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Numerical simulations of the competition between the effects of inertia and viscoelasticity on particle migration in Poiseuille flow

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ABSTRACT

In this work, we present 2D numerical simulations on the migration of a particle suspended in a viscoelastic fluid under Poiseuille flow at finite Reynolds numbers, in order to clarify the simultaneous effects of viscoelasticity and inertia on the lateral particle motion.

The governing equations are solved through the finite element method by adopting an Arbitrary Lagrangian–Eulerian (ALE) formulation to handle the particle motion. The high accuracy provided by such a method even for very small particle–wall distances, combined with proper stabilization techniques for viscoelastic fluids, allows obtaining convergent solutions at relatively large flow rates, as compared to previous works. As a result, the detailed non-linear dynamics of the migration phenomenon in a significant range of Reynolds and Deborah numbers is presented.

The simulations show that, in agreement with the previous literature, a mastercurve relating the migration velocity of the particle to its ‘vertical’ position completely describes the phenomenon. Remarkably, we found that, for comparable values of the Deborah and Reynolds numbers, inertial effects are negligible: migration is in practice driven by fluid viscoelasticity only. At moderate Reynolds numbers ($20 < Re < 200$) and by lowering De , the transition from viscoelasticity-driven to inertia-driven regimes occurs through two intermediate regimes characterized by multiple stable solutions, i.e. attractors of particle trajectories at different vertical positions across the gap. At low but non-zero Reynolds numbers, only two stable solutions are found for any non-zero Deborah number in the investigated range. In particular, the wall is always an attractor for the migrating particle.

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1. Introduction

Cross-streamline particle migration is a well-known and widely studied phenomenon occurring in flowing suspensions [1–3]. It consists of a motion of the suspended particles transversally to the main flow direction, which can be induced by several factors, e.g. through inertia [1,4,2,5] or viscoelasticity [3,6,7].

This problem received great interest over the last fifty years as particle migration can determine unexpected inhomogeneities in the suspension concentration thus affecting those processes/materials that require uniform distributions of particles (e.g. fluid–solid

reactions, filler-loaded materials). Furthermore, with the recent development of microfluidic chips, the need of controlling particle trajectories has directed the scientific interest in designing novel devices able to induce the lateral motion [8].

The first accurate experimental studies on the migration phenomenon have been reported by Segré and Silberberg [1,4]. They found that non-interacting, neutrally buoyant spheres suspended in a Newtonian fluid flowing in a tube move away from both the wall and the channel centerline, and are attracted towards an ‘equilibrium’ radial position of about 0.6 times the tube radius. This relevant phenomenology has been confirmed in several experimental [9,2,5], theoretical [10–12] and numerical [13–15] works. The lateral motion has been explained as an inertial effect [10,12].

Migration can also occur, at vanishing Reynolds numbers, in viscoelastic fluids [3,16,6,7]. The experimental results show that a particle suspended in a viscoelastic medium subjected to a

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Poiseuille flow migrate towards the minimum shear-rate direction (i.e. the centerline) [3,6,7], whereas shear-thinning promotes migration towards the walls [17].

Migration towards the minimum shear-rate region has been analytically deduced by Ho and Leal [16] through a perturbative method by considering a Second Order Fluid as suspending medium, and is ascribable to the existence of normal stresses.

Recently, Villone et al. [18,19], by means of 2D and 3D numerical simulations, have extensively studied the effects of both viscoelasticity and shear thinning on particle migration under inertialess conditions. They found that the sole shear thinning does not determine transversal motion; on the other hand, if coupled with viscoelasticity, it determines a multistability condition, where the particles migrate towards the axis of the channel or the walls depending on their initial positions. In other words, looking for simplicity to the 2D case, three equilibrium positions in each half gap are identified along the gradient direction: the centerline and the wall (stable), and a ‘separatrix’ (unstable) at some vertical position in the gap. These points are nodes of a *mastercurve* where the particle trajectories for different initial positions are shown to collapse on, and which completely describes the migration dynamics. In addition, it is found that large Deborah numbers lead to a faster migration, and shear thinning promotes the displacement of the separatrix towards the centerline, thus increasing the fraction of particles that approach the walls.

In summary, both inertia and viscoelasticity promote particle migration in Poiseuille flow, but they work in opposite directions: the former drives the particles towards an equilibrium position between the channel centerline and the walls (‘Segré–Silberberg effect’), whereas the latter induces a lateral motion away from an unstable equilibrium position and towards the centerline or the walls (‘inversion’ of the Segré–Silberberg effect).

Few works have addressed the simultaneous effects of inertia and viscoelasticity on particle migration [20–22]. 2D direct numerical simulations have been performed by modeling the fluid with the Oldroyd-B constitutive equation with a Bird-Carreau shear rate viscosity dependence. The main focus of the simulations was on the effect of the buoyancy on the particle dynamics, resulting in empirical correlations for the particle lift-off to equilibrium. However, due to numerical problems [20], the computations were limited to low Deborah numbers (in most of the cases $De < 0.1$, with some spot results at $De = 0.25$, according to the definition of De used in this work and given in the next section), thus inertial effects prevail over the elastic ones. In general, the results show that the migration direction depends in a complex way on the interplay among inertia, blockage ratio, elasticity and shear thinning of the fluid. In particular, in Poiseuille flow, the elasticity of the fluid drives the particles towards the axis of the channel, whereas shear thinning and confinement make them to migrate towards the closest wall. Interestingly, the simulation results show the existence of multiple equilibrium positions through the channel [22].

Therefore, a study on the detailed dynamics of particle migration in Poiseuille flow induced by inertia and viscoelasticity, in a significant range of Reynolds and Deborah numbers, is missing. Understanding the effect of those two driving forces on the particle lateral motion would be useful in optimizing novel microfluidic technologies where exploitation of the competition between inertia and elasticity effects has been suggested as a method to perform 3D particle focusing and separation [23,24].

