

Chapter 2

Complex Flows of Micro/Nano Structured Fluids: Reinforced Polymer Composites

Abstract The motion of an ellipsoidal particle immersed in a Newtonian fluid was studied in the pioneering work of Jeffery in 1922. Suspensions of industrial interest usually involve particles with a variety of shapes. Moreover, suspensions composed of rods (a limit case of an ellipsoid) aggregate, leading to clusters with particular shapes that exhibit, when immersed in a flow, an almost rigid motion. In this chapter, we revisit the modeling and simulation of suspensions involving rods throughout the different scales of description (microscopic, mesoscopic and macroscopic) and the different concentration regimes (dilute, semi-dilute, semi-concentrated and concentrated), involving gradually richer physics.

2.1 Introduction

Suspensions involving particles can be described at the microscopic scale by tracking the motion of each one of the particles involved in the system. This approach is based on three main elements: (i) the knowledge of the equation governing the particle motion in the fluid flow; (ii) the introduction of the particle effects on the flow kinematics if coupled simulations are envisaged; and (iii) the availability of computational resources for tracking efficiently millions of particles.

In dilute suspensions, the motion of ellipsoidal particles can be accurately described by using Jeffery's equation [1]. When the concentration becomes large enough, interactions cannot be neglected any longer and the calculation becomes more complex from the computational point of view. At this scale, currently available simulations remain quite far from the scenarios of industrial interest.

For circumventing the difficulties related to simulations at the microscopic scale, these being more computational than conceptual, coarser models were introduced. The interested reader can refer to [2] and the references therein for a review on multi-scale approaches in the context of computational rheology.

Mesoscopic kinetic theory models result from coarsening microscopic descriptions. In kinetic theory models the individuality of the particles is lost in favour of a statistical description that substitutes the entities by a series of conformation coordinates [3, 4]. For example, when considering a suspension of rods, the

mesoscopic description consists in giving the fraction of rods that at position $\mathbf{x}$ and time t are oriented along direction $\mathbf{p}$. This information is contained in the probability distribution function—pdf—whose conservation balance results in the so-called Fokker-Planck equation governing its evolution. Fokker-Planck equations involve the flow induced conformation evolution. In the case of a suspension of rods, the flow induced conformation (orientation) evolution is given, as indicated above, by Jeffery's equation. Since the pdf depends on the physical coordinates (space and time) and a series of conformational coordinates, the associated Fokker-Planck equation is multidimensional. Standard mesh-based discretization techniques fail when addressing multidimensional models. This issue is known as the curse of dimensionality and it explains the few number of existing works addressing the solution of kinetic theory models within the Fokker-Planck framework.

For circumventing the curse of dimensionality at the mesoscopic scale, several techniques based on the use of particles were proposed and widely employed. Here the particles are not real particles, but rather should be viewed as computational particles that allow one to describe the main suspension features (rheology, properties related to the particles conformation, etc.). Despite the fact of considering a discrete description, the level of detail in the description and the richness of the physics is exactly the same that the one associated with the use of Fokker-Planck descriptions, and obviously the solutions computed by using both descriptions are in the limit of convergence exactly the same.

The use of the continuous description based on the solution of the Fokker-Planck equation remains challenging because of the high dimensionality that it involves. On the other hand, when employing its discrete counterpart, the main difficulty is related to the extremely large number of particles to be considered. This number depends on the model output of interest. When only the moments of the distribution are concerned, a moderate number of particles is enough. However, when one is interested in the pdf itself, the number of computational particles could become extremely large.

Solution procedures based on the use of particles at the mesoscopic scale have been extensively employed by many authors [5–13]. On the other hand, there are few works focusing on the solution of Fokker-Planck equations by using standard discretization techniques [7, 14]. We proposed some years ago a new solution technique called Proper Generalized Decomposition based on the use of separated representations in order to ensure that the complexity scales linearly with the model dimensionality [15, 16]. This technique consists in expressing the unknown field as a finite sum of functional products, i.e. expressing a generic multidimensional function $u(x_1, \dots, x_d)$ as:

$$u(x_1, \dots, x_d) \approx \sum_{i=1}^{i=N} F_i^1(x_1) \cdots F_i^d(x_d). \quad (2.1)$$

The interested reader can refer to [17–19] and the references therein for a deep analysis of this technique and its applications in computational rheology.

At the macroscopic scale, the pdf is substituted by some of its moments. Here the level of detail and the involved physics are sacrificed in favour of computational efficiency. The equations governing the time evolution of these moments usually involve closure approximations whose impact on the results is unpredictable [20, 21]. Alternatively, macroscopic equations are carefully postulated, within a top-down approach, in order to guarantee the model objectivity and its thermodynamical admissibility.

In the case of dilute suspensions of short fibers, the three scales have been extensively considered to model the associated systems without major difficulties. However, difficulties appear as soon as the concentration increases. In the semi-dilute and semi-concentrated regimes, fiber-fiber interactions occur, but in general they can be accurately modeled by introducing a sort of randomizing diffusion term [22]. There is a wide literature concerning dilute and semi-dilute suspensions, addressing modeling [23–27], flows [28–32] and rheology [33, 34]. These models describe quite well the experimental observations. When the concentration increases, rod interactions cannot be neglected anymore and appropriate models addressing these intense interactions must be considered, as for example the one proposed in [35]. Recent experiments suggest that short fibers in concentrated suspensions align more slowly as a function of strain than models based on Jeffery’s equation predict [36]. For addressing this issue Wang et al. [36] proposed the use of a strain reduction factor, however this solution violates objectivity. Later, the same authors proposed an objective model by decoupling the time evolution of both the eigenvalues and the eigenvectors of the second-order orientation tensor [37]. In [38] an anisotropic rotary diffusion is proposed for accounting for the fiber-fiber interactions and the model parameters were selected by matching the experimental steady-state orientation in simple shear flow and by requiring stable steady states and physically realizable solutions.

