Cross-stream migration of non-spherical particles in a second-order fluid – theories of particle dynamics in arbitrary quadratic flows

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Particle migration in viscoelastic suspensions is vital in many applications in the biomedical community and the chemical/oil industries. Previous studies have provided insight into the motion of spherical particles in simple viscoelastic flows, yet the combined effect of more complex flow profiles and particle shapes is under-explored. Here, we develop approximate analytical expressions for the polymeric force and torque on an arbitrarily shaped particle in a second-order fluid, subject to a general quadratic flow field. This model is exact for the case when the first and second normal stress coefficients satisfy $\psi_1 = -2\psi_2$. Under this assumption, we examine how particle shape alters cross-stream particle migration (i.e. lift) and particle orientation in both shear- and pressure-driven flows. In shear-driven flows, we observe that spheroidal particles adjust their orientation to align their longer axis along the vorticity direction, although significant deviations from slender-body theories occur for finite aspect ratios. In a slit-like pressure-driven flow, we identify scaling theories to quantify how the particle lift depends on shape for a wide variety of shapes. We find that prolate particles slowly transition to a log-rolling state as they approach the flow centre, with the lift initially being larger than that of an equal-volume sphere, but then becoming smaller as log-rolling emerges. The net effect is a smaller average migration speed for particles with larger aspect ratio. Lastly, we discuss future directions for experimental studies on particle dynamics as well as directions to extend the current work towards more complicated systems.

\textbf{Key words:} microfluidics, viscoelasticity

1. Introduction

Particle focusing refers to the cross-streamline migration of particles and the formation of specific patterns in channels due to flow forces. Cross-flow migration may arise due to fluid inertia (Segré & Silberberg 1961) or viscoelastic forces developed by non-Newtonian fluids (Karnis & Mason 1966). The phenomenon has received much attention in recent years due to its potential in a wide range of applications, such as developing high-throughput, marker-free particle separation techniques in microfluidic platforms (Yang \textit{et al.} 2011; Li \textit{et al.} 2016; Nam \textit{et al.} 2016; Liu \textit{et al.} 2017) and

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designing compact, high-accuracy microfluidic flow cytometers for particle and cell characterization (Bhagat et al. 2010; Asghari et al. 2017). In many cases, viscoelastic focusing can be advantageous due to its tendency to form a single focusing line in the channels (D’Avino, Greco & Maffettone 2017). Here we focus our discussions on particle migration in such fluids.

Fluid rheology and particle properties (e.g. size, morphology and deformability) are major factors that affect the particle migration behaviour in non-Newtonian fluids. Currently there are numerous experimental studies that provide detailed information on the effects of fluid rheology on particle focusing (Leshansky et al. 2007; Lee et al. 2013; Del Giudice et al. 2015; Kim & Kim 2016). In general, particles migrate to regions of lowest normal stress difference in channel flows. In pure elastic fluids, this corresponds to the channel centre, while for shear-thinning fluids, the focusing position is closer to the channel wall (Lim et al. 2014; Seo et al. 2014; Del Giudice et al. 2017). For the effect of particle properties on focusing behaviour, however, many questions remain unanswered. For example, recent experiments have shown that particle shape has a significant effect on cross-stream migration (Lu & Xuan 2015; Lu et al. 2015; D’Avino et al. 2017; Yuan et al. 2018), yet the vast majority of previous theories examine the motion of spherical particles in viscoelastic flows (Ho & Leal 1976; Brunn 1976, 1977; Ardekani, Rangel & Joseph 2007), with limited information available on rods and disks (Gauthier, Goldsmith & Mason 1971; Bartram, Goldsmith & Mason 1975; Leal 1975).

For an ellipsoid particle, which is the simplest deviation from sphericity, previous theories provided solutions for the polymeric force and torque on a slightly deformed sphere in shear flow (Brunn 1979) and an ellipsoid under sedimentation (Kim 1986), all using a second-order fluid model. Several numerical studies were also conducted on the dynamics of a settling ellipsoid in a second-order fluid under the influence of weak inertial and viscoelastic effects using a double perturbation expansion on the Reynolds number $Re$ and Deborah number $De$ (Feng et al. 1995; Dabade, Marath & Subramanian 2015). For the sedimentation problem, the steady orientation of the settling spheroid due to the fluid viscoelasticity has been studied in terms of the particle geometry (i.e. aspect ratio) for arbitrary ratios between the first and second normal stress coefficients (Dabade et al. 2015). More recent works simulated the motion of an ellipsoid in a three-dimensional shear flow (D’Avino et al. 2014) and a pressure-driven slit flow (D’Avino et al. 2019) using a Giesekus fluid model (i.e. a fluid that exhibits shear-thinning). With the notable exception of D’Avino et al. (2019), we note that almost all previous theories of non-spherical particles examine their motions in linear flow fields, but neglect higher-order (i.e. pressure-driven) flows where gradients in shear rate would exist, and hence normal stress gradients and lateral migration would occur. Studies providing such information will be vital in a wide range of applications, such as particle separation in microfluidic devices as well as fibre migration in viscoelastic flows found in the chemical and oil/gas industries.

In this work, we investigate the motion of a rigid, arbitrarily shaped particle in a viscoelastic fluid subject to a general quadratic flow field (i.e. linear plus quadratic flow in an unbound space). By assuming steady flow with negligible fluid and particle inertia, we apply the second-order fluid model to characterize the fluid viscoelasticity, which faithfully describes the rheological behaviour of any non-Newtonian fluid in the slow flow limit (Weissenberg number $Wi \ll 1$) (Coleman & Noll 1960; Bird, Curtiss & Armstrong 1987; Rivlin & Ericksen 1997). For the two model constants $\psi_1$ and $\psi_2$ (first and second normal stress coefficients), we further assume the relationship $\psi_1 = -2\psi_2$. Under this condition, the dynamics will behave as a Stokes flow with a
modified fluid pressure, which allows one to qualitatively capture the essential physics and greatly simplifies the mathematical procedure. We use a multipole expansion for Stokes flow as well as a symmetry analysis to derive the analytical solutions for the polymeric force and torque on an arbitrarily shaped particle. We establish a boundary element method (BEM) numerical framework to verify our calculations, and we apply our model to study the motion of general ellipsoids in a second-order fluid. The work here will allow one to gather vital insights as to how particle orientability and aspect ratio alter their tumbling dynamics and cross-stream migration in pressure-driven flows.

The outline of this paper is as follows. Section 2 provides the problem set-up, methodology and solution strategy. Section 3 studies the migration behaviour of general ellipsoids (sphere, spheroid and ellipsoid) in a quadratic flow of a second-order fluid. In § 3.2, we first verify that our theory matches the exact solutions of spheres in a linear flow (Brunn 1977) and numerical solutions of spheres in a quadratic flow. In § 3.3, we show that our theories qualitatively capture the experimental orientation dynamics of spheroidal particles under shear flows, such as tumbling and log-rolling (Bartram et al. 1975; Gunes et al. 2008). In § 3.4.1, we examine the translation and rotation of force-free, torque-free ellipsoids in a pressure-driven flow under different particle orientations, to help identify scaling theories for particle mobility under different morphologies (tumbling versus log-rolling). In § 3.4.2, we track the migration and orientation trajectories of ellipsoids in a pressure-driven flow, to see which regime (tumbling versus log-rolling) dominates in the overall cross-stream migration process. Our results are checked using our BEM numerical framework. Section 4 summarizes the current work and discusses the future directions towards more complicated systems.

2. Dynamics of an arbitrarily shaped particle in a second-order fluid

2.1. System set-up and definitions

We consider a rigid, arbitrarily shaped particle in a general quadratic flow field as shown below:

\[ u_i^\infty = u_i^c + \Gamma_{ij}^{(2)} x_j + \frac{1}{2} \Gamma_{ijk}^{(3)} x_j x_k. \]  

(2.1)

In this equation, the first, second and third terms on the right-hand side represent the constant, linear and quadratic parts of the flow profile, respectively. The position vector pointing from the particle’s centre of mass is \( x_i \), and the flow parameters \( u_i^c \), \( \Gamma_{ij}^{(2)} \) and \( \Gamma_{ijk}^{(3)} \) are given by

\[ u_i^c = u_i^\infty |_{x_i=0}, \quad \Gamma_{ij}^{(2)} = \left. \frac{\partial u_i^\infty}{\partial x_j} \right|_{x_i=0}, \quad \Gamma_{ijk}^{(3)} = \left. \frac{\partial u_i^\infty}{\partial x_j \partial x_k} \right|_{x_i=0}, \]  

(2.2a–c)

where the quantities are evaluated at \( x_i = 0 \).