In this work, we present 2D numerical simulations on the migration of a neutrally buoyant particle suspended in a viscoelastic fluid under Poiseuille flow, with inertia effects included. The explored ranges of the Reynolds and Deborah numbers are $Re \in [0 - 200]$ and $De \in [0 - 1]$. As compared to previous studies, the upper limit of the Deborah number is one order of magnitude higher, so that the detailed dynamics from the inertia- to the

viscoelasticity-driven regime is addressed. The achievement of convergent solutions at finite De -values is assured by implementing proper stabilization techniques in the momentum balance and constitutive equations. An Arbitrary Lagrangian–Eulerian (ALE) method is employed for the particle motion that allows to accurately solve the flow fields around the particle, even at relatively small particle–wall distances. Results are presented in terms of particle trajectories and migration velocities in the whole channel gap, highlighting the complex non-linear dynamics arising when both inertia and viscoelasticity are relevant.

2. Governing equations

In Fig. 1 a schematic diagram of the problem is presented: a single, rigid, non-Brownian, circular particle (2D problem) moves in a channel filled by a viscoelastic fluid in Poiseuille flow. The particle with diameter d_p , denoted by $P(t)$ and boundary $\partial P(t)$, moves in a rectangular domain Ω with dimensions L and H along the x - and y -axis, respectively, and external boundaries denoted by Γ_i ($i = 1, \dots, 4$). The Cartesian x and y coordinates are selected with the origin at the center of the domain. The fluid flows along the x -direction with a flow rate Q imposed on the left boundary, and the upper and lower boundaries are walls.

The vector $\mathbf{x}_p = (x_p, y_p)$ gives the position of the center of the particle, whereas the particle angular rotation is denoted by θ_p . The particle moves according to the imposed flow and its rigid-body motion is completely defined by the translational and angular velocities, denoted by $\mathbf{u}_p = (u_p, v_p) = d\mathbf{x}_p/dt$ and $\omega_p = \omega_p \mathbf{k} = d\theta_p/dt$, respectively, where $\mathbf{k}$ is the unit vector in the direction normal to the $x - y$ plane.

The governing equations for the fluid domain, $\Omega - P(t)$, read as follows:

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

$$\rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \cdot \boldsymbol{\sigma} \quad (2)$$

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

Eqs. (1)–(3) are respectively the mass balance (continuity), the momentum balance and the expression for the total stress. In these equations $\boldsymbol{\sigma}$, $\mathbf{u}$, p , $\mathbf{I}$, ρ_f , η_s , $\mathbf{D}$, are the stress tensor, the velocity vector, the pressure, the 2×2 unity tensor, the fluid density, a Newtonian viscosity, and the rate-of-deformation tensor $\mathbf{D} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2$. The viscoelastic stress tensor, $\boldsymbol{\tau}$, is written in terms of the ‘conformation tensor’ $\mathbf{c}$ as:

$$\boldsymbol{\tau} = \frac{\eta_p}{\lambda} (\mathbf{c} - \mathbf{I}) \quad (4)$$

where η_p is a viscosity constant (polymer viscosity), and λ is the relaxation time.

The viscoelastic fluid is modeled by the Giesekus constitutive equation (for $\mathbf{c}$) [25]:

$$\lambda \overset{\nabla}{\mathbf{c}} + \mathbf{c} - \mathbf{I} + \alpha(\mathbf{c} - \mathbf{I})^2 = \mathbf{0} \quad (5)$$

Fig. 1. Sketch of the flow cell and of the adopted coordinate system.

where α is the so-called mobility parameter that modulates the shear thinning behavior. The symbol (∇) denotes the upper-convected time derivative, defined as:

$$\overset{\nabla}{\mathbf{c}} \equiv \frac{\partial \mathbf{c}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{c} - (\nabla \mathbf{u})^T \cdot \mathbf{c} - \mathbf{c} \cdot \nabla \mathbf{u} \quad (6)$$

No-slip conditions are imposed on the walls and on the particle boundary:

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_1 \text{ and } \Gamma_3 \quad (7)$$

$$\mathbf{u} = \mathbf{u}_p + \boldsymbol{\omega}_p \times (\mathbf{x} - \mathbf{x}_p) \quad \text{on } \partial P(t) \quad (8)$$

where the latter equation expresses the rigid-body motion. Periodic boundary conditions are imposed on the left (inflow) and right (outflow) boundaries, along with a flow rate Q in inflow:

$$\mathbf{u}|_{\Gamma_4} = \mathbf{u}|_{\Gamma_2} \quad (9)$$

$$\boldsymbol{\sigma}|_{\Gamma_4} = \boldsymbol{\sigma}|_{\Gamma_2} - \Delta p \mathbf{i} \quad (10)$$

$$-\int_{\Gamma_4} \mathbf{u} \cdot \mathbf{n} dy = Q \quad (11)$$

In Eq. (10) Δp is the pressure drop along the channel in between Γ_4 and Γ_2 and $\mathbf{i}$ is the unit vector in the x direction; in Eq. (11) $\mathbf{n}$ is the outwardly directed unit normal vector. The flow rate in Eq. (11) is imposed through a constraint where the associated Lagrange multiplier is identified as the unknown pressure difference $\Delta p = p|_{\Gamma_4} - p|_{\Gamma_2}$ [26].

To close the set of equations, the hydrodynamic force and torque acting on the particle needs to be specified. Under the assumptions of no 'external' forces and torques, such balance equations are given by:

$$m_p \frac{d\mathbf{u}_p}{dt} = \mathbf{F} = \int_{\partial P(t)} \boldsymbol{\sigma} \cdot \mathbf{n} ds \quad (12)$$

$$I_p \frac{d\boldsymbol{\omega}_p}{dt} \mathbf{k} = \mathbf{T} = \int_{\partial P(t)} (\mathbf{x} - \mathbf{x}_p) \times (\boldsymbol{\sigma} \cdot \mathbf{n}) ds \quad (13)$$

where $\mathbf{F} = (F_x, F_y)$ and $\mathbf{T} = T\mathbf{k}$ are the total force and torque on the particle boundary, m_p and I_p are the particle mass and moment of inertia (relative to the z -axis; it is $I_p = m_p d_p^2/8$), and $\mathbf{n}$ is the outwardly directed unit normal vector on ∂P .

