yy}$ on the xy -plane and on one-half of the particle surface for different times is shown, for the case $y_{p,0} = 0.294$ (orange curve in Fig. 3a). Previous works on spherical particles have reported that the migration phenomenon is related to an imbalance of N_1 around the particle surface [5, 6, 7]. The snapshots in Fig. 4 show that highest N_1 -values always occur in the fluid

Figure 4: Distribution of the first normal stress difference N_1 at different times. The particle major axis is initially aligned along the y -axis. The initial particle position is $y_{p,0} = 0.294$.

region between the particle and its nearest wall, where the local largest shear rate gradient is found (compare the red regions near the upper and lower wall where the flow field is more and less undisturbed by the particle). Hence, similarly to spheres, the interplay between viscoelasticity and confinement might be likely responsible for the migration phenomenon.

We run further simulations by changing the initial particle orientation, but still maintaining the major axis on the flow-gradient plane. Results (not shown) are qualitatively similar to those just discussed. Hence, we can conclude that, for the fluid, flow, and geometrical parameters chosen, a

Figure 5: Trajectories of the spheroid barycenter for different initial positions. The initial orientation is $\mathbf{p}_0 = (0, 0, 1)$ (a) and $\mathbf{p}_0 = (0, \sqrt{3}/2, 1/2)$ (b). In both panels, the green shaded area is the channel region not accessible by the particle relatively to its initial configuration.

spheroid with its major axis on the xy -plane always migrates towards the channel centerplane and aligns along the flow direction, regardless of its initial position and orientation.

The just discussed dynamics of a particle with its major axis in the flow-gradient plane is a very special case. The more general case with an initial orientation out of the xy -plane is now investigated. Of course, in this general case, the orientational dynamics needs the three components of the orientation vector to be characterized.

We first study the migration phenomenon. Let us start with the case of

a particle initially aligned along the vorticity axis, i.e., $\mathbf{p}_0 = (0, 0, 1)$. For symmetry, such initial orientation cannot change with time, and the particle undergoes the so-called ‘log-rolling’ motion around the z -axis. We carried out several simulations by varying the initial particle position $y_{p,0}$. The results are reported in Fig. 5a. At variance with the case of the major axis lying on the xy -plane, here we observe the coexistence of migration towards the centerplane and migration towards the wall. The separatrix is identified around $y_p = 0.34$. The long-time regimes are, then, expected to be a non-rotating particle with barycenter on the channel centerplane (for initial positions lower than the separatrix), and a particle in contact with the wall experiencing likely a rolling motion, similar to that one found for circular objects [23] (for initial positions between the separatrix and the wall).

Let us now consider the case of a particle initially oriented in the yz -plane. In this case, $\mathbf{p}_0$ is identified by a single angle θ_0 between the z -axis and $\mathbf{p}_0$, see Fig. 6b. Figure 5b shows the results for $\theta_0 = 60^\circ$ corresponding to an

initial orientation vector $\mathbf{p}_0 = (0, 3/2, 1/2)$. Similarly to the case of the spheroid initially aligned with the y -axis, the particle always migrates towards the centerplane. Of course, for this initial configuration, the orientational dynamics is more complex as compared to the log-rolling motion since the orientation vector goes out the yz -plane (see below).

By varying the angle θ_0 , we can compute the value of the separatrix (if any) and build the state diagram shown in Fig. 6a. The locus of points of the separatrix, denoted by the dashed-dotted red curve, is obtained according to the following procedure: (i) an angle θ_0 is fixed, (ii) several simulations by varying the initial position are run, (iii) two limiting initial positions such

that the migration has opposite direction are detected, (iv) the position of the separatrix is taken as the average of these two limiting initial positions. Since the step used to vary the initial positions is set (in dimensionless terms) to 0.01, the separatrix is detected within a tolerance of ± 0.005 .

The state diagram in Fig. 6a shows that an initial configuration $(\theta_0, y_{p,0})$ corresponding to a point below the dashed-dotted red line leads to migration towards the centerplane. On the contrary, in the region between the red and green curves (that, as above, delimits the channel region inaccessible by the particle), the particle migrates towards the wall. It can be readily seen that the spheroid prevalently migrates to the channel centerplane and, for angles θ_0 larger than about 30° , this is the only stable solution. For lower θ_0 -values, wall attraction is possible, although it is restricted to initial particle positions quite close to the wall. Notice that the dashed-dotted red curve is symmetric around the value $\theta_0 = 0^\circ$ since, for particles lying in the yz -plane, orientations at θ_0 and $-\theta_0$ are equivalent.

