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**Scuola Politecnica e
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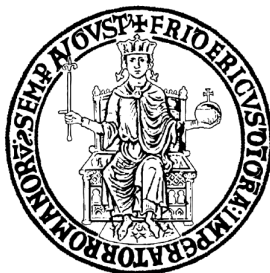


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Particle Dynamics in Elastoviscoplastic Fluids: Effect of Shape and Confinement



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Prof. Pier Luca Maffettone

Candidate's declaration

I hereby declare that this thesis submitted to obtain the academic degree of Philosophiæ Doctor (Ph.D.) in PhD program is my own unaided work, that I have not used other than the sources indicated, and that all direct and indirect sources are acknowledged as references.

Parts of this dissertation have been published in international journals and/or conference articles (see list of the author's publications at the end of the thesis).

Napoli, December 11, 2024

Alie Abbasi Yazdi

To my dear husband, whose unwavering support, patience, and love have been my anchor throughout this journey. Thank you for always believing in me and standing by my side.

To my beloved parents, who endured the pain of being away from me and constantly surrounded me with love, encouragement, and prayers.

I would also like to express my gratitude to my supervisors, Prof. Gaetano D'Avino and Prof. Pier Luca Maffettone, for their guidance, support, and mentorship. Your knowledge and encouragement have been instrumental in shaping this work.

*Lastly,
to the brave women of my homeland, Iran....*

Abstract

This thesis explores the dynamics of particles within elastoviscoplastic (EVP) fluids, which exhibit both yield-stress and viscoelastic properties. These unique characteristics of EVP fluids are essential in various industrial and geophysical applications, where controlling particle behavior can enhance process efficiency. This research investigates the settling, migration, and orientation dynamics of a particle with different shapes and under varying confinement conditions in EVP fluids. Using finite element method, the study investigates the behavior of a particle in an EVP fluid modeled through the Saramito-Giesekus constitutive equation, addressing key factors such as the effect of the Bingham and Weissenberg numbers on particle motion

We start by studying the dynamics of a spherical particle settling near a flat wall in an EVP fluid. Direct numerical simulations reveal that particle-wall distance and the yield stress of the fluid significantly impact sedimentation and lateral migration. Additionally, the study identifies regions of yielded and unyielded fluid around the particle and examines the negative wake phenomenon in comparison to a purely viscoelastic case, highlighting how elasticity and plasticity interact to alter particle behavior near the boundary.

Then, the investigation is extended to prolate spheroidal particle settling in an unbounded EVP material. The results indicate that particle shape strongly affects settling, lift, and angular velocities. With increasing aspect ratio, particle exhibits slower rotational dynamics and a higher sensitivity to the yield-stress properties. The study further explores the flow field around the particle, presenting results for the drag correction coefficient as a function of aspect ratio, Bingham number, and Weissenberg number, which collectively define the settling patterns and particle stoppage.

Finally, the dynamics of circular and elliptical particles suspended in an EVP fluid flowing in a channel flow are examined. The main focus is on the particle migration and orientation, and interaction with yielded and unyielded fluid regions. The study demonstrates that the initial position, shape, and yield-stress characteristics of the fluid influence the equilibrium position and orientation attained by the particle.

Keywords:Elastoviscoplastic fluids, Yield stress, Particle dynamics, Sedimentation, Migration, Numerical simulations, Saramito-Giesekus constitutive equation

Sintesi in lingua italiana

Questo lavoro di tesi studia la dinamica di particelle all'interno di fluidi elastoviscoplastici (EVP) che presentano sia uno sforzo di soglia che elasticità. Queste caratteristiche uniche dei fluidi EVP sono essenziali in varie applicazioni industriali e geofisiche, dove il controllo del comportamento delle particelle può migliorare l'efficienza dei processi. Questa ricerca indaga le dinamiche di sedimentazione, migrazione e orientamento di particelle con forme diverse e in condizioni di confinamento variabili. Attraverso simulazioni agli elementi finiti, lo studio si incentra sul comportamento di particelle sospese in fluidi EVP modellato attraverso l'equazione costitutiva di Saramito-Giesekus, esaminando fattori chiave come l'effetto dei numeri adimensionali di Bingham e Weissenberg sul moto delle particelle.

Il primo problema investigato riguarda la dinamica di una particella sferica che sedimenta vicino a una parete in un fluido EVP. Le simulazioni numeriche mostrano che la distanza particella-parete e lo sforzo di soglia del fluido influenzano significativamente la sedimentazione e la migrazione laterale. Inoltre, lo studio identifica regioni yielded e unyielded attorno alla particella ed esamina il fenomeno della 'negative wake' rispetto ad un caso puramente viscoelastico, evidenziando come l'elasticità e la plasticità interagiscano alternando il comportamento delle particelle vicino alla parete.

Successivamente, lo studio viene esteso a particelle sferoidali prolatti che sedimentano in un fluido EVP inconfinato. I risultati indicano che la forma della particella influisce fortemente sulla sedimentazione, la velocità di lift e la velocità angolare. All'aumentare dell'aspect ratio, le particelle mostrano dinamiche rotazionali più lente e una maggiore sensibilità alle proprietà plastiche del materiale. Lo studio esplora il campo di moto attorno alla particella, presentando risultati per il coefficiente di correzione del drag in funzione dell'aspect ratio, del numero di Bingham e del numero

di Weissenberg.

Infine, l'ultimo problema affrontato riguarda la dinamica di particelle circolari ed ellittiche sospese in un fluido EVP che fluisce in un canale. L'obiettivo principale è studiare la migrazione e l'orientazione delle particelle, e l'interazione con le regioni yielded e unyielded del materiale. Lo studio mostra che la posizione iniziale, la forma e le proprietà plastiche del fluido influenzano la posizione e l'orientazione di equilibrio delle particelle.

Parole chiave: Fluidi elastoviscoplastici (EVP), Yield stress, Dinamica di particelle, Sedimentazione, Migrazione, Simulazioni numeriche, Equazione costitutiva di Saramito-Giesekus

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List of abbreviations

The following abbreviations are used throughout the thesis.

Re	Reynolds number
Bn	Bingham number
Wi	Weissenberg number
EVP	Elastoviscoplastic

Author's Publications

The contents of this thesis are the results of the research of the author, Alie Abbasi Yazdi, during her PhD studies at UNINA, under the supervision of Prof. Gaetano D'Avino and co-supervision of Prof. Pier Luca Maffettone. The following papers have been published and/or are in progress:

1. Yazdi, A.A. and D'Avino, G., 2023. Sedimentation and migration dynamics of a spherical particle in an elastoviscoplastic fluid near a wall. *Journal of Non-Newtonian Fluid Mechanics*, 314, p.105004.

(<https://doi.org/10.1016/j.jnnfm.2023.105004>)

2. Abbasi Yazdi, A. and D'Avino, G., 2024. Sedimentation of a spheroidal particle in an elastoviscoplastic fluid. *Physics of Fluids*, 36(4).

(<https://doi.org/10.1063/5.0199919>)

3. Yazdi, A.A. and D'Avino, G., Dynamics of a circular or elliptical particle in an EVP fluid in a channel flow (under preparation)

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Chapter 1

Introduction

This thesis investigates the motion of particles in elastoviscoplastic (EVP) fluids, i.e., materials that exhibit both yield stress and viscoelastic properties. While the contributions presented are primarily advances in understanding fundamental physics, the thesis is strongly motivated by industrial applications where EVP fluids are relevant. In these fluids, yield stress refers to a threshold in stress that must be exceeded for the material to deform. A fluid exhibiting this behavior is known as a yield stress fluid. When such a material also shows elastic behavior, it is classified as an elastoviscoplastic fluid. In practical terms, small or light particles tend to remain suspended in EVP fluids due to the support provided by the unyielded (solid-like) regions, while larger or heavier particles can settle or sediment through the fluid, overcoming the yield stress. Between these two behaviors, a complex interplay of parameters defines the boundary between flow and no-flow conditions, commonly called the yield limit. Understanding this boundary is essential for predicting particle behavior under different flow and stress conditions.

The geometry and shape of a particle, as well as proximity to a wall, directly play crucial roles in particle dynamic behavior within EVP fluids. For instance, ellipsoidal particles might encounter different resistance compared to spherical ones. Particles close to a solid boundary might act differently due to the confinement effect of the wall on the yielded and unyielded regions. These factors, while intuitively impactful, require a systematic mechanical analysis to fully understand and predict their effects

on particle migration, orientation, and settling within EVP material.

This thesis, therefore, provides a comprehensive investigation of these scenarios, exploring the fundamental behaviors of particles in elastoviscoplastic fluids and addressing critical questions. By studying these factors, we aim to deepen our understanding of particle-fluid interactions in EVP materials. This knowledge is crucial because the ability to control particle motion can improve the efficiency, quality, and effectiveness of various processes.

In this chapter, we first discuss the industrial applications and motivations for this study. Next, we introduce the concept of yield stress, followed by an overview of elastoviscoplastic materials. We then review previous studies on particle dynamics in yield stress fluids and viscoelastic fluids and present the available literature on particle dynamics in EVP materials. Finally, we close the chapter with an outline of the thesis, highlighting the research questions and objectives of the subsequent chapters.

1.1 Industrial applications

Elastoviscoplastic materials exhibit a complex combination of elastic, viscous, and plastic behavior, making them essential in various applications across multiple industrial processes due to their unique properties. In construction and civil engineering, elastoviscoplastic models are utilized to describe the behavior of clay and other cohesive soils under loading, aiding in the design of foundations and earth structures. Additionally, concrete and asphalt exhibit elastoviscoplastic behavior, particularly under varying temperature and loading conditions, which influences their performance and longevity [3, 4].

In the automotive industry, elastoviscoplastic materials are employed as damping materials in automotive components to reduce vibrations and noise, enhancing ride comfort and minimizing fatigue on vehicle structures [5, 6]. These materials are also used in seals and gaskets, where their yield stress and viscoelastic behavior help maintain a seal under fluctuating pressures and temperatures.

The aerospace sector utilizes elastoviscoplastic materials in the design of lightweight structures requiring a combination of strength and flexibility. These materials contribute to reduce failure and deformation under

loads in composite and structural applications. In biomedical applications, elastoviscoplastic behavior is essential for tissue engineering, aiding in the development of scaffolds that mimic natural tissue properties [7, 8]. Additionally, prosthetics rely on these materials to respond to dynamic loading conditions while ensuring user comfort.

The food industry also benefits from elastoviscoplastic materials, particularly in food processing. Many food products, such as dough and cheese, behave as elastoviscoplastic materials, and understanding their behavior helps optimize processing, packaging, and storage [9, 10, 11].

Particles are suspended in yield-stress fluids in important industrial applications such as the flow of food suspensions and the mixture of additives in the cosmetic and drug industries [12]. For instance, toothpaste often contains particles such as hydroxyapatite, silver (for antibacterial properties), and titanium dioxide. The stability of these particles is a crucial concern; Liu et al. [13] studied the stability of chitosan and active nanoparticles in toothpaste using scanning electron microscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. The pH of the toothpaste is particularly important since higher pH values can increase particle size (Figure 1.1).

Particle stability is also significant in cosmetics (Figure 1.1), where adding particles is common. The size of these particles affects how the product feels on the skin, which is vital for product development [14]. For example, particle sizes smaller than 10 μm lead to reduced skin feel and improved viscosity, while sizes exceeding 200 μm can form silicon elastomer gel balls on the skin. Additionally, food industries face challenges with yield-stress fluids and particle motions, such as chocolate chips in cookies. While there are numerous empirical models to describe the behavior of emulsions or suspensions, most of them focus on fluids without yield stress (Newtonian or viscoelastic suspensions). Recently, there has been growing interest in suspensions of yield-stress materials, evidenced by some experimental studies and few in-depth theoretical or numerical works.

In polymer science, foams and gels exhibit elastoviscoplastic properties, making them suitable for cushioning and packaging applications where energy absorption is critical. Adhesives and sealants frequently show yield stress and viscoelastic behavior, which are crucial for effective bonding under various conditions. The oil and gas industry employs elastoviscoplastic



Figure 1.1. Some examples of particles in yield-stress fluids in different industries

fluids in drilling operations to stabilize boreholes and manage pressure, adapting to different geological conditions [15, 16].

Several materials exemplify elastoviscoplastic behavior, including clays and mud, which naturally exhibit these properties due to their structure and moisture content. Biopolymers such as gelatin and alginate also demonstrate elastoviscoplastic behavior, particularly in gel form. Various blends and alloys of polymers can exhibit yield stress and viscoelastic characteristics, while concrete and cementitious materials can be modeled as elastoviscoplastic due to their setting behavior. Certain metallic alloys, especially at elevated temperatures, can show elastoviscoplastic behavior, affecting their formability and performance under stress [17].

In conclusion, elastoviscoplastic materials play a vital role in many industries by combining the advantages of elastic, viscous, and plastic behaviors. Understanding their properties allows for improved design and functionality in diverse applications, from construction to biomedical devices.

1.2 Yield-stress fluids

The term *yield-stress fluid* is used to categorize a range of non-Newtonian fluids that behave as rigid solids when the imposed stress is below a threshold (called the yield stress). Otherwise, these materials flow (i.e., deform) when the level of imposed stress exceeds the yield stress [18]. Describing materials that exhibit yield stress behavior is one of the most difficult tasks in rheology, as one of the aims is to minimize the number of material parameters while respecting the complex rheological behavior of these types of materials. To achieve a realistic description of the behavior of yield stress materials, several simplifying assumptions have been made in the formulation of constitutive equations.

About a century ago, Bingham, in his seminal work on plasticity [19], assumed a threshold pressure drop below which a pipe full of viscoplastic material would not flow, and a linear increase in pressure drop with a flow rate above this threshold. This led to the development of the Bingham fluid constitutive equation that, for a simple shear flow, reads as:

$$\begin{cases} \tau = \tau_y + K\dot{\gamma} & \text{if } |\tau| > \tau_y \\ \dot{\gamma} = 0 & \text{if } |\tau| \leq \tau_y \end{cases} \quad (1.1)$$

where τ is the shear stress, K the plastic viscosity, τ_y the yield stress, and $\dot{\gamma}$ the shear rate. This model assumes that yield-stress materials are rigid when unyielded and exhibit a linear flow curve when yielded. It should be noted that in Eq. (1.1), the von Mises yield criterion has been used implicitly. Indeed, it states that if the stress does not exceed τ_y , then the material is unyielded (i.e., the shear rate vanishes).

After Bingham, a few years later, Herschel and Bulkley [20] added a power-law dependency to the Bingham model to account for the shear-thinning behavior in the rheological measurements of yield stress materials:

$$\begin{cases} \tau = \tau_y + K\dot{\gamma} & \text{if } |\tau| > \tau_y \\ |\dot{\gamma}|^{n-1} = 0 & \text{if } |\tau| \leq \tau_y \end{cases} \quad (1.2)$$

This modification allows the rheology of more materials to be fitted, as many yield-stress fluids exhibit shear-thinning behavior. Other models proposed over the years include the Casson and Robertson-Stiff models,

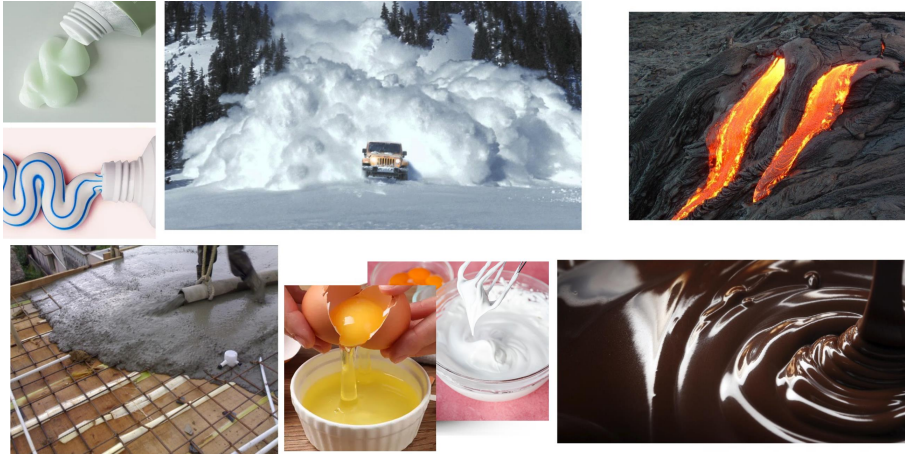


Figure 1.2. Some examples of yield-stress fluids.

both of which exhibit a yield-stress and shear-thinning behavior. While these are not as widely used as the Bingham and Herschel-Bulkley fluids, they have their specific applications (Figure 1.2).

The Bingham and Herschel-Bulkley (HB) models have been extensively utilized to study the flow problems of yield-stress fluids, with several papers published on the topic [12, 21].

1.3 Elastoviscoplastic fluid

Elastoviscoplastic (EVP) fluids are increasingly significant in both geophysical and industrial applications due to their unique mechanical behavior, which combines elastic, viscous, and plastic properties. In geophysical contexts, EVP fluids are crucial for modeling natural phenomena like mudslides and tectonic movements. Industrial applications also rely on EVP materials, notably in sectors such as mining, biomass-to-fuel conversion, and petroleum extraction. Moreover, biological and adaptive materials often exhibit EVP behavior, making their study relevant for physiology, biolocomotion, tissue engineering, and other biomedical fields. Many of these applications involve complex multiphase flows, underscoring the need to study and predict EVP fluid behavior.

EVP fluids deform elastically under low strain but undergo irreversible plastic deformation and start to flow once the strain reaches a certain threshold. Unlike ideal yield-stress fluids (e.g., Bingham or Herschel-Bulkley models), EVP materials require more sophisticated modeling to capture their combined elastic, viscous, and plastic responses accurately. In this regards, Saramito [22] proposed a tensorial constitutive model based on Bingham viscoplastic and Oldroyd viscoelastic models, ensuring compliance with thermodynamic laws. In this model, the material behaves as a Kelvin-Voigt viscoelastic solid until yielding, which occurs when a critical strain energy level—defined by the von Mises criterion—is surpassed. Upon yielding, the stress field follows a nonlinear viscoelastic constitutive equation. This model was further refined to account for shear-thinning viscosity and a more enhanced plasticity criterion, enabling the prediction of behaviors such as the first normal stress difference in simple shear flow due to combined viscoelastic and viscoplastic effects.

Saramito model, however, assumes an ideal Hookean response before yielding, resulting in a zero-phase difference between strain oscillation and shear stress, leading to a prediction of zero loss modulus G'' . This discrepancy was addressed by introducing an isotropic kinematic hardening approach, as proposed by Dimitriou et al. [18]. This approach allows yield stress to evolve over time and flow conditions, making it possible to predict a non-zero loss modulus at small strain amplitudes, aligning the model more closely with experimental observations in large-amplitude oscillatory shear tests. Additionally, recent developments in isotropic kinematic hardening have enabled the modeling of thixotropic behaviors in EVP materials, such as those observed in waxy crude oils.

Several alternative constitutive models have been proposed to describe EVP fluids. De Souza Mendes [23] presented a model based on modifying the Oldroyd-B equation by allowing parameters like relaxation and retardation times, and viscosity, to vary with the deformation rate. Another model by Bénito et al. [24] simplifies the EVP description with a fully tensorial, rheological constitutive equation predicting substantial deformation before yielding. Recently, systematic comparisons of these models have demonstrated their performance against experimental data in standard viscometric flows, providing insights into their applicability across different EVP fluid behaviors.

Despite the progress in EVP fluid modeling, numerical studies on these materials are limited due to the complex, nonlinear nature of their governing equations. Simulation of EVP fluids is critical for gaining quantitative insights that are challenging to obtain experimentally, such as velocity and stress fields. Notably, simulations have shown elastic effects in fluids like liquid foams and Carbopol, revealing phenomena like the negative wake—an overshoot in velocity behind an obstacle. Initial experiments by Dollet and Graner [25] showed a velocity overshoot in liquid foam flow around a circular obstacle, an observation confirmed through EVP model simulations by Cheddadi et al. [26], which demonstrated that the negative wake is an elastic effect. Recent numerical studies using Saramito EVP model successfully captured this effect around a sedimenting particle in Carbopol solutions [1], aligning with experimental observations. Other simulations have explored elasticity impact on yield surfaces, finding that elasticity can significantly alter these surface shape and position [27].

The growing interest in EVP fluids has led to advancements in modeling and simulating their interactions in multiphase systems, such as particle-laden flows. As a result, the study of EVP fluids continues to expand, with models evolving to capture these material complex behaviors more accurately. The continued development of models and computational methods for EVP fluids is essential for advancing our understanding of complex, real-world fluid dynamics across a range of geophysical, industrial, and biological applications.

1.4 Particle dynamics in EVP fluids

The transport of particles in non-Newtonian fluids has been the subject of a vast literature. However, most of the works are limited to generalized Newtonian fluids, viscoelastic or viscoplastic liquids. Only few works exploring the dynamics of rigid particles in EVP materials are available. In the following sections, we review the existing literature for the sedimentation and channel flow.

1.4.1 Sedimentation of particles in non-Newtonian fluids

The transport of solid particles in non-Newtonian fluids is fundamental in a huge number of industrial and biological applications. The peculiar rheological properties of the suspending liquid are responsible for drastic variations of the particle dynamics as compared to Newtonian suspensions. Experiments, theoretical predictions, and numerical simulations have highlighted the importance of typical non-Newtonian properties as shear-thinning, elasticity, plasticity on the particle settling dynamics, affecting the flow field surrounding the particles and, in turn, the drag coefficient [28, 29, 30, 1].

A sphere sedimenting in a quiescent unconfined viscoelastic fluid, for instance, exhibits a variation of the steady-state drag correction factor (defined as the ratio between the drag coefficient of the particle in the viscoelastic fluid and in the Newtonian one) as the degree of elasticity is varied [30], and the appearance of the ‘negative wake’ behind the particle, i.e., a region downstream the fluid velocity has a direction opposite to the gravity [31, 32]. The presence of confining walls strongly affects both the drag coefficient and the negative wake phenomenon [30]. Furthermore, a particle sufficiently close to a wall may also experience a motion orthogonal to the force direction referred as ‘lateral migration’ [33, 34]. The migration phenomenon has been studied in other flow fields such as shear, Couette, channel flows, with the latter case of special interest for microfluidic applications [35]. The presence of a wall has a strong influence on the migration velocity and is even necessary to observe the lateral motion in a linear flow field [35]. A significant number of studies have focused on the effect of viscoelasticity on the motion of the suspended particles in a variety of flow fields [36].

As previously discussed, another relevant property of non-Newtonian fluids is the existence of the yield-stress [37, 38]. Several works have investigated the settling dynamics of spherical particles in yield-stress materials both experimentally [39, 40, 41, 42, 43, 44, 45] and numerically [28, 46, 47, 48, 49, 50, 51]. The results show that the drag correction factor increases as the yield stress increases, i.e., a sphere settles slower in a viscoplastic fluid rather than in a Newtonian fluid. Criteria for the stopping of the particle and the shape of the yielded/unyielded region as the relevant parameters are varied are also investigated.

In a variety of real fluids, both elasticity and yield-stress are present. Elasticity must be considered in order to justify some phenomena observed in yield-stress materials that are typical of viscoelastic fluids. This is the case of the loss of the fore-aft symmetry of the flow field around a settling particle under creeping conditions and the formation of the negative wake [41, 43], both phenomena that are not predicted in viscoplastic fluids with negligible elasticity.

Despite their relevance, studies on the dynamics of particles in elasto-viscoplastic fluids are relatively few. Fragedakis et al. [1] incorporated elastic effects in a pure viscoplastic fluid using the constitutive equation proposed by Saramito [22, 52]. They solved the problem of a sphere sedimenting in a large container by a 2D axisymmetric finite element method. They found that typical phenomena such the negative wake and the loss of the fore-aft symmetry under creeping flow conditions are due to elasticity and not to thixotropy. The simulation results agree very well with the available experimental measurements [53]. They also propose a relation for the drag correction coefficient as a function of the material plasticity for different levels of elasticity and the criteria for particle entrapment. The settling dynamics of a spherical particle in an unconfined EVP fluid has been later investigated by fully-resolved 3D numerical simulations in the absence and presence of a cross-shear flow orthogonal to the settling direction under weak inertia [54]. They found that, in the presence of a cross-shear flow, the drag on the sphere is reduced and the negative wake behind the particle disappears. and demonstrates that it is necessary to consider elasticity in laboratory yield-stress fluids to quantitatively describe the flow characteristics and the dynamics of a particle settling in EVP materials.

As previously mentioned, the presence of a confining wall strongly affects the particle dynamics giving rise to new phenomena such as the cross-stream lateral migration. It is interesting, then, to investigate the interplay between wall effect, fluid viscoelasticity and plasticity on the dynamics of particles. Sarabian et. al. [2] numerically investigated the confinement effect on the sedimentation of a single spherical particle in elastoviscoplastic fluids between two parallel walls under weak inertial conditions. The fluid is modelled through the Saramito constitutive equation and the immersed boundary method is used to handle the rigid particle motion. The results

show that, by increasing the confinement, the fluid velocity relaxes faster and the location of the negative wake moves towards the sphere, resulting in a lower sedimentation rate. The minimum value of the confinement ratio such that the wall effect becomes negligible and the maximum variation of the drag correction coefficient with confinement ratio are weakly dependent on the fluid elasticity and plasticity for a certain range of parameters. Also, they propose an expression of the drag coefficient as a function of the Bingham number and confinement ratio. It is important to point out that the particle is always initially located with center on the centerplane between the two walls, thus for symmetry does not migrate.