We would like to evaluate the polymeric force and torque on a freely suspended particle (i.e. polymeric force/torque is balanced by the Newtonian force/torque). We assume the surrounding fluid to be incompressible, and the inertia of the fluid and particle to be negligible. Far away from the particle, the fluid velocity field is \( u_i \to u_i^\infty \). At finite distances from the particle, the fluid velocity satisfies

\[ \frac{\partial u_i}{\partial x_j} = 0, \]  

(2.3)
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\[
\frac{\partial T_{ij}}{\partial x_j} = 0, \quad (2.4)
\]

where \( T_{ij} \) is the total stress tensor of the fluid. For a second-order fluid, the total stress tensor \( T_{ij} \) is given by

\[
T_{ij} = -P \delta_{ij} + \mu \dot{\gamma}_{ij} - \frac{\psi_1}{2} \frac{\gamma_{ij}}{\gamma^2} \left[ \frac{D \gamma_{ij}}{Dt} + \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} - \frac{\partial u_j}{\partial x_k} \frac{\partial u_i}{\partial x_k} \right], \quad (2.5)
\]

where \( P \) is the fluid pressure, \( \mu \) is the zero-shear total viscosity and \( \dot{\gamma}_{ij} \) is twice the strain rate of the flow,

\[
\dot{\gamma}_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}. \quad (2.6)
\]

In the above, \( \gamma_{ij} \) represents the upper-convected time derivative of \( \dot{\gamma}_{ij} \), defined as

\[
\frac{\gamma_{ij}}{\gamma^2} = \frac{D \dot{\gamma}_{ij}}{Dt} - \dot{\gamma}_{jk} \frac{\partial u_i}{\partial x_k} - \dot{\gamma}_{ik} \frac{\partial u_j}{\partial x_k}, \quad (2.7)
\]

where \( D/Dt = \partial/\partial t + u_i \partial/\partial x_i \) is the substantial derivative.

The quantities \( \psi_1 \) and \( \psi_2 \) are the first and second normal stress coefficients, which monitor the normal stress differences in flow–shear and shear–vorticity directions, respectively. For example, let \( x, y \) and \( z \) directions represent the flow, shear gradient and vorticity directions, respectively. In a simple shear flow defined by \( u_x = \dot{\gamma} y \), the normal stress coefficients are defined by

\[
\psi_1 = \frac{T_{xx} - T_{yy}}{\dot{\gamma}^2}, \quad \psi_2 = \frac{T_{yy} - T_{zz}}{\dot{\gamma}^2}. \quad (2.8a,b)
\]

For most realistic polymer solutions, \( \psi_1 \) is experimentally found to be positive and \( \psi_2 \) to be negative (Bird & Wiest 1995). The magnitude of \( \psi_2 \) is also found to be much smaller than \( \psi_1 \), with a typical value \(-1/6 < \psi_2/\psi_1 < 0 \) (Ho & Leal 1976). In our analysis, we make the simplifying assumption \( \psi_1 = -2\psi_2 \), i.e. the Weissenberg approximation (Ardekani, Rangel & Joseph 2008). Despite the fact that the assumption overestimates the second normal stress difference, this nevertheless allows one to make significant analytical progress and qualitatively extract the essential physics.

The expression for \( T_{ij} \) is now

\[
T_{ij} = -P \delta_{ij} + \mu \dot{\gamma}_{ij} - \frac{\psi_1}{2} \frac{\gamma_{ij}}{\gamma^2} \left[ \frac{D \gamma_{ij}}{Dt} + \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} - \frac{\partial u_j}{\partial x_k} \frac{\partial u_i}{\partial x_k} \right], \quad (2.9)
\]

By (2.9), for a system with characteristic velocity \( u^m \), characteristic length \( L \) and pressure \( \mu u^m/L \), we define the polymer relaxation time \( \lambda \) to be \( \lambda = \psi_1/2\mu \) and the Weissenberg number of the system to be \( Wi = \psi_1 u^m/\mu L \). We note that the second-order fluid model is valid only when \( Wi < 1 \) (i.e. flow time scale is longer than polymer relaxation time). In the following studies, we will make such restriction to ensure the validity of the model.

By substituting (2.9) into (2.4), we get

\[
\frac{\partial}{\partial x_i} \left[ -P + P^N - \frac{\psi_1}{2} \left( \frac{1}{\mu} \frac{DP^N}{Dt} + \frac{1}{4} \dot{\gamma}_{ij} \dot{\gamma}_{jk} \right) \right] = 0, \quad (2.10)
\]
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where $P^N$ is the pressure in a Newtonian fluid, satisfying

$$\frac{\partial P^N}{\partial x_i} = \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \quad (2.11)$$

Equation (2.10) implies:

$$P = P^N - \frac{\psi_1}{2} \left( \frac{1}{\mu} \frac{D P^N}{D t} + \frac{1}{4} \dot{\gamma}_{kj} \dot{\gamma}_{jk} \right). \quad (2.12)$$

The above equation indicates that, under the assumption $\psi_1 = -2\psi_2$, the flow $u_i$ around the particle is the same as that in Stokes flow, but with a modified fluid pressure $P$.

2.2. Integral expressions for polymeric force/torque on particle

To evaluate the polymeric force $F^p_i$ and torque $T^p_i$ on the particle (i.e. the force/torque in excess of the Newtonian contribution), we first construct a control volume $V$ containing the particle with its surface denoted as $S_\infty$. We also define the particle surface to be $S_p$. The outward normals on $S_\infty$ and $S_p$ are denoted as $n^\infty_i$ and $n^p_i$, respectively. Figure 1 shows the system set-up.

From (2.4) we know that

$$\int_V \frac{\partial T_{ij}}{\partial x_j} \, dV = 0. \quad (2.13)$$

By the divergence theorem, we get

$$\int_{S_\infty} T_{ij} n^\infty_j \, dS = \int_{S_p} T_{ij} n^p_j \, dS. \quad (2.14)$$

Equation (2.14) indicates that the force on the particle can be evaluated over any closed surface $S_\infty$ as long as it completely contains the particle. This statement is true for torque as well. Next, we extract the polymeric contribution to the total stress tensor $T_{ij}$ and perform integration over a spherical surface $S_\infty$ containing the particle:
\[ \frac{2}{\psi_1} F_i^p = \int_{S_\infty} \left( \frac{1}{\mu} \frac{\partial P^N}{\partial t} \delta_{ij} - \frac{\partial \gamma_{ij}}{\partial t} \right) n_j^\infty \, dS + \int_{S_\infty} \left( \frac{1}{\mu} \frac{\partial P^N}{\partial x_m} \delta_{ij} - \frac{u_m}{\partial x_m} \frac{\partial \gamma_{ij}}{\partial x_m} \right) n_j^\infty \, dS, \]
\[ + \int_{S_\infty} \left( \frac{1}{4} \gamma_{km} \gamma_{mk} \delta_{ij} - \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} + \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \right) n_j^\infty \, dS, \tag{2.15} \]
\[ \frac{2}{\psi_1} T_i^p = \int_{S_\infty} \varepsilon_{ijk} \left( \frac{1}{\mu} \frac{\partial P^N}{\partial \delta_{kp}} - \frac{\partial \gamma_{kp}}{\partial t} \right) n_p^\infty \, dS \]
\[ + \int_{S_\infty} \varepsilon_{ijk} \left( \frac{1}{\mu} \frac{\partial P^N}{\partial x_m} \delta_{kp} - u_m \frac{\partial \gamma_{kp}}{\partial x_m} \right) n_p^\infty \, dS \]
\[ + \int_{S_\infty} \varepsilon_{ijk} \left( \frac{1}{4} \gamma_{nm} \gamma_{m} \delta_{kp} - \frac{\partial u_m}{\partial x_k} \frac{\partial u_m}{\partial x_p} + \frac{\partial u_k}{\partial x_m} \frac{\partial u_p}{\partial x_m} \right) n_p^\infty \, dS. \tag{2.16} \]