Finally, initial conditions for the fluid velocity and the conformation tensor as well as for the translational and angular velocities of the particle need to be specified:

$$\mathbf{c}|_{t=0} = \mathbf{I} \quad (14)$$

$$\mathbf{u}|_{t=0} = \mathbf{u}_p|_{t=0} = \mathbf{0}; \quad \boldsymbol{\omega}_p|_{t=0} = 0 \quad (15)$$

Eq. (14) defines a stress-free state in the whole fluid domain whereas Eq. (15) denote fluid and particle at rest.

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:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p, \quad \mathbf{x}_p|_{t=0} = \mathbf{x}_{p,0} \quad (16)$$

$$\frac{d\boldsymbol{\theta}_p}{dt} = \boldsymbol{\omega}_p, \quad \boldsymbol{\theta}_p|_{t=0} = \boldsymbol{\theta}_{p,0} \quad (17)$$

The equations are made dimensionless by choosing the following characteristic quantities: H for length, Q/H for velocity, H^2/Q for time and $\eta_p Q/H^2$ for stress. Then, the following dimensionless parameters appear in the governing equations: the fluid Reynolds number $Re = \rho_f Q/\eta_p$, the Deborah number $De = \lambda Q/H^2$, the density ratio ρ_p/ρ_f , and the viscosity ratio η_s/η_p . By specifying the blockage ratio $\beta = d_p/H$ and the mobility parameter of the consti-

tutive equation α the problem is completely defined. In what follows, all the symbols refer to dimensionless quantities.

3. Weak form, implementation and code validation

3.1. Weak form

The system of Eqs. (1)–(6) with boundary conditions (7)–(11), initial conditions (14) and (15) and the force and torque balances (12) and (13) are solved by the finite element method. Each time step the flow fields are evaluated along with the rigid-body unknowns. Then, the kinematic Eqs. (16) and (17) are integrated to update the particle position and rotation.

Proper stabilization techniques which, in respect to previous works, allow obtaining convergent solutions even at relatively high Deborah and Reynolds numbers are used. The momentum balance is discretized through the DEVSS-G mixed finite element method [27,28] that is one of the most robust formulations currently available. The viscoelastic constitutive equation is stabilized by implementing the SUPG technique, with a log-representation for the conformation tensor [29,30]. The original equation for the conformation tensor $\mathbf{c}$, Eq. (5), is transformed to an equivalent equation for $\mathbf{s} = \log(\mathbf{c})$:

$$\dot{\mathbf{s}} = \frac{\partial \mathbf{s}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{s} = \mathbf{g}(\nabla \mathbf{u}^T, \mathbf{s}) \quad (18)$$

An expression for the function $\mathbf{g}$ for a Giesekus fluid can be found in [30]. Solving the equation for $\mathbf{s}$ instead of the equation for $\mathbf{c}$ leads to a substantial improvement of stability for high Deborah numbers. Finally, an Arbitrary Lagrangian–Eulerian (ALE) formulation is adopted to manage the particle motion [31].

With these premises, the weak formulation of the equation system for the fluid domain $\Omega_f \equiv \Omega \setminus P(t)$ reads as follows: For $t > 0$, find $\mathbf{u} \in U$, $p \in P$, $\mathbf{s} \in S$, $\mathbf{G} \in G$, $\mathbf{u}_p \in \mathbb{R}^2$, $\boldsymbol{\omega}_p \in \mathbb{R}$, $\lambda \in L^2(\partial P(t))$ such that:

$$\begin{aligned} & \int_{\Omega_f} \mathbf{v} \cdot \rho_f \left(\frac{\delta \mathbf{u}}{\delta t} + (\mathbf{u} - \mathbf{u}_m) \cdot \nabla \mathbf{u} \right) dA + \int_{\Omega_f} 2\eta_s \mathbf{D}(\mathbf{v}) : \mathbf{D}(\mathbf{u}) dA \\ & - \int_{\Omega_f} \nabla \cdot \mathbf{v} p dA + \int_{\Omega_f} a(\nabla \mathbf{v})^T : \nabla \mathbf{u} dA - \int_{\Omega_f} a(\nabla \mathbf{v})^T : \mathbf{G}^T dA \\ & + \int_{\partial P(t)} [\mathbf{v} - (\mathbf{V} + \boldsymbol{\chi} \times (\mathbf{x} - \mathbf{x}_p))] \cdot \lambda ds + \mathbf{V} \cdot m_p \frac{d\mathbf{u}_p}{dt} + \boldsymbol{\chi} \cdot I_p \frac{d\boldsymbol{\omega}_p}{dt} \\ & = - \int_{\Omega_f} \mathbf{D}(\mathbf{v}) : \boldsymbol{\tau} dA, \end{aligned} \quad (19)$$

$$\int_{\Omega_f} q \nabla \cdot \mathbf{u} dA = 0, \quad (20)$$

$$\int_{\Omega_f} \mathbf{H} : \mathbf{G} dA - \int_{\Omega_f} \mathbf{H} : (\nabla \mathbf{u})^T dA = 0, \quad (21)$$

$$\int_{\Omega_f} (\mathbf{S} + \tau(\mathbf{u} - \mathbf{u}_m) \cdot \nabla \mathbf{S}) : \left(\frac{\delta \mathbf{s}}{\delta t} + (\mathbf{u} - \mathbf{u}_m) \cdot \nabla \mathbf{s} - \mathbf{g}(\mathbf{G}, \mathbf{s}) \right) dA = 0, \quad (22)$$

$$\int_{\partial P(t)} \boldsymbol{\mu} \cdot [\mathbf{u} - (\mathbf{u}_p + \boldsymbol{\omega}_p \times (\mathbf{x} - \mathbf{x}_p))] ds = 0, \quad (23)$$

$$\mathbf{s} = \mathbf{s}_0 \quad \text{at } t = 0 \quad (24)$$

for all $\mathbf{v} \in U$, $q \in P$, $\mathbf{S} \in S$, $\mathbf{H} \in G$, $\mathbf{V} \in \mathbb{R}^2$, $\boldsymbol{\chi} \in \mathbb{R}$ and $\boldsymbol{\mu} \in L^2(\partial P(t))$, where U , P , S , G are suitable functional spaces. Eq. (21) is the combined fluid-particle momentum equation [31]. In Eqs. (19) and (22), $\mathbf{u}_m$ is the velocity of the mesh nodes and $\delta/\delta t$ denotes the grid derivative, both coming from the ALE formulation [31].