Despite the obvious relevance, studies on the sedimentation of non-spherical particles in complex liquids are even more limited as compared to spheres. Experiments reported that axisymmetric bodies (e.g., cylinders) falling in a viscoelastic fluid at negligible inertia rotate up to reach an orientation with major axis aligned with the force direction [55, 56], regardless of fluid rheology, aspect ratio of the particle, and initial orientation. Theoretical calculations and numerical simulations [57, 58, 59, 60, 61, 62] showed that fluid elasticity generates a non-zero torque on the particle with opposite sign with respect to the one induced by inertia. Studies on spheroidal particles highlighted that the torque is such that both prolate and oblate shapes attain a stable orientation with major axis along the applied force [62, 63]. A similar behavior has been found for triaxial ellipsoidal particles where the shape affects the settling dynamics and the steady drag coefficient but not the final orientation [63]. Recent numerical simulations have reported the existence of a mastercurve governing the settling dynamics of prolate/oblate spheroids (and a mastersurface for triaxial ellipsoids) after the initial transient due to the viscoelastic stress development, i.e., the settling dynamics only depends on the current orientation regardless of the history to reach it [63]. This behavior is expected whether the characteristic time for the stress development (the fluid relaxation time) is small compared with the characteristic time of the particle rotation, the latter depending on the applied force and the particle shape.

Few recent studies have investigated the sedimentation of non-spherical particles in viscoplastic (inelastic) fluids. Sobhani et al.[64] carried out Lattice-Boltzmann simulations to study the sedimentation of a rigid, elliptical (2D) particle in a biviscous, yield stress fluid contained in a finite,

closed-ended channel. They reported that the trajectory of the particle is strongly affected by the presence of the yield stress, giving rise to new settling modes. Specifically, a particle initially released at the channel centerline and inclined with respect to the force direction first migrates towards the wall and then moves back towards the centerline, reaching an equilibrium distance from the wall and keeping a non-horizontal orientation while sedimenting. The offset position depends on the Bingham number and the density ratio, and is independent of the initial inclination angle. Da Hui et al.[65] employed a graphics processing unit accelerated immersed boundary Lattice-Boltzmann method to study the sedimentation of elliptical particles in a Bingham fluid. The single particle case was considered for validation purposes, confirming the results of Sobhani et al.[64]. The settling of a pair, a chain, and of a cluster of elliptical particles is addressed, highlighting the appearance of a variety of sedimentation dynamics due to the fluid yield stress. The sedimentation of (3D) prolate and oblate spheroidal particles in a Bingham liquid has been studied by Romanus et al. [66] by numerical simulations. The particle aspect ratio is varied between $1/4$ to 4 . Creeping flow conditions are first analyzed, then the study is extended including inertial effects. In the former case, the critical conditions for particle stoppage are evaluated for spheroids oriented with major axis parallel and orthogonal to the force direction. A quantitative match with previous data obtained by the augmented Lagrangian method [50] is found. As inertia becomes relevant, the spheroids reach an equilibrium angle depending on the aspect ratio and sediment following a trajectory inclined with respect to the force direction. The analysis of the yielded/unyielded regions reveals that the yielded envelope follows the spheroid extremities during the rotation. A ‘belt’ of plastic material surrounding the particle is found, with dimension depending on the particle shape and orientation. For an inclined prolate spheroid, the plastic belt acts as a lever arm of length dependent on the aspect ratio. For oblate spheroids, two large domes of plastic material form near the flat sides, leading to a stronger rotation resistance. We would like to remark that the just mentioned studies consider (2D or 3D) particles in purely viscoplastic fluids without accounting for elastic effects. To the best of our knowledge, works dealing with the dynamics of non-spherical particles in elastoviscoplastic fluids are not available.

1.4.2 Particle motion in EVP fluids flowing in a channel

In a Newtonian fluid under creeping flow conditions (where inertia is completely neglected in the equations of motion), a single particle does not migrate in a unidirectional flow [67, 68]. However, in an inertialess viscoelastic channel flow, a particle migrates either towards the center or the walls based on various factors, such as its initial position and shear-thinning effects [69, 70, 71]. Inertia also promotes particle migration, but in a different manner: it pushes the particles towards an equilibrium position in the middle of the channel half-width, whereas the elasticity of the fluid induces lateral motion towards the centerline or the walls. Thus, in the inertial channel flow of a viscoelastic fluid, the balance between these two competing effects results in different equilibrium positions, depending on the Reynolds number and the Weissenberg number. This analysis is not trivial; as shown by Di Carlo et al. [72], the lateral force on the particle in a viscous inertial flow collapses onto ‘master curves’ (which differ close to the wall and in the vicinity of the channel centerline with various scalings). However, when fluid elasticity is considered, the lateral force distribution becomes markedly more complicated [73]. Additionally, multiple stable and unstable final positions for particles may occur, which is largely attributed to the combined effects of shear-thinning and fluid elasticity. Consequently, the final position is influenced not only by the Reynolds number and the Weissenberg number but also by the initial position of the particles [74]. The complexity of this problem dramatically increases in three-dimensional flows, as discussed in Li et al. [75].

The mechanisms of particle migration within a Poiseuille flow of a yield-stress fluid and the entrapment of particles in the core unyielded plug are not well understood. Recently, Siqueira and de Souza Mendes [76] investigated particle migration in an ‘apparent’ yield-stress fluid by integrating the regularized effective viscosity of a viscoplastic material with models for suspension viscosity and shear-induced particle migration. Their findings indicate that there is a high concentration of particles in the plug region at short time scales; however, due to the models used, this plug zone eventually becomes entirely depleted of particles over longer time scales.

Chaparian et. al. [77] performed a numerical study of the dynamics of a neutrally buoyant rigid spherical particle carried by an elastoviscoplastic fluid in a pressure-driven flow between two infinite flat walls. The

Saramito constitutive equation [22] is employed. The Reynolds number is fixed to 20, the Weissenberg number is varied between 0.1 and 1, and the Bingham number between 0 and 0.4. They observed two sheared yielded regions near the walls and a core unyielded region. Particles initially released in the core region translate at the same velocity as the plug without migrating and rotating. On the other hand, the dynamics of the particles in the yielded regions depend on the relative weight of elasticity and plasticity. In the viscoelastic limit, inertia is dominant and the particle migrates towards a position in between the centerline and the wall. In the viscoplastic limit, a similar behaviour is observed, with the yield surface taking the role of the centerline, so the migration occurs in the sheared regions only. Finally, when both elasticity and plasticity are relevant, for a certain range of Weissenberg numbers, the particle enters the plug region and moves towards the centreline. This behavior is also observed for non-neutrally buoyant particles, although these particles tend to lose stability with a smaller buoyancy than what is needed for sedimentation in a quiescent yield-stress fluid [78, 79, 80]. Some of these characteristics have been observed experimentally by Merkak et al. [81, 82] in inertialess viscoplastic pipe flows, where the maximum particle Reynolds number is approximately $O(10^{-1})$.

Outline

This thesis is composed of four main chapters.

Chapter 2 We begin by formulating the problem of particle dynamics in elastoviscoplastic (EVP) fluids. We examine three main symmetric geometries: a large box containing a single particle near a wall, a spherical domain containing particles with different aspect ratios, and Poiseuille flow in a long channel. The governing and constitutive equations used to model the computational domain are presented. Additionally, the numerical methodology employed in this thesis is explained in detail.

Chapter 3 We study the dynamics of a spherical particle settling in an elastoviscoplastic fluid near a flat wall, under inertialess conditions. The sedimentation and migration phenomena are analyzed by varying the

particle-wall distance and relevant dimensionless numbers. We investigate the yielded/unyielded fluid regions, the shear rate distribution around the particle, and the negative wake phenomenon, and we relate these to the observed dynamics. A comparison with the purely viscoelastic case is also discussed.

Chapter 4 This chapter addresses the dynamics of a prolate spheroidal particle settling in an unbounded elastoviscoplastic fluid under inertialess conditions. The sedimentation, lift, and angular velocities are computed as the relevant fluid, flow, and geometrical parameters vary. We investigate the flow fields around the particle, including the yielded/unyielded fluid regions and the viscoelastic stress distribution. Results for the drag correction coefficient as a function of the aspect ratio, Weissenberg number, and Bingham number are presented.

Chapter 5 In this chapter, we investigate the dynamics of circular and elliptical particles suspended in EVP fluids, focusing on their migration, orientation, and interaction with the yielded and unyielded regions of the suspension in a channel flow. As in previous chapters, the fluid is modeled using the Giesekus constitutive equation, modified according to Saramito to account for yield stress. Results are provided at a fixed Weissenberg (Wi) number, with varying Bingham (Bn) numbers, distances from the channel centerline, and, for elliptical particles, initial orientations. The purely viscoelastic case is also simulated to understand the effect of plasticity on particle dynamics.

Chapter 6 Finally, this chapter provides a summary of the research conducted, draws conclusions, and offers recommendations for future research.

Mathematical model and numerical method

In this section, the governing equations for the fluid dynamics of a particle immersed in a non-Newtonian fluid are introduced. The particle is considered rigid and non-Brownian, with the system being isothermal. Additionally, the equations are presented in dimensionless form to enable comparison with results from the literature

2.1 Governing equations

Let us consider a system consisting of one particle suspended in a non-Newtonian fluid. The suspension (fluid and particle) occupies a volume Ω with external boundaries $\partial\Omega$ and the particle occupies a volume $P(t)$ with boundaries $\partial P(t)$. Assuming incompressible and inertialess flow conditions, the motion of the fluid domain $\Omega - P(t)$ is governed by the continuity and momentum balance equations:

$$\nabla \cdot \mathbf{u} = 0 \tag{2.1}$$

$$\nabla \cdot \mathbf{T} = \mathbf{0} \tag{2.2}$$

where $\mathbf{u}$ is the fluid velocity and $\mathbf{T}$ is the total stress tensor given by:

$$\mathbf{T} = -p\mathbf{I} + 2\eta_s\mathbf{D} + \boldsymbol{\tau} \tag{2.3}$$

In this equation, p is the pressure, $\mathbf{I}$ is the unity tensor, η_s is the viscosity of a Newtonian solvent, $\mathbf{D}$ is the rate of deformation tensor defined as $\mathbf{D} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$, and $\boldsymbol{\tau}$ represents the extra stress due to the non-Newtonian nature of the fluid. Therefore, the total stress tensor is given by an isotropic contribution, a Newtonian solvent contribution and a non-Newtonian stress contribution. The extra stress tensor needs to be specified through a constitutive equation that relates $\boldsymbol{\tau}$ to the velocity gradient. The constitutive equations used in this project will be discussed in the next section.

If no external forces or torques act on the particle and assuming inertialess conditions, the particle is force- and torque-free:

$$\int_{\partial P(t)} \mathbf{T} \cdot \mathbf{n} dS = \mathbf{0} \quad (2.4)$$

$$\int_{\partial P(t)} (\mathbf{x} - \mathbf{X}) \times (\mathbf{T} \cdot \mathbf{n}) dS = \mathbf{0} \quad (2.5)$$

where the left-hand sides are the total force and torque acting on the particle surface. $\mathbf{X}$ is the particle centroid, $\mathbf{x}$ is the position vector of a point on the boundary $\partial P(t)$, and $\mathbf{n}$ is the outward unit normal vector on $\partial P(t)$ and dS is the local surface area.

To solve the above system of equations, boundary conditions are required. No-slip conditions are generally assumed to hold on the particle boundaries $\partial P(t)$, thus the fluid velocity is related to the kinematic particle quantities through the rigid-body motion equation:

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X}) \quad (2.6)$$

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

Due to the inertialess assumption, no initial condition for the velocity is needed. In case the constitutive equation contains a time derivative (as in the viscoelastic or elasto-viscoplastic case, see later), an initial condition is required for the stress tensor. A stress-free condition, i.e., $\boldsymbol{\tau}|_{t=0} = \mathbf{0}$, is considered.

The conditions on the external boundaries $\partial\Omega$ depend on the specific problem. For a spherical or spheroidal particle sedimenting in a fluid (chap-

ters 3 and 4), no-slip is applied at the external boundaries. In addition, for these two problems, Eq. (2.4) is replaced by:

$$\mathbf{F} = (F, 0, 0) = \int_S \mathbf{T} \cdot \mathbf{n} dS \quad (2.7)$$

assuming that a force $\mathbf{F}$ is applied on the particle along the x -direction.

For a particle freely transported by the fluid in a channel (chapter 5) we impose no-slip at the channel walls and periodic conditions between the inflow (Ω_{in}) and the outflow (Ω_{out}) boundaries together with a flow rate in the inflow:

$$\mathbf{u}|_{\Omega_{\text{in}}} = \mathbf{u}|_{\Omega_{\text{out}}} \quad (2.8)$$

$$\mathbf{t}|_{\Omega_{\text{in}}} = \mathbf{t}|_{\Omega_{\text{out}}} - \Delta p \mathbf{n} \quad (2.9)$$

$$\int_{\Omega_{\text{in}}} \mathbf{u} \cdot \mathbf{n} dS = Q \quad (2.10)$$

In Eq. (2.9), $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$ is the traction on the inflow/outflow curves, and $\Delta p = \frac{dp}{dx}L$, where $\frac{dp}{dx}$ is the pressure gradient, L is the channel length, and $\mathbf{n}$ is the outwardly directed unit normal vector. The flow rate in Eq. (2.10) is imposed through a constraint, where the associated Lagrange multiplier is identified as the pressure difference, which is an unknown quantity determined by Eq. (2.10) [?].

Finally, once the fluid velocity, pressure, and stress fields are calculated along with the particle kinematic quantities, the particle centroids $\mathbf{X}$ and the orientations $\boldsymbol{\Theta}$ are updated by integrating the following equations:

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}, \quad \mathbf{X}|_{t=0} = \mathbf{X}_0 \quad (2.11)$$

$$\frac{d\boldsymbol{\Theta}}{dt} = \boldsymbol{\omega}, \quad \boldsymbol{\Theta}|_{t=0} = \boldsymbol{\Theta}_0 \quad (2.12)$$

where $\mathbf{X}_0$ and $\boldsymbol{\Theta}_0$ are the initial particle position and orientation.

2.2 Constitutive equations

Non-Newtonian fluids show several peculiar rheological properties compared to Newtonian liquids. Several constitutive equations are available in

the literature [83]. As stated in the Introduction, the aim of the present project is to carry out numerical simulations on the dynamics of a particle in an EVP fluid. The developed numerical code has been first set-up and tested for a viscoelastic and a viscoplastic fluid. In what follows, the adopted constitutive equations for these kinds of non-Newtonian fluids are presented.

2.2.1 Viscoelastic fluids

One of the simplest constitutive equations for viscoelastic fluids is:

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} + \boldsymbol{\tau} = 2\eta_p \mathbf{D} \quad (2.13)$$

where λ is the relaxation time and η_p is the polymer contribution to the viscosity. The symbol $(\overset{\nabla}{\boldsymbol{\tau}})$ denotes the upper-convected time derivative, defined as:

$$\overset{\nabla}{\boldsymbol{\tau}} \equiv \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\tau} - (\nabla \mathbf{u})^T \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \nabla \mathbf{u} \quad (2.14)$$

In planar shear flow with x as the flow direction, y the gradient direction, and z the vorticity axis, this model predicts a constant viscosity and a quadratic dependence of the first normal stress difference $N_1 = T_{xx} - T_{yy}$ on the shear rate. No second normal stress difference $N_2 = T_{yy} - T_{zz}$ is predicted in shear flow. If the solvent viscosity η_s in Eq. 2.3 is zero, the model is referred to as the Upper Convected Maxwell (UCM) model, otherwise it is denoted as the Oldroyd-B (OB) model.

To account for the typically observed shear-thinning behavior, i.e., the viscosity decreases with increasing shear rate, the Giesekus (GSK) constitutive equation is commonly used:

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} + \frac{\alpha \lambda}{\eta_p} \boldsymbol{\tau} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} = 2\eta_p \mathbf{D} \quad (2.15)$$

where α (dimensionless) is the so-called ‘mobility’ parameter. Beyond an initial plateau at low shear rates, this model predicts a viscosity η , and first and second normal stress difference coefficients, $\Psi_1 = N_1/\dot{\gamma}^2$ and $\Psi_2 = N_2/\dot{\gamma}^2$, that thin as the shear rate increases. Higher values of the parameter α lead to earlier onset of shear-thinning. The value of

Ψ_2 is negative (as it is for real fluids), and the ratio Ψ_2/Ψ_1 at low shear rates depends on the mobility parameter α . A limiting case is $\alpha = 0$, corresponding to the UCM model.

For both constitutive equations, the zero-shear viscosity is given by $\eta_0 = \eta_s + \eta_p$. For future reference, it is also convenient to introduce the conformation tensor $\mathbf{c}$, which for the models just presented, is linearly related to the viscoelastic stress tensor:

$$\mathbf{c} = \mathbf{I} + \frac{\lambda}{\eta_p} \boldsymbol{\tau} \quad (2.16)$$

2.2.2 Viscoplastic fluids

The simplest equation to model viscoplastic fluids is the Bingham model, where $\eta_s = 0$ in Eq. 2.3, and $\boldsymbol{\tau}$ is given by:

$$\boldsymbol{\tau} = 2 \left(\frac{\tau_y}{\dot{\gamma}} + K \right) \mathbf{D} \quad \text{if } |\boldsymbol{\tau}| > \tau_y, \quad (2.17)$$

$$\mathbf{D} = 0 \quad \text{if } |\boldsymbol{\tau}| \leq \tau_y. \quad (2.18)$$

where $\dot{\gamma}$ and $|\boldsymbol{\tau}|$ are the square root of the negative of the second invariant of the tensor $2\mathbf{D}$ and $\boldsymbol{\tau}$, respectively:

$$\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}, \quad (2.19)$$

$$|\boldsymbol{\tau}| = \sqrt{\frac{1}{2} \boldsymbol{\tau} : \boldsymbol{\tau}}. \quad (2.20)$$

The constitutive parameters τ_y and K are the yield stress of the fluid and the viscosity index, respectively. Such a model predicts flow if the magnitude of the stress is higher than the yield stress.

The Herschel-Bulkley constitutive equation is similar to the Bingham model but accounts for viscosity thinning:

$$\boldsymbol{\tau} = 2 \left(\frac{\tau_y}{\dot{\gamma}} + K \dot{\gamma}^{n-1} \right) \mathbf{D} \quad \text{if } |\boldsymbol{\tau}| > \tau_y, \quad (2.21)$$

$$\mathbf{D} = 0 \quad \text{if } |\boldsymbol{\tau}| \leq \tau_y. \quad (2.22)$$

where n is the power-law index.

The two equations presented above exhibit a discontinuity when the stress field passes through the yield stress value. To handle such discontinuities numerically, ‘regularization’ techniques have been proposed, such as the one introduced by Papanastasiou [84], in which the Bingham model is modified as follows:

$$\boldsymbol{\tau} = 2 \left(\frac{\tau_y}{\dot{\gamma}} [1 - \exp(-m\dot{\gamma})] + K \right) \mathbf{D} \quad (2.23)$$

where m is a regularization parameter that should be chosen sufficiently large to closely reproduce the original Bingham model. A similar regularization can be applied to the Herschel-Bulkley constitutive model as well.

2.2.3 Elastoviscoplastic fluids

To account for both elasticity and yield-stress, Saramito proposed a modification of the UCM/OB model [22]. In this work, we model the EVP fluid with the Giesekus constitutive equation modified as proposed by Saramito [22] to account for the yield stress:

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} + \max \left(0, \frac{|\boldsymbol{\tau}_d| - \tau_y}{|\boldsymbol{\tau}_d|} \right) \left(\boldsymbol{\tau} + \frac{\alpha \lambda}{\eta_p} \boldsymbol{\tau} \cdot \boldsymbol{\tau} \right) = 2\eta_p \mathbf{D}, \quad (2.24)$$

where $|\boldsymbol{\tau}_d|$ is given by:

$$|\boldsymbol{\tau}_d| = \sqrt{\frac{1}{2} \hat{\boldsymbol{\tau}} : \hat{\boldsymbol{\tau}}}, \quad (2.25)$$

with:

$$\hat{\boldsymbol{\tau}} = \boldsymbol{\tau} - \frac{1}{3} \text{Tr} \boldsymbol{\tau} \mathbf{I}. \quad (2.26)$$

with ‘Tr’ the trace operator.

Similarly, the equivalent elastoviscoplastic version of the Herschel-Bulkley model is obtained as [52]:

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} + K \left(\max \left(0, \frac{|\boldsymbol{\tau}_d| - \tau_y}{K |\boldsymbol{\tau}_d|^n} \right) \right)^{1/n} \boldsymbol{\tau} = 2\eta_p \mathbf{D} \quad (2.27)$$

2.3 Dimensionless equations

It is useful to present the set of equations discussed above in dimensionless form. For a spherical particle suspended in a fluid (chapter 3), the particle radius R is chosen as the characteristic length. Following Fraggadakis et al. [1] and Sarabian et al. [2], we selected the characteristic velocity as the one obtained by balancing viscous and buoyancy forces $U_c = 3F/(4\pi R\eta_0)$. Consequently, the characteristic time is $t_c = R/U_c$. The characteristic stress is $\tau_c = \eta_0/t_c$ where $\eta_0 = \eta_s + \eta_p$ is the zero-shear viscosity.

Denoting with starred symbols the dimensionless quantities, Eqs. (2.1)-(2.2) can be expressed in dimensionless form as:

$$\nabla^* \cdot \mathbf{u}^* = 0 \quad (2.28)$$

$$-\nabla^* p^* + \eta_r \nabla^{*2} \mathbf{u}^* + \nabla^* \cdot \boldsymbol{\tau}^* = \mathbf{0} \quad (2.29)$$

Notice that the expression of the total stress tensor in Eq. (2.2) has been substituted in the momentum balance. The dimensionless constitutive equation is:

$$Wi \nabla^* \boldsymbol{\tau}^* + \max \left(0, \frac{|\boldsymbol{\tau}_d^*| - Bn}{|\boldsymbol{\tau}_d^*|} \right) \left(\boldsymbol{\tau}^* + \frac{\alpha Wi}{1 - \eta_r} \boldsymbol{\tau}^* \cdot \boldsymbol{\tau}^* \right) = 2(1 - \eta_r) \mathbf{D}^* \quad (2.30)$$

In the above equations, the Weissenberg and Bingham numbers, and the viscosity ratio appear:

$$Wi = \frac{\lambda}{t_c} = \frac{\lambda F}{\frac{4}{3}\pi R^2 \eta_0}, \quad (2.31)$$

$$Bn = \frac{\tau_y R}{\eta_0 U_c} = \frac{\tau_y \frac{4}{3}\pi R^2}{F}, \quad (2.32)$$

$$\eta_r = \frac{\eta_s}{\eta_0}. \quad (2.33)$$

For a spheroidal particle (chapter 4), we choose the characteristic

length R_c as the radius of the sphere with the same volume of the spheroid, the characteristic velocity U_c as the settling velocity of a sphere with radius R_c in a Newtonian fluid with the same zero-shear viscosity η_0 of the EVP fluid, and the characteristic stress as $\eta_0 U_c / R_c$. We made these choices to be consistent with previous literature results. The dimensionless governing equations are the same as above, with the following definitions of Wi and Bn :

$$Wi = \lambda \frac{F}{6\pi\eta_0 R^2}, \quad (2.34)$$

$$Bn = \frac{\tau_y 6\pi R^2}{F}. \quad (2.35)$$

In the case of non-spherical particles, other parameters are needed to characterize the shape of the particle. For a spheroid, the aspect ratio is generally used:

$$\beta = \frac{a}{b} \quad (2.36)$$

defined as the ratio between the semi-major axis a and the semi-minor axis b .

Finally, for the (2D) problem of a particle in Poiseuille flow (chapter 5), we choose the height of the channel, H , as characteristic length, $U_c = Q/H$ as characteristic velocity and $\eta_0 U_c / H$ as characteristic stress. The Weissenberg and Bingham numbers are defined as:

$$Wi = \lambda \frac{Q}{H^2}, \quad (2.37)$$

$$Bn = \frac{\tau_y H^2}{\eta_0 Q}. \quad (2.38)$$

In all this work, we fix $\alpha = 0.2$ (denoting a shear-thinning fluid) and $\eta_r = 0.1$. From now on, we remove the starred symbols, and all the quantities are intended to be dimensionless.

2.4 Numerical method and weak formulation

The simulation of viscoelastic fluids and elasto-viscoplastic fluids is a difficult task due to the well-known High Weissenberg Number Problem [85], i.e., the arising of numerical instabilities at high values of Wi due to the mathematical nature of the constitutive equations. Several stabilization techniques have been proposed to alleviate this problem. The code developed in this project implements some of these techniques.