By employing the divergence theorem, the polymeric force and torque expressions can be modified to
\[ \frac{2}{\psi_1} F_i^p = \int_{S_\infty} \left( \frac{1}{\mu} \frac{\partial P^N}{\partial t} \delta_{ij} - \frac{\partial \gamma_{ij}}{\partial t} \right) n_j^\infty \, dS \int_{S_\infty} \frac{1}{\mu} \frac{\partial u_m}{\partial x_j} (P^N \delta_{ij} - \mu \gamma_{ij}) n_m^\infty \, dS \]
\[ + \int_{S_\infty} \left( \frac{1}{4} \gamma_{km} \gamma_{mk} \delta_{ij} - \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} + \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \right) n_j^\infty \, dS, \tag{2.17} \]
\[ \frac{2}{\psi_1} T_i^p = \int_{S_\infty} \varepsilon_{ijk} \left( \frac{1}{\mu} \frac{\partial P^N}{\partial \delta_{kp}} - \frac{\partial \gamma_{kp}}{\partial t} \right) n_p^\infty \, dS \int_{S_\infty} \varepsilon_{ijk} \frac{\partial u_m}{\partial x_p} \left( \frac{1}{\mu} P^N \delta_{kp} - \gamma_{kp} \right) n_m^\infty \, dS \]
\[ - \int_{S_\infty} \varepsilon_{Imk} \left( \frac{1}{\mu} P^N \delta_{kp} - \gamma_{kp} \right) u_m n_p^\infty \, dS \]
\[ + \int_{S_\infty} \varepsilon_{ijk} \left( \frac{1}{4} \gamma_{nm} \gamma_{m} \delta_{kp} - \frac{\partial u_m}{\partial x_k} \frac{\partial u_m}{\partial x_p} + \frac{\partial u_k}{\partial x_m} \frac{\partial u_p}{\partial x_m} \right) n_p^\infty \, dS. \tag{2.18} \]

Equations (2.17) and (2.18) allow us to solve for the polymeric force and torque once we acquire information on the velocity field \( u \) and pressure field \( P^N \), which are the velocity and pressure fields for the Stokes flow past the particle in the same geometry. In §2.3 we employ a multipole expansion to obtain these fields and hence simplify the analytical expressions for the polymeric force and torque.

### 2.3. Multipole expansion and symmetry analysis – analytical solution to resistance functions for arbitrarily shaped particles

For a Newtonian fluid in the creeping flow regime, the fluid disturbance velocity and pressure fields far away from the particle surface can be expressed using a multipole expansion (Kim & Karrila 2013) as
\[ \begin{align*}
    u_i - u_i^\infty &= -\frac{1}{8\pi \mu} F^{(1)}_j G_{ji} + \frac{1}{8\pi \mu} F^{(2)}_j \frac{\partial G_{ij}}{\partial x_k} - \frac{1}{16\pi \mu} F^{(3)}_{jkm} \frac{\partial G_{ij}}{\partial x_k \partial x_m} + \cdots, \\
    P^N - P^{N\infty} &= -\frac{1}{8\pi} F^{(1)}_j \pi_j + \frac{1}{8\pi} F^{(2)}_j \frac{\partial \pi_j}{\partial x_k} - \frac{1}{16\pi} F^{(3)}_{jkm} \frac{\partial \pi_j}{\partial x_k \partial x_m} + \cdots,
\end{align*} \tag{2.19, 2.20} \]

where \( G_{ij} \) and \( \pi_j \) are the Green’s functions for velocity and pressure, respectively. The expressions \( F^{(n)}_{k_1 \ldots k_n} \) are the force moments (i.e. monopole, dipole, etc.) on the particle
in Stokes flow. Thus

\[
G_{ij} = \frac{\delta_{ij}}{r} + \frac{x_i x_j}{r^3}, \quad \pi_i = \frac{2x_i}{r^3}, \quad r = (x_i x_i)^{1/2},
\]

\[
F_{x_{k_1} \ldots x_{k_n}}^{(n)} = \int_{S_p} (\sigma_{k_1 m}^{N} n_m^o) x_{k_2} \cdots x_{k_n} \, dS,
\]

\[
\sigma_{ij}^N = -P^N \delta_{ij} + \mu \dot{\gamma}_{ij},
\]

\[
- \frac{\partial P^N}{\partial x_i} + \mu \frac{\partial^2 u^\infty}{\partial x_j \partial x_j} = 0.
\]

Equations (2.19) and (2.20) hold for any particle shape as long as the position is far away from the particle surface.

We will evaluate an analytical expression for the polymer force and torque in (2.17) and (2.18) by substituting the far-field velocity and pressure fields in (2.19) and (2.20). To simplify the mathematics, we note that only a small number of terms will contribute to the integrals. Since the integrals are evaluated on a spherical surface far away from the particle (i.e. \( r \to \infty \)), one should expect only the terms of \( O(r^{-1}) \) in the integrand of (2.17) and (2.18) to contribute to the polymeric force and torque since the surface element \( dS \) is proportional to \( r^2 \).

For the integrals in (2.17), we find that the following vector and tensor combinations will contribute to the polymeric force:

\[
\frac{\partial F^{(1)}_{ij}}{\partial t}, \quad \Gamma^{(2)}_{ij} F^{(1)}_k, \quad \Gamma^{(3)}_{ijk} F^{(2)}_{mp},
\]

Following the same ideas, we expect the terms of \( O(r^{-2}) \) in the integrand of (2.18) will contribute to the polymeric torque:

\[
\frac{\partial T^N}{\partial t}, \quad F^{(3)}_{imk} \Gamma^{(3)}_{pqj}, \quad F^{(2)}_{ik} \Gamma^{(2)}_{mj}, \quad u^c_i F^{(1)}_{ij}.
\]

Next we perform tensor decomposition of the force moments \( F^{(2)}_{ij}, F^{(3)}_{ijk} \) and external velocity gradients \( \Gamma^{(2)}_{ij}, \Gamma^{(3)}_{ijk} \) into irreducible forms:

\[
\Gamma^{(2)}_{ij} = E_{ij} - \varepsilon_{ijk} \Omega_k, \tag{2.22}
\]

\[
F^{(2)}_{ij} = S_{ij} - \frac{1}{2} \varepsilon_{ijk} T^N_i, \tag{2.23}
\]

\[
\Gamma^{(3)}_{ijk} = \Gamma^{(3)'}_{ijk} - \frac{1}{6} \Omega_{im} \varepsilon_{mjk} - \frac{1}{3} \Omega_{km} \varepsilon_{mij} + \frac{1}{10} (-\tau_k \delta_{ij} - \tau_j \delta_{ik} + 4 \tau_i \delta_{jk}), \tag{2.24}
\]

\[
F^{(3)}_{ijk} = F^{(3)'}_{ijk} - \frac{1}{6} \Theta_{im} \varepsilon_{mjk} - \frac{1}{3} \Theta_{km} \varepsilon_{mij} + \frac{1}{10} (-H_k \delta_{ij} - H_j \delta_{ik} + 4 H_i \delta_{jk})
\]

\[
+ \frac{1}{10} (3 B_k \delta_{ij} + 3 B_j \delta_{ik} - 2 B_i \delta_{jk}). \tag{2.25}
\]

The right-hand sides of (2.22)–(2.25) are the irreducible elements of the force moments and the external velocity gradients. For example, \( E_{ij} \) and \( \Omega_i \) are the rate of strain and angular velocity of the external flow, while \( S_{ij} \) and \( T^N_i \) are the stresslet and torque in a Newtonian fluid. The definitions of each of the irreducible elements are detailed in tables 1 and 2.