The τ parameter in Eq. (22) is given by $\tau = Bh/2U_e$, where B is a dimensionless constant, h is a typical size of the element and U_e is a characteristic velocity for the element. In our simulations, we have chosen $B = 1$ and for U_e we take the average of the magnitude of the velocities in all integration points. In addition, the parameter a in Eq. (19) is chosen as $a = \eta_p$. Finally, we take the initial value $\mathbf{s}_0 = \mathbf{0}$, corresponding to zero initial stress.

The rigid-body motion on the particle boundary is imposed through Lagrange multipliers λ . Thus, the particle kinematic quantities are considered as additional unknowns that are directly obtained by solving the full system of equations.

The y -component of the mesh velocity $u_{m,y}$ is obtained by solving a Laplace equation:

$$\nabla \cdot (\epsilon \nabla u_{m,y}) = 0 \quad (25)$$

with boundary conditions:

$$u_{m,y} = u_{p,y} \quad \text{on } \partial P(t) \quad (26)$$

$$u_{m,y} = 0 \quad \text{on } \Gamma_i, \quad (i = 1, \dots, 4) \quad (27)$$

that guarantees a smooth mesh motion [31]. In Eq. (25), the parameter ϵ is taken equal to the inverse of the local element area in order to let the largest elements adsorb the most part of deformation. Following [32], the mesh grid is moved along the flow at the same x -velocity of the particle, in order to limit particle motion only in the gradient direction and substantially reduce mesh distortion. Therefore, the x -component of the mesh velocity is given by the x -component of the particle translational velocity $u_{m,x} = u_{p,x}$. The weak form for Eq. (25) can be derived in a standard way.

3.2. Implementation

For the discretization of the weak form, we use triangular elements with continuous quadratic interpolation (P_2) for the velocity $\mathbf{u}$ and linear continuous interpolation (P_1) for the pressure p , velocity gradient $\mathbf{G}$ and log-conformation tensor $\mathbf{s}$.

Following D'Avino et al. [32], the mass and momentum balances are decoupled from the constitutive equation. Initially, the viscoelastic stress is set to zero in the whole domain. The following procedure is adopted at each time step:

Step 1. The particle position is updated by integrating the kinematic Eq. (16) by an explicit second-order Adams–Bashforth method:

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \left(\frac{3}{2} \mathbf{u}_p^n - \frac{1}{2} \mathbf{u}_p^{n-1} \right) \quad (28)$$

with Δt the time step size.

Step 2. The mesh nodes, $\mathbf{x}_m$, are updated according to:

$$\mathbf{x}_m^{n+1} = \mathbf{x}_m^n + \Delta t \left(\frac{3}{2} \mathbf{u}_m^n - \frac{1}{2} \mathbf{u}_m^{n-1} \right) \quad (29)$$

Step 3. The log-conformation tensor is computed by integrating the constitutive Eq. (22). A second-order semi-implicit Gear scheme is used:

$$\begin{aligned} \int_{\Omega_t^{n+1}} (\mathbf{S} + \tau \dot{\mathbf{u}}^{n+1} \cdot \nabla \mathbf{S}) : \left(\frac{3}{2} \frac{\mathbf{s}^{n+1}}{\Delta t} + \dot{\mathbf{u}}^{n+1} \cdot \nabla \mathbf{s}^{n+1} \right) dA \\ = \int_{\Omega_t^{n+1}} (\mathbf{S} + \tau \dot{\mathbf{u}}^{n+1} \cdot \nabla \mathbf{S}) \\ : \left(\frac{2\mathbf{s}^n - \frac{1}{2}\mathbf{s}^{n-1}}{\Delta t} + 2\mathbf{g}(\mathbf{G}^n, \mathbf{s}^n) - \mathbf{g}(\mathbf{G}^{n-1}, \mathbf{s}^{n-1}) \right) dA, \end{aligned} \quad (30)$$

where $\dot{\mathbf{u}}^{n+1} = 2(\mathbf{u}^n - \mathbf{u}_m^n) - (\mathbf{u}^{n-1} - \mathbf{u}_m^{n-1})$. Notice that in Eq. (30) (and in Eq. (31) below) many fields are evaluated at times t^n and t^{n-1} , although the integration domain is at time t^{n+1} . In the ALE method adopted in the present work, all the fields are convected with the mesh (see the grid derivatives in Eqs. (19) and (22)). Hence, a field labeled n (and $n-1$) in a point P^{n+1} (of the domain Ω_t^{n+1}) is simply that same field in the point P^n (P^{n-1}), which was the point of the domain Ω_t^n (Ω_t^{n-1}) that has moved to P^{n+1} according to the mesh velocity. In other words, values at previous times should be evaluated in the previous domains, but at the same grid points.