The momentum balance is modified according to the DEVSS (Discrete Elastic Viscous Splitting Scheme), whereby a viscous term is added to the momentum equation and subtracted again using a projection of the symmetric part of the velocity gradient [86]. A slightly different variant proposed by Bogaerds et al. [87] is implemented, which uses the velocity gradient directly.

The convective term of the constitutive equation is stabilized through the SUPG (Streamline Upwind Petrov-Galerkin) method [88]. This technique uses a modified test function that assigns more weight to the upwind direction of the streamline. Finally, the log-representation of the conformation tensor is adopted [89, 90], i.e., the original constitutive equation is transformed into an equivalent equation for the logarithm of the conformation tensor, leading to a stability improvement.

The governing equations are solved through the finite element method (FEM). The solution of the continuity and momentum balance equations is decoupled from the constitutive equation. At each time step, the constitutive equation is first solved using the velocity field from the previous step. Then, the computed stress tensor is used as a known source term in the momentum balance equation.

The particle motion is handled using an Arbitrary-Lagrangian Eulerian (ALE) moving mesh method [91]. At every time step, the mesh nodes are moved to follow the particle motion. The mesh displacement (in terms of velocity) is calculated by solving a Laplace equation to ensure smooth variation [91]. To account for the relative motion of the mesh nodes concerning the fluid velocity, the node velocities must be subtracted from the convective term of the constitutive equation (since inertia is neglected, no convective term appears in the momentum balance).

In what follows, we present the weak form of the governing equations

presented in the previous section. We refer to the general case of an elasto-viscoplastic fluid with a particle. The weak form for a pure EVP fluid (without particle) can be straightforwardly recovered as described below.

Considering the stabilization techniques previously mentioned, the weak form can be stated as follows: For $t > 0$: Find $\mathbf{u} \in U, p \in P, \mathbf{s} \in S, \mathbf{U} \in \mathbb{R}^3, \boldsymbol{\omega} \in \mathbb{R}^3$, such that:

$$\begin{aligned} & \int_{\Omega-P(t)} 2\eta_s \mathbf{D} : \mathbf{D}(\mathbf{u}) dV - \int_{\Omega-P(t)} (\nabla \cdot \mathbf{u}) p dV + \int_{\Omega-P(t)} \eta_p (\nabla \mathbf{u})^T : \\ & \nabla \mathbf{v} dV - \int_{\Omega-P(t)} \eta_p (\nabla \mathbf{u})^T : \mathbf{G}^T dV + \int_{\partial P(t)} [\mathbf{u} - (\mathbf{V} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X}))] \cdot \boldsymbol{\lambda} dS \\ & = - \int_{\Omega-P(t)} \mathbf{D} : \mathbf{s} dV, \end{aligned} \quad (2.39)$$

$$\int_{\Omega-P(t)} q (\nabla \cdot \mathbf{u}) dV = 0, \quad (2.40)$$

$$\int_{\Omega-P(t)} \mathbf{H} : \mathbf{G} dV - \int_{\Omega-P(t)} \mathbf{H} : (\nabla \mathbf{u})^T dV = 0, \quad (2.41)$$

$$\int_{\Omega-P(t)} (\mathbf{S} + \tau \mathbf{u} \cdot \nabla \mathbf{S}) : \left(\frac{\partial \mathbf{s}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{s} - g(\mathbf{G}, \mathbf{s}) \right) dV = 0, \quad (2.42)$$

$$\int_{\partial P(t)} \mu \cdot [\mathbf{u} - (\mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X}))] dS = 0, \quad (2.43)$$

with the initial condition:

$$\mathbf{s} = \mathbf{s}_0 \quad \text{at } t = 0 \text{ in } V. \quad (2.44)$$

Here, $\mathbf{U}, \mathbf{P}, \mathbf{S}, \mathbf{H}$ are suitable functional spaces. The parameter τ in Eq. (2.42) is given by:

$$\tau = \beta \frac{h}{2U_e},$$

where β is a dimensionless constant, h is the element size, and U_e is a characteristic velocity for the element. The function $g(\mathbf{G}, \mathbf{s})$ in Eq. (2.42) contains the non-linear terms of the constitutive equation, and $\mathbf{s} = \log \mathbf{c}$. Finally, we take the initial value of $\mathbf{s}_0 = \mathbf{0}$, corresponding to zero initial stress.

Notice that the particle kinematic quantities $\mathbf{U}$ and $\boldsymbol{\omega}$ are treated as additional unknowns and are included in the weak form of the momentum equation. The force- and torque-free conditions are imposed through the Lagrange multipliers, $\boldsymbol{\lambda}$.

For the case of an EVP fluid without a particle, the corresponding weak form is modified by removing the last term of the left-hand side in Eqs. (2.39) and (2.43).

Time-integration is done by decoupling the continuity/momentum balance from the constitutive equation. At each time step, the former system of equations is solved by taking the divergence of the viscoelastic stress tensor from the previous step. Then, the constitutive equation is solved by using the velocity and gradient fields just computed. A second-order Gear scheme is employed for time-integration.

Compared to other methods, the main advantage of the ALE formulation is the use of a boundary-fitted mesh throughout the simulation, leading to high accuracy around the particle where the largest gradients are expected. However, as the particle moves, the mesh becomes increasingly distorted, reducing the solution accuracy. Therefore, a new mesh is generated, and the fields from the old mesh are projected onto the new one.

The code for a viscoelastic suspending fluid has been extensively validated in numerous previous publications (see, e.g., Refs. [92, 71, 93]). The Saramito-Giesekus constitutive equation employed in this work is a modified Giesekus model where a factor (that contains the viscoelastic stress components through $\boldsymbol{\tau}_d$) multiplies the term $(\boldsymbol{\tau} + \alpha\lambda/\eta_p \boldsymbol{\tau} \cdot \boldsymbol{\tau})$. In our implementation, such a term is treated explicitly [94], i.e., the viscoelastic stress components are taken from the previous time step. Hence, the Saramito factor is straightforwardly implemented in the discretization of the constitutive equation. We have first validated the code without particle by solving the transient flow field of an EVP fluid in a 2D periodic domain with an applied shear flow. The original Saramito model (obtained

by setting $\alpha = 0$ in Eq. (2.24)) is employed. The results show an excellent agreement between the analytical and numerical solution for all the investigated combinations of Wi and Bn .

Chapter 3

Sedimentation and migration
dynamics of a spherical
particle in an EVP fluid near
a wall

3.1 Introduction

As previously mentioned, the presence of a confining wall strongly influences the particle dynamics, giving rise to new phenomena such as cross-stream lateral migration. It is therefore interesting to investigate the interplay between wall effects, fluid viscoelasticity, and plasticity on the dynamics of particles.

In this chapter, we study the dynamics of a spherical particle settling in an elastoviscoplastic fluid near a flat wall through direct numerical simulations under inertialess conditions. The sedimentation and migration phenomena are investigated by varying the particle-wall distance and the relevant dimensionless numbers. The yielded/unyielded fluid regions, the shear rate distribution around the particle, and the negative wake phenomenon are analyzed and related to the observed dynamics. A comparison with the purely viscoelastic case is also discussed. In the following sections, the applied geometry, time, and mesh convergence are explained. Then, results are presented in detail for a spherical particle settling near the wall in EVP material.

3.2 Geometry, validation, and convergence

The dynamics of a spherical particle settling in an EVP fluid near a wall is simulated in the domain shown in Fig. 3.1a. A Cartesian reference frame is selected with origin at the center of the physical wall with axes oriented as in figure. A force acting along the x -direction is applied on the spherical particle with radius R . The distance between the particle center and the wall is denoted by Γ . The domain size is chosen sufficiently large in order to avoid any influence of the box boundaries (except, of course, the boundary representing the physical wall) on the particle motion. From preliminary tests by progressively increasing the domain size, we found that a box with side lengths of $160R \times 80R \times 160R$ in the x , y and z directions, respectively, fulfills the previous condition for any set of parameters investigated in this work. In this computational domain, no-slip conditions are imposed. The symmetry boundary condition is applied at the symmetry plane. Due to the inertialess assumption, no initial condition for the velocity is needed. The stress-free condition, i.e., $\boldsymbol{\tau}|_{t=0} = \mathbf{0}$, is considered as initial condition

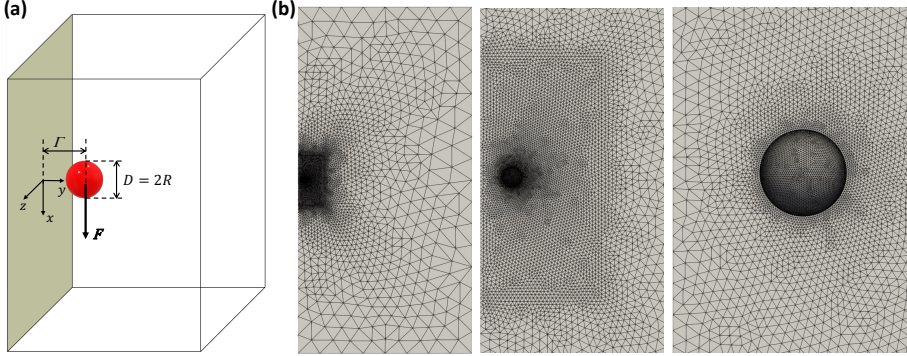


Figure 3.1. (a) Schematic representation of the computational domain: a spherical particle with diameter D subjected to a constant force settles in an EVP fluid near a wall; the origin of a Cartesian reference frame is set on the wall with x the direction of the applied force; the distance between the particle center and the wall is denoted by Γ . (b) Typical mesh used in the simulations. The panels show the mesh over the particle surface and on the symmetry plane with the particle progressively zoomed from the left to the right.

for the viscoelastic stress.

The code is validated for the case of a sedimenting sphere in an EVP fluid. The simulations are done through the Saramito constitutive equation in an infinite medium. The computed steady-state settling velocity U_s is used to evaluate the Stokes drag coefficient defined as:

$$C_S = \frac{F}{6\pi\eta_0 U_s R} \quad (3.1)$$

Figure 3.2 compares the numerical results between the present work, Fraggadakis et al. [1] and Sarabian et al. [2] for $Wi = 1$ and three values of the Bingham number. The agreement is quantitatively good and the small deviations may be attributed to the different numerical methods employed in these works.

Finally, mesh and time convergence are verified for all the simulations. Figure 3.1b displays a typical mesh employed in this work. The images show the mesh over the particle surface and on the symmetry plane, with the particle progressively zoomed from the left to the right. Notice that

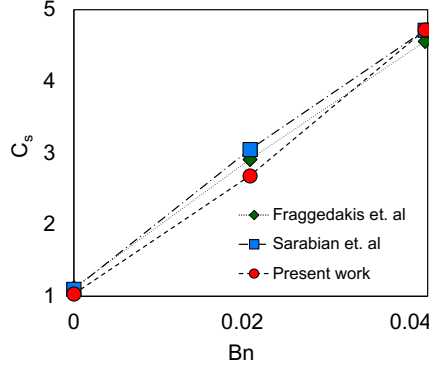


Figure 3.2. Stokes drag coefficient of a spherical particle sedimenting in an unconfined EVP fluid as a function of the Bingham number for $Wi = 1$ computed in Fraggedakis et al. [1], Sarabian et al. [2], and the present work. The fluid is modeled by the Saramito constitutive equation obtained by setting $\alpha = 0$ in Eq. (2.24).

the particle is ‘surrounded’ by a box (clearly visible in the middle image of Fig 3.1b) with a finer resolution. We need such a refinement in order to accurately capture the yielded/unyielded regions as discussed later. Typical results of convergence tests are reported in Fig. 3.3 where the sedimentation U_s , migration U_m , and angular velocity ω are reported as a function of time for two mesh resolutions and two time step sizes. The parameters are: $Wi = 2$, $Bn = 0.01$, $\Gamma = 1.5$. For all the kinematic quantities, the curves fairly overlap. As expected, the required mesh resolution and time step size to get convergent results depend on Wi and Bn . For Wi up to 2 and Bn up to 0.01, about 45000 tetrahedral elements are needed in the domain, with about 1000 triangular elements over the particle surface. A (dimensionless) time step size of 0.005 is used. At higher values of Wi and Bn , the number of elements need to be increased up to 75000, with about 1600 triangular elements over the particle, and the time step size reduced to 0.0025.

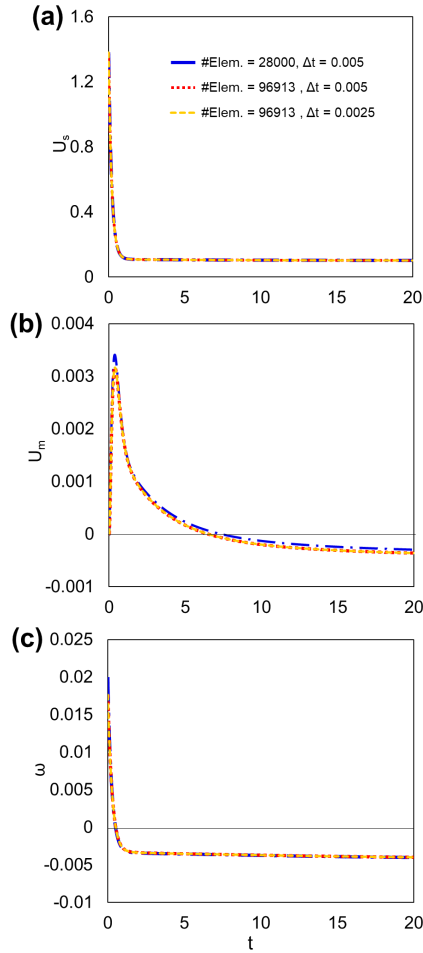


Figure 3.3. Sedimentation (a), migration (b), and angular (c) velocities of a spherical particle in an EVP fluid near a wall as a function of time for different mesh resolutions and time step sizes. The parameters are: $Wi = 2$, $Bn = 0.01$, $\Gamma = 1.5$.

3.3 Results and discussion

The particle dynamics in terms of the translational and rotational velocities is first addressed, with a special focus on the migration phenomenon

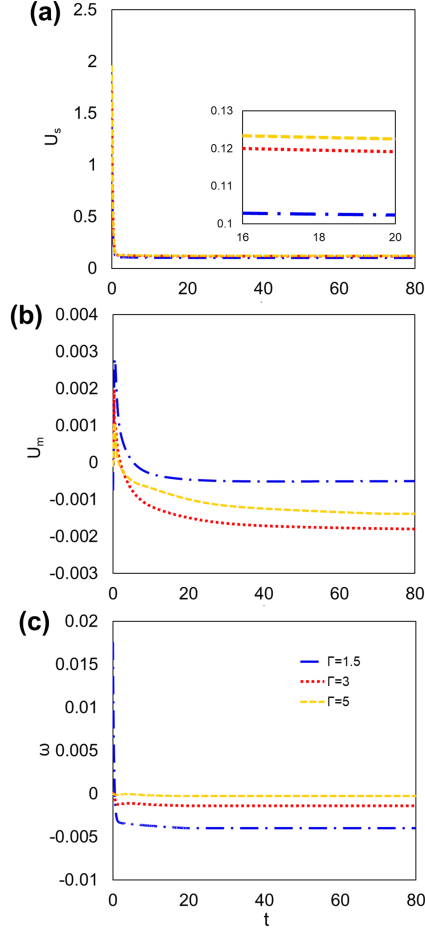


Figure 3.4. Sedimentation (a), migration (b), and angular (c) velocities of a spherical particle in an EVP fluid as a function of time for different particle-wall distances. The Weissenberg number is $Wi = 2$ and the Bingham number is $Bn = 0.01$. The inset in panel (a) shows a zoom of the three curves at long times once the trends are nearly horizontal.

as the particle-wall distance, Weissenberg and Bingham numbers are varied. The flow field around the particle and the yielded/unyielded regions are then presented. The purely viscoelastic case is also simulated to un-

derstand the effect of plasticity on the particle motion.

The sedimentation velocity of the particle as a function of time is displayed in Fig. 3.4a for $Wi = 2$ and $Bn = 0.01$, and for three values of the particle-wall distance, $\Gamma = 1.5$, $\Gamma = 3$, and $\Gamma = 5$. At the initial time, the viscoelastic stresses are zero so the system is equivalent to a Stokes flow. The first point on the curves is, in fact, the settling velocity of a sphere in a Newtonian liquid with viscosity η_s at a certain distance from a flat wall. Since we set $\eta_s/\eta_0 = 0.1$, the Newtonian sedimentation velocity is one order of magnitude higher than the one in a viscoelastic fluid after the stress development (where the characteristic viscosity is η_0). Indeed, after the initial transient, the settling velocity rapidly reduces and the trend becomes nearly horizontal. As expected, the long-time value of the sedimentation rate depends on the particle-wall distance as visible in the inset of the figure. It has to be pointed out, however, that the value reached at long times is not constant as the particle-wall distance is changing due to the migration phenomenon (see below). This behavior is similar to what observed for the translational velocity of a particle suspended in a viscoelastic fluid under planar shear [92] or pressure-driven flow [95]. In the present case, indeed, we find that the curves taken after the initial stress development at different particle-wall distances superimpose and identify a mastercurve. As thoroughly discussed in previous works [92, 94, 95], the existence of a mastercurve suggests that the settling velocity (but this holds for the other kinematic quantities as well, see below) is uniquely related to the particle-wall distance once the viscoelastic stresses fully develop.

Figure 3.5 shows the mastercurves of the particle sedimentation rate for four values of the Weissenberg number. In each plot, four values of the Bingham number are considered. The case at $Bn = 0$ corresponds to the purely viscoelastic case. It can be readily observed that: i) the presence of a confining wall hinders the sedimentation speed, as also found for a Newtonian fluid [96], ii) higher Bingham numbers slow down the sedimentation, in agreement with unconfined systems [1, 2], iii) at a particle-wall distance of about 10 radii, the curves become nearly horizontal denoting that the wall has a negligible effect in the settling phenomenon, i.e., the system can be considered unconfined, iv) increasing the Weissenberg number speeds up the sedimentation although the effect is quantitatively small. Regard-

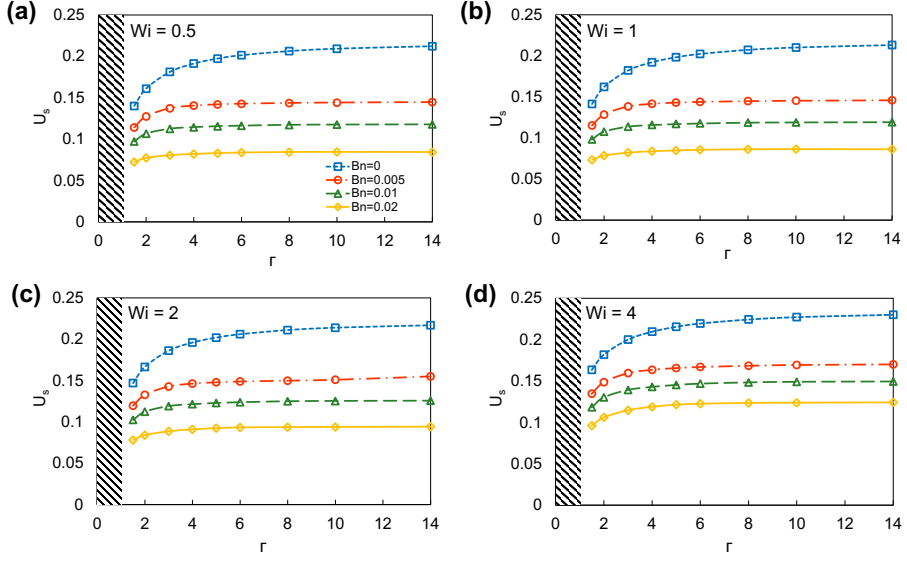


Figure 3.5. Sedimentation velocity of the particle as a function of the particle-wall distance for different values of the Weissenberg and Bingham number. The shaded area is the region inaccessible to the particle due to its finite size.

ing the effect of the Weissenberg number on the sedimentation speed, a vast literature exists for a spherical particle in a viscoelastic fluid (see, e.g., Ref. [30]). Previous simulation results in a variety of fluids show that the fluid viscoelasticity reduces the drag coefficient as Wi increases, i.e., the sphere settles faster in a viscoelastic fluid, in agreement with the data shown in Fig. 3.5. In these works, the characteristic flow time used to define the Weissenberg number is the particle radius divided by the steady-state sedimentation speed. By using this definition, the range of Wi corresponding to the purely viscoelastic case in an unbounded domain (rightmost black point in the panels of Fig. 3.5) is between 0.1 and 0.9. In this range, the effect of Wi on the sedimentation speed is relatively weak [97], as confirmed by our simulation results.

As mentioned in the Introduction, a particle immersed in a viscoelastic fluid near a wall and subjected to a force parallel to the wall experiences

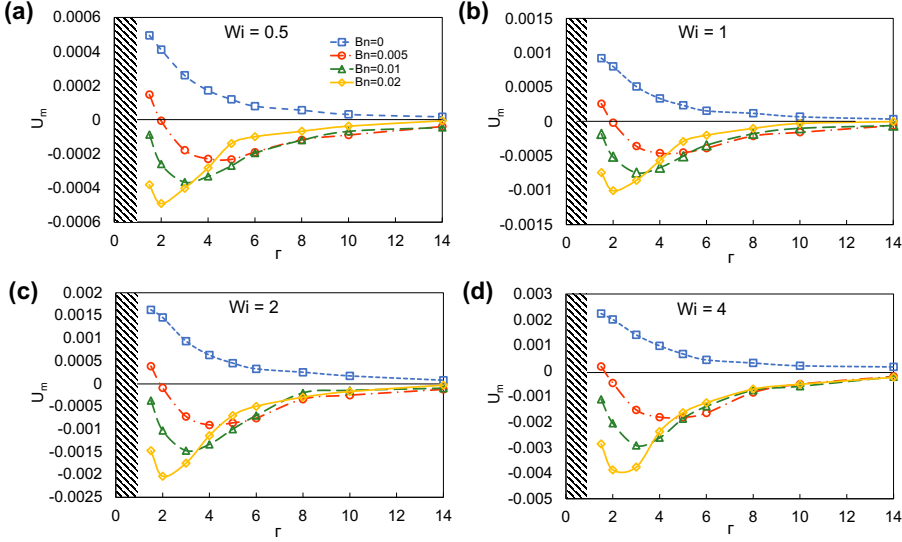


Figure 3.6. Migration velocity of the particle as a function of the particle-wall distance for different values of the Weissenberg and Bingham number. The shaded area is the region inaccessible to the particle due to its finite size.

a lateral motion termed ‘migration’ [33, 34]. Figure 3.4b reports the transient migration velocity (denoted as U_m) for $Wi = 2$, $Bn = 0.01$ and three distances from the wall. The three curves start at the origin as for a sphere in a Newtonian inertialess fluid no migration occurs. As soon as the viscoelastic stresses start develop, a maximum is achieved after which the curves attain a nearly constant trend. Similarly to the sedimentation velocity previously discussed, the curves taken after the initial stress development at different particle-wall distances superimpose describing a mastercurve. Figure 3.6 shows the mastercurves of the migration velocity at different values of the Weissenberg and Bingham numbers. Positive or negative values of the migration velocity indicate a lateral motion of the particle away or towards the wall, respectively. In a purely viscoelastic case ($Bn = 0$), the migration velocity is positive for any particle-wall distance. The trend is monotonic and decreasing as the particle moves away from the wall. At the largest investigated distance ($r = 14$), the migration velocity is nearly zero denoting a negligible effect of the confinement

(in an unbounded domain a spherical particle does not migrate). The curves at varying Wi are qualitatively similar. These results agree with those reported by Spanjaards et al. [34] for a Couette flow cell. In this regard, it should be remarked that the simulation results reported in the aforementioned paper show that the migration velocity is positive (wall repulsion) for Wi below a threshold and becomes negative (wall attraction) for large Wi -values. The maximum Weissenberg number explored in the present work is lower than the threshold reported in Spanjaards et al. [34], confirming the wall repulsive behavior. (Notice that the definition of the Weissenberg number in Spanjaards et al. [34] is different from the one adopted in this paper; specifically, for the same set of parameters, our Wi is nine times lower than the one given in Spanjaards et al. [34].) Higher values of the Weissenberg number lead to a faster migration rate as previously found for different flow fields [92, 95, 94].