Based on the decomposition, the following combinations of the irreducible tensors can possibly contribute to the polymeric force:
The polymeric force and torque will be a linear combination of the terms listed above. To determine the coefficients for each possible combination, for instance \( E_{ij} F_j^{(1)} \), we choose the force moments and external velocity gradients such that the only contribution to the polymeric force and torque will come from \( E_{ij} F_j^{(1)} \), and then directly integrate (2.17) and (2.18). Repeating this procedure for all possible tensor combinations, we have the following expressions for the polymeric force and torque:

\[
\frac{2\mu}{\psi_1} F_i^p = \frac{\partial F_i^{(1)}}{\partial t} - E_{ij} F_j^{(1)} - \varepsilon_{ijk} F_j^{(1)} \Omega_k - \Gamma_{ijk}^{(3)} \frac{\partial S_{ij}}{\partial t} - \frac{3}{10} S_{ij} \tau_j \]

\[
+ \frac{1}{6} \varepsilon_{ijk} \Omega_{jm} S_{mk} + \frac{1}{4} \varepsilon_{ijk} T_j^N \tau_k - \frac{1}{4} \Omega_{ij} T_j^N,
\]

\[
\frac{2\mu}{\psi_1} T_i^p = \frac{\partial T_i^{(1)}}{\partial t} + \varepsilon_{ijk} u_j^p F_k^{(1)} + 2 \varepsilon_{ijk} E_{jm} S_{mk} - \varepsilon_{ijk} T_j^N \Omega_k + \frac{3}{2} \varepsilon_{ijk} \Gamma_{jpq}^{(3)} F_p^{(3)}
\]

\[
+ \frac{1}{2} \varepsilon_{ijk} \tau_j H_k - \frac{1}{10} \varepsilon_{ijk} \tau_j B_k + \frac{1}{6} \varepsilon_{ijk} \Omega_{jm} \Theta_{mk}.
\]
This is one of the main results of this paper. The effect of particle shape comes through the force moments \( F_i^{(1)}, S_{ij}, T_i^{N} \) on the particle in Stokes flow, which are related to the external flow fields \( (u_i^e, E_{ij}, \Omega_i, \ldots) \) through a resistance matrix. For example, if we are examining a sphere of radius \( R \) in an external flow, the force moments come from the Stokes drag/torque/stresslet formulae: 
\[
F_i^{(1)} = 6 \pi \mu R (u_i^e - U_i), \quad T_i^{N} = 8 \pi \mu R^3 (\Omega_i - \omega_i), \quad S_{ij} = (20 \pi / 3) \mu R^3 E_{ij}, \quad \text{etc.}
\]
where \( U_i \) and \( \omega_i \) are the translational and rotational velocities of the particle. If we are examining a slender body of length \( L \), aspect ratio \( A_R \) and orientation vector \( p_i \), the force moments come from slender-body theory: 
\[
F_i^{(1)} = (4 \pi \mu L / \ln(2A_R)) [\delta_{ij} - \frac{1}{2} p_i p_j] (u_i^e - U_i), \quad T_i^{N} = (\pi \mu L^3 / (3 \ln(2A_R))) [\delta_{ij} - \frac{1}{2} p_i p_j] (\Omega_j - \omega_j) - \epsilon_{ijk} p_j E_{kn} p_m, \quad \text{etc.}
\]
The main point to take away from this section is that, if one knows the force/torque/stresslet, etc. on an arbitrarily shaped particle in a Newtonian fluid, one can determine the polymeric force and torque on the same particle using formulae (2.26) and (2.27). We note that the methodologies applied in this and the following section are only valid when we impose the assumption \( \psi_1 = -2 \psi_2 \), under which the flow dynamics can be analysed using the linear superposition techniques developed from the Stokes flows. The analysis techniques are not valid for the general case \( \psi_1 \neq -2 \psi_2 \), where the flow dynamics are nonlinear. We further note that the time-dependent terms \( \partial F_i^{(1)} / \partial t \) and \( \partial T_i^{N} / \partial t \) in (2.26) and (2.27) will be negligible for a force/torque-free particle. In § 2.4 we perform a perturbation expansion analysis to clarify this idea.

### 2.4. Perturbation expansion analysis

For a system as defined in § 2.1, when force/torque-free, the total force and torque on the particle are identically zero:
\[
F_i^{(1)} + F_i^0 = 0, \quad T_i^{N} + T_i^0 = 0. \tag{2.28a,b}
\]
We perform a perturbation expansion on the particle’s translational and rotational velocities \( (U_i, \omega_i) \) using the small parameter \( Wi \):
\[
\begin{align*}
U_i & = U_i^{[0]} + Wi U_i^{[1]} + \cdots, \\
\omega_i & = \omega_i^{[0]} + Wi \omega_i^{[1]} + \cdots
\end{align*}
\tag{2.29}
\]
where \( U_i^{[n]} \) and \( \omega_i^{[n]} \) represent the particle’s translational and rotational velocities at \( O(Wi^n) \). Our goal is to obtain the \( O(Wi) \) correction to the particle motion.

If we scale all velocities by a characteristic scale \( u_m \), all lengths by a characteristic length \( L \), times and rotational velocities by \( L / u_m \), forces by \( \mu u_m L \) and torques by \( \mu u_m L^2 \), the force/torque-free requirement indicates that the Newtonian force and torque at leading order are identically zero:
\[
F_i^{(1),[0]} = 0, \quad T_i^{N,[0]} = 0. \tag{2.30a,b}
\]
At \( O(Wi) \), the Newtonian force/torque evaluated using \( U_i^{[1]} \) and \( \omega_i^{[1]} \) are in balance with the polymeric force/torque evaluated using \( U_i^{[0]} \) and \( \omega_i^{[0]} \):
\[
\begin{align*}
F_i^{(1),[1]} + F_i^{p,[0]} & = 0, \\
T_i^{N,[1]} + T_i^{\psi,[0]} & = 0.
\end{align*}
\tag{2.31}
Owing to the Newtonian force/torque vanishing at \(O(1)\), the time-dependent terms \(\partial F_i^{(1)} / \partial t\) and \(\partial T_i^{(1)} / \partial t\) will vanish in the polymeric force and torque expression in (2.31). Thus, for a viscoelastic fluid in the limit of small Weissenberg number (\(Wi \ll 1\)) and co-rotational limit (\(\psi_1 = -2\psi_2\)), the polymer stresses and pressures will be unsteady, but the unsteady effects will cancel out when computing the polymer force and torque to \(O(Wi)\). This argument is consistent with Brunn (1977), where he also investigated the dynamics of a rigid particle under these same assumptions and found that the force and torque appear steady at \(O(Wi)\).

In § 2.5, we will introduce the resistance matrix of a general ellipsoid in Stokes flow, and use (2.26) and (2.27) to calculate its motion in a second-order fluid when \(\psi_1 = -2\psi_2\) under a general quadratic flow field. We will use boundary element simulations in § 2.6 to verify the results shown here.

### 2.5. Resistance matrix for a general ellipsoid in Stokes flow

We extend the original resistance relationship in Kim & Karrila (2013) to consider the motion of an arbitrarily shaped particle in a quadratic flow:

\[
\begin{pmatrix}
F^{(1)} \\
T^{(1)} \\
S \\
F^{(3)}
\end{pmatrix} = \mu \begin{pmatrix}
A & B & G & O \\
B & C & M & Q \\
G & M & N & R \\
O & Q & R & V
\end{pmatrix} \begin{pmatrix}
u^t - U \\
\Omega - \omega \\
E \\
\Gamma^{(3)}
\end{pmatrix},
\]

where \(U\) and \(\omega\) denote the translation and rotation of the particle, respectively. Specifically, the resistance matrix can be written in index notation:

\[
\begin{align*}
F_i^{(1)} &= \mu A_{ij}(u_i^t - U_j) + \mu B_{ij}(\Omega_j - \omega_j) + \mu G_{ijk}E_{jk} + \mu O_{ijkl}\Gamma^{(3)}_{ijkl}, \\
T_i^{(1)} &= \mu B_{ij}(u_i^t - U_j) + \mu C_{ij}(\Omega_j - \omega_j) + \mu M_{ijk}E_{jk} + \mu Q_{ijkl}\Gamma^{(3)}_{ijkl}, \\
S_{ij} &= \mu G_{ijk}(u_k^t - U_k) + \mu M_{ijk}(\Omega_k - \omega_k) + \mu N_{ijkl}E_{kl} + \mu R_{ijklw}\Gamma^{(3)}_{klw}, \\
F_{ij}^{(3)} &= \mu O_{ij}(u_i^t - U_j) + \mu Q_{ijkl}(\Omega_l - \omega_l) + \mu R_{ijklw}E_{lw} + \mu V_{ijklw}\Gamma^{(3)}_{lw}.
\end{align*}
\]