Step 4. After computing $\mathbf{c}^{n+1} = \exp(\mathbf{s}^{n+1})$, the remaining unknowns $(\mathbf{u}, p, \mathbf{G}, \mathbf{u}_p, \omega_p, \lambda)^{n+1}$ are calculated by solving Eqs. (19)–(21) and (23). The following scheme is adopted:

$$\begin{aligned} \int_{\Omega_t^{n+1}} \mathbf{v} \cdot \rho_f \frac{3}{2} \frac{\mathbf{u}^{n+1}}{\Delta t} dA + \int_{\Omega_t^{n+1}} 2\eta_s \mathbf{D}(\mathbf{v}) : \mathbf{D}(\mathbf{u}^{n+1}) dA \\ - \int_{\Omega_t^{n+1}} \nabla \cdot \mathbf{v} p^{n+1} dA + \int_{\Omega_t^{n+1}} a(\nabla \mathbf{v})^T : \nabla \mathbf{u}^{n+1} dA \\ - \int_{\Omega_t^{n+1}} a(\nabla \mathbf{v})^T : (\mathbf{G}^{n+1})^T dA \\ + \int_{\partial P(t^{n+1})} \left[\mathbf{v} - (\mathbf{V} + \boldsymbol{\chi} \times (\mathbf{x} - \mathbf{x}_p^{n+1})) \right] \cdot \boldsymbol{\lambda}^{n+1} ds \\ + \mathbf{V} \cdot m_p \frac{3}{2} \frac{\mathbf{u}_p^{n+1}}{\Delta t} + \boldsymbol{\chi} \cdot l_p \frac{3}{2} \frac{\omega_p^{n+1}}{\Delta t} \\ = \int_{\Omega_t^{n+1}} \mathbf{v} \cdot \rho_f \left(\frac{2\mathbf{u}^n - \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} - 2(\mathbf{u}^n - \mathbf{u}_m^n) \cdot \nabla \mathbf{u}^n \right. \\ \left. + (\mathbf{u}^{n-1} - \mathbf{u}_m^{n-1}) \cdot \nabla \mathbf{u}^{n-1} \right) dA + \mathbf{V} \cdot m_p \frac{2\mathbf{u}_p^n - \frac{1}{2}\mathbf{u}_p^{n-1}}{\Delta t} \\ + \boldsymbol{\chi} \cdot l_p \frac{2\omega_p^n - \frac{1}{2}\omega_p^{n-1}}{\Delta t} - \int_{\Omega_t^{n+1}} \mathbf{D}(\mathbf{v}) : \boldsymbol{\tau}(\mathbf{c}^{n+1}) dA, \end{aligned} \quad (31)$$

$$\int_{\Omega_t^{n+1}} q \nabla \cdot \mathbf{u}^{n+1} dA = 0, \quad (32)$$

$$\int_{\Omega_t^{n+1}} \mathbf{H} : \mathbf{G}^{n+1} dA - \int_{\Omega_t^{n+1}} \mathbf{H} : (\nabla \mathbf{u}^{n+1})^T dA = 0, \quad (33)$$

$$\int_{\partial P(t^{n+1})} \boldsymbol{\mu} \cdot \left[\mathbf{u}^{n+1} - (\mathbf{u}_p^{n+1} + \omega_p^{n+1} \times (\mathbf{x} - \mathbf{x}_p^{n+1})) \right] ds = 0, \quad (34)$$

Notice that the momentum balance is discretized through a mixed explicit–implicit scheme [33]. Although it might be less stable than a fully implicit treatment of the convective term, it requires the solution of a linear system each time step. As shown in the validation tests below, the required Δt to get convergent results is acceptable, thus this scheme is preferred over implicit ones. Finally, the time derivative of the particle translational and angular velocities is discretized through a second-order backward differencing scheme.

Step 5. Finally, the Laplace equation is solved:

$$\nabla \cdot (\epsilon \nabla u_{m,y}^{n+1}) = 0 \quad (35)$$

with boundary conditions:

$$u_{m,y} = u_{p,y}^{n+1} \quad \text{on } \partial P(t^{n+1}) \quad (36)$$

$$u_{m,y} = 0 \quad \text{on } \Gamma_i, \quad (i = 1, \dots, 4) \quad (37)$$

and the mesh velocity $\mathbf{u}_m^{n+1} = (u_{p,x}^{n+1}, u_{m,y}^{n+1})$ are obtained.

All the second-order schemes in the equations above are replaced by the corresponding first-order schemes at the first time step.

3.3. Code validation

Preliminary simulations have been performed to properly select the length L of the domain. Indeed, because of the imposed periodic boundary conditions, Eqs. (9) and (10), the domain length needs to be chosen sufficiently larger than the particle size to avoid hydrodynamic interactions of the particle with its periodic images. We found that $L/d_p = 40$ is sufficient to satisfy such a condition.

Mesh and time convergence are checked for all the results reported in this work (a typical mesh is shown in Fig. 2). As an example, the migration velocity v_p and position y_p of the particle as function of time t for different mesh resolutions (see Table 1) and time step sizes are reported in Fig. 3a and b, respectively. The fair superposition of the data indicates that, for the chosen parameters, both mesh and time convergence are satisfied.

In general, it is found that a mesh with 80 elements on the particle boundary is sufficient to achieve convergence, although an extra refinement between the particle and the upper boundary is needed when the particle starts quite close to the wall. For this reason, the total element number varies from about 15,000 to 30,000. Notice that the meshes used in our computation are much more refined than those required for convergence in both the inertialess viscoelastic and inertial inelastic cases. As an example, in the inertial inelastic case, an appropriate mesh is typically composed of around 4000 elements.

Regarding the time convergence, we found that a smaller step size is required as the particle starts close to the wall, due to fast dynamics involved, or for low Deborah numbers ($De < 0.1$) to assure code stability. Specifically, all the simulations to be presented are performed by choosing a constant time step size $\Delta t = 0.005$ when the particle is far from the wall and $\Delta t = 0.001$ when the particle is close to it (with a distance less than one particle diameter).

To verify the ability of our numerical code to predict the pure inertial and viscoelastic behavior, we carried out some simulations under the same operative conditions used in previous studies [13,34,35,18]. The results for the inertial (inelastic) case in terms of position of the particle along the gap y_p as a function of the position along the flow direction x_p are shown in Fig. 4a. In Fig. 4b, the particle y -velocity v_p as a function of position y_p is reported for the viscoelastic (inertialess) case. In both figures, our data are in good

Table 1
Mesh parameters.