As the Bingham number increases, the migration velocity progressively decreases and changes sign, i.e., the particle inverts its migration direction and moves towards the wall. The trend becomes non-monotonic with the migration velocity that achieves a minimum as the particle-wall distance increases, and approaches to zero for large distances. Interestingly, for $Bn = 0.005$, the migration velocity crosses the horizontal axis at a particle-wall distance of about $\Gamma = 2$. This is a stable equilibrium point, i.e., the particle settles maintaining a fixed distance from the wall. A similar behavior could occur for $Bn = 0.01$ too since the extrapolated curves likely cross the horizontal axis at a finite (although very small) particle-wall distance. For higher values of Bn , the migration velocity becomes negative for any Γ -value thus the particle sediments near the wall (in theory, in contact with the wall). In this regard, we mention that the simulations break down for very low particle-wall distances so we were unable to investigate the particle dynamics close to the wall (the minimum initial distance simulated is $\Gamma = 1.5$ corresponding to one-half radius between the wall and the particle surface). A variation of the Weissenberg number speeds up the migration velocity also for an elastoviscoplastic fluid, although the trends of the migration velocity curves are essentially unaffected. The only visible difference is that the curve at $Bn = 0.005$ for $Wi = 4$ crosses the x -axis at about $\Gamma = 1.5$, thus the wall repulsive region is narrower as compared to lower Wi -values. Higher values of the Weissenberg number are expected

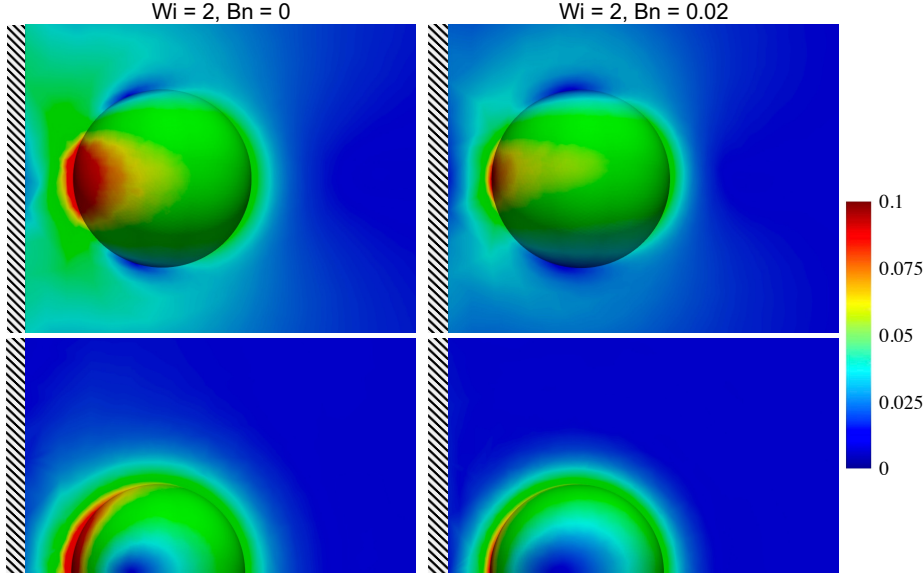


Figure 3.7. Shear rate distribution on the xy -plane and on the spherical surface (top), and on the yz -plane (bottom). The purely viscoelastic case ($Bn = 0$) is considered on the left. On the right the EVP case is shown at $Bn = 0.02$. In both cases, the Weissenberg number is $Wi = 2$. The shaded area is the region inaccessible to the particle due to its finite size.

to further reduce this region and lead to a fully repulsive dynamics from the wall for smaller values of the Bingham number.

The results just discussed show that fluid plasticity has a relevant effect on the migration phenomenon as the particle lateral motion reverts direction. Previous works on the dynamics of particles on viscoelastic fluids in shear and Poiseuille flows attributed the migration mechanism to an imbalance of normal stresses due to the shear rate gradients around the particle that generates a net force displacing the particle trajectory [35]. The shear rate distribution around the particle, indeed, can provide useful information about the migration dynamics. The top panels of Fig.3.7 display the distribution of the (dimensionless) shear rate $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$ on the symmetry xy -plane and on the spherical surface. The bottom panels report the same quantity on the yz -plane. On the left, the purely viscoelastic case ($Bn = 0$) is considered at Weissenberg number $Wi = 2$.

The right panels refer to the elastoviscoplastic fluid with $Bn = 0.02$ and the same value of Wi as in the left figures. In both cases, the distance from the channel inlet is $\Gamma = 1.5$. The first case corresponds to the leftmost data point of the blue curve in Fig.3.6c, showing a positive value of the migration velocity, i.e., the particle is moving away from the wall. On the contrary, the migration velocity for the EVP fluid case is represented by the leftmost data point of the yellow curve in Fig.3.6c which is negative, i.e., the particle is moving towards the wall.

As expected, the highest shear rate region is found in between the particle and the wall where the gap is small. Specifically, the shear rate is higher for the viscoelastic case (see the large red region on the left side of the particle surface). This is a consequence of the higher sedimentation speed of the particle in a viscoelastic fluid rather than in an elastoviscoplastic one, as previously discussed (see Fig.3.5). Nevertheless, the migration velocity has a similar magnitude in the two cases (around 0.0015, as shown in Fig.3.6c), although opposite in sign. Recalling that the migration phenomenon is related to the shear rate gradient around the particle, Fig.3.7 shows that the spatial variation of the shear rate on the left side of the particle from the surface to the wall is larger for the viscoelastic fluid as compared to the EVP one. This generates, in turn, a stronger net force away from the wall in the viscoelastic case. On the contrary, the shear rate gradient on the right side of the particle is higher for the EVP case. Indeed, the shear rate value at the particle surface is the same for the two cases (denoted by a green color corresponding to about 0.05). However, it becomes near zero (blue color) in a shorter distance from the sphere in the EVP case, as visible from the narrower green band at the right side of the particle in the right panels of Fig. 3.7. This generates a force towards the wall that is stronger for the EVP fluid. Such a force overcomes the (small) force from the left side, pushing the particle towards the wall. The larger shear rate gradient on the right side observed in the EVP case is likely induced by the presence of the unyielded region that ‘confines’ the sphere on the right (see below). As the Bingham number increases, the yielded region moves closer to the particle, further increasing the shear rate gradient on the unconfined side, leading to a faster migration towards the wall. By further increasing the Bingham number, we expect that the unyielded region touches the particle leading to the blockage (no sedimentation [1]

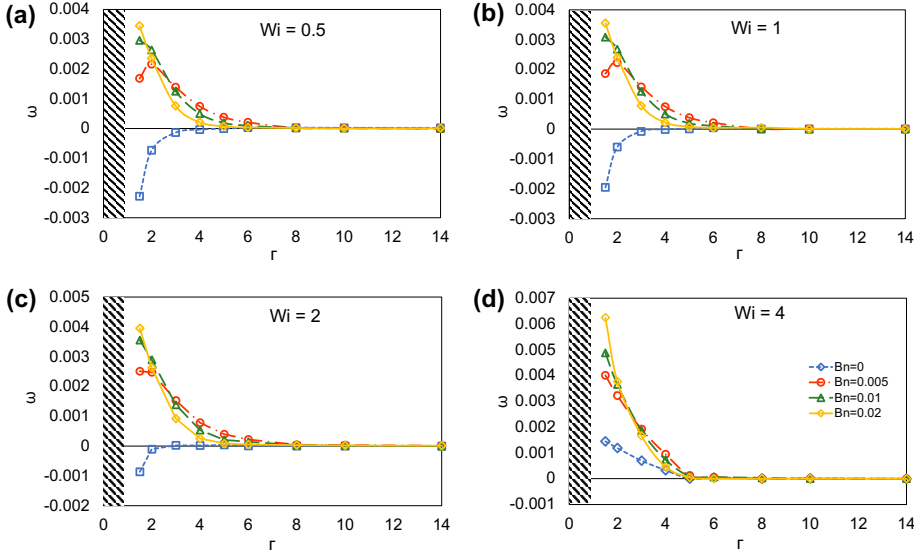


Figure 3.8. Angular velocity of the particle as a function of the particle-wall distance for different values of the Weissenberg and Bingham number. The shaded area is the region inaccessible to the particle due to its finite size.

and no migration).

Finally, we report in Fig. 3.4c and 3.8 the transient and mastercurves of the particle angular velocity. For a purely viscoelastic fluid at low Wi -values, the angular velocity is negative at any distance from the wall, denoting a clockwise rotation with respect to the z -direction, in agreement with the Newtonian case [96]. As the Weissenberg number increases, the angular velocity decreases and changes sign at $Wi = 4$, as discussed in previous works [33, 98]. For an elastoviscoplastic suspending fluid, the rotation is always counterclockwise. Notice also that the angular velocity becomes nearly zero at a particle-wall distance of about 5-6 radii, that is shorter as compared to the distance such that the migration velocity becomes nil or the settling velocity constant.

An interesting feature of suspensions of particles in EVP fluids is the shape and extension of the yielded/unyielded zones around the particle, i.e., the regions in the fluid domain where $|\tau_d|$ is higher (fluid behavior)

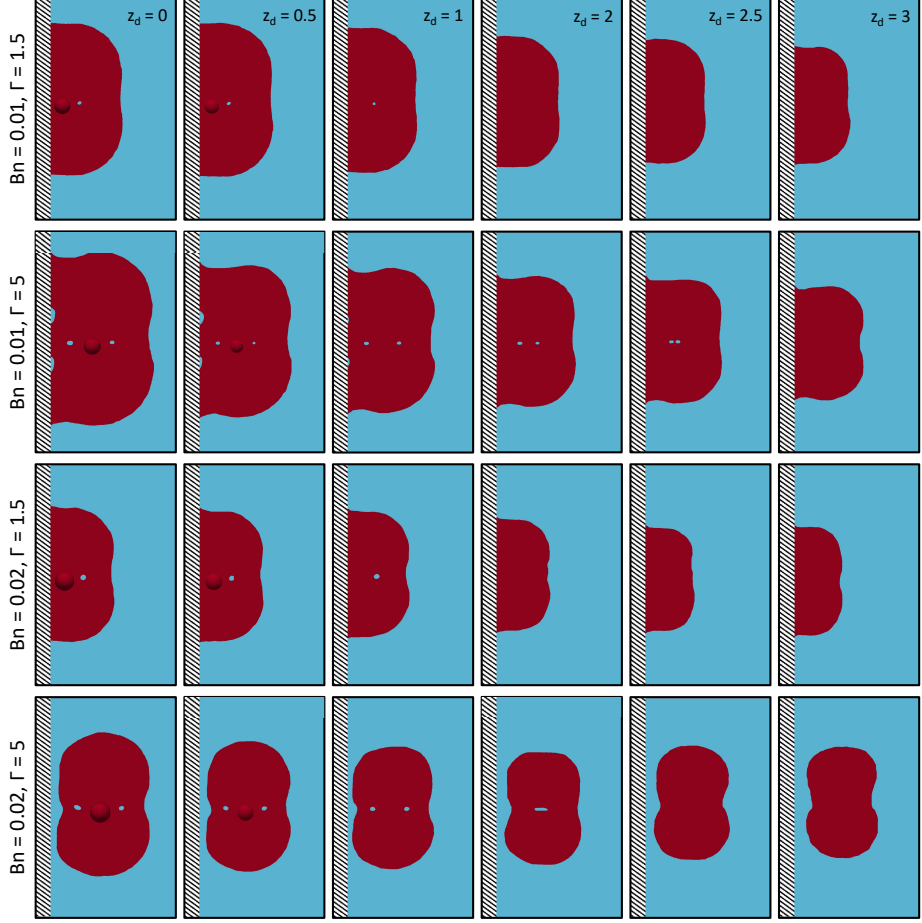


Figure 3.9. Yielded (red) and unyielded (cyan) regions around the particle on slices parallel to the xy -plane at different dimensionless depth z_d . The slice at $z_d = 0$ corresponds to the symmetry plane. Two values of the Bingham number and two particle-wall distances are considered. The Weissenberg number is $Wi = 2$. The shaded area is the region inaccessible to the particle due to its finite size. The force is applied from top to bottom.

or lower (solid behavior) than the yield stress. Figure 3.9 displays the yielded (red) and unyielded (cyan) regions around the particle on some slices parallel to the symmetry xy -plane at different depths z_d from such a

plane. The Weissenberg number is fixed to $Wi = 2$. The first and second rows refer to a particle-wall distance of $\Gamma = 1.5$ and $\Gamma = 5$, respectively, at a Bingham number of $Bn = 0.01$. The same distances are set in the third and fourth rows, with the Bingham number increased to $Bn = 0.02$.

A yielded zone surrounds the particle because of the high stress region due to the particle motion. As displayed in the leftmost panels (corresponding to the symmetry plane), at least two unyielded regions are visible in the examined cases. The first one is the external region surrounding the fluid zone. The second region is the small circle appearing at one or both sides of the particle. The existence of these isolated unyielded regions has been reported in Sabarian et al. [2] for the case of a sphere settling in an EVP material at the centerplane between two parallel walls and at different confinement ratios. However, as visible in Fig. 3.9, our results indicate that the small unyielded region in the gap disappears for a sufficiently low particle-wall distance. An inspection of the unyielded region shape inside the domain reveals that, at $\Gamma = 5$, the two circles get closer and form a connected domain at $z_d \approx 2.5$ for $Bn = 0.01$ and at $z_d \approx 2$ for $Bn = 0.02$ (see the sequence of slices at increasing depth from the symmetry plane). Hence, the internal unyielded region is a ring surrounding the particle, as also found in Sabarian et al. [2]. On the other hand, at $\Gamma = 1.5$, the unyielded region is an island with angular extension of about 30° from the symmetry plane situated at the unconfined side of the particle. Indeed, by looking at the slices inside the domain, we observe that the circle disappears from $z_d = 1$ to $z_d = 2$ for both Bingham numbers. Sabarian et al. [2] found the ring for all the considered confinement ratios. It should be mentioned that the lowest confinement ratio studied in their work corresponds to a particle-wall distance of $\Gamma = 2$ and the two circles are visibly smaller than the cases of less confined systems. It is likely to assume that, by further reducing the confinement ratio, the ring disappears (probably leaving two isolated islands on the forth and back of the sphere). Two more unyielded regions are visible in the second row of Fig. 3.9 close to the wall. These two regions are present only in a specific range of distances, provided that the particle is not too close to the wall and the boundary of the yielded region touches the wall. These regions are islands embedded in the yielded region, as confirmed by the sequence of slices for $Bn = 0.01$ and $\Gamma = 5$ showing that these two regions progressively reduce and disappear

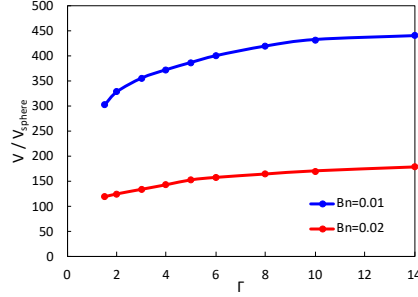


Figure 3.10. Volume of the yielded region as a function of the particle-wall distance for $Bn = 0.01$ and $Bn = 0.02$. The volume is normalized by the particle volume.

at about $z_d = 1$.

As reported in the literature [1, 2], the extension of the yielded region reduces by increasing the Bingham number. The presence of the wall does not significantly affect the extension of the unconfined side of the yielded region, which is also similar to the extension in the neutral z -direction. Finally, we show in Fig. 3.10 the volume of the yielded region, normalized by the particle volume, by varying the distance of the particle from the wall. As expected, the volume increases for increasing particle-wall distances up to reaching a constant value corresponding to the unconfined case, and a lower volume is found for the highest Bn -value.

Regarding the shape of the yielded region, some similarities can be noticed with the shapes reported in Sabarian et al. [2] for the confined cases. However, our results indicate a more symmetric shape in the fluid region above and below the sphere, whereas the top boundary of the yielded region reported in Sabarian et al. [2] and Fraggadakis et al. [1] is closer to the particle.

Another interesting feature is the negative wake phenomenon behind the sphere. The blue curve in Fig. 3.11a shows the component of the fluid velocity along the sedimentation direction, u_x , on a line passing through the center of the sphere and parallel to the x -direction for the purely viscoelastic case ($Bn = 0$) at $\Gamma = 1.5$ and $Wi = 4$. In Fig. 3.11b, the xx -component of the viscoelastic stress, τ_{xx} , is reported. Both quantities are taken just after the initial transient due to the stress development. The

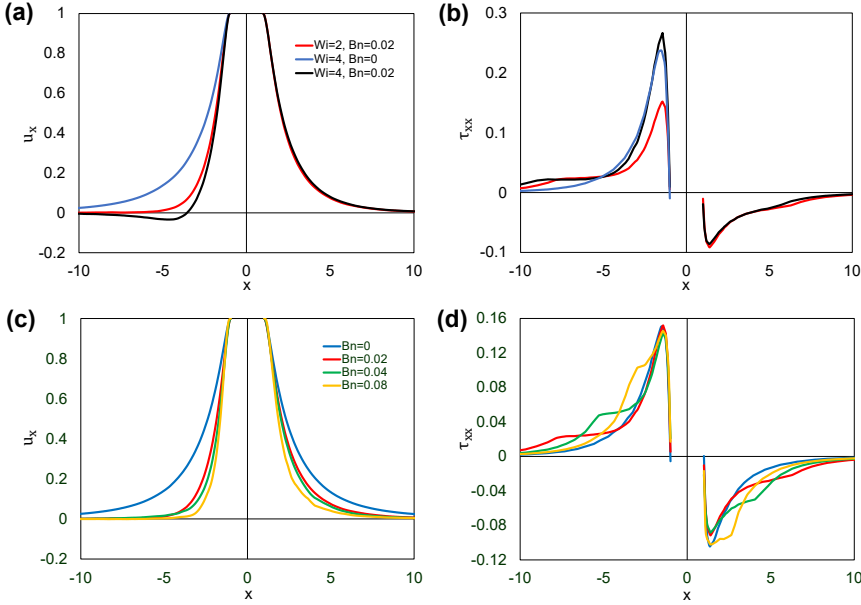


Figure 3.11. Fluid velocity (left) and axial stress component (right) along the line passing through the particle center and parallel to the sedimentation direction for different values of the Weissenberg and Bingham numbers. The initial distance is $\Gamma = 1.5$ and the profiles are taken after the initial transient due to the stress development. The fluid velocity is normalized by the sedimentation velocity of the particle taken at the same instant.

fluid velocity is normalized by the sedimentation velocity of the particle taken at the same instant. The fluid velocity is always positive, denoting no negative wake behind the sphere. The red curves refer to the EVP fluid for $\Gamma = 1.5$, $Wi = 2$, and $Bn = 0.02$. Despite the lower value of the Weissenberg number, the fluid velocity decays faster due to the plasticity effect. Indeed, the distribution of τ_{xx} , qualitatively similar to that reported in Fraggedakis et al. [1], shows an abrupt change of the trends (at around $x = -8$) due to the transition from the yielded to the unyielded region. As discussed in Fraggedakis et al. [1], the residual normal stresses in the solid-like region pull the solid away from the sphere, possibly leading to the backflow motion, promoting the negative wake. Finally, by increasing the

Weissenberg number to $Wi = 4$ (black curves), the axial stress behind the sphere is both higher in magnitude and has a steeper slope as compared to the red curve that, together with the pulling effect of the solid-like region, leads to an even faster decay of the fluid velocity downstream with the appearance of the negative wake.

The effect of the Bingham number on the flow field behind the sphere is displayed in the bottom panels of Fig. 3.11. The Weissenberg number fixed to $Wi = 2$. The blue curve corresponds to the purely viscoelastic case, $Bn = 0$, and the red one is the same of the top panels, i.e., for $Bn = 0.02$. As the Bingham number increases, the abrupt change in τ_{xx} approaches the sphere as the yielded region surrounding the particle becomes smaller. The trends of the axial stress in the fluid layer just behind and in front of the sphere (i.e., from the maximum/minimum of τ_{xx} up to the particle surface) are, however, unaffected. Hence, both the magnitude and the gradient of the axial stress do not change as Bn increases. Nevertheless, the fluid velocity decays faster at higher Bingham numbers due to the aforementioned ‘pulling effect’ of the solid region. Although not clearly visible, the yellow curve Fig. 3.11c, corresponding to $Bn = 0.08$, is below the x -axis in a small region, denoting the onset of the negative wake phenomenon. Notice that the velocity decay is observed upstream the sphere too where a similar abrupt change of the axial stress occurs due to the transition from yielded to unyielded region. This is at variance with the purely viscoelastic case where a much weaker variation of the velocity field upstream the sphere is observed as the Weissenberg number is increased (see, e.g., Su et al. [99]).

We conclude this section by showing some simulation results at $\alpha = 0$, i.e., for the original Saramito model. The sedimentation, migration, and angular particle velocities are reported in Fig.3.12 for several particle-wall distances and $Wi = 2$ as solid lines. For comparison, the same quantities at $\alpha = 0.2$ are shown as symbols (the data are those already presented in the previous figures). It is readily observed that the sedimentation and migration velocities are very weakly affected by the mobility parameter. Specifically, only a slight decrease of these two quantities is found, in agreement with the purely viscoelastic case [71, 99]. A more relevant quantitative deviation at $\alpha = 0$ is observed for the angular velocity at small particle-wall distances and for low Bingham numbers. However, the

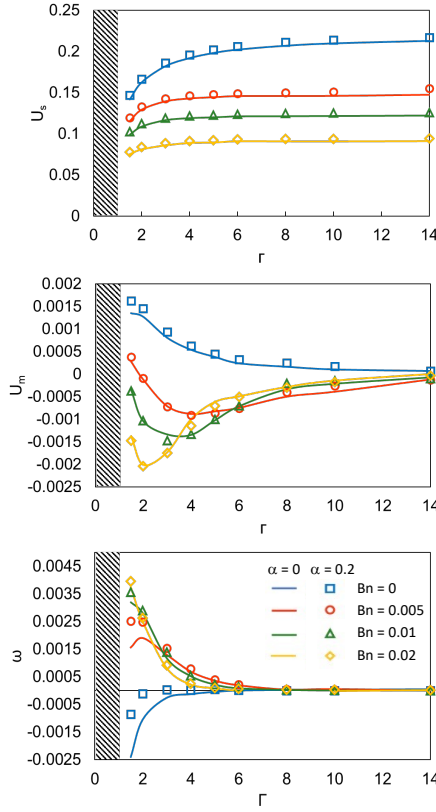


Figure 3.12. Sedimentation, migration, and angular velocity of the particle as a function of the particle-wall distance for the different values of the Weissenberg and Bingham number. The solid lines refer to the Saramito model ($\alpha = 0$) and the symbols to the Saramito-Giesekus model with $\alpha = 0.2$. The shaded area is the region inaccessible to the particle due to its finite size.

trends and the sign of the angular velocity are the same as the case at $\alpha = 0.2$. To justify the quantitative similar behavior of the particle dynamics between the Saramito and Saramito-Giesekus model, we evaluated the effective Weissenberg number, $Wi_{\text{eff}} = \lambda \dot{\gamma}$, in the fluid domain around the particle. It turns out that, even for the highest Wi -value investigated in this work, the largest effective Weissenberg number is lower than 1. Hence, as visible in the plots reported in the Appendix, a variation of

the mobility parameter α does not produce any significant change in the rheological functions. The only difference between the two models is that the Giesekus variant predicts a non-zero second normal stress difference in shear flow. This, however, does not seem to have any relevant effect on the particle dynamics. As a final comment, we mention that, despite no relevant change is observed between $\alpha = 0$ and $\alpha = 0.2$, we experienced some numerical issues in the former case at $Bn = 0$ and $Bn = 0.005$, and for low particle-wall distances. Specifically, both the mesh and the time step needed to be refined to get convergent solutions. Recalling that the Saramito model predicts a divergent extensional viscosity (see Fig.A.3), numerical instabilities can be likely due to high elongational stress regions around the particle

3.4 Conclusions

The dynamics of a rigid spherical particle in an elastoviscoplastic fluid in proximity of a flat wall subjected to a force parallel to the wall and under inertialess conditions is studied by direct finite element numerical simulations. The Giesekus-Saramito constitutive equation is employed to model the fluid. The Arbitrary Lagrangian-Eulerian formulation is used to handle the particle motion. The code is validated by simulating the settling dynamics of a sphere in an EVP fluid using the Saramito constitutive equation in an infinite medium. Mesh and time convergence are verified by comparing the time evolution of the particle kinematic quantities for different mesh resolutions and time step sizes.

The particle dynamics in terms of the translational and rotational velocities is studied for various particle-wall distances, Weissenberg and Bingham numbers. The purely viscoelastic case is also simulated to understand the effect of plasticity on the particle motion. The sedimentation slows down as the Weissenberg number decreases and the Bingham number increases. The mastercurves of the migration velocity indicate a lateral motion of the particle away from the wall in the purely viscoelastic case. However, as the Bingham number increases, the migration velocity progressively decreases and the particle inverts its migration direction and approaches to the wall. The inversion of the migration direction from the purely viscoelastic to the EVP case is due to a different shear rate distribu-

tion around the particle induced by the yield stress. In the EVP material, indeed, the shear rate gradient in the particle-wall gap reduces to the lower sedimentation speed and, at the same time, the presence of the unyielded region leads to a larger shear rate gradient at the particle side far from the wall, generating, in fact, a net force towards the wall.

Regarding the flow field, two unyielded regions are found: an external region surrounding the fluid zone around the particle, and isolated small regions at one or both sides of the particle. No negative wake is observed up to $Wi = 2$ and $Bn = 0.04$. However, as Bn increases, the yielded region becomes smaller and the solid region approaches the particle. The residual normal stresses in this region pull the solid away from the particle, leading to a faster decay of the fluid velocity behind the sphere. Indeed, at $Bn = 0.08$, a zone in the wake with inverted velocity is observed. Such a phenomenon is more pronounced at $Wi = 4$.