For a general triaxial ellipsoid, one obtains

\[
\begin{align*}
\tilde{B}_{ij} &= B_{ij} = 0, \\
\tilde{G}_{ijk} &= G_{ijk} = 0, \\
\tilde{Q}_{ijkl} &= Q_{ijkl} = 0, \\
\tilde{R}_{ijklw} &= R_{ijklw} = 0.
\end{align*}
\]

Therefore, the resistance relationship can be simplified as

\[
\begin{align*}
F_i^{(1)} &= \mu A_{ij}(u_i^t - U_j) + \mu \tilde{O}_{ijkl}\tilde{\Gamma}^{(3)}_{ijkl}, \\
T_i^{(1)} &= \mu C_{ij}(\Omega_j - \omega_j) + \mu M_{ijk}E_{jk}, \\
S_{ij} &= \mu M_{ijk}(\Omega_k - \omega_k) + \mu N_{ijkl}E_{kl}, \\
F_{ij}^{(3)} &= \mu O_{ij}(u_i^t - U_j) + \mu V_{ijklw}\Gamma^{(3)}_{lw}.
\end{align*}
\]

In (2.34), the coefficients \(A_{ij}, C_{ij}\) and \(M_{ijk}\) have been detailed in Kim & Karrila (2013); and \(O_{ijkl}\) and \(V_{ijklw}\) are provided in Wang, Martin & Kim (2019). For completeness, the relationships are provided as follows:

\[
F_i^{(1)} = \mu \frac{16\pi abc}{\chi_0 + \alpha_0 a^2} (u_i^t - U_i) + \mu \frac{16\pi abc a_k^2\Gamma^{(3)}_{ijkl}}{\chi_0 + \alpha_0 a^2},
\]
The quadrature scheme is given in Pozrikidis (2002).

\[
T_z^N = \mu \frac{16\pi abc}{3(a^2\alpha_o + b^2\beta_o)} \left[ (a^2 + b^2)(\Omega_z - \omega_z) + (a^2 - b^2)E_{xy} \right],
\]
(2.36)

\[
S_{xx} = \frac{16\pi abc}{9(\beta''_o\gamma''_o + \gamma''_o\alpha''_o + \alpha''_o\beta''_o)} \left[ 2\alpha''_o E_{xx} - \beta''_o E_{yy} - \gamma''_o E_{zz} \right],
\]
(2.37)

\[
S_{xy} = S_{yx} = \frac{8\pi abc}{3(a^2\alpha_o + b^2\beta_o)} \left[ (a^2 - b^2)(\Omega_z - \omega_z) + \frac{\alpha_o + \beta_o}{\gamma'_o} E_{xy} \right],
\]
(2.38)

where

\[
\chi_o = abc \int_0^\infty \frac{dt}{\Delta(t)}, \quad \alpha_o = abc \int_0^\infty \frac{dt}{(a^2 + t)\Delta(t)},
\]
(2.39a,b)

\[
\alpha'_o = \frac{\gamma_o - \beta_o}{b^2 - c^2}, \quad \alpha''_o = \frac{b^2\beta_o - c^2\gamma_o}{b^2 - c^2},
\]
(2.39c,d)

\[
\Delta(t) = \sqrt{(a^2 + t)(b^2 + t)(c^2 + t)}.
\]
(2.39e)

and \(a, b\) and \(c\) are the length of the semi-axes of an ellipsoid in \(x, y\) and \(z\) directions, respectively. Note that other components can be realized by index cycling.

### 2.6. Boundary element simulations

We will use the BEM to determine the polymeric force and torque on a force/torque-free particle in a second-order fluid under the assumption \(\psi_1 = -2\psi_2\). The strategy is as follows. We first perform a boundary element simulation to solve for the Newtonian velocity field \(u_i\) and pressure field \(P^N\) around an arbitrarily shaped particle. Using these fields, we construct the polymeric force and torque on a particle using the integral expressions in (2.17) and (2.18). We compare these numerical results to the analytical expressions derived for the particle resistance in (2.26) and (2.27).

We consider a rigid, arbitrarily shaped particle with its surface denoted by \(S_p\) under an external flow described by \(u_i^\infty\). In Stokes flow, the tractions \(f_i\) on the particle surface can be solved from the following equation:

\[
u_i(x) - u_i^\infty(x) = -\frac{1}{8\pi \mu} \int_{S_p} G_{ij}(x - \xi)f_j(\xi)\,dS(\xi),
\]
(2.40)

where \(G_{ij}\) is the Oseen tensor as defined in (2.21), \(\xi\) denotes a position on the particle surface, while \(x\) is a position in the fluid surrounding the particle. When \(x\) approaches the particle surface, the velocity \(u_i \to U_i + \varepsilon_{ijk}\omega_j x_k\), where \(U_i\) and \(\omega_i\) are the translational and rotational velocities of the particle.

Next we approximate the particle surface as a triangular mesh using the procedures provided in Pozrikidis (2002). We let \(x\) approach the particle surface and rewrite the integral in (2.40) as a summation over all the surface elements:

\[
U_i + \varepsilon_{ijk}\omega_j x_k - u_i^\infty(x) = -\frac{1}{8\pi \mu} \sum_{n=1}^N \sum_{q=1}^{N_q} G_{ij}(x - \xi^{(n,q)})f_j(\xi^{(n,q)})dS(\xi^{(n,q)})w^{(n,q)}.
\]
(2.41)

In the above equation, \(N\) is the total number of elements and \(N_q\) is the total number of quadrature points, \(w^{(n,q)}\) is the quadrature weight and \(\xi^{(n,q)}\) is the position of the \(q\)th quadrature point on the \(n\)th element. We assume the traction \(f_i\) to be piecewise constant on each element and we solve for these values through a collocation method. The quadrature scheme is given in Pozrikidis (2002).
After obtaining the surface traction, we can evaluate the velocity field $u_i$ and pressure field $P^N$ at any arbitrary point outside the particle utilizing (2.40). Following the mechanism discussed in §2.1, we can solve for the polymeric force and torque on a force-free and torque-free particle using (2.17) and (2.18).

3. Results

In this section we first verify our analytical solutions in (2.26) and (2.27) by comparing to previous experimental and theoretical studies of spherical and non-spherical particles in viscoelastic flows, as well as to our boundary element simulations. We will then study the cross-stream migration of general ellipsoids in a quadratic flow of a second-order fluid.

In general, we find that our theories are able to capture the detailed orientation transitions of spheroidal particles in any slow, viscoelastic fluid. We are also able to identify scaling relationships that quantify how particle lift depends on particle shape for a wide variety of particle shape families.

3.1. Particle geometry definitions

We will restrict our study to the following family of particle shapes: spheres, prolate with $F_ω$ velocity $aA$ can examine. In particular, we will focus on the geometry $ψ$ and (3.2) match with the results in Brunn (1977) under the assumption $R$ are $a$ of each of these particles as $R$, which is the radius of a sphere with the same volume as the particle – i.e. $V = \frac{4}{3} \pi R^3$. We quantify particle asphericity by aspect ratio $A_R$, and the semi-axes lengths of the particle as $a$, $b$ and $c$. The dimensions of the prolatones are $a/R = A_R^{2/3}$, $b = c = a/A_R$. The dimensions of the oblates are $a/R = A_R^{-2/3}$, $b = c = aA_R$. For prolate-like ellipsoids, there are many families of particle shapes that one can examine. In particular, we will focus on the geometry $a/R = A_R$, $a/b = b/c = A_R$.