Mesh label	M1	M2	M1	M2
Particle y -position	0.30	0.30	0.44	0.44
#el. on the particle boundary	80	100	120	180
#el. in the mesh	13,864	20,472	28,182	48,736

Fig. 3. Migration velocity v_p (a) and position y_p (b) of the particle as function of time t for different mesh resolutions (see Table 1) and time step sizes, for the case $y_{p,0} = 0.3$, $De = 1.0$, $Re = 40$.

agreement with those obtained from previous studies, with the remaining small differences likely ascribable to differences in the numerical approaches.

4. Results

Aim of this paper is to investigate on the simultaneous effect of inertia and viscoelasticity on particle migration in Poiseuille flow. Therefore, we present simulations by systematically varying the Reynolds and Deborah numbers and keeping the other parameters fixed to the following values: $\beta = 0.1$, $\alpha = 0.2$, $\rho_p/\rho_f = 1$, $\eta_s/\eta_p = 0.1$. The chosen value for the confinement ratio is generally met in microfluidic experiments [23,24]. The non-zero constitutive parameter α denotes a shear-thinning fluid. Finally, the unitary density ratio indicates a neutrally-buoyant particle. The choice for those parameter values is consistent with our previous work

Fig. 2. Typical mesh used in the simulations. In the inset, a close view of the mesh around the particle is shown.

Fig. 4. Comparison with previous studies. (a) Inertial inelastic case ($De = 0$) [13,35]: position of the particle along the gap y_p as a function of the position along the flow direction x_p . The 'geometric' parameters are: $\beta = 0.25$, $L/d_p = 4$. (b) Inertialess viscoelastic case ($Re = 0$) [18]: migration velocity of the particle v_p as function of its position y_p after the transient extinguished (mastercurve). The shaded area represents the region where the center of the particle cannot access.

[18], and allows for a direct comparison with results obtained in the inertialess viscoelastic case.

We start our analysis by setting the same value for the Reynolds and Deborah numbers, that is $Re = De = 1$. In Fig. 5a, the temporal trends of the migration velocities $v_p(t)$ for different particle initial positions $y_{p,0}$ are reported, whereas in Fig. 5b the trajectories $y_p(t)$ corresponding to those same initial positions are shown. Because of symmetry, from now on, we only report the curves which refer to the upper half of the channel (from $y = 0$ to $y = 0.5$). The shaded area in these and the following figures represents the portion of the channel that cannot be accessed by the center of the particle, due to its finite dimension.

As in the inertialess viscoelastic case [18], a 'critical' unstable equilibrium position y_N is found (see Fig. 5b) that identifies two basins of attraction, corresponding to the stable equilibrium positions $y = 0$ (axis) and $y = 0.5 - \beta/2$ (wall). For $0 < y_{p,0} < y_N$, the particles migrate towards the axis (blue curves in Fig. 5b). On the contrary, for $y_{p,0} > y_N$, the particles move to the wall (red curves in Fig. 5b). Notice that both those behaviors occur after an early time transient, where an inversion of the sign of the migration velocity can also be present (see Fig. 5a). The initial velocity oscillations are due to the stress build-up around the particle in the start-up of the process, as well as to inertial effects. The duration

Fig. 5. Migration velocity v_p (a) and position y_p (b) of the particle as function of time t for six different values of its initial position $y_{p,0}$ in the case $De = 1.0$ and $Re = 1.0$. The red dash-dotted lines represent particles migrating towards the wall, whereas the others correspond to the migration towards the channel centerline. y_N identifies the separatrix, i.e. the unstable equilibrium position of the particle. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

of this transient phase has indeed been shown to grow with increasing the fluid inertia and relaxation time (not reported). Such initial transients are very short, however, and the particles experience for the most part of their motion a negative/positive y -velocity, for $0 < y_{p,0} < y_N$ and $y_{p,0} > y_N$, respectively. At long times, all the velocity trends approach zero, although the dynamics is much faster as the particles tend to the wall. More specifically, as the particle is close to the solid boundary, v_p achieves a maximum before steeply decreasing to zero, whereas the migration velocity smoothly changes in time as the particles move to the channel center. Finally, it seems worth mentioning that, by shifting in time the trajectories of Fig. 5b, a fair superposition of all curves is obtained (not shown). Two 'master trajectories' $y_p(t)$ are then found to fully describe the migration phenomenon in the whole channel, one leading the particle to the channel axis, and the other to the wall.

Following previous works [32,18,19], we can combine the information on velocities and trajectories supplied in Fig. 5a and b. This is done by running several simulations with different initial particle positions $y_{p,0}$ and by taking the values of $v_p(t)$, together with y_p at the same time, where the curves coming from different initial position overlap, that is, after the (fast) initial transients. As a matter of fact, this overlapping identifies the mastercurve. By plotting the pairs $(y_p(t), v_p(t))$ and by interpolating the data around y_N , we

get then a unique curve of v_p as a function of y_p , reported as a dashed green line in Fig. 6. Such a curve crosses the axis $v_p = 0$ at three points: the channel axis ($y_p = 0$), the point corresponding to the particle that touches the wall ($y_p = 0.5 - \beta/2$), and the point y_N defining the separatrix ($y_N \approx 0.36$). As it can be deduced from the sign of the migration velocities around those three points, the first two are stable whereas the third one is unstable. Finally, notice that the maximum velocity is achieved very close to the wall, with a steep trend to a zero velocity as the particle further approaches the boundary.

The just described v_p vs y_p behavior is quite similar to the one previously found in the inertialess viscoelastic case [18]. In Fig. 6, we added with a blue solid line the v_p vs y_p mastercurve at $De = 1$ (and $Re = 0$) taken from that work: matching between the green and blue curves is quantitative. Hence, we conclude that, for the case $Re = De = 1$, inertia does not in fact have any influence on migration dynamics.