The results of this study show that the interplay of confinement, elasticity, and plasticity significantly affects the settling dynamics of a spherical particle as well as the shape and extension of the yielded/unyielded regions. This suggests that the critical value of the Bingham number leading to the blockage of the particle depends on the confinement.

Chapter 4

Sedimentation of a spheroidal particle in an EVP fluid

4.1 Introduction

Studies on the sedimentation of non-spherical particles in viscoplastic fluids are limited, with most research focusing on either 2D or 3D particles in purely viscoplastic environments, neglecting the role of elastic effects. While the behavior of spherical particles in elastoviscoplastic fluids has been explored, investigations on the dynamics of non-spherical particles in EVP media are not available. In this chapter, we study the dynamics of a prolate spheroidal particle settling in an unbounded elastoviscoplastic fluid through direct numerical simulations under inertialess conditions. The sedimentation, lift, and angular velocities are computed as the relevant fluid, flow, and geometrical parameters are varied. The flow fields around the particle, including the yielded/unyielded fluid regions and the viscoelastic stress distribution, are investigated. Results for the drag correction coefficient as a function of the aspect ratio, Weissenberg and Bingham numbers are provided.

4.2 Geometry, time and mesh convergence

Figure 4.1a displays the computational domain considered in this work. A prolate spheroidal particle with semi-major and semi-minor axes a and b is placed at the center of a spherical domain with radius R . As discussed later, the choice of a spherical domain is convenient from a numerical point of view. The domain between the particle and the spherical surface is filled by an EVP fluid. Since our aim is to study the settling dynamics of the particle in an unbounded domain, the radius R is chosen much larger than the characteristic particle size. A Cartesian reference frame is selected with origin at the center of the particle with axes oriented as in figure. A force acting along the x -direction is applied on the particle. Without loss of generality, the spheroid major axis is initially placed on the xy -plane. Because of the symmetry, the major axis remains on this plane during the sedimentation process and the particle rotates around the z -direction. Hence, the angle ϕ , defined as the angle between the force and the major axis direction (see Fig. 4.1b) suffices to describe the particle rotational dynamics. Due to the axisymmetric shape of the particle, we can consider one-half of the computational domain where the xy -plane

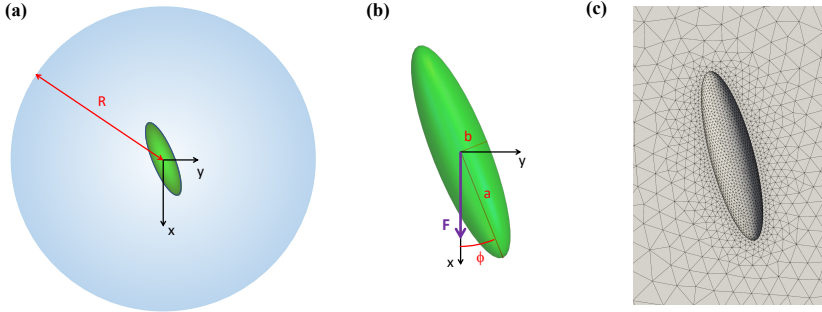


Figure 4.1. (a) Schematic representation of the computational domain: a prolate spheroidal particle is placed at the center of a sphere with radius R with major axis lying on the xy -plane of a Cartesian reference frame with origin at the center of the spherical domain. (b) A force F is applied on the particle along the direction of the x -axis; the angle between the major axis and the x -axis is denoted by ϕ . (c) Typical mesh around the particle used in the simulations.

passing through the particle center is a symmetry plane. At the external boundaries of the fluid domain (i.e., over the semi-spherical surface in Fig. 4.1a) we apply no-slip conditions. The numerical method has been validated in the previous works for spheroidal particles in viscoelastic fluids [100, 63] and in the previous chapter for spherical particles in EVP fluids. In this work, we have verified mesh and time convergence for all the investigated parameters. The required mesh resolution and time step size to get convergent results depend on Wi , Bn , and the particle aspect ratio. We found that about 50000 tetrahedral elements assure spatial-independent solutions for the most critical cases. The (dimensionless) typical time step size is 0.005 that must be reduced to 0.001 for the highest values of Wi and Bn . Finally, the value of the radius R of the spherical domain is a delicate choice. Indeed, as pointed out by Moschopoulos et al. [101], because of the adopted constitutive equation, a variation of the velocity field in the unyielded area travels through the domain up to reach the external boundary, disturbing the numerical solution. Hence, we selected a very large domain ($R = 100R_c$) so that a stationary condition is reached before the numerical solution is affected by this issue.

4.3 Results and discussion

The dynamics of a spheroidal particle in an EVP fluid is presented in terms of the translational and rotational velocities as the aspect ratio, initial orientation, Weissenberg and Bingham numbers are varied. Simulation results for the purely viscoelastic case are also included to highlight the effect of fluid plasticity on the particle motion. The diagrams presented in Fig. 4.2 show the sedimentation velocity U_s (the velocity component along the force direction), the lift velocity U_l (the velocity component orthogonal to the force direction), and the angular velocity ω around the z -axis as a function of orientation angle ϕ of a prolate spheroid with aspect ratio $\beta = 2$ and $Wi = 1$ for different values of the Bingham number. Each curve represents a different initial orientation, denoted by ϕ_0 , changing from 0 to $\pi/2$ with $\pi/12$ increment. For a better visualization of the results, we split the curves in two plots: the left column of Fig. 4.2 reports the data up to $Bn = 0.1$ and the right one from $Bn = 0.3$ up to $Bn = 1$. Each curve shows the evolution of the particle kinematic quantities as a function of the particle orientation, i.e., time runs along the curves. The first point of each curve corresponds to a spheroid in a Newtonian fluid under creeping flow conditions due to the stress-free initial condition [63]. Because of the small solvent viscosity contribution used in this work, the sedimentation and lift velocities are initially very large (and beyond the selected range for the y -axes of the diagrams) whereas the angular velocity is zero. Similarly to the purely viscoelastic case, the kinematic quantities rapidly change due to the build-up of the viscoelastic stresses, as denoted by the almost vertical trends of the curves. Then, depending on the Bingham number, different behaviors can be observed.

First of all, for all the cases, the angular velocity is negative denoting a clockwise rotation leading the spheroid to align with major axis along the force direction. Furthermore, the sedimentation velocity increases from $\phi = \pi/2$ to $\phi = 0$, i.e., the fastest sedimentation rate corresponds to the spheroid aligned with the longest axis along the applied force. For a purely viscoelastic case ($Bn = 0$), once the elastic stresses fully develop, the curves overlap indicating the presence of a mastercurve denoted by the dotted lines in Fig. 4.2 [63]. The same behavior is observed at $Bn = 0.01$. In this case, the sedimentation velocity is lower than the viscoelastic

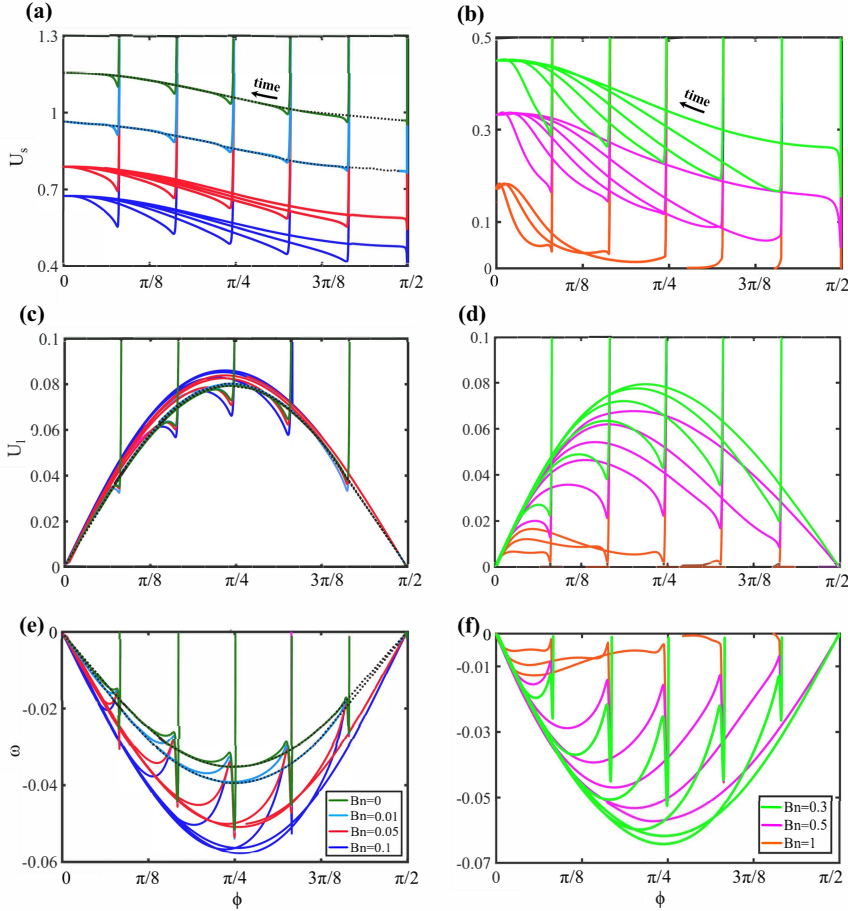


Figure 4.2. Sedimentation velocities (a-b), lift velocities (c-d), and angular velocities (e-f) of a prolate spheroid with an aspect ratio $\beta = 2$ settling in an elastoviscoplatic fluid at $Wi = 1$ as a function of the orientation angle and for different values of the Bingham number. The curves correspond to different initial orientations.

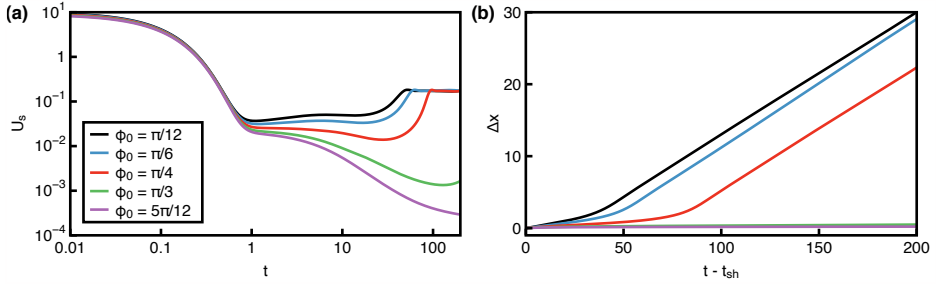


Figure 4.3. (a) Sedimentation velocity and (b) distance travelled by the spheroid along the force direction as a function of time for a particle with aspect ratio $\beta = 2$, $Bn = 1$, $Wi = 1$ for different initial orientation angles. In panel (b), $t_{sh} = 2$ is the time needed to almost completely extinguish the initial stress build-up.

case due to the effect of fluid plasticity. The lift velocity is only barely affected, whereas the angular velocity increases in magnitude. At $Bn = 0.05$ and $Bn = 0.1$, the settling velocity further reduces and the trends for different initial orientations visibly do not overlap anymore. While the lift velocity does not significantly change, the angular velocity further increases in magnitude. Hence, from $Bn = 0$ to $Bn = 0.1$, the spheroid settles slower but rotates faster, reaching the stable orientation in a shorter time. Notice also that all the angular velocity curves in Fig. 4.2e show an undershoot followed by a overshoot in a very short time (in about one dimensionless relaxation time). After the overshoot, the angular velocity of the purely viscoelastic case remains quantitatively similar to the overshoot itself, whereas it becomes larger and larger as Bn increases. A larger ω implies that, during the transient of the stress build-up, the spheroid changes its orientation faster at high Bn and the curves overlap at later times or not overlap at all. The faster rotation rate at high Bn -values is likely induced by the existence of the yielded region surrounding the particle that acts as a confinement. As discussed later, such a region is not symmetric and changes shape with the particle orientation.

The behavior just discussed is even more pronounced at higher Bingham numbers as shown in the right column panels of Fig. 4.2. At $Bn = 0.3$, the magnitude of the angular velocity further increases and, indeed, the yellow curves overlap only when the spheroid has almost reached the equi-

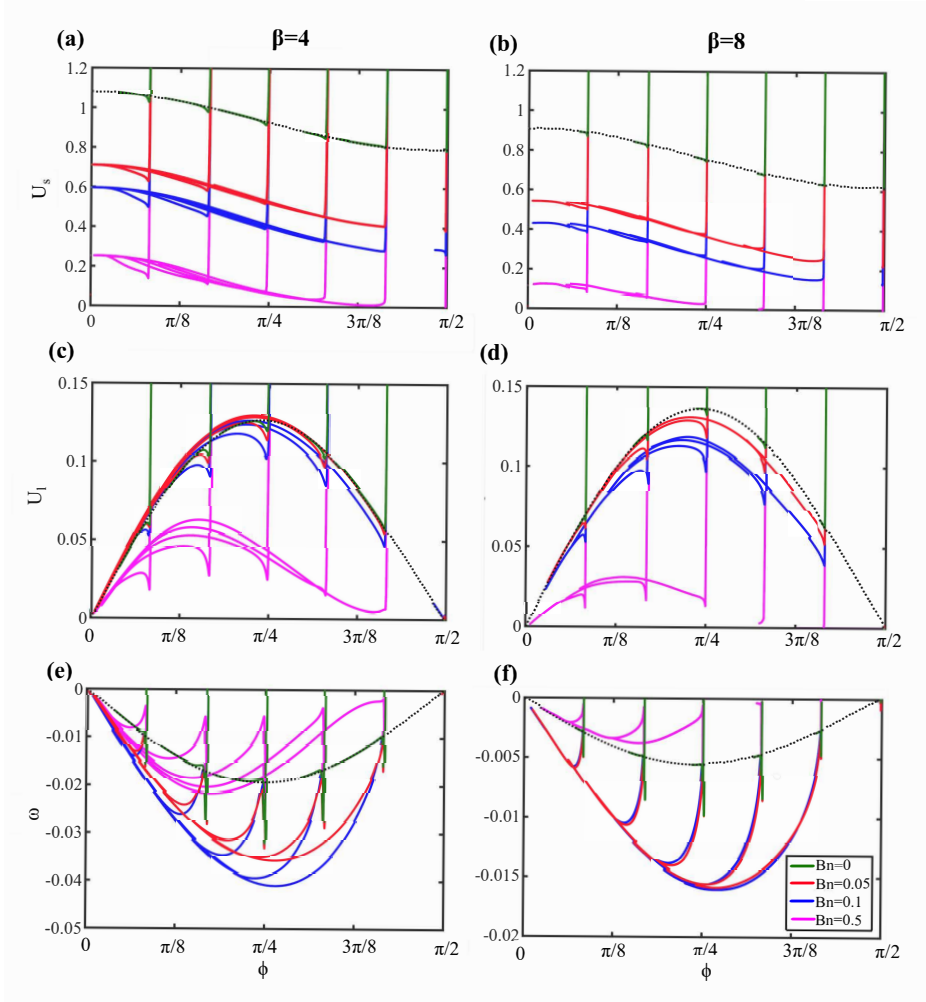


Figure 4.4. Sedimentation velocities (top), lift velocities (middle), and angular velocities (bottom) of a prolate spheroid settling in an elastoviscoplastic fluid at $Wi = 1$, $\beta = 4$ (left) and $\beta = 8$ (right) as a function of the orientation angle. The curves correspond to different initial orientations.

librium orientation. A similar behavior is observed at $Bn = 0.5$. However, in this case, the angular velocity is starting decreasing as the yielded region is approaching the particle (see later). Despite the lower angular velocity, the curves at different initial orientations follow different trends and overlap only when the spheroid almost aligned along the force. This behavior is due to the longer and longer transient dynamics observed at high Bingham numbers.

At $Bn = 1$, all the kinematic quantities significantly reduce since the particle is going towards the stoppage condition. It is interesting to note that the curves corresponding to initial orientation $\phi_0 = \pi/4$ or lower show a similar trends to those at smaller Bn -values, i.e., the particle (slowly) rotates to the vertical equilibrium position with an increasing sedimentation rate; on the contrary, for $\phi_0 = \pi/3$ or higher, all the kinematic quantities (in magnitude) are close to zero so the settling dynamics is extremely slow or even the particle is expected to be blocked at some orientation. All the red curves correspond to the same final simulation time (200 dimensionless times). Due to the very low angular velocity, the curve at $\phi_0 = \pi/3$ ends before the others since the particle changes its orientation ϕ very slowly. A more detailed investigation on the dynamics at $Bn = 1$ is reported in Fig. 4.3a where the sedimentation velocity U_s is plotted as a function of time for different initial orientation angles. After the initial transient due to the stress build-up, the curves for $\phi_0 \leq \pi/4$ reach the same plateau corresponding to the vertical alignment. At $\phi_0 = \pi/3$ (green curve), the settling rate achieves a minimum at around $t = 100$ and then starts increasing. At longer times, we expect that particle rotates to attain the stable vertical orientation and the sedimentation velocity curve reaches the plateau observed at lower ϕ_0 . However, since the minimum of U_s is two orders of magnitude lower than the steady-state value, the time needed to achieve the stable orientation is very long. This is confirmed in Fig. 4.3b where the dimensionless distance travelled by the spheroid along the force direction is reported as a function of time. To neglect the effect of the initial viscoelastic stress transient, the time is shifted by t_{sh} (set equal to 2) which is the time needed to almost completely extinguish the stress build-up. The green curve at $\phi_0 = \pi/3$ remains nearly horizontal within the investigated time window denoting no appreciable motion of the particle, in contrast with the curves at lower ϕ_0 where the travelled distance

is up to 30 times the characteristic particle size. At $\phi_0 = 5\pi/12$ (purple curves in Fig. 4.3), the settling rate is one order of magnitude smaller at long times, further slowing down the sedimentation dynamics. We cannot assess whether the settling velocity rises towards the steady-state value. If this is the case, however, we expect that the time to achieve an appreciable settling rate is so long that the particle can be considered blocked for any practical purpose.

In summary, at $Bn = 1$, a critical initial orientation angle $\phi_{0,\text{cr}}$ can be identified such that particles released at $\phi_0 < \phi_{0,\text{cr}}$ (slowly) settle and rotate towards the stable vertical orientation. Such particles coexist with spheroids released at $\phi_0 > \phi_{0,\text{cr}}$ that experience a larger drag and are blocked in the fluid (or settle extremely slow). For these particles, the instantaneous Bingham number, i.e., the Bingham number defined with the current sedimentation velocity, is lower than the critical value for particle stoppage and the spheroid is not able to settle and rotate. Particles with major axis closer to the force direction settle sufficiently fast to overcome the critical Bingham number and follow the expected sedimentation dynamics. By further increasing Bn , the critical initial orientation reduces and more and more particles oriented with major axis near the force are blocked. Above a critical Bingham number Bn_{cr} , all the spheroids stop translating and rotating regardless of the initial orientation. Such a critical value is the one corresponding to the blockage of the spheroid with longest axis along the force, and will be discussed later.

The effect of aspect ratio on the settling dynamics is shown in Fig. 4.4 where the sedimentation, lift and angular velocities of spheroids with aspect ratio $\beta = 4$ and $\beta = 8$ are reported for $Wi = 1$. As the aspect ratio increases, the settling velocity reduces for a fixed Bingham number. Whereas for $\beta = 4$ the existence of a mastercurve is visible only at relatively low Bn -values (like the case at $\beta = 2$), the curves for $\beta = 8$ at different initial orientations fairly overlap up to $Bn = 0.5$. Indeed, at high aspect ratios, the particle rotates slower (compare the angular velocity values between Fig. 4.4f, Fig. 4.4e and Figs. 4.2e-4.2f) and the stress build-up ends while the spheroid did not significantly change its orientation. Because of the enhanced drag, a spheroid with higher aspect ratio stop translating and rotating at a lower Bingham number. This is clearly visible for $\beta = 8$ where, at $Bn = 0.5$ (purple curves), spheroids that (slowly) rotate towards

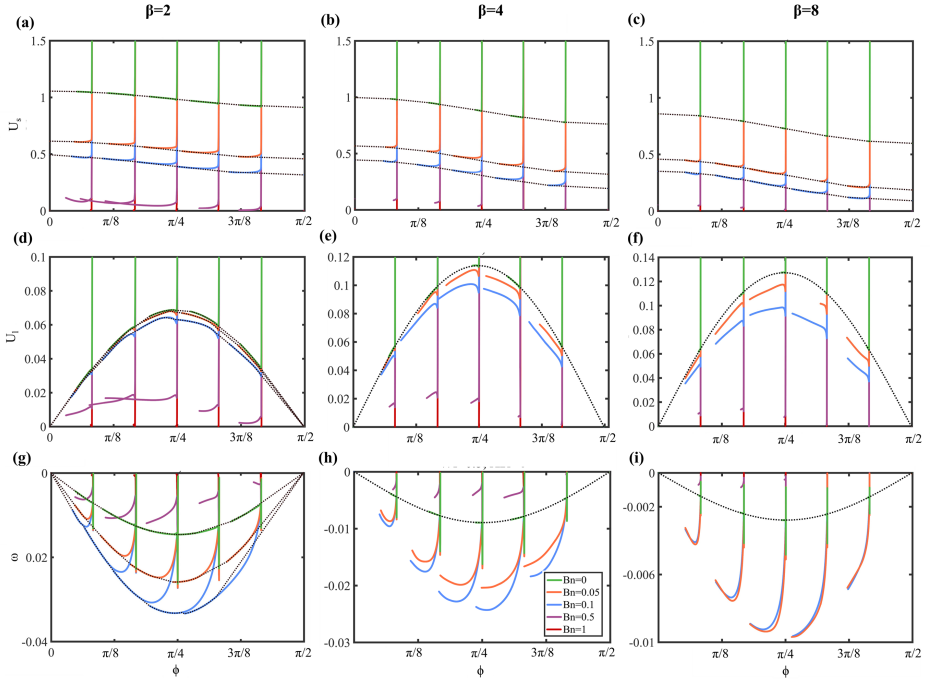


Figure 4.5. Sedimentation velocities (top), lift velocities (middle), and angular velocities (bottom) of a prolate spheroid settling in an elastoviscoplastic fluid at $Wi = 0.5$, $\beta = 2$ (left), $\beta = 4$ (middle) and $\beta = 8$ (right) as a function of the orientation angle. The curves correspond to different initial orientations.

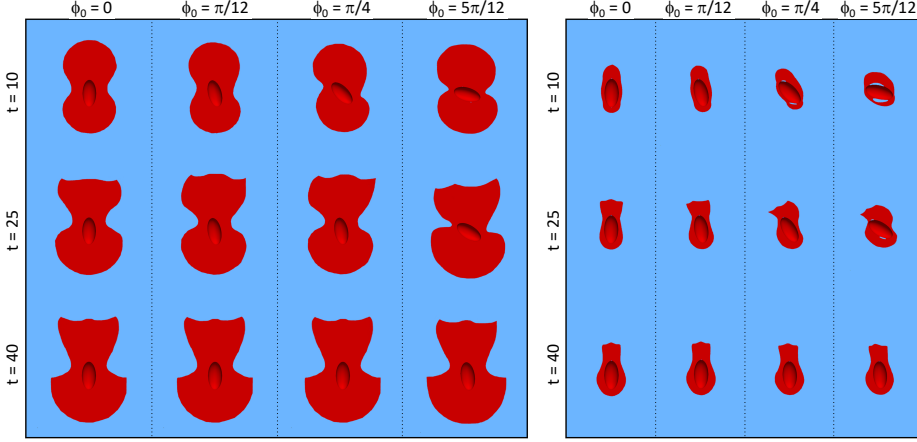


Figure 4.6. Snapshots of the yielded (red) and unyielded (cyan) regions on the symmetry plane around a spheroid with aspect ratio $\beta = 2$ and $Wi = 1$. Four values of the initial orientation angle and three (dimensionless) time instants are considered. The left and right images refer to $Bn = 0.1$ and $Bn = 0.5$, respectively.

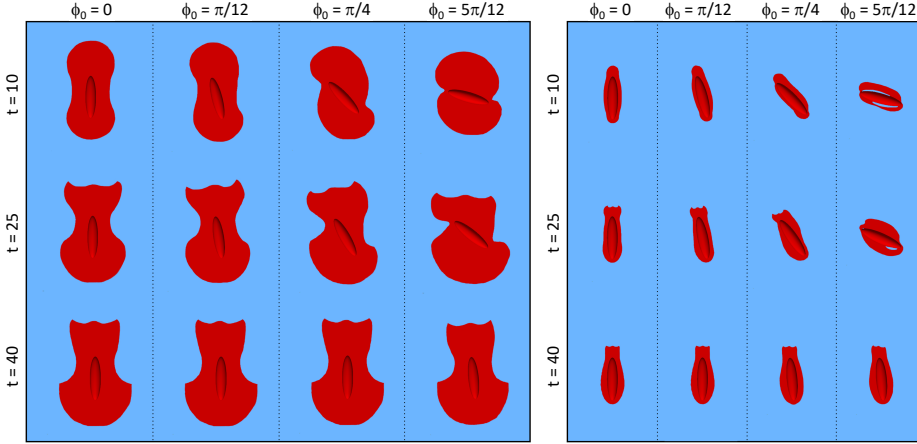


Figure 4.7. Snapshots of the yielded (red) and unyielded (cyan) regions on the symmetry plane around a spheroid with aspect ratio $\beta = 4$ and $Wi = 1$. Four values of the initial orientation angle and three (dimensionless) time instants are considered. The left and right images refer to $Bn = 0.1$ and $Bn = 0.5$, respectively.