3.2. Verification: spheres in linear and quadratic flows of second-order fluids

3.2.1. Spheres in a general linear flow

Consider a spherical particle of radius $R$ translating in a second-order fluid with total viscosity $μ$. Let the particle migrate at a translational velocity $U_i$ and angular velocity $Ω_i$ in a linear flow with uniform velocity $u_i$, fluid angular velocity $Ω_i$, and rate of strain $E_{ij}$. The polymeric force $F_i^p$ and torque $T_i^p$ on the particle can be derived according to (2.26) and (2.27):

$$ F_i^p = -\frac{ψ_1}{2μ} \left( \frac{∂F^{(1)}_i}{∂t} + ε_{ijk}F^{(1)}_jΩ_k + E_{ij}F^{(1)}_j \right), $$

$$ T_i^p = -\frac{ψ_1}{2μ} \left( \frac{∂T^{(1)}_i}{∂t} + ε_{ijk}F^{(1)}_jU_k + ε_{ijk}T^{(1)}_jΩ_k + 2ε_{ijkm}E_{km}S_{mj} \right), $$

with $F^{(1)}_i = 6πμR(u'_i - U_i)$, $T^{(1)}_i = 8πμR^3(Ω_i - ω_i)$ and $S_{ij} = \frac{20}{3} πμR^3E_{ij}$. Equations (3.1) and (3.2) match with the results in Brunn (1977) under the assumption $ψ_1 = -2ψ_2$. Under the same condition, the total force and torque (Newtonian and polymeric) exerted by the fluid on the particle can be written as

$$ F_{tot}^i = 6πμR(u'_i - U_i) \left[ δ_{ij} - \frac{ψ_1}{2μ} ε_{ijk}(Ω_k - ω_k) - \frac{ψ_1}{2μ} E_{ij} \right] $$

$$ + \frac{ψ_1}{2μ} \left[ 6πμRε_{ijk}ω_j(u'_i - U_i) \right] - 3πRψ_1 \frac{∂}{∂t} (u'_i - U_i), $$

(3.3)
\[ T_i^{\text{tot}} = 8\pi \mu R^3 (\Omega_i - \omega_i) - \frac{\psi_1}{2\mu} e_{ijk} [6\pi \mu R (u_j' - U_j) u_k'] \]
\[ - \frac{\psi_1}{2\mu} e_{ijk} [8\pi \mu R^3 (\Omega_j - \omega_j) \Omega_k] + \frac{\psi_1}{\mu} e_{ijk} E_{jm} S_{mk} - 4\pi R^3 \psi_1 \frac{\partial}{\partial t} (\Omega_i - \omega_i), \quad (3.4) \]

where we recover the results by Brunn (1976).

### 3.2.2. Spheres in a pressure-driven flow

Consider a spherical particle of radius \( R \) in a pressure-driven flow defined by

\[ u_\infty^x = u^m \left[ 1 - \left( \frac{y}{L} \right)^2 \right], \quad u_\infty^y = u_\infty^z = 0, \quad (3.5a,b) \]

where \( u^m \) is the maximum velocity. We denote the coordinate of the particle’s centre of mass by \( (x_0, y_0) \). Figure 3(a) shows a schematic of the set-up. Let the particle migrate at a velocity such that, at each point, \( u_\infty - U = -\hat{e}_x - \hat{e}_y \) and \( \Omega - \omega = 0 \). We calculate the polymeric force and torque at various \( y_0 \) values using (2.26) and (2.27). The results compare well to our BEM simulation.

### 3.3. Spheroids under shear flow in a second-order fluid

We consider two different types of spheroids (prolate and oblate) that freely rotate under shear flow in a viscoelastic fluid. In previous experimental and theoretical studies, it was observed that such particles experience distinct orientation regimes at different shear rates. At relatively low shear rates with \( \tilde{W}_i \ll 0.1 \), where \( \tilde{W}_i \) is defined as \( \tilde{W}_i = \psi_1 \dot{\gamma}/\mu \), the rotational behaviour of both prolate and oblate particles will be similar to those in Newtonian fluids due to the weak viscoelastic effect present in the system. A gradual transition in rotational behaviour is experimentally observed when the shear rate is increased \( (\tilde{W}_i = 0.1 - 1) \). Prolates tend to perform a log-rolling motion with the long axis aligned with the vorticity direction of the flow, while oblates or disk-shaped particles perform a tumbling motion with the short axis perpendicular to the vorticity axis (Gauthier et al. 1971; Bartram et al. 1975; Johnson, Salem & Fuller 1990; Gunes et al. 2008). At even higher shear rates \( (\tilde{W}_i > O(1)) \), Gunes et al. (2008) reported that prolates will reorient the long axis along the flow direction when they are in a fluid with both high elasticity and shear-thinning. However, this reorientation transition is not observed when shear-thinning is absent even at extreme shear rates \( (\dot{\gamma} > 200 \text{ s}^{-1}, \tilde{W}_i > 30) \). Bartram et al. (1975) reported that the reorientation state is metastable in Boger fluids (i.e. no shear-thinning) and the particle will perform log-rolling once subject to any perturbation such as a Brownian force or an imperfect flow field.

A previous theoretical study by Leal (1975) employing the slender-body approximation \( (A_R \to \infty) \) predicted the reorientation transition for slender rods. The critical shear rate \( \dot{\gamma}_c \) for the reorientation to occur on a slender rod is predicted to be \( (\text{Leal 1975; Gunes et al. 2008}) \)

\[ \dot{\gamma}_c = \frac{16}{A_R} \left( \frac{\mu}{4\psi_1 - \psi_2} \right). \quad (3.6) \]
However, the critical shear rate of this transition does not quantitatively match experimental observations by Gunes et al. (2008) on finite-aspect-ratio particles.

In this study, equations (2.26) and (2.27) are employed to investigate three-dimensional particle orientations in shear flow. The flow field is defined by

\[ u_\infty^x = \frac{y}{L}, \quad u_\infty^y = u_\infty^z = 0, \quad (3.7a,b) \]

where the shear rate of the flow is \( \dot{\gamma} = \partial u_\infty^y / \partial y = 1/L \). Similar to the experiments in Gunes et al. (2008), we set the aspect ratio to be \( A_R = 3.8 \) for both oblate and prolate particles. The particle orientation angles \( \phi \) and \( \theta \) are defined based on the direction of the particle’s major axis as shown in figure 2(a). Therefore, the transition of orientation regimes can be captured solely by \( \theta \): for example, log-rolling of prolate particles corresponds to \( \theta = 0^\circ \), while tumbling of oblate particles in the \( x-y \) plane corresponds to \( \theta = 90^\circ \). Figure 2(b–d) shows the schematics of various possible rotation modes for prolate and oblate particles. We set the initial orientations of the particle at \( \theta_0 = 45^\circ \) and \( \phi_0 = 10^\circ \). Figure 4(a,b) shows the temporal evolution of angle \( \theta \) under various shear rates, described by Weissenberg number \( Wi = \psi_1 \dot{\gamma} / \mu \). In Newtonian flows (\( Wi = 0 \)), both particles perform the Jeffery orbit, i.e. a tumbling motion without any drift in \( \theta \) observed. When viscoelasticity is present at a very low shear rate (\( Wi = 0.025 \)), the evolution in \( \theta \) is similar to the Newtonian case, with a slight deviation observed in the later part of the simulation. As we increase the shear rate (\( Wi = 0.50 \)), a significant drift in \( \theta \) is observed for both particles. The oblate drifts towards the tumbling state in the \( x-y \) plane (\( \theta = 90^\circ \)) while the prolate drifts towards the log-rolling state (\( \theta = 0^\circ \)). We find that, as long as prolate particles do not start in the \( x-y \) plane (\( \theta = 90^\circ \)), the long-time configuration (\( t \to \infty \)) will always be the log-rolling state (\( \theta = 0^\circ \)), consistent with the experimental observations of Bartram et al. (1975) for particles in Boger fluids.
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\( u_\infty^m = u_\infty^m [1 - (y/L)^2] \)

\( y = 0 \)

\( u_\infty^m = u_\infty^m \frac{1 - (y/L)^2}{L} \)

\( y_0/L \)

\( y_0/L \)

\( F_{yp} / \mu u_\infty^m L Wi \)

\( T_{zp} / \mu u_\infty^m L^2 Wi \)

\( (a) \) Set-up for a spherical particle in a pressure-driven flow. (b) Non-dimensionalized polymeric force in the \( y \) direction for different values of \( y_0 \). (c) Non-dimensionalized polymeric torque in the \( z \) direction for different values of \( y_0 \). The parameters are \( R = 1, L = 10, u_\infty^m = 1, \mu = 1, \psi_1 = 1 \) and \( Wi = 0.1 \). The Weissenberg number is defined by \( Wi = \psi_1 u_\infty^m / L \mu \).