The issue we want to address now is how large should the Reynolds number be so that, for a given De , inertia effects start to affect particle migration. To this aim, we perform simulations at increasing values of Re , keeping fixed $De = 1$. In what follows, we will present the results in terms of mastercurves $v_p(y_p)$.

As it can be seen in Fig. 6, by increasing the Reynolds number up to $Re = 40$, the separatrix moves towards the wall and the positive migration velocity peak decreases. In addition, at $Re = 10$, a minimum in v_p appears that is more and more pronounced as Re is higher. However, the overall phenomenology stays qualitatively similar to that described above, i.e. the particles are driven towards the axis or the wall, although the ‘attraction region’ around the wall becomes quite limited for high Reynolds numbers.

Since for $De = 1$ and up to $Re = 40$ inertia does not produce any qualitative change in the dynamics, we investigate now in the ‘reverse’ direction, i.e. how the purely inertial case is essentially recovered by progressively reducing the Deborah number at a given Reynolds number ($Re = 40$). As reported in Fig. 7, the situation at $De = 0.5$ is still similar to that at $De = 1$. In contrast, at $De = 0.25$ (red short dashed curve), one additional intersection with the horizontal line $v_p = 0$ appears, at about $y_p \approx 0.18$. Notice that the migration velocity around the channel axis has now become positive, i.e. the particle moves away from the axis. Thus, two stable equilibrium points still coexist, but they are no more the axis and the wall, as it was for higher De values. Rather, the axis

now becomes an unstable position for the particle, and a novel equilibrium height appears in between the axis and the wall. By further reducing the Deborah number to 0.1 (green long dashed curve), the intersection with the horizontal line $v_p = 0$ near the wall moves very close to it but not disappears, thus the wall is still stable. For this reason, this case does not precisely correspond to the purely inertial case $De = 0$ (blue solid curve), for which the wall is unstable. However, such near-wall intersection at small De is so close to the wall that, from a practical point of view, the migration dynamics can be assumed to be actually the one observed for the purely inertial case. We did not investigate further how the aforementioned near-wall intersection disappears, i.e. whether the purely inertial case is exactly recovered only for $De = 0$ or at some small but finite De -value.

The transition observed at around $De = 0.25$ is studied in details by reducing De from 0.28 to 0.25 (for values $De > 0.28$, the scenario is, indeed, qualitatively similar to the case at $De = 0.5$). The corresponding curves are reported in Fig. 8. For sake of clarity, only the region around the channel axis is shown. Passing from $De = 0.28$ to $De = 0.27$, the mastercurve crosses the zero in two points and becomes positive in a small interval, leading to the appearance of one new equilibrium point. The intersection closer to the axis channel is unstable and the other is stable. Therefore, for this set of parameters, five fixed points are present in each half gap, three are stable (axis, wall and one between them) and two are unstable, the latter separating the basins of attraction of the stable equilibrium points. A similar situation is also observed for $De = 0.26$ (dashed-dotted purple curve in Fig. 8), where the interval of positive migration velocity is wider. At $De = 0.25$, the curve goes up and the unstable equilibrium point close to the axis disappears, with the simultaneous stability change of the channel axis, as described above.

To summarize, for $Re = 40$, by decreasing the Deborah number from 1 to 0.1, four different scenarios are observed: (i) for $De \gtrsim 0.28$, the purely viscoelastic behavior is found with two attractors (axis and wall) and one intermediate unstable separatrix; (ii) for $0.26 \lesssim De \lesssim 0.28$, five equilibrium points appear, three are stable (axis, intermediate height, wall) and two are unstable (that separate the three stable regions); (iii) for $De \lesssim 0.26$, the equilibrium points become four, two stable (intermediate height and wall) and two unstable (axis and one in between the two stable points); (iv) finally, for a very small (or even zero) Deborah

Fig. 6. Migration velocity of the particle v_p as function of its position y_p after the transient extinguished (mastercurve), for $De = 1.0$ and different values of the Reynolds number Re in the range $[0-40]$. The blue solid line represents a purely viscoelastic inertialess case. The shaded area represents the region where the center of the particle cannot access. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 7. Migration velocity of the particle v_p as function of its position y_p after the transient extinguished (mastercurve), for $Re = 40$ and different values of the Deborah number De in the range $[0-0.5]$. The blue solid line represents a purely inertial inelastic case. The shaded area represents the region where the center of the particle cannot access. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 8. Mastercurves of v_p vs y_p for $Re = 40$ and different values of the Deborah number De around the axis-stability transition.

number, the purely inertial behavior is found with one attractor (in between the axis and the wall) and two unstable points (axis and wall).

The trajectories (in terms of mastercurves) corresponding to the two intermediate scenarios are reported in Fig. 9. The data in Fig. 9a, corresponding to $De = 0.27$, clearly show the three attractors separated by two unstable heights at $y_{N1} \approx 0.09$ and $y_{N2} \approx 0.43$. In Fig. 9b, obtained for $De = 0.25$, the axis becomes an unstable separatrix and only two attractors are found.

The complex non-linear dynamic behavior just discussed can be conveniently represented in a solution diagram where the equilibrium points (stable and unstable) are reported as a function of the Deborah number. Such solution diagrams, parametric in the Reynolds numbers, are shown in Fig. 10. Stable/unstable equilibrium points are reported as blue filled symbols and solid lines, and as open red symbols and dashed lines, respectively. For sake of clarity, the stability of the axis is not explicitly reported in this figure (see below Fig. 11, for $Re = 10$ and $Re = 40$). The cases at higher Re are qualitatively similar to that for $Re = 40$.