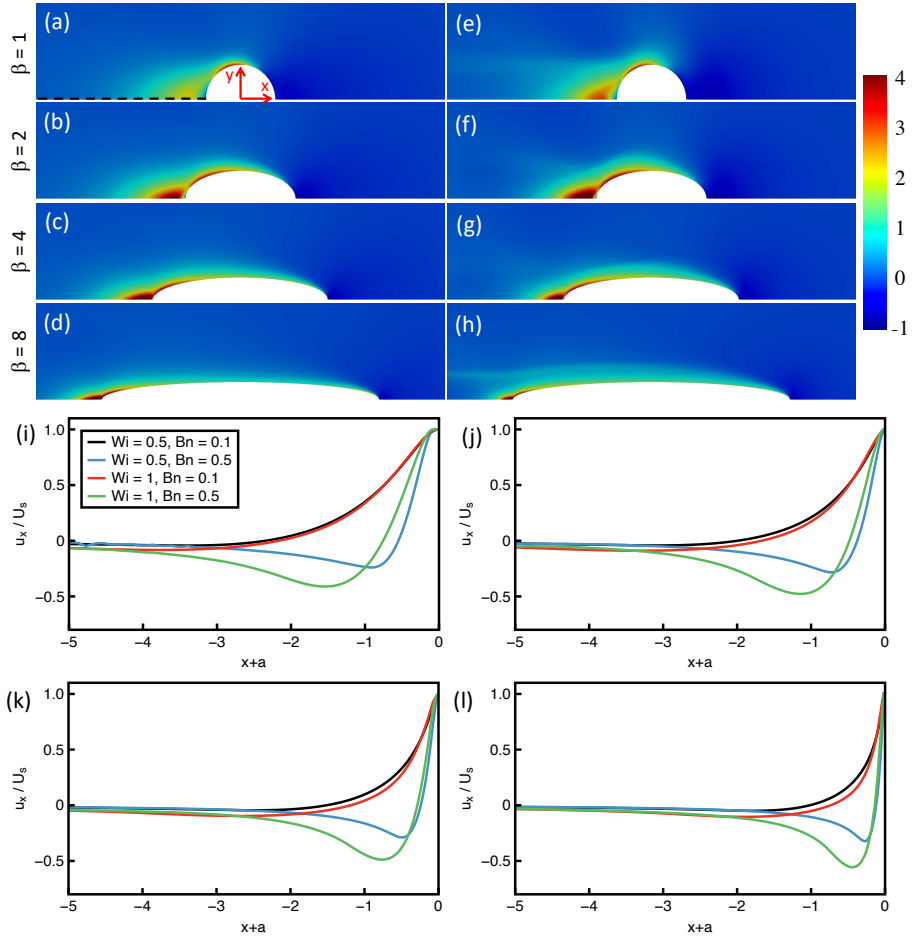


Figure 4.8. (a)-(h) Distribution of τ_{xx} around a spheroid with the major axis aligned with the force direction at two Bingham numbers $Bn = 0.1$ (left column) and $Bn = 0.5$ (right column), and four aspect ratios. The Weissenberg number is $Wi = 1$. (i)-(l) x -component of the fluid velocity normalized by the steady-state settling velocity along the axis of symmetry behind the particle indicated as the dashed line in panel (a). In panels (i)-(l), the axial coordinate x is translated by the semi-major axis, thus the point at $x = 0$ coincides with the particle tip.

the stable orientation coexist with blocked particles.

The settling dynamics of a spheroid with different aspect ratio is also studied at $Wi = 0.5$. The results (not reported) show that, as the Weissenberg number decreases, both the translational and rotational velocities reduce, leading to a slower overall settling dynamics. Because of the smaller angular velocity and the shorter characteristic time for the stress build-up, mastercurves are observed for all the investigated cases. The trends of the kinematic quantities are qualitatively similar to those at $Wi = 1$ and only quantitative differences are observed. Specifically, the slower settling velocity leads to a smaller critical Bingham number for particle stopping.

The shape and extension of the yielded/unyielded zones surrounding a particle in elastoviscoplastic suspensions, i.e., the regions in the fluid domain where $|\tau_d|$ is higher (indicating fluid behavior) or lower (indicating solid behavior) than the yield stress, is an intriguing characteristic of yield stress materials. Figure 4.6 displays the yielded (red) and unyielded (cyan) regions around a spheroidal particle on the xy -plane (the symmetry plane). The Weissenberg number is fixed at $Wi = 1$, and the aspect ratio is $\beta = 2$. Panels (a) and (b) refer to Bingham numbers of $Bn = 0.1$ and $Bn = 0.5$, respectively. Three time instants and four initial particle orientations are considered. The same plots for a spheroid with aspect ratio $\beta = 4$ are shown in Fig. 4.7.

As expected, from $Bn = 0.1$ to $Bn = 0.5$ the yielded region reduces. For particles aligned with the force direction, the shape of the yielded region is qualitatively similar to spheres (see, e.g., Fraggidakis et al. [1]) with the loss of the fore-aft symmetry due to the fluid elasticity. As pointed out by Romanus et al. [66], the shape of the yielded region changes during the settling dynamics, following the particle orientation. Specifically, for particles oriented transversely to the flow direction, the yielded region ‘shrinks’ towards the tips of the spheroid, as visible in the snapshots at $\phi_0 = 5\pi/12$ for $Bn = 0.1$. This phenomenon is likely related to the fact that, because of the elongated shape, the fluid stress is enhanced in the region very close to the tip but decays faster far from the particle, as observed for the purely viscoelastic case [63]. Hence, as the particle is more elongated, the fluid stress becomes lower than the yield stress at a shorter distance from the tip. This behavior is confirmed in Fig. 4.7

where, for $\phi_0 = 5\pi/12$, the unyielded region is almost in contact with the particle tips until the spheroid major axis is nearly perpendicular to the force direction. At $Bn = 0.5$, the effect of the particle orientation is even more relevant. Indeed, for spheroids nearly oriented along the force direction, the yielded region surrounds the particle similarly to the case at $Bn = 0.1$. On the contrary, the yielded fluid zone around particles with major axis transversal to the force contains unyielded regions, as visible in the rightmost snapshots in Figs. 4.6 and 4.7. These embedded unyielded regions are rather thin and extend along the flatter surface of the spheroid. During the settling dynamics, the particle rotates to reach the vertical stable orientation and these zones reduce up to disappear at some orientation. These regions are similar to the solid caps at the front and back of a spherical particle where the stress is very low due to the stagnation point [28]. For an elongated particle oriented transversal to the flow, the low stress region is more extended as compared to spheres and the solid regions are wider. We do not observe embedded unyielded regions for vertically aligned particles as the stresses around the particle tip are large.

The results just discussed show that, if the spheroid is not blocked at some orientation, the angular velocity is such that the particle, while settling, rotates to align the major axis along the force regardless of the aspect ratio, Weissenberg and Bingham numbers. In the rest of the paper, we provide additional results assuming that the particle has reached the equilibrium orientation. In this regards, we adopt an axisymmetric version of our code that allows to explore a wide range of parameters at reduced computational cost. The results in terms of particle velocities, yielded/unyielded region, fluid velocity and stress fields, are preliminary compared with those obtained by the 3D version of the code under same conditions showing an excellent quantitative agreement.

Figures 4.8a-4.8h display the color map of the axial component of the viscoelastic stress τ_{xx} around the spheroid (the particle is settling from the left to the right) for different aspect ratio at $Wi = 1$. The left and right panels refer to $Bn = 0.1$ and $Bn = 0.5$, respectively. Similarly to the viscoelastic case, as the aspect ratio increases, the axial stress reduces along the particle side, while it increases in the wake due to the high curvature of the shape, denoting a stronger extensional flow behind the

particle. The extension of the high stress region, however, decreases as the particle is more elongated. Interestingly, the effect of the Bingham number depends on the aspect ratio: at $\beta = 1$ and $\beta = 2$, higher Bingham numbers increase τ_{xx} in the particle wake, whereas, at $\beta = 4$ and $\beta = 8$, the opposite is found.

As reported for viscoelastic fluids [102, 63], higher values of τ_{xx} and its axial gradient lead to a more rapid variation of the fluid axial velocity, possibly leading to the negative wake phenomenon [32]. Figures 4.8i-4.8l show the fluid velocity u_x normalized by the steady-state particle settling velocity along the symmetry axis (the x -coordinate of the graphs is translated by the particle semi-major axis a so that the rightmost point identifies the particle tip). Four combinations of Wi and Bn are considered. We recall that the fluid behind a sphere/spheroid in a purely viscoelastic case does not show a negative velocity up to $Wi = 2$ [63]. On the contrary, the negative wake phenomenon is observed for all the examined cases. Even at $Wi = 0.5$ and $Bn = 0.1$ (black curves), the fluid velocity is slightly negative in a wide region behind the particle, regardless of the aspect ratio. The negative wake phenomenon is enhanced at $Wi = 1$ although the effect is relatively small. A much stronger negative velocity is observed as Bn is increased to 0.5 (blue and green curves). In this case, the minimum fluid velocity is about one-half of the settling speed. As the aspect ratio increases, such a minimum is (in magnitude) larger and moves towards the particle tip.

The faster decay of the stresses and the consequent shrinkage of the high stress region in the wake of the particle discussed above affect the extension of the yielded region behind the particle. Such effect, partially shown in Figs. 4.6 and 4.7, is clearly visible in Fig. 4.9 where the yielded/unyielded regions are compared for different Weissenberg numbers and aspect ratios. The Bingham number is fixed to $Bn = 0.1$. As β increases, the yielded interface behind the spheroid approaches the particle surface. A similar behavior occurs at the front of the particle. The shape of the yielded region shows the same features as the aspect ratio is varied, with the lateral concavity that is smoother and moves backwards as the particle is more elongated. Figure 4.9 displays the effect of the Weissenberg number as well. As Wi increases, the yielded envelope is closer to the front of the particle surface and farther from its back. This is a consequence of the

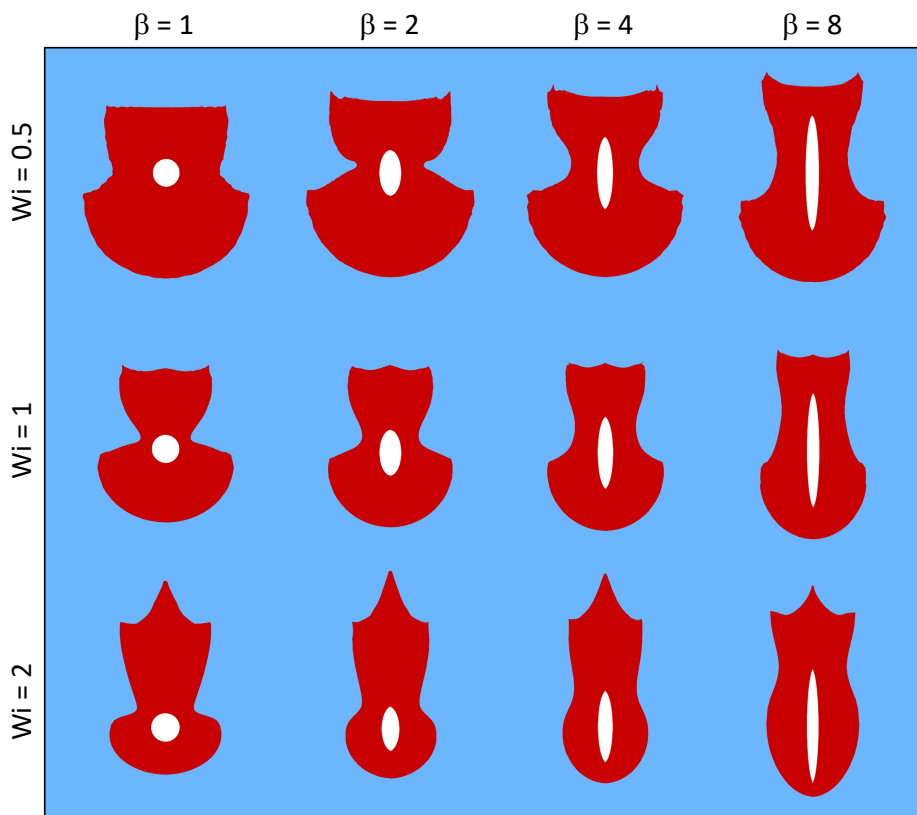


Figure 4.9. Snapshots of the yielded (red) and unyielded (cyan) regions on the symmetry plane around a spheroid aligned with the force direction for different aspect ratios and Weissenberg numbers. The Bingham number is $Bn = 0.1$.

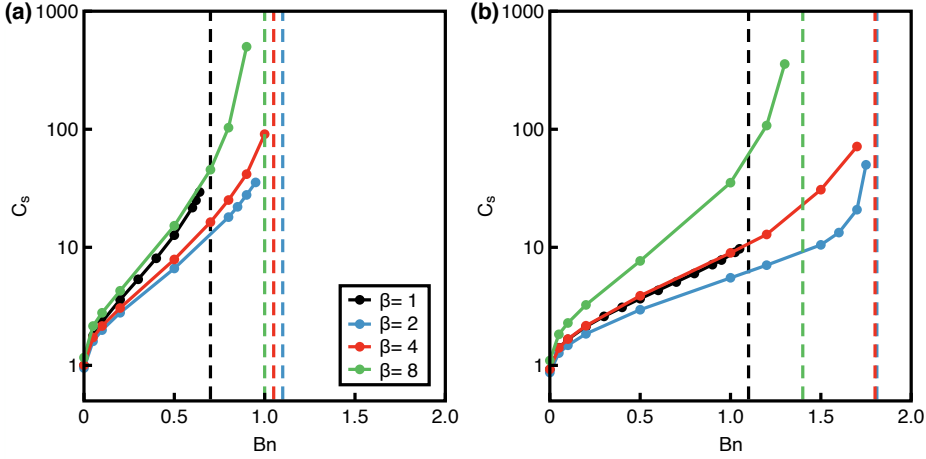


Figure 4.10. Drag correction coefficient as a function of the Bingham number for different values of the aspect ratio. The Weissenberg number is $Wi = 0.5$ in panel (a) and $Wi = 1$ in panel (b).

different stress region around the particle as Wi is varied [63]. Specifically, at higher Weissenberg values, the stresses behind the particle increase in magnitude and decay slower. Hence, a wider fluid region experiences a stress higher than the yield stress. The opposite happens ahead the particle where the stress decreases in magnitude and decays faster as Wi increases, thus reducing the extension of the yielded region. Increasing the Weissenberg number also changes the shape of the yielded envelope, leading to a narrower fluid region alongside the spheroid and the appearance of a central ‘horn’ on the axis of symmetry behind the particle.

We finally investigate the drag correction coefficient defined as $C_s = F/(6\pi\eta_0 R_c U_s)$ representing the deviation from the Stokes drag (valid for an isolated sphere in a Newtonian fluid under creeping flow conditions). Figure 4.10 reports C_s as a function of the Bingham number for four values of the aspect ratio and for $Wi = 0.5$ and $Wi = 1$. The point at $Bn = 0$ denotes the purely viscoelastic case which is slightly lower than 1 as elasticity reduces the drag compared to a Newtonian fluid [99, 63]. The points of the curves correspond to the values of the drag correction coefficient once a steady-state is reached. In this regards, we found that, as the Bingham number increases, the time needed to reach a stationary

condition increases as well. The vertical dashed lines denote the lowest values of the Bingham number such that, after 5000 dimensionless times, the sedimentation velocity did not reach a steady-state but decreases in time, similarly to the purple curve in Fig. 4.3, and reaches values lower than 10^{-5} . As previously commented, we cannot assess whether the trend will increase at longer times. In any event, the sedimentation phenomenon is extremely slow so that the particle can be considered stopped for practical applications. Our numerical method is not able to directly compute the exact value of the critical Bingham number corresponding to the stoppage condition and special techniques are required [50]. However, we expect that the critical Bingham number does not differ too much from the values denoted by the dashed lines. For Bn -values between the rightmost point of the curves and the dashed lines, we found that a steady-state is not reached in 5000 dimensionless times, although the sedimentation rate attained or is attaining a plateau and, then, is likely to rise so the corresponding Bn is lower than the critical value. Regardless of the aspect ratio, the drag increases for increasing values of the Bingham number, i.e., the particle sediments slower. The drag correction coefficient and the values of the critical Bingham number are a non-monotonic function of the aspect ratio, decreasing from the sphere to the spheroid with $\beta = 2$ and then increasing for more elongated particles. This result agrees with the Newtonian and viscoelastic cases where the minimum drag coefficient is observed for a prolate spheroid with aspect ratio of about 2. Hence, as previously discussed, a more elongated particle gets stopped at a lower Bingham number. Finally, from $Wi = 0.5$ to $Wi = 1$, the drag correction coefficient reduces for a fixed value of Bn and the critical Bingham number is larger due to the aforementioned drag reduction induced by fluid elasticity.

4.4 Conclusions

The settling dynamics of a prolate spheroidal particle in an unbounded elastoviscoplastic fluid is studied by direct numerical simulations under inertialess flow conditions. The Saramito-Giesekus constitutive equation is employed to model the suspending liquid. The equations governing the fluid and particle dynamics are solved through the finite element method.

The Arbitrary Lagrangian-Eulerian formulation is used to handle the particle motion.

Similarly to the purely viscoelastic case, a spheroid in an EVP fluid rotates up to attain a stable orientation with major axis along the force direction, corresponding to the fastest sedimentation. As the Bingham number increases, the settling rate reduces. On the contrary, the angular velocity first increases (in magnitude) and then decreases. This non-monotonic behavior might be attributed to the yielded region surrounding the particle that acts as a confinement, speeding up the rotational dynamics. However, as the Bingham number further increases, the yielded region approaches the particle leading to the stoppage condition, thus slowing down the rotation rate.

The initial orientation has a relevant qualitative effect on the settling dynamics when the Bingham number is close to the critical one, leading to the coexistence of particles initially oriented with the longest axis close to the direction perpendicular to the force that experience a large drag and are not able to translate/rotate, and particles with major axis more aligned with the force which (slowly) rotate towards the stable orientation. As the aspect ratio increases, the drag experienced by the particle increases too, thus the spheroid stops translating and rotating at a lower Bingham number. Also, a more elongated particle rotates slower and the stress build-up ends while the spheroid did not change too much its orientation, leading to the appearance of a mastercurve for the kinematic quantities as a function of the current particle orientation, like for the purely viscoelastic case. At higher Weissenberg numbers, the drag reduces speeding up the particle sedimentation and moving the critical Bingham number at higher values.

The shape of the yielded region depends on the Bingham number and the aspect ratio, and changes as the particle rotates. For particles oriented transversely to the force, the yielded region shrinks near the tips of the spheroid due to the fast spatial decay of the stresses in that regions. As the Bingham number increases, unyielded regions appear along the surface of the particles, similar to the solid caps observed at the front and back of a sphere. While rotating towards the stable orientation, these unyielded regions disappear as the stresses behind the spheroid are larger due to the particle tip. Such larger stresses are responsible for the negative wake

phenomenon that, in an EVP fluid, is observed at Weissenberg number values significantly lower than the purely viscoelastic case.

Chapter 5

Dynamics of a circular or
elliptical particle in an EVP
fluid in a channel flow

5.1 Introduction

Particle suspensions often exhibit unique behaviors that are strongly influenced by the nature of the flow and the rheological properties of the suspending medium. One such phenomenon is particle migration in channel flow, where particles move orthogonally to the direction of the main flow. This effect has been studied extensively over the past 50 years due to its relevance in various industrial and natural processes. While much attention has been given to particle migration in Newtonian and viscoelastic fluids, less is known about this behavior in more complex fluids, such as elastoviscoplastic fluids, which exhibit both elasticity and plasticity.

In this chapter, we aim to investigate the dynamics of circular and elliptical particles suspended in EVP fluids, focusing on their migration, orientation, and interaction with the yielded and unyielded regions of the suspension in a channel flow. As for the previous chapters, the fluid is modeled using the Giesekus constitutive equation, modified as proposed by Saramito to account for the yield stress. Results are provided at a fixed Weissenberg (Wi) number, different Bingham (Bn) numbers, distances from the channel centerline and (for elliptical particles) initial orientations. The purely viscoelastic case is also simulated to understand the effect of plasticity on the particle dynamics.

5.2 Geometry, mesh and convergence tests

The dynamics of a rigid circular particle with a diameter D and an elliptical particle with semi-major and semi-minor axes a and b suspended in an EVP fluid are simulated in a channel flow. The channel height is denoted by H . The position of the center of the particle along the gap is denoted by y_p . A Cartesian reference frame is selected with its origin at the center of the channel, and the x -axis is aligned with the centerline of the channel. Figures 5.1a and 5.1b display the 2D computational domain considered in this work. On the upper and lower boundaries, no-slip conditions are applied, and periodicity is imposed on the left and right boundaries along with a flow rate Q (see chapter 2).

Mesh and time convergence are verified for all the simulations. Figure 5.1c displays a typical mesh employed in this work. The images show

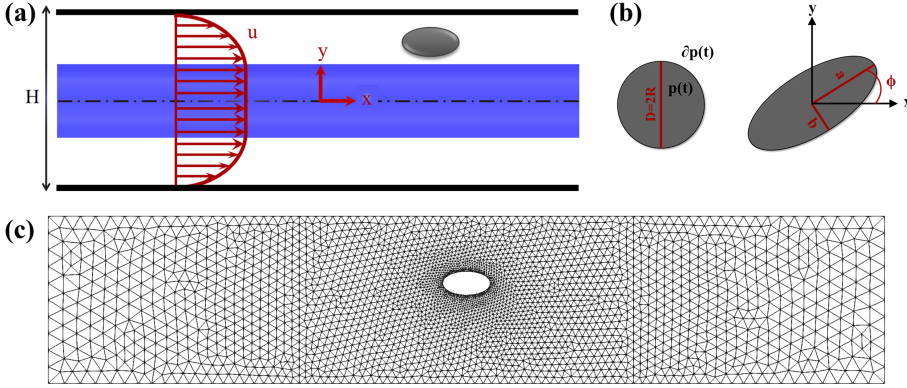


Figure 5.1. (a) Schematic representation of the computational domain: The x -axis is aligned with the centreline of the channel that is formed by the two infinite parallel plates separated by the gap H . The origin of the Cartesian reference frame is set at the center of the channel. A circular/elliptical particle is suspended in an elastoviscoplastic fluid flowing in the channel. The core unyielded region is illustrated in blue. (b) A circular particle with diameter D and an elliptical particle with semi-major a and semi-minor b axes are considered. The angle between the major axis and the x -axis is denoted by ϕ . (c) Typical mesh used in the simulations.

the mesh over the particle and in the channel. Notice that the particle is ‘surrounded’ by a box with finer resolution.

The results of the convergence tests are reported in Fig. 5.2, where the migration velocity of the particle V_p (the particle’s motion towards the channel centerline or the wall) and the angular velocity of the particle ω_p are shown as a function of time for two mesh resolutions and three time-step sizes. In Figs. 5.2a and 5.2b, mesh convergence is addressed for $\beta = 2$, $Wi = 1$, $Bn = 1$ for two initial particle positions $y_{p0} = 0.1$ with orientation angle $\phi = 0$, and $y_{p0} = 0.2$ with orientation angle $\phi = 90^\circ$. Figures 5.2c and 5.2d illustrate the time convergence of migration velocity and angular velocity as a function of time, respectively, at $\beta = 2$, $Wi = 1$, $Bn = 1$ for the initial particle position $y_p = 0.1$ with orientation angle $\phi = 0$. For all the kinematic quantities, the curves overlap fairly well. For the 2D computational domain used in this study, about 4000 elements with a time step size of 0.005 are used.

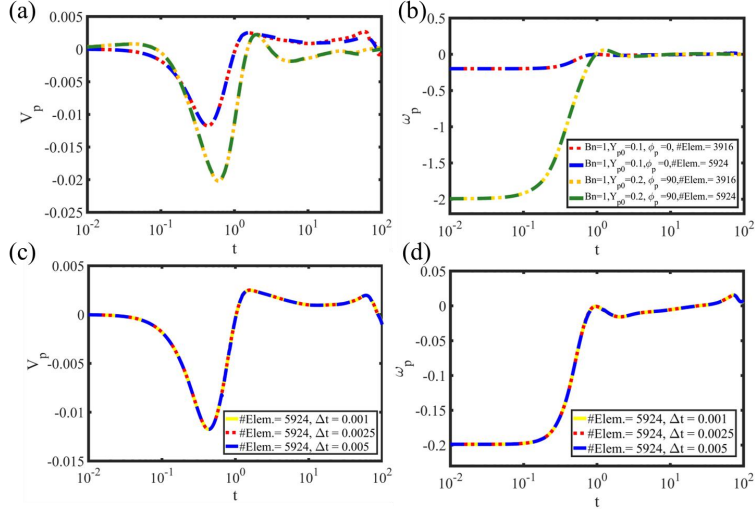


Figure 5.2. Migration and angular velocities of an elliptical particle in an EVP fluid as a function of time for two different mesh resolutions (panels a and b) and three time step sizes (panels c and d). The considered parameters are: $y_{p0} = 1$, $\phi = 90$, $Bn = 1$, $\beta = 2$, and $Wi = 1$.