\( \theta_0 = 45^\circ \), \( \phi_0 = 10^\circ \). The Weissenberg number in the shear flow is defined as \( Wi = \psi_1 \dot{\gamma} / \mu \). The case of \( Wi = 0 \) corresponds to a Newtonian flow with \( \psi_1 = 0 \).

When prolate particles are restricted to lie in the \( x-y \) plane (metastable regime), the particles can either tumble or align along the flow direction (\( \theta = 90^\circ, \phi = 0^\circ \)).
Figure 5 shows the phase diagram of prolate orientation modes under various flow conditions $Wi$ and particle aspect ratios $AR$. We observe a transition from tumbling to reorientation (i.e. flow alignment) above a critical shear rate, with no transition occurring for aspect ratios $3 \leq AR \leq 6$ under the tested conditions. The critical shear rate predicted by (3.6) (dashed line in figure 5) is quantitatively inconsistent with our results especially in the low-$AR$ regime. The equation will provide better consistency (not shown here) at extreme $AR$ such as $AR = 100$, indicating the limited applicability of (3.6) to slender-body systems. The observations here are in qualitative agreement with previous studies by Bartram et al. (1975), Johnson et al. (1990) and Gunes et al. (2008). Quantitatively, Gunes et al. (2008) observed that transition occurs for $AR = 3.8$ in the regime where $Wi > 1$. In such a flow regime the second-order fluid model will lose its validity and therefore a quantitative discussion of the phenomenon would require extending the current model to more general conditions as well as considering more complex physics such as shear-thinning effects.

3.4. General ellipsoids in quadratic flows

We consider general ellipsoids (sphere, prolate, oblate and prolate-like ellipsoid) in a second-order fluid under a parabolic profile defined by (3.5). We follow the particle geometry definitions in § 3.1. We investigate the effect of particle orientation, position and morphology on particle migration. We also examine the translational and rotational trajectories in a quadratic flow. The common parameters are $R = 1$, $L = 4$, $\mu = 1$ and $\psi_1 = 1$. We vary the maximum flow velocity $u''$, and hence can vary the flow Weissenberg number $Wi \equiv \psi_1 u'' / L\mu$. 
3.4.1. Effect of particle orientation, position and morphology

We first study cross-stream particle migration under different particle orientations. We set the particle aspect ratio to be $A_R = 3$ and their initial position at $(x_0, y_0) = (0, -3.5)$. We calculate the particle lateral velocity $U_y$ and rotational velocity $\omega_z$ at different particle orientations $\phi$ and $\theta$. For lateral migration velocity $U_y$, it can be seen in figure 6(a) that all non-spherical particles show similar behaviour with respect to $\phi$, with the fastest migration occurring at $\phi = 45^\circ$ and $135^\circ$. The prolate-like ellipsoid shows the fastest lateral migration among all the particles. Figure 6(d) shows the lateral migration velocity at various $\theta$ angles. The prolate and prolate-like ellipsoids show maximum $U_y$ at $\theta = 90^\circ$ and minimum at $\theta = 0^\circ$, since particles in these configurations yield the largest and smallest span along the shear-gradient direction ($y$ direction), respectively. The oblate shows the opposite behaviour due to its morphology.

For the rotational dynamics, figures 6(b) and 6(d) show the rotational velocity $\omega_z$ at various $\phi$ and $\theta$ angles, respectively. In figure 6(b) the prolate and prolate-like ellipsoids perform nearly identical sinusoidal behaviour in rotational velocity $\omega_z$ throughout the tested range of $\phi$, with the fastest rotation appearing at $\phi = 90^\circ$. The oblate shows a $90^\circ$ phase lag in $\omega_z$ compared to that of the prolate and ellipsoid. In figure 6(d), the rotational velocity $\omega_z$ decreases for prolate and ellipsoid particles as the angle $\theta$ increases, due to the fact that the particle’s moment of inertia in the vorticity direction ($z$ direction) increases. The opposite trend in $\theta$ is observed for the oblate particle due to the same physics.

We next study the particle migration behaviour at different positions in the flow. We first fix the particle orientation at $\theta = 90^\circ$, $\phi = 45^\circ$ and calculate the particle lateral velocity $U_y$ and rotational velocity $\omega_z$ at various initial positions $y_0$. Figure 7(a) shows that all particles tend to migrate towards the centre of the flow profile regardless of their position in the flow. The lateral velocity $U_y$ and rotational velocity $\omega_z$ show a linear dependence with respect to $y_0$. The prolate-like ellipsoid shows the most significant lateral migration among all particles. A similar linear trend of $U_y$ is also observed as we change the $\theta$ orientation, as shown in figure 7(b).

To explain these observations, we refer to the scaling analysis by Leshansky et al. (2007). In their paper, Leshansky et al. (2007) proposed that the polymeric force on a particle of characteristic radius $R$ scales linearly with the normal stress gradients as $F^D_y \sim R^3 \psi_1 (\partial/\partial y)(\partial u^2/\partial y)^2 |_{y=y_0}$. When force-free, the polymeric force should balance the Stokes drag $F^D_y$ in the opposite direction: $F^D_y \sim -\mu RU_y$. The lateral migration velocity $U_y$ should thus scale as $U_y \sim (\psi_1 R^2 (u^m)^2 / \mu) y_0 / L^4$, which shows a linear dependence on $y_0$ as in our calculations.

We next extend the scaling analysis above to study the influence of particle shape on the particle mobility. We define the proportionality constant for the $U_y$ scaling relation to be the mobility constant $M_D$:  

$$U_y = M_D \frac{\psi_1 R^2 u^m^2 y_0}{\mu L^4} = M_D \frac{\psi_1 R^2 u^m y_0}{\mu L^3},$$  

where $Wi$ is the Weissenberg number, defined as $Wi = \psi_1 u^m / L \mu$. We apply this relation to calculate the mobility $M_D$ for different particle shapes.

Here we specifically investigate two different sets of particle orientations, $\theta = 90^\circ$, $\phi = 45^\circ$ and $\theta = 0^\circ$, $\phi = 45^\circ$, and the results are presented in figure 8(a,b). The insets of both panels show the particle relative mobility with respect to a sphere, $M_D / M^\text{sphere}_D$, at different particle aspect ratios $A_R$. When $\theta = 90^\circ$, all three types of
particles have higher mobility at higher $A_R$ and the prolate-like ellipsoid shows the most significant increase in the mobility among the three. In the case of $\theta = 0^\circ$, only the oblate gains higher mobility at higher $A_R$, while the prolate and ellipsoid show decreasing mobility. However, when we plot the mobility data against the longest possible particle axis length in the shear gradient direction $L_{sg}$, the mobility curves for all three particles collapse onto one major curve as shown in figure 8. This indicates that the effective length spanned along the velocity gradient is the major factor that affects the particle mobility in the flow. In the case when $\theta = 90^\circ$, the major axis length of the particle acts as the determining factor for the migration velocity in the velocity gradient direction, while in the case of $\theta = 0^\circ$, the shorter axes of prolate and ellipsoid and the long axis of oblate will be the dominant factors. This also explains the decreasing trend in mobility with respect to $A_R$ for prolate and ellipsoid when $\theta = 0^\circ$. For $0^\circ < \theta < 90^\circ$, the dominant length will be a mixture of long and short particle axes.
3.4.2. Particle migration trajectories

In figure 9(a,b), we first restrict the particle orientation in the flow–shear gradient plane (θ = 90°) and track the trajectories of tumbling particles in a pressure-driven flow as they migrate to the flow centre. The particles are released at (x₀, y₀) = (0, −3.5) with an initial orientation φ₀ = 45°. It can be seen from figure 9(a) that the prolate-like ellipsoids and the oblate particles exhibit the fastest and the slowest migration speeds, respectively. Particles tend to stay near the flow centre once they reach the region since the polymeric force is zero. Figure 9(b) shows the evolution of particle orientation angle φ with respect to the dimensionless time t/uₚ/L. The non-spherical particles perform a clockwise tumbling motion during migration and attain a steady orientation once they reach the flow centre. At the flow centre, the particles align their longest axis with the flow (φ = 0° for prolate and prolate-like ellipsoid, φ = 90° for oblate). These observations qualitatively agree with the results from D’Avino et al. (2019) when particles are restricted to the x–y plane.