The just discussed ‘migration state diagram’ in Fig. 6a refers to a spheroid initially oriented in the yz -plane. Let us now consider the general case, where the particle can have an arbitrary initial orientation in space. The initial orientation must now be specified by two angles, which we choose as illustrated in Fig. 6c: ϕ_0 identifies the projection of $\mathbf{p}_0$ on the xz -plane, and θ_0 is the angle between such projection and $\mathbf{p}_0$ itself. We repeated the analysis of migration dynamics for various values of ϕ_0 by running, for each ϕ_0 , several simulations with different values of θ_0 and $y_{p,0}$. Results for the case $\phi_0 = 45^\circ$ are reported in Fig. 6a. It is found that the ‘migration state diagram’ stays essentially unaltered: the two bistability windows for $\phi_0 = 0^\circ$

Figure 6: (a) State diagram of particle migration. The dashed-dotted and dashed red curves, corresponding to $\phi_0 = 0^\circ$ and $\phi_0 = 45^\circ$ separate the plane of possible initial configurations in channel centerplane and wall attraction. The green shaded area is the channel region not accessible by the particle. (b)-(c) The two initial configurations considered in the state diagram.

and 45° almost coincide, with the separatrix for $\phi_0 = 45^\circ$ (dashed red line) very close to the one for $\phi_0 = 0^\circ$. Notice that, by further increasing the angle ϕ_0 , the wall attraction region must shrink since, for $\phi_0 = 90^\circ$, i.e., with the spheroid major axis lying in the xy -plane, no separatrix at all is found, as discussed in the previous section. At variance with the case $\phi_0 = 0$, initial orientations corresponding to two opposite angles θ_0 (i.e., with the spheroid major axis above or below the xz -plane) are not equivalent and, indeed, the particle trajectories (not shown) are qualitatively different. Nevertheless,

Figure 7: Snapshots of the dynamics of a spheroid initially orientated with the major axis on the yz -plane with $\theta_0 = 85^\circ$ and at a distance $y_{p,0} = 0.15$ from the centerplane. The Weissenberg number is $Wi = 0.5$. The red line denotes the trajectory of the particle barycenter. The green line is the orbit described by the tip of the orientation vector represented by the black line. For the sake of clarity, the x -axis has been shrunk.

the position of the separatrix nearly coincides, at least within the chosen tolerance. Hence, the dashed red line is not strictly symmetric around the value $\theta_0 = 0^\circ$ although deviations from the symmetric trend are extremely low. We can conclude that, for the parameters chosen here, a spheroid in a viscoelastic fluid flowing between two parallel plates under a pressure-driven flow migrates towards the channel centerplane for the most of its initial positions and orientations. Wall attraction is possible, but is restricted to a narrow set of initial configurations.

Two examples of the orientational dynamics for a spheroid with major axis out of the flow-gradient plane are shown in Figs. [7](#) and [8](#). In the first figure, the initial orientation vector lies on the yz -plane at an angle $\theta_0 = 85^\circ$

from the z -axis, i.e., very close to the y -axis. The initial distance from the channel centerplane is $y_{p,0} = 0.15$. The spheroid migrates towards the centerplane experiencing a tumbling-like motion. During the migration, the orientation vector slowly rotates and finally aligns along the flow direction. Figure 8 refers to an initial orientation vector still lying on the yz -plane but at an angle $\theta_0 = 25^\circ$ from the z -axis. The initial distance from the channel centerplane is $y_{p,0}$, the same as in the previous case, and migration is again towards the centerplane. Despite the initial orientation is now rather close to the z -axis, after few small-amplitude rotations around such axis, the particle tends to re-orient towards the flow direction. The re-orientation dynamics is extremely slow however. At the end of the simulations, the orientation vector is still far from being aligned with the x -axis.

The plots in Fig. 9 report the particle trajectories and the evolution of the orientation vector components for the two just discussed cases. Notice that the abscissa in these plots is the (dimensionless) coordinate of the particle barycenter along the flow direction. Panel (a) in Fig. 9 shows that, for both initial configurations, the migration occurs relatively fast: at a distance from the channel inlet of about 100 channel gaps, the particle barycenter reaches the centerplane. On the other hand, the channel length needed to attain the final orientation, which is along the x -axis in both cases, is strongly dependent on the initial orientation. A spheroid initially near to the velocity-gradient axis aligns to the flow direction in few hundreds of channel gaps. A much longer alignment distance is, instead, required for a spheroid initially oriented near to the ‘neutral’ z -axis. Panel (b) in Fig. 9 shows that, after a distance from the channel inlet of more than 600 channel gaps, the particle is still far from

Figure 8: Snapshots of the dynamics of a spheroid initially orientated with the major axis on the yz -plane with $\theta_0 = 25^\circ$ and at a distance $y_{p,0} = 0.15$ from the centerplane. The Weissenberg number is $Wi = 0.5$. The red line denotes the trajectory of the particle barycenter. The green line is the orbit described by the tip of the orientation vector represented by the black line. For the sake of clarity, the x -axis has been shrunk.