Let us analyze first the case at $Re = 40$ (square symbols) corresponding to Figs. 7–9. Two bifurcations are now evident: one saddle-node bifurcation where the intermediate stable and unstable branches near the axis collapse (at $De \approx 0.28$) and one subcritical pitchfork where the intermediate unstable branch near the axis collapses onto the stable one at $y_p = 0$ (at $De \approx 0.26$), see Fig. 11. For Deborah numbers higher than the saddle-node, the purely viscoelastic case is found (axis and wall attraction). In the narrow range between the saddle-node and the pitchfork bifurcations, there are three stable solutions, whereas between the pitchfork and some Deborah number value very close (or equal) to zero the stable solutions are two. Finally, in a narrow interval close to $De = 0$ (or just for $De = 0$), the purely inertial regime is recovered (one stable solution in between the axis and the wall).

A similar scenario around the centerline is also observed for $Re = 100$ and $Re = 200$. In general, by increasing Re , both bifurcations shift at higher De . In addition, the range of De where the axis and the intermediate height are stable is wider. However, in contrast with the $Re = 40$ case, the wall is now an unstable equilibrium point so that the particle can migrate towards the axis or towards the intermediate height.

Finally, by reducing the Reynolds number to $Re = 10$, the pitchfork bifurcation passes from subcritical to supercritical, as reported in Fig. 11. Indeed, the two symmetric unstable branches starting from the pitchfork point at $Re = 40$ (red dashed lines in the right panel of Fig. 11) disappear and are replaced by two stable

Fig. 9. Master trajectories $y_p(t)$ in the multistability case of $Re = 40$ and $De = 0.27$ (a) or $De = 0.25$ (b). For $De = 0.27$ there are three stable positions: the wall, the axis and an intermediate height. For $De = 0.25$ the stable positions become two: the wall and the intermediate height.

(symmetric) branches (blue solid lines in the left panel of Fig. 11). In addition to those stable branches, the wall is an attractor as for the $Re = 40$ case, as shown by the upper blue curve in Fig. 10. In conclusion, in each half-gap, two stable equilibrium solutions coexist for any De -value in the explored range. More specifically, beyond the pitchfork bifurcation, the particle can migrate towards the axis or the wall, whereas, for Deborah numbers lower than the bifurcation value, the stable position moves from the axis to an intermediate height that approaches the middle of the half-gap for decreasing De -values.

As final remark, the coexistence of the subcritical pitchfork and the saddle-node bifurcations at $Re = 40$, shown in the right panel of Fig. 11, leads to a hysteresis loop. Indeed, by varying the bifurcation parameter De , the regime achieved by the particle evolves in a different way depending on the starting point. When crossing one of the two bifurcations, a ‘jump’ occurs in the equilibrium position (that is, however, reached by a transient with a characteristic time depending on Reynolds and Deborah numbers). This is not the case at $Re = 10$, where slow changes in the Deborah number lead to smooth variations in the neutral height.

We conclude this section by emphasizing that our 2D simulations can only give qualitative results on the inertio-elastic particle migration phenomenon. For instance, the present simulations cannot account for secondary flows that may arise in viscoelastic fluids

Fig. 10. Bifurcation diagram as function of the Deborah number $De \in [0 - 1]$ for different values of the Reynolds number $Re \in [0 - 200]$. The lines (blue solid for stable and red dashed for unstable equilibrium positions) are a guide to the eye. The stability of the axis is not reported but can be readily inferred, being the opposite of the nearest equilibrium solution. By increasing Re the separatrix moves towards the wall, the pitchfork on the axis goes from supercritical to subcritical and a saddle-node appears. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 11. Supercritical (left) and subcritical (right) pitchfork on the axis. The blue solid/red dashed lines represent stable/unstable equilibrium positions. For the subcritical case, hysteresis in between $De \approx 0.26$ and $De \approx 0.28$ is apparent. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

with a non-zero second normal stress difference flowing in non-circular channels (see, e.g., Refs. [36,37]).

5. Conclusions

In this work, the effects of inertia and viscoelasticity on the cross-streamline migration of a single solid particle in a viscoelastic shear thinning fluid under Poiseuille flow have been investigated through 2D direct numerical simulations.

The model equations have been solved through the finite element method. A DEVSS-G/SUPG formulation with a log-representation of the conformation tensor is used to guarantee numerical convergence at relatively large Reynolds numbers, and for Deborah numbers up to unity. The ALE method is adopted to manage the particle motion, assuring high accuracy around the particle surface. The code has been validated by comparison with previous numerical

results (also obtained by other groups), demonstrating the ability to correctly predict the purely inertial and purely viscoelastic behaviors, which represent our limiting situations.

The migration dynamics has been found to depend on the competition between inertia, that drives the particles towards a certain position along the gap, and viscoelasticity, that promotes migration to the wall and the centerline, depending on the initial position of the particle. For comparable values of Deborah and Reynolds numbers, the migration is dominated by fluid viscoelasticity. Our simulations show that inertial effects start to become relevant as the Reynolds number is at least two order of magnitudes higher than the Deborah number.

For moderate and high Reynolds numbers, the transition from the viscoelasticity-driven to the inertia-driven regimes occurs through two intermediate regimes, characterized by multiple stable equilibrium positions. The solution diagram shows the existence of two bifurcations, a saddle-node and a pitchfork, that determine the establishment of a hysteresis loop.

In contrast, at low Reynolds numbers, the saddle-node bifurcation disappears and, by reducing the Deborah number, the stable equilibrium point moves from the axis towards intermediate positions in the midgap.

The results presented in this work point out the complex dynamic behavior of a particle migrating in a fluid under Poiseuille flow as both inertia and viscoelasticity are relevant. The simulations carried out require highly refined meshes and small time steps to assure spatial and time independence, especially at high Reynolds and Deborah numbers. Hence, a similar detailed analysis through 3D simulations would require huge computational resources (e.g. high performance computing environment) and code parallelization. Although limited to 2D, the analysis qualitatively highlights the appearance of new regimes that are not possible when only one of the two effects is present. Therefore, care must be taken when dealing with technological applications exploiting particle migration in an inertio-elastic regime. On the other hand, the increasing number of stable positions might suggest novel technologies for particle manipulation.

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