In order to quantify the tumbling motion, we define n as the number of times a particle performs a 180° flip and Δtn as the time required for the nth flip to occur. The plot of 1/Δtn with respect to n for the three non-spherical particles is shown in figure 9(c). In general, particles will rotate at a slower rate as they approach the flow centre. The prolate-like ellipsoid achieved the least number of flips (n = 5) due to its fastest migration towards the flow centre. The oblate, on the other hand, spent more time in the off-centre region and therefore shows the highest number of flips (n = 12) among the three particles. Jeffery (1922) proposed that, for a general ellipsoidal particle in a Newtonian fluid under shear rate γ, the tumbling period T' of the particle follows

\[ T' = \frac{2\pi}{\dot{\gamma}} \left( A_R + \frac{1}{A_R} \right). \]  

(3.9)

We sample the shear rate at the averaged y position during each flip to estimate the local Jeffery orbit period. The calculated half-period data are also shown in
When \( \theta \) we choose \( L \) (i.e. \( \theta \) orientations) non-spherical particles in the off-centre region of the flow are in good agreement with Jeffery orbits, with only less than 4% of error from \( \mathcal{T} \). Deviation from Jeffery orbit is only observed as the particles approach the flow centre, where the quadratic part of the flow dominates the particle motion. The results indicate that, under the above flow condition, the polymeric effect does not greatly alter the rotation dynamics of the particle’s initial orientation spans the largest distance in the shear gradient direction as it moves towards the flow centre. Generally, the migration speed is fastest when the particle’s initial orientation spans the largest distance in the shear gradient direction (i.e. \( \theta = 0^\circ \) for oblate, \( \theta = 90^\circ \) for prolate). This state corresponds to the metastable configuration for both prolates and oblates. Lastly, figure 12 plots how the migration time \( t_m \) towards the flow centre varies with initial orientation \( \theta_0 \), initial position \( y_0 \), init and aspect ratio \( A_R \). In these plots, \( t_m \) is defined as the time it takes for the particle to
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reach \( y_0 < 0.01L \) from the flow centre. In figure 12(a), both oblate and prolate particles have a slight variation in \( t_m \) when \( \theta_0 \) is close to their stable orientation. A steep drop in \( t_m \) is observed near the metastable orientation. Figure 12(b) shows the plot of \( t_m \) with respect to various initial \( y_{0,\text{init}} \). The initial \( \theta \) orientation was set to be 0° and 90° for oblates and prolates, respectively. Oblate particles show a monotonic decrease in \( t_m \) with decreasing \( y_{0,\text{init}} \). On the other hand, prolate particles show a non-monotonic trend in \( t_m \), mainly due to the fact that tumbling motion (thus change in \( \phi \) angle) also plays a role in their migration dynamics. We note that such effects do not occur for oblates with \( \theta_0 = 0° \) since different \( \phi \) angles correspond to the same state of orientation. Figure 12(c) shows the variation of \( t_m \) with respect to particle aspect ratio \( A_R \) for prolate and oblate particles. Both particles show longer migration time with increasing \( A_R \). Prolate particles always transition into a log-rolling state and thus have migration time \( t_m \) increasing monotonically with \( A_R \). On the other hand, oblate particles tend to perform tumbling motion (\( \theta = 90° \)) during their migration. The migration time is affected by both long and short axes, and therefore the trend is not monotonic.

4. Conclusion and future directions

We studied the dynamics of non-spherical particles in an inertialess, steady flow of a second-order fluid. The assumption of \( \psi_1 = -2\psi_2 \) allows us to reduce the fluid dynamics to a Stokes flow with a modified total pressure. By utilizing a multipole expansion, we derived an analytical solution for the polymeric force and torque on an arbitrarily shaped particle in a general quadratic flow field (i.e. quadratic...
Figure 10. (a) Plot of oblate $\theta$ trajectory with respect to simulation time $t$ under various initial orientations $\theta_0$. (b) Plot of prolate $\theta$ trajectory with respect to simulation time $t$ under various initial orientations $\theta_0$. The common parameters are $R = 1$, $L = 4$, $AR = 3$, $u^m = 1$, $\mu = 1$, $\psi_1 = 1$ and $Wi = 0.25$. The particles are released at $(x_0, y_0) = (0, -3.5)$. Time is non-dimensionalized by the average, inverse shear rate $L/u^m$. The duration of the simulation is $tu^m/L = 1000$.

Figure 11. (a) Plot of oblate migration trajectories from various $\theta_0$. (b) Plot of prolate migration trajectories from various $\theta_0$. The particles are released at $(x_0, y_0) = (0, -3.5)$. The common parameters are $R = 1$, $L = 4$, $AR = 3$, $u^m = 1$, $\mu = 1$, $\psi_1 = 1$ and $Wi = 0.25$. The simulation duration is $tu^m/L = 1000$.

plus linear flow in an unbound domain). The solutions are in good agreement with previous studies on spherical particle dynamics in viscoelastic flows as well as our boundary element simulations. We also verified that our theory can qualitatively
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Figure 12. (a) The migration time $t_m$ required for aspect ratio $A_R = 3$ oblate and prolate particles to reach $y_0 < 0.01L$ from different initial $\theta$ orientations. Particles are released at $(x_0, y_0) = (0, -3.5)$ with initial $\phi_0 = 45^\circ$. (b) The migration time $t_m$ required for $A_R = 3$ oblate and prolate particles to reach $y_0 < 0.01L$ from different lateral positions $y_{0,\text{init}}$. The initial $\theta$ orientation is set to be $\theta_0 = 0^\circ$ and $\theta_0 = 90^\circ$ for oblates and prolates, respectively. Initial $\phi_0$ is set at $45^\circ$. (c) The migration time $t_m$ required for oblate and prolate particles to reach $y_0 < 0.01L$ for different particle aspect ratios. Particles were released at $(x_0, y_0) = (0, -3.5)$ with initial orientation $\theta_0 = 45^\circ$, $\phi_0 = 45^\circ$. The common parameters are $R = 1$, $L = 4$, $u_m = 1$, $\mu = 1$, $\psi_1 = 1$ and $Wi = 0.25$.

capture the experimentally observed orientation transitions of spheroids under various flow conditions.

We applied our model to investigate the dynamics of spheres, spheroids (oblate and prolate) and ellipsoids in a slit-like pressure-driven flow of second-order fluid. In general, the particles slowly migrate to the centre of the pressure-driven flow, with their dynamics governed by the position, orientation and particle morphology. We develop scaling theories to quantify how the particle shape affects the migration velocity. The length $L_{\text{sg}}$ spanned by the particles in the velocity gradient direction determines the lift velocity for a wide range of particle family shapes. Our trajectory studies show that spheroidal particles slowly adjust their orientation towards a favoured configuration (e.g. log-rolling for prolates, tumbling for oblates). The effect of initial orientation, initial position and particle aspect ratio on the migration time is also identified in this paper.

This work provides a preliminary understanding of non-spherical particle dynamics in viscoelastic flows from an analytical standpoint. For future directions, investigations towards more general conditions (e.g. $\psi_1 \neq -2\psi_2$) are necessary for a better understanding of particle dynamics in a viscoelastic flow. It is also our interest to investigate more complicated systems such as wall-bounded flows and three-dimensional flows to understand the particle dynamics in realistic systems such as microfluidic platforms. Experimental studies on particle dynamics in viscoelastic flow will also provide insight on the validity of the developed model to real systems.

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Declaration of interests

The authors report no conflict of interest.

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