5.3 Results and discussion

The dynamics of both circular and elliptical particles is first addressed, with a special focus on the final particle position as the initial particle position and Bingham number vary. Due to yield stress, the flow is divided into two main regions: the core unyielded region and two yielded regions near the walls, which are analyzed in the presence of particles in these areas. The purely viscoelastic case is also simulated to understand the effect of plasticity on particle motion.

While an inertialess particle immersed in a Newtonian and inertialess fluid in Poiseuille flow does not migrate and keeps its initial position [68, 67], a particle in an inertialess viscoelastic channel flow migrates either towards the center or the walls based on various factors, such as its initial position and shear-thinning effects [69, 70, 71]. Villone et al. [71] observed that particles move towards either the centerline or the walls depending on their initial position and there is a critical' position y_N along the gap,

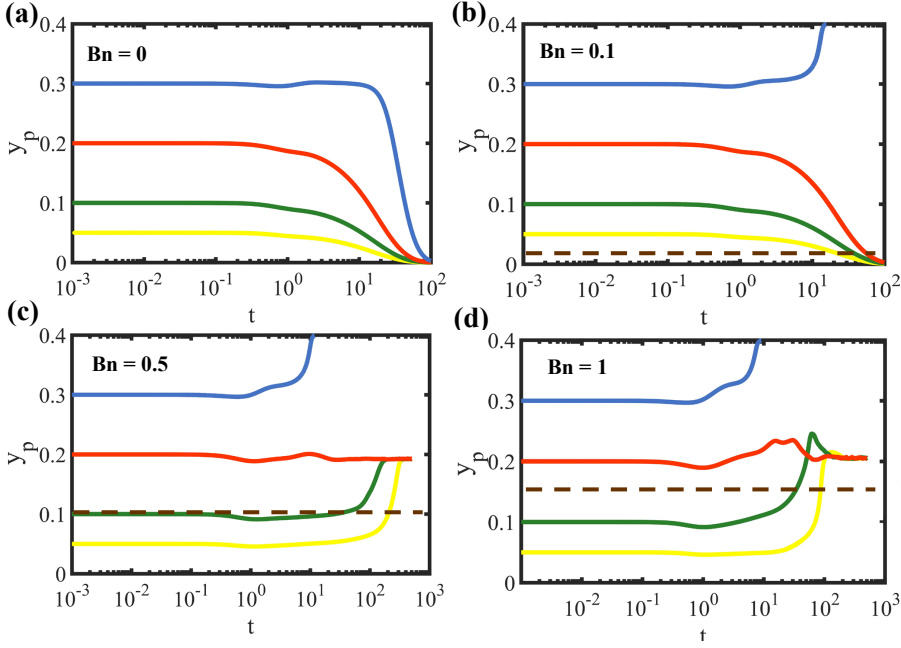


Figure 5.3. Particle position as a function of time for a circular particle for four initial positions and four different Bingham numbers.

above which the particle migrates towards the wall, and below which it migrates towards the center of the channel.

Chaparian et al. [77] considered the individual and combined effects of elasticity and plasticity of the suspending fluid on particle migration, discussing only the cases in which the particles are initially in the yielded regions. Within the specified range of parameters, in the viscoelastic regime, inertia is dominant, leading to particles finding their equilibrium position between the centerline and the walls. In the viscoplastic regime, a similar pattern is observed; however, in this regime, the yield surface acts as the centerline, restricting particle movement to the yielded areas. As the Bingham number increases, the equilibrium position of the particles shifts closer to the wall due to the expansion of the plug region, with the distance between the final particle position and the plug surface remaining constant. In the intermediate regime, where the suspending fluid exhibits

both elastic and plastic behavior, it is observed that particles can be focused at the centerline. Specifically, for a certain range of Weissenberg numbers in elastoviscoplastic fluids, particles can enter the plug region and move toward the center. This phenomenon is linked to the rotation of the particles, which partially yields the plug region, and the subsequent interplay of elastic forces and Magnus lift forces that drive the particles to the center, where all forces effectively balance.

The position of the circular particle as a function of time is displayed in Fig. 5.3 in the viscoelastic and elastoviscoplastic fluids, considering three values of the Bingham number and four different initial particle positions: $y_{p0} = 0.05, 0.1, 0.2, 0.3$. The Weissenberg number is fixed to $Wi = 1$. The largest value of the y-axis ($=0.4$) corresponds to the position of the center of the particle when in contact with the wall. The brown dashed line shows the boundary of the unyielded region. In this and all the subsequent figures, due to symmetry, we only present the curves in the upper half of the channel.

In Fig. 5.3a, the trajectories $y_p(t)$ for different initial values are reported for the viscoelastic case. It is observed that, in this range of parameters, a particle with an initial position up to 0.3 finds its equilibrium position at the center of the channel. Figure 5.3b shows the case at $Bn = 0.1$, which exhibits a similar behavior of the viscoelastic case for initial positions of 0.05, 0.1, and 0.2, where the particle migrates into the unyielded region and finds a stable position at the centerline. However, when the initial position is 0.3, the particle settles near the wall in the yielded area.

Figures 5.3c and 5.3d illustrate results for $Bn = 0.5$ and $Bn = 1$, respectively. It is observed that the particle attains an equilibrium position at around $y_{p0} = 0.2$ for initial positions of 0.05, 0.1, and 0.2 in both $Bn = 0.5$ and $Bn = 1$, which are in the yielded region. At $y_{p0} = 0.3$, the migration is towards the wall. It is evident that, by increasing plasticity, raises the height of the equilibrium position of the circular particle, in agreement with the results of Chaparian et al. [77]. However, there is no direct relationship between the height of the unyielded area and the equilibrium position. Notice that, once the final position is reached, the particle is fully immersed in the yielded region at $Bn = 0.5$, whereas it is partially embedded in the unyielded region at $Bn = 1$. The shapes of the yielded/unyielded regions will be discussed later.

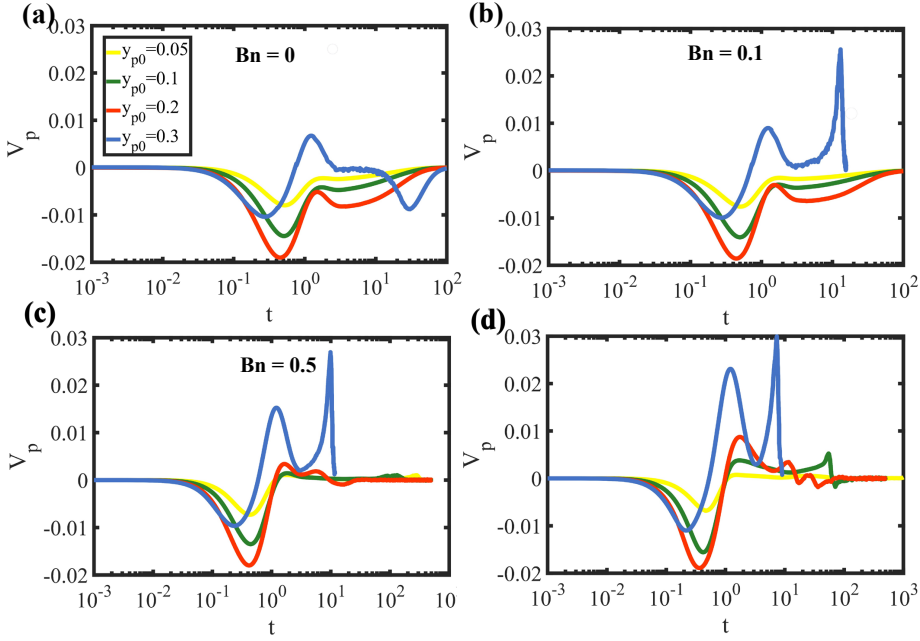


Figure 5.4. Particle migration velocity as a function of time for a circular particle for four initial positions and four different Bingham numbers.

In Fig. 5.4, the temporal trends of V_p related to the trajectories y_p shown in Fig. 5.3 are illustrated. The parameters and values used are the same of those in Fig. 5.3. It can be noted that the migration direction is influenced by the initial position of the particle. The initial oscillations in migration velocity result from the stress development around the particle. As the Bingham number and the initial particle position increase, both the amount and height of the oscillations rise. In the elastoviscoplastic cases, when the particle is near the wall, V_p reaches a peak before quickly dropping to zero when reaching the solid boundary. Interestingly, as Bn increases, damped oscillations appear before attaining the equilibrium position, likely due to the crossing of the unyielded region.

In Fig. 5.5, the particle angular velocity is presented for a circular particle with the same parameters described in Fig. 5.3. The angular velocity is negative at any distance from the wall and for any Bingham number,

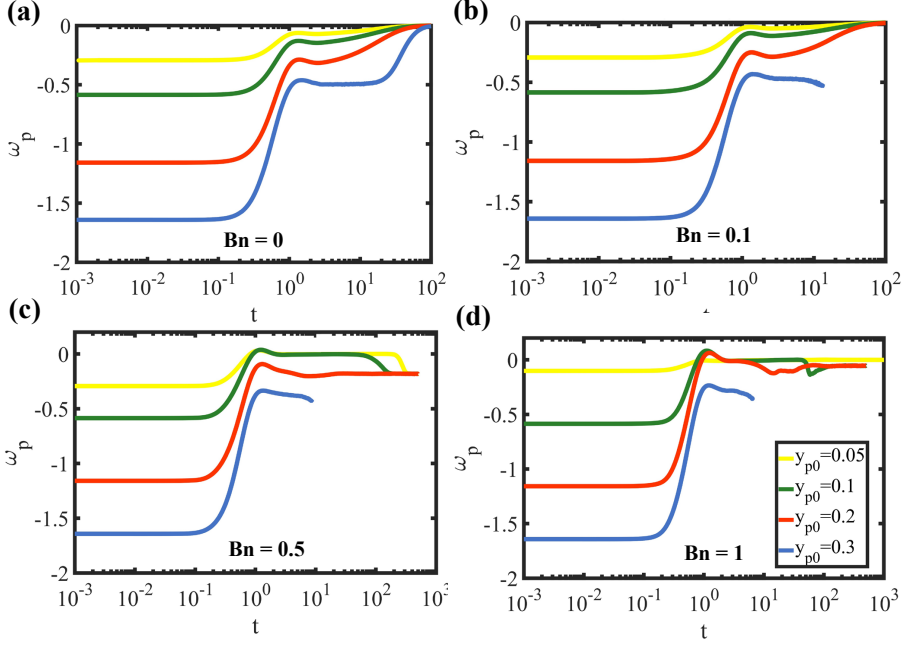


Figure 5.5. Particle angular velocity as a function of time for a circular particle for four initial positions and four different Bingham numbers.

indicating a counterclockwise rotation induced by the flow field. The angular velocity attained by the particle when reaching the wall corresponds to the rolling motion along the wall.

Figure 5.6 shows the graphs of particle position as a function of time for an elliptical particle with $\beta = a/b = 2$. The value of the major axis is chosen to have the same area of the circular particle. As before, four values of the Bingham number and four different initial positions are considered. The Weissenberg number is $Wi = 1$ and the initial orientation angle is $\phi = 90^\circ$. The orientation angle is defined as the angle between the major axis of the ellipse and the x-axis, hence, the particle is initially released with major axis along the gradient direction. It can be observed that, as the Bingham number increases, significant changes occur in the final equilibrium position of the particle as compared to the circular case. For the purely viscoelastic case, the particle finds its stable position at the

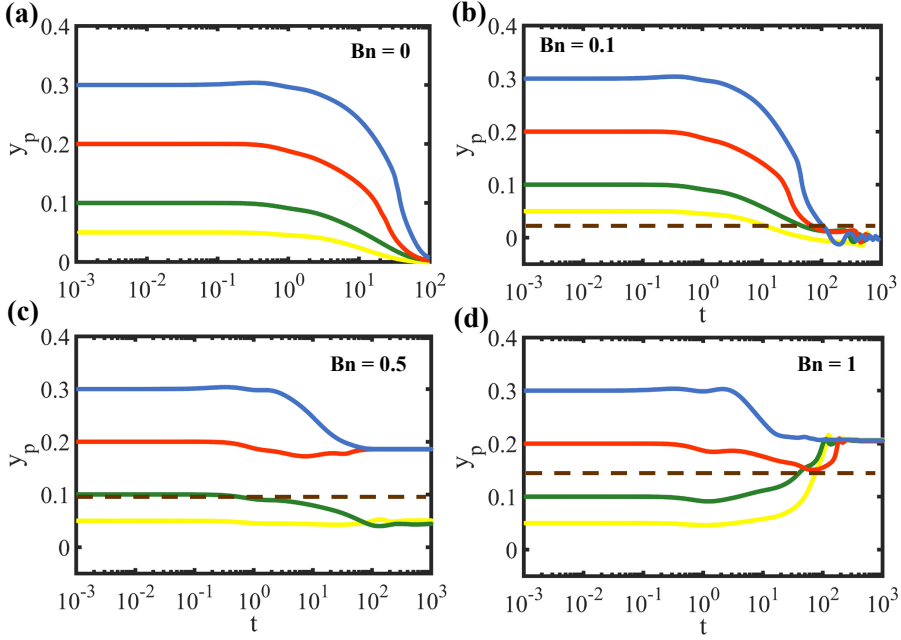


Figure 5.6. Particle position as a function of time for an elliptical particle ($\beta = 2$) for four initial positions and four different Bingham numbers. The initial orientation angle is $\phi_0 = \pi/2$.

center of the channel, similarly to the results for $\beta = 1$.

For $Bn = 0.1$, the particle migrates towards the wall regardless of its initial position, at variance with the circular particle where the wall is a stable position for particles released near the wall. Notably, as the particle center enters the unyielded zone, several damped oscillations are observed in the particle position. These are connected with the deformation of the shape of the yielded/unyielded region induced by the presence of the particle as discussed later.

As the Bingham number is increased to $Bn = 0.5$, two stable equilibrium positions are observed as visible in Fig. 5.6c. A particle that has an initial position in the unyielded region or at the boundary of the yielded/unyielded region migrates towards a stable position between the centerline and the yielded/unyielded boundary (around $y_p = 0.05$). On the contrary, a particle with an initial position in the yielded area reaches an

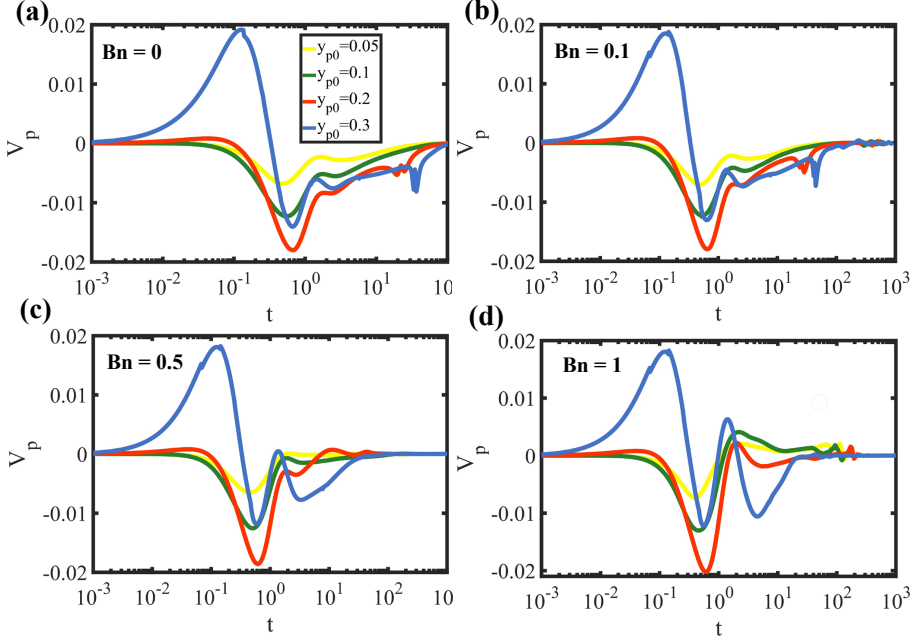


Figure 5.7. Particle migration velocity as a function of time for an elliptical particle ($\beta = 2$) for four initial positions and four different Bingham numbers. The initial orientation angle is $\phi_0 = \pi/2$.

equilibrium position in the yielded region in between the yielded boundary and the wall (around $y_p = 0.2$). Finally, Fig. 5.6d indicates that as the Bingham number increases to $Bn = 1$, the equilibrium position in the unyielded region disappears, and the particle migrates to the one in between the yielded/unyielded boundary and the wall, regardless of the initial position.

The migration velocity of the elliptical particle corresponding to the parameters in Fig. 5.6 is reported as a function of time in Fig. 5.7. The trends of the velocity curves are not only similar for all Bingham numbers, but they also resemble the trend of migration velocity of a circle in EVP fluid discussed in Fig. 5.4. Specifically, after viscoelastic stress development, particle migration in the purely viscoelastic case and for EVP at $Bn = 0.1$ and $Bn = 0.5$ is negative for all the initial positions. It indicates that the particle equilibrium position is lower than its initial

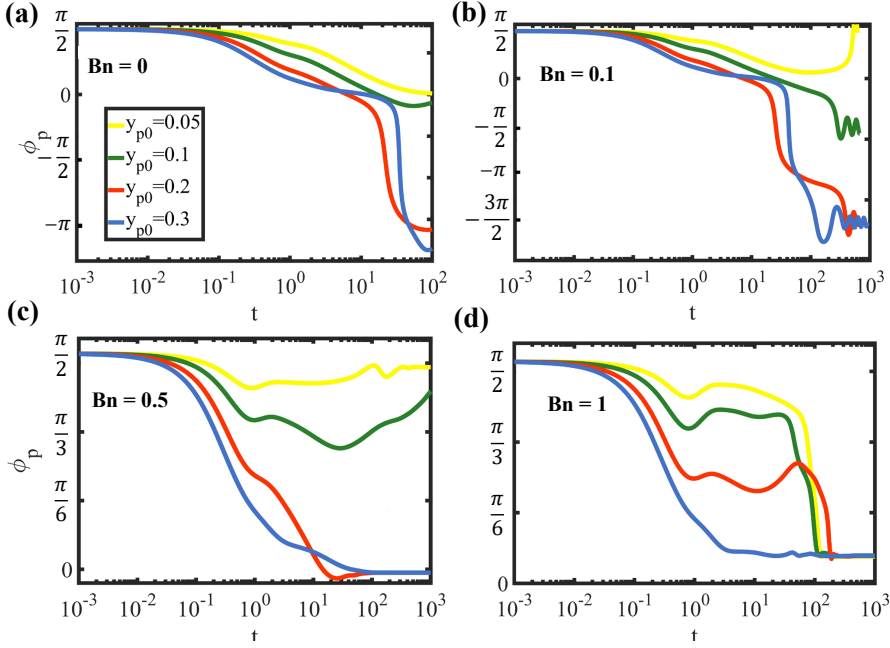


Figure 5.8. Particle orientation angle as a function of time for an elliptical particle ($\beta = 2$) for four initial positions and four different Bingham numbers. The initial orientation angle is $\phi_0 = \pi/2$.

position, even for small values like $y_{p0} = 0.05$, which is located in the unyielded area when $Bn = 0.5$. At $Bn = 1$, the migration velocity is positive for initial positions $y_{p0} = 0.05$ and $Bn = 0.1$, meaning that the equilibrium position is situated higher than the initial position.

The orientation of a non-circular particle is another important parameter that should be considered. The particle orientation angle as a function of time is reported in Fig. 5.8, with the same parameters as in Fig. 5.6. In this figure, the initial orientation angle is considered to be 90 degrees, so the particle has its major axis orthogonal to the x-axis. Figure 5.8a shows the orientation angle in a viscoelastic fluid, where the final stable orientation for the ellipse at any initial position is zero or $-\pi$, i.e., at long times the major axis is along the flow direction. Notice that the red and the blue curves do not exactly reach $-\pi$ because of the relatively short simulation time. More specifically, the particle at initial positions $y_{p0} = 0.05$ and

0.1 rotates by 90 degrees and finds a stable position at $\phi = 0$. The particles at higher initial positions $y_{p0} = 0.2$ and 0.3 experience a larger rotation because of the higher shear rate and rotates by 135 degrees and then stops at a (about) 180-degree orientation. All the rotation are counterclockwise. Notably, as $Bn = 0.1$, the equilibrium orientation changes from flow- to gradient-alignment. Furthermore, the final orientation is reached through damped oscillations around the equilibrium position, similarly to a pendulum. Similar oscillations have been observed for the equilibrium particle position at $Bn = 0.1$ in Fig. 5.6. At $Bn = 0.5$, the particle at higher initial positions, $y_{p0} = 0.2$ and 0.3 , finds an equilibrium orientation angle of zero (flow alignment), while at initial positions $y_{p0} = 0.05$ and 0.1 , the final orientation angle is close to 90° . Finally, at $Bn = 1$, and all the initial particle positions, one equilibrium orientation angle is observed close (but not coincident) to the flow direction. In addition, we examined the particle behavior at other initial orientations of $\phi_0 = 0^\circ$ and 45° . Similar translational and orientational dynamics are observed so the results are not reported.

The angular velocity as a function of time displayed in Fig. 5.9 reflects the just discussed orientational behavior of the particle. The spikes visible at $Bn = 0$ and $Bn = 0.1$ are due to the fast change of the orientation vector from 0 to $-\pi$ for the viscoelastic case, and from 0 to $-3\pi/2$ for the EVP case at $Bn = 0.1$. Notice the (vey small) oscillations around 0 of the angular velocity for the blue and green curves at $Bn = 0.1$, denoting the pendulum-like behavior.

Except these small oscillations, the angular velocity remains negative for all the initial positions at $Bn = 0$ and $Bn = 0.1$. On the contrary, an overshoot is observed for some initial position at $Bn = 0.5$ and $Bn = 1$ where the angular velocity becomes positive (clockwise rotation) indicating that the particle does not consistently rotate following fluid velocity profile. This is induced by the presence of the unyielded region around the particle.

Indeed, an interesting feature of suspensions of particles in EVP fluids is the shape and extent of the yielded and unyielded zones around the particle, i.e., the regions in the fluid domain where $|\tau_d|$ is higher (fluid behavior) or lower (solid behavior) than the yield stress. The shapes of the yielded (red) and unyielded (blue) zones at four time instants are displayed in Fig. 5.10 for two initial particle positions, $y_{p0} = 0.1$ and 0.3 ,

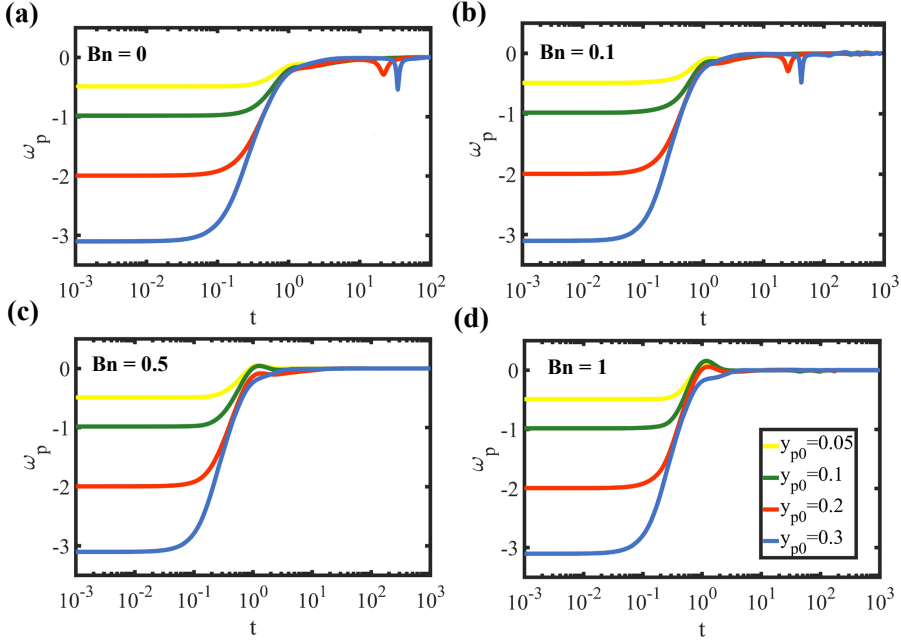


Figure 5.9. Particle angular velocity as a function of time for an elliptical particle ($\beta = 2$) for four initial positions and four different Bingham numbers. The initial orientation angle is $\phi_0 = \pi/2$.

and two values of the Bingham number $Bn = 0.5$ and $Bn = 1$. As before, the Weissenberg number is fixed at $Wi = 1$, and a circular particle ($\beta = 1$) is considered. Similar plots with the same parameters for an ellipse with $\beta = 2$ are presented in Fig. 5.11. In these two figures, the first column panels show the initial particle position and orientation and are included to better understand particle motion at the other time instants.