being reached its final orientation. i.e., the flow direction. Of course, a slow orientational dynamics has important implications in microfluidic applications. Just to give some figures, assuming a channel gap of 100 microns, a distance of 6 centimeters is not enough to observe a complete orientation of the spheroid starting at $\theta_0 = 25^\circ$. Extrapolating the trends in Fig. 9d, at least 15 centimeters are needed to achieve the orientation to the flow. Such alignment distance is expected to increase for spheroids with initial orientation vector closer to the z -axis, i.e., with $\theta_0 < 25^\circ$. The orientational dynamics has been also investigated for the general case of $\phi_0 > 0$. Similar trends to those shown in the previous figures are found. This is not unexpected since each point of the green orbits in Figs. 7 and 8 (except the first one) correspond to

Figure 9: (a) Trajectories of the barycenter of a spheroid with initial orientation vector on the yz -plane and an angle from the vorticity axis of $\theta_0 = 25^\circ$ and $\theta_0 = 85^\circ$. (b)-(c) Evolution of the orientation vector components for $\theta_0 = 25^\circ$ (b) and $\theta_0 = 85^\circ$ (c).

orientations out of the yz -plane. Thus, a particle initially oriented out of such plane feels about the same velocity field and undergoes a very similar dynamics (the only difference being that the viscoelastic stress tensor is in a free-state condition whereas, in the simulations in Figs. [7](#) and [8](#), it is to some

Figure 10: (a) Trajectories of the spheroid barycenter for different initial positions. The inset shows a closer look at initial times. The particle major axis is initially aligned along the y -axis. The Weissenberg number is $Wi = 1$. The green shaded area is the channel region not accessible by the particle relative to its initial configuration. (b)-(c) Evolution of the orientation vector components p_x and p_y for an initial position $y_{p,0} = 0.15$ (b) and $y_{p,0} = 0.25$ (c).

extent developed).

Finally, we have performed some simulations for $Wi = 1$. The results for a spheroid initially oriented with its major axis along the y -axis are shown in Fig. 10, which is the analogous of Fig. 3. A behavior qualitatively similar to the case $Wi = 0.5$ is found: the spheroid migrates towards the centerplane for any initial position in the gap, and experiences tumbling around the vorticity axis. The trajectories in Fig. 10a show that the migration phenomenon is, in dimensional terms, faster as compared to the case $Wi = 0.5$. Indeed, by comparing the time evolution of the orientation vector components between Figs. 10b-10c and Figs. 3b-3c, we observe that the spheroid experiences a lower number of complete rotations before aligning near to the flow direction, due to a faster transversal motion across the channel section.

We have also carried out some spot simulations (not shown) for initial orientations out of the flow-gradient plane. The results, again, qualitatively agree with those obtained for $Wi = 0.5$, confirming that the migration is mainly towards the centerplane and the particle slowly tends to align along the flow direction.

4. Conclusions

In this work, the dynamics of a spheroidal particle suspended in a viscoelastic, shear-thinning liquid flowing in a wide-slit microchannel is studied by direct numerical simulations. An Arbitrary Lagrangian-Eulerian formulation is used to manage the particle motion. Remeshing and projection are employed to account for mesh distortion.

Similarly to a spherical particle, the spheroid migrates transversally to

the flow direction. In some situations, migration can be towards the channel centerplane or the closest wall, depending on the initial distance from the centerplane and the initial particle orientation. The centerplane of the channel, however, is by far the most probable final destination of the spheroid migration. Specifically, wall attraction is limited to a narrow set of initial configurations, with particles close to the wall, and oriented with their major axis around the ‘neutral’ direction z of the Poiseuille flow. Regarding orientational dynamics, for the parameters and initial orientations considered in our simulations, we found that the particle always tends to align along the flow direction. Such alignment process is much slower than migration and, for initial orientations close to the neutral direction, many hundreds of channel gaps are required to reach the final orientation.

The results presented in this work have been carried out for low and moderate values of the Weissenberg number. For those cases, the translational and rotational dynamics are qualitatively similar. However, previous studies in (unconfined) shear flow evidenced that, by increasing the Weissenberg number, the orientational behavior of the spheroid changes, with a rich dynamical scenario [24, 16]. Hence, we plan to extend the present simulations to higher Weissenberg numbers. Geometrical properties (confinement and particle aspect ratio) and fluid rheology (e.g., shear-thinning) are also expected to have an influence on the spheroid motions, and their effects deserve further investigation. Simulations at high Weissenberg numbers as well as at higher confinements or aspect ratios will likely require finer meshes. Optimization of the existing code and evaluation of more efficient solvers will then also be part of future work.

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