Fig. 5.10 shows that the particle movement significantly deforms the unyielded zone. Even when the particle is initially far from the unyielded zone ($y_{p0} = 0.3$), its presence disturbs the shape of the unyielded region. When the particle is located within the unyielded zone ($y_{p0} = 0.1$), it starts migrating out of the unyielded region, changing the shape of the unyielded region around it, and eventually finds a stable position in the yielded region. This behavior is similar to what reported in Chaparian et al. [77] and it can be explained considering the the unyielded region acts

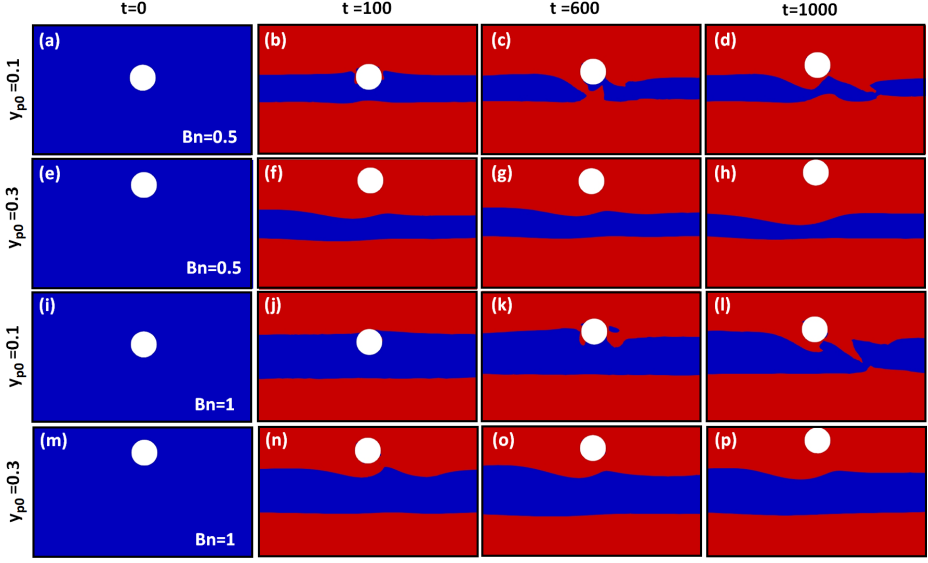


Figure 5.10. Snapshots of the yielded (red) and unyielded (blue) regions in the channel for a circular particle ($\beta = 1$) and $Wi = 1$ at different dimensionless times. Two values of the Bingham number and two initial particle positions are considered.

as a ‘rigid boundary’. For the same reason, a particle released at $y_{p0}0.3$ that in a viscoelastic fluid migrates to the centerline, it migrates to the wall in an EVP liquid.

Figure 5.11 shows the motion of an elliptical particle ($\beta = 2$) in an elastoviscoplastic suspension. For $y_{p0} = 0.1$ and $Bn = 0.5$ (Fig. 5.11a-d), the elliptical particle is located inside the unyielded zone. Due to the particle motion, the stress around the particle is higher than the yield stress; therefore, when the particle approaches the unyielded region, it ‘fluidifies’ the surrounding EVP material, creating an unstable yielded region near the particle, while we still observe the unyielded region farther from the particle when the flow is less perturbed by the presence of the particle. After reaching the x-axis, the particle remains trapped between two unstable unyielded regions on the left and right sides. Since the height of the unyielded regions is smaller than the particle length, the confinement effect from the unyielded region applies only to the body of the particle, while its

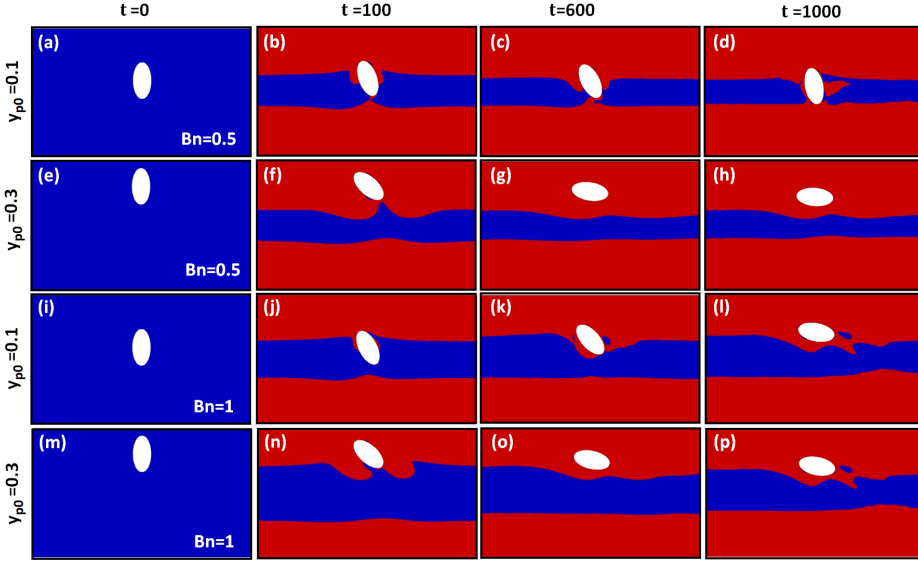


Figure 5.11. Snapshots of the yielded (red) and unyielded (blue) regions in the channel for an elliptical particle ($\beta = 2$) and $Wi = 1$ at different dimensionless times. Two values of the Bingham number and two initial particle positions are considered. The initial orientation angle is $\phi_0 = 90^\circ$.

tips are completely within the yielded area. Hence, in this case, an exact equilibrium position is not observed, and the particle oscillates in a small range between the center of the channel and the unyielded boundary, as previously reported.

The elliptical particle is also located inside the unyielded zone in panels at $y_{p0} = 0.1$ and $Bn = 1$ (Fig. 5.11i-l). Here, however, the particle is pushed out the unyielded region and finally reaches an equilibrium position in the yielded region. At $y_{p0} = 0.3$ for both Bingham numbers, the particle center is initially outside the unyielded zone, but as it starts rotating, the particle tip touches the boundary of the yielded/unyielded zone and deforms the unyielded area around it. The particle then migrates toward the wall and finds an equilibrium position in the yielded region. Here, although the particle is located farther away from the unyielded zone, it still affects the surrounding regions, but the impact is more localized. In general, the elliptical particle induces more complex deformations in the

surrounding unyielded zone compared to a circular particle due to its shape and orientation.

5.4 Conclusion

In this chapter, the dynamics of rigid circular and elliptical particles within an elastoviscoplastic (EVP) fluid in channel flow is studied. The fluid is modeled using the Giesekus constitutive equation, modified as proposed by Saramito, to account for the yield stress. The governing equations under inertialess conditions are solved using the finite element method. An Arbitrary Lagrangian-Eulerian method is employed to manage particle motion. Different initial particle positions, ranging from the center of the channel to the wall, are considered in both the plug region and the sheared regions at various Bingham numbers, with a fixed Weissenberg number. Additionally, three different initial orientation angles for the elliptical particles are considered to study the effect of particle orientation. The purely viscoelastic case is also simulated to understand the effect of plasticity on particle motion.

In the viscoelastic case, the particle migrates towards the centerline, while in the EVP material, the migration behavior of both circular and elliptical particles depends on their initial positions and the flow characteristics, highlighting the influence of yield stress on particle dynamics. Due to the presence of yield stress, an unyielded region at the center of the channel and two yielded regions close to the walls appear. As the Bingham number increases, the area of the unyielded region expands, further affecting the particle dynamics.

The results show that, for both circular and elliptical particles, plasticity affects the equilibrium position and the final orientation of the ellipse. The migration and rotation of the particles also affect the shape of the yielded/unyielded region around them. The main conclusions can summarized as follows: i) plasticity induces a migration to the wall at initial positions such that the particle migrates to the centerline in a viscoelastic fluid, ii) as Bn increases, a circular particle attains an equilibrium position in between the centerline and wall (induced by the presence of the central unyielded region), iii) for an elliptical particle wall migration is suppressed, iv) the final orientation is along the flow for a viscoelastic fluid and orthog-

onal or close to the flow in an EVP liquid, and the former is reached though damped oscillations like a pendulum.

In conclusion, the simulations reveal that elliptical particles induce more intricate deformations in the yielded and unyielded zones compared to circular particles. This behavior can be attributed to their shapes and orientations, which complicate the flow dynamics around them.

Chapter 6

Conclusions

In this thesis, we have investigated the dynamics of particles in elastoviscoplastic fluids, focusing on the effects of confinement and particle shape. Two flow fields have been considered, i.e., sedimentation and channel flow. The study is carried out through finite element direct numerical simulations with the Arbitrary Lagrangian-Eulerian (ALE) formulation to handle the particle motion. The Saramito-Giesekus constitutive equation is used to model the behavior of the elastoviscoplastic fluid.

This concluding chapter provides a summary of the key findings from each of the previous chapters, followed by the computational challenges and limitations we found. Directions for future research are suggested at the end of the chapter.

6.1 Sedimentation of a spherical particle near a wall

The movement of a rigid spherical particle in an elastoviscoplastic fluid near a flat wall is investigated in chapter 3. A force parallel to the wall is applied to the particle and inertialess conditions are assumed. The accuracy of the simulations is tested by comparing with known results for the sedimentation of a sphere in an infinite EVP medium, using the Saramito equation. The simulations are further validated through mesh and time step convergence tests, ensuring that the particle kinematic behavior remains consistent across different resolutions and time steps.

The study focuses on the particle translational and rotational velocities, considering different distances between the particle and the wall, as well as by varying the Weissenberg and Bingham numbers. Additionally, a purely viscoelastic case is simulated to better understand how plasticity influences the particle motion. The results show that as the Weissenberg number decreases and the Bingham number increases, the particle sedimentation slows down. For the purely viscoelastic case, the particle migrates laterally away from the wall. However, as the Bingham number increases, this migration slows down and eventually reverts its direction, with the particle moving towards the wall. This reversal is attributed to changes in the shear rate distribution around the particle caused by the yield stress. Specifically, in the particle-wall gap, the reduced shear rate leads to a slower sedimentation, while a larger shear rate gradient on the other side of the particle generates a net force pushing it toward the wall. Regarding the flow field, two unyielded regions are found: an external region surrounding the fluid zone around the particle, and isolated small regions at one or both sides of the particle.

Overall, our results reveal that the interaction between confinement, elasticity, and plasticity significantly impacts the particle settling dynamics, as well as the shape and extent of the yielded and unyielded regions around the particle. This suggests that the critical value of the Bingham number leading to the blockage of the particle depends on the confinement.

Computational challenges and limitations

The methodology adopted for the present study includes some limitations. One computational challenge we faced in this part of the study was the size of the gap between the particle center and the wall, which made impossible to examine distances extremely close to the wall. Another challenge was the difficulty of numerical calculations at high Weissenberg and Bingham numbers due to the appearance of numerical instabilities, arising from the mathematical nature of the constitutive equations.

6.2 Sedimentation of a spheroidal particle in an unconfined flow

The settling dynamics of a prolate spheroidal particle in an unbounded elastoviscoplastic fluid is analyzed in chapter 4 of this thesis. Similar to the purely viscoelastic case, the spheroid in an EVP fluid rotates until it reaches a stable orientation, where its major axis aligns with the direction of the applied force, leading to the fastest sedimentation. However, as the Bingham number increases, the sedimentation rate decreases. Interestingly, the angular velocity first increases (in magnitude) and then decreases, showing a non-monotonic trend. This behavior is likely due to the yielded region around the particle, which acts like a confinement, initially accelerating the rotation. As the Bingham number rises further, the yielded region moves closer to the particle, ultimately causing it to slow down and approach a stoppage condition.

The initial orientation of the spheroid also plays a significant role in the dynamics, especially when the Bingham number is near its critical value. Particles that begin with their longest axis nearly perpendicular to the force experience high drag, making them unable to translate or rotate effectively. In contrast, particles that start with their major axis more aligned with the force gradually rotate toward the stable orientation. As the aspect ratio of the particle increases, the drag force it experiences also increases, meaning that more elongated particles stop moving at lower Bingham numbers. Additionally, elongated particles rotate more slowly, and the stress build-up ends before the particle significantly changes its orientation. This leads to the emergence of a master curve for the kinematic quantities, based on the particle's current orientation, similar to what is seen in purely viscoelastic fluids. At higher Weissenberg numbers, the drag decreases, allowing the particle to sediment more quickly and shifting the critical Bingham number to higher values.

The shape of the yielded region around the particle depends on both the Bingham number and the particle aspect ratio, and it changes as the particle rotates. For particles that are oriented transversely to the force, the yielded region shrinks near the tips of the spheroid due to the rapid decrease in stress in these areas. As the Bingham number increases, unyielded regions appear along the surface of the particle, resembling the

solid caps seen at the front and back of a sphere. As the particle rotates toward its stable orientation, these unyielded regions vanish because the stresses behind the particle are greater near the tips. These larger stresses cause a negative wake phenomenon, which occurs at lower Weissenberg numbers in an EVP fluid compared to a purely viscoelastic case.

Overall, the study demonstrates the complex interactions between particle shape, orientation, and the properties of the surrounding EVP fluid, providing valuable insights into how these factors influence settling behavior and fluid dynamics.

Computational challenges and limitations

One of the interesting features of yield-stress fluid flows is the critical Bingham value and particle stoppage. A limitation of our approach is determining the exact critical Bingham number at different particle orientations and for varying parameters in elastoviscoplastic fluid. The Saramito-Giesekus model is a complex constitutive equation used to model EVP materials, as it includes several parameters that capture elasticity, plasticity, and shear-thinning behavior. The evaluation of the exact critical Bingham number corresponding to the stoppage condition requires special techniques. The method used in this work is based on a ‘mobility’ approach, i.e., the particle is driven by a body force (the sedimentation force) and the resulting translational and angular velocities are computed by solving the flow field. The detection of the critical condition for particle stoppage requires the solution of the fluid dynamics equations by progressively increasing the Bingham number to approach the yield limit. The main issue is that, as the Bingham number gets closer to the critical one, the time needed to (possibly) get a steady-state solution increases, making the simulations longer. This complexity posed several challenges, making the investigation of a precise particle stoppage condition in our computational framework the most difficult part of the work.

6.3 Particle dynamics of circular/elliptical particles in channel flow

In chapter 5, we analyzed the behavior of rigid circular and elliptical particles in an elastoviscoplastic fluid flowing in a channel. Various initial particle positions were considered in both the plug region and the sheared regions, at different Bingham numbers, while keeping the Weissenberg number constant. To further explore the dynamics, three different initial orientation angles were examined for elliptical particles. Additionally, the purely viscoelastic case was simulated to investigate the role of plasticity on the particle motion.

In the viscoelastic case, particles mainly migrated towards the centerline of the channel. However, in the EVP material, the migration behavior of both circular and elliptical particles varies based on their initial positions and the flow characteristics, emphasizing the impact of yield stress on particle dynamics. Due to the presence of yield stress, an unyielded region formed at the center of the channel, surrounded by two yielded regions closer to the walls. As the Bingham number increases, the size of the unyielded region grows, further influencing the particle dynamics. Specifically, plasticity induces a migration to the wall at initial positions such that the particle migrates to the centerline in a viscoelastic fluid. As the Bingham number increases, a circular particle attains an equilibrium position in between the centerline and wall (induced by the presence of the central unyielded region) whereas for an elliptical particle wall migration is suppressed. The final orientation for an elliptical particle is along the flow for a viscoelastic fluid and orthogonal or close to the flow in an EVP liquid, and the former is reached through damped oscillations like a pendulum.

Hence, the results highlight that the interaction between particle position, elasticity, and plasticity has a profound impact on the migration and rotational behavior of both circular and elliptical particles.

Computational challenges and limitations

In this chapter, we focused only on 2D simulations. The main reason is that 3D computations are significantly slower and more demanding in terms of computational resources. Additionally, we used a mesh refinement

technique to refine the mesh around the particle during the simulations. For 3D cases, this approach would result in even higher computational costs. The main consequence of the 2D assumption is that orientation out of the flow-gradient plane cannot be considered.

6.4 A discussion on the challenges of elastoviscoplastic versus viscoelastic simulations

Since this numerical study has focused on the dynamics of particles in elastoviscoplastic fluids, it is important to highlight the significant computational and theoretical challenges that distinguish simulations of EVP materials from those of viscoelastic fluids. These challenges arise due to the additional complexity introduced by the yield-stress behavior in EVP fluids.

Numerical instabilities

Numerical instabilities are more prominent in EVP simulations, especially at high Weissenberg and Bingham numbers, due to the inherent non-linearity and stiffness of the governing equations. In contrast, viscoelastic simulations, while challenging, do not involve yield surfaces, making their numerical solution relatively more stable.

Detection of yielded/unyielded regions

One of the defining characteristics of EVP materials is the yield stress value, separating yielded and unyielded regions. Accurately capturing these regions requires fine spatial and temporal resolutions as well as advanced numerical techniques. For viscoelastic fluids, the absence of yield stress simplifies the flow field and reduces the need for such high-resolution techniques.

Evaluation of the critical conditions

As discussed in previous chapters, determining the critical Bingham number corresponding to particle stoppage is particularly challenging.

This requires iterative simulations and convergence analyses to pinpoint the yield limit.

Computational Cost

Simulating EVP fluids is computationally expensive, especially for 3D cases. Mesh refinement is necessary to calculate accurately yielded/un-yielded regions and particle-fluid interactions, leading to a significant increase in computational resources. In viscoelastic cases, the computational costs are less than elasto- viscoplastic cases due to the absence of plasticity.

6.5 Future perspectives

The present results can be extended in several directions. First, studying the sedimentation of non-spherical particles, including non-symmetric particle geometries (e.g., triaxial ellipsoids or fractal aggregates), in EVP fluids near a flat wall could provide insights into the rotational dynamics and the effect of the aspect ratio of the particles. The effect of the anisotropic shape is particularly interesting in channel flow where, although limited to 2D systems, the results revealed new dynamics induced by the complex interplay between particle shape and fluid rheology. This has a direct application in microfluidic devices where many biological particles are not spherical. In this regards, extending the simulations to 3D systems is mandatory to fully capture the rotational particle dynamics.

In this thesis we have considered a single particle suspended in the liquid. The effect of the interparticle hydrodynamic interactions is, of course, important and may lead to new dynamics, as already shown for bubbles in EVP materials. Hence, extending the study to systems with an increased number of particles could provide valuable insights into the collective behavior of the EVP suspension, potentially revealing new phenomena that are not evident in simpler configurations.

Finally, an interesting topic when dealing with yield-stress fluids is to identify the criteria for particle stoppage, i.e., the critical Bingham number such that the particle is ‘frozen’ in the fluid. As discussed in chapter 4, the exact evaluation of the critical conditions is not trivial and requires special numerical techniques, so far applied to viscoplastic fluids. More

investigation in this direction is then needed.

Appendix A

Appendix

The rheological properties predicted by the Saramito-Giesekus model, Eq.(2.14), under shear and uniaxial elongational flows are shown in this Appendix. For comparison, the same properties for the original Saramito model are reported as well. In all the cases, we do not consider the viscosity solvent contribution, i.e., $\eta_s = 0$ in Eq.(2.13). FigureA.1 displays the shear and normal stresses for the Saramito model at various values of the yield stress. Specifically, the black curve is for a zero yield stress, recovering the Upper-Convected Maxwell (UCM) equation. Notice that the stresses (including the yield stress) are made dimensionless by the elastic modulus $G = \eta_p/\lambda$ and the abscissa is the Weissenberg number defined as $\lambda\dot{\gamma}$.

The same quantities for the Saramito-Giesekus model with $\alpha = 0.2$ are shown in Fig. A.2. The third panel reports the (negative values of the) second normal stress difference which is not zero in this constitutive equation (as for the original Giesekus model). Apart from the existence of a second normal stress difference, other differences from the Saramito model are the shear-thinning behavior of the viscosity and of the first and second normal stress difference coefficients (beyond a typical shear rate value, the shear stresses increase less than linear and the normal stresses less than quadratic), similarly to what observed by comparing the Giesekus and UCM models.

Finally, in Fig. A.3, the uniaxial extensional viscosity normalized by $3\eta_0$ is shown as a function of the Weissenberg number defined as $\lambda\dot{\epsilon}$ with $\dot{\epsilon}$ the elongational rate. Curves at different Bingham numbers, defined

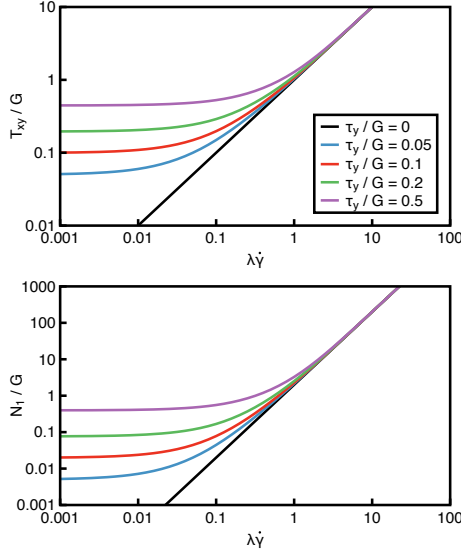


Figure A.1. Shear stress (top) and first normal stress difference (bottom) as a function of the Weissenberg number for the Saramito model in simple shear flow at different values of the yield stress. The stresses are made dimensionless with the elastic modulus $G = \eta_p/\lambda$.

as $Bn = \tau_y/(\eta_0\dot{\epsilon})$, are reported. The left and right panels refer to the Saramito and Saramito-Giesekus model with $\alpha = 0.2$. As it is well-known [22], the Saramito model predicts a divergent extensional viscosity at $Wi = 0.5$ (as for the UCM model), regardless of the value of the Bingham number. The Giesekus variant has a bounded extensional viscosity (as for the Giesekus model) at high Weissenberg numbers with an horizontal asymptote depending on the Bingham number. As a final remark, we point out that the rheological predictions for the Saramito-Giesekus model are qualitatively similar to those of the Phan-Thien-Tanner (PTT) variant of the Saramito model, proposed in the original paper [22], with the only difference being $N_2 = 0$ in the Saramito-PTT (just like the original PTT model).

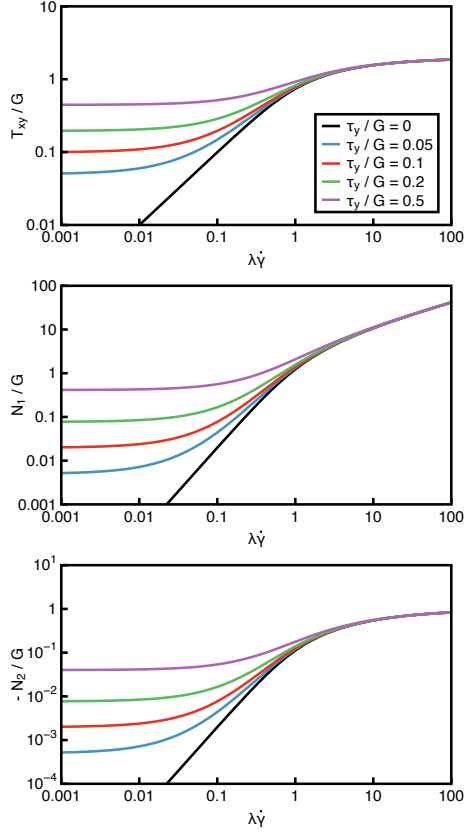


Figure A.2. Shear stress (top), first normal stress difference (middle), and second normal stress difference as a function of the Weissenberg number for the Saramito-Giesekus model in simple shear flow at different values of the yield stress. The mobility parameter is set to $\alpha = 0.2$. The stresses are made dimensionless with the elastic modulus $G = \eta_p/\lambda$.

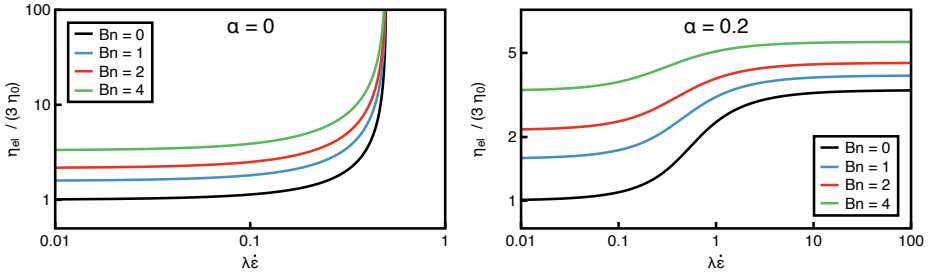


Figure A.3. Extensional viscosity for the Saramito (left) and Saramito-Giesekus (right) models in uniaxial extensional flow as a function of the Weissenberg number for different values of the Bingham number. The mobility parameter for the Saramito-Giesekus model is set to $\alpha = 0.2$. The extensional viscosity is normalized by $3\eta_0$.

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