The worst scenario concerns concentrated suspensions involving entangled clusters exhibiting aggregation/disaggregation mechanisms. A first approach in that sense was proposed in [39]. The first natural question is how to describe such systems. At the macroscopic scale, one could try to fit some power-law constitutive equation, however, this description does not hold for the microstructure. At the microscopic scale, direct numerical simulations describing complex fiber-fiber interactions can be carried out in small enough representative volumes [40–42]. A natural candidate to be a reasonable compromise between (fine) micro and (fast) macro descriptions consists in considering again a kinetic theory description.

The main issue with such an approach lies in the fact that it must include two scales, the one involving the aggregates and the one related to the rods composing the aggregates. What are the appropriate conformational coordinates? How to determine the time evolution of these conformational coordinates? How to represent simultaneously both scales, the one related to the aggregates and the other related to the fibers? How to derive the interaction mechanisms?

In [43], the authors propose a first attempt to describe such clusters from a micro-mechanical model. Later in [44], the authors compared the model predictions with direct numerical simulation in the case of rigid and deformable clusters. An enriched

description taking into account the polydispersity of fibers constituting the cluster within a multi-scale framework was addressed in [45] in the case of rigid clusters.

In this chapter, we start by revisiting in Sect. 2.2 the multi-scale description of dilute and semi-dilute suspensions of rigid rods, whose numerical solution is addressed in Sect. 2.3. More concentrated regimes involving rod clustering are considered in Sect. 2.4, and finally in Sect. 2.5 we consider some advanced topics related to work in progress.

Remark 1 In the present chapter we consider the following tensor products, where Einstein's summation convention is assumed:

- if $\mathbf{a}$ and $\mathbf{b}$ are first-order tensors, the single contraction “ $\cdot$ ” reads $(\mathbf{a} \cdot \mathbf{b}) = a_j b_j$;
- if $\mathbf{a}$ and $\mathbf{b}$ are first-order tensors, the dyadic product “ $\otimes$ ” reads $(\mathbf{a} \otimes \mathbf{b})_{jk} = a_j b_k$;
- if $\mathbf{a}$ and $\mathbf{b}$ are first-order tensors, the cross product “ $\times$ ” reads $(\mathbf{a} \times \mathbf{b})_j = \varepsilon_{jmn} a_m b_n$, where ε_{jmn} are the components of the Levi-Civita tensor ε (also known as permutation tensor);
- if $\mathbf{a}$ and $\mathbf{b}$ are respectively second and first-order tensors, the single contraction “ $\cdot$ ” reads $(\mathbf{a} \cdot \mathbf{b})_j = a_{jm} b_m$;
- if $\mathbf{a}$ and $\mathbf{b}$ are second-order tensors, the single contraction “ $\cdot$ ” reads $(\mathbf{a} \cdot \mathbf{b})_{jk} = a_{jm} b_{mk}$;
- if $\mathbf{a}$ and $\mathbf{b}$ are second-order tensors, the double contraction “ $:$ ” reads $(\mathbf{a} : \mathbf{b}) = a_{jk} b_{kj}$;
- if $\mathbf{a}$ and $\mathbf{b}$ are third-order tensors then the triple contraction “ $\cdot$ ” reads $(\mathbf{a} \cdot \mathbf{b}) = a_{jkm} b_{mkj}$;
- if $\mathbf{a}$ and $\mathbf{b}$ are fourth-order tensors then the fourth contraction “ $::$ ” reads $(\mathbf{a} :: \mathbf{b}) = a_{jkmn} b_{nmkj}$.

2.2 Dilute and Semi-dilute Suspensions

2.2.1 Multi-scale Description of Non-brownian Rod Suspensions

We consider a suspending medium consisting of a Newtonian fluid of viscosity η in which there are suspended rigid and non-Brownian rods. We assume as first approximation that their presence and orientation do not affect the flow kinematics that is defined by the velocity field $\mathbf{v}(\mathbf{x}, t)$, with $\mathbf{x} \in \Omega \in \mathbb{R}^d$, $d = 2, 3$. The multi-scale modeling involves nine main conceptual bricks, the first three related to the microscopic description (conformation, kinematics and dynamics), the next three related to the mesoscopic scale (conformation, kinematics and dynamics) and the last three to the macroscopic description (conformation, kinematics and dynamics). We describe all of them in what follows.

2.2.1.1 Particle Conformation

The conformation of each rod $\mathcal{R}$ of length $2L$ can be described from its orientation given by the unit vector $\mathbf{p}$ located at the rod center of gravity $\mathcal{G}$ and aligned along the rod axis. Inertial effects are neglected in the sequel.

2.2.1.2 Particle Conformation Evolution

The orientation evolution of an ellipsoidal particle is described by Jeffery's equation [1]. This equation can be derived in a very simple way illustrated in Fig. 2.1. We consider a system consisting of a rod and two beads located at both rod ends where we assume that hydrodynamic forces apply. We assume that the forces that apply on each bead $\mathbf{F}$ depend on the difference of velocities between the fluid and the bead, the first one given by $\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L$ and the second one by $\mathbf{v}_G + \dot{\mathbf{p}}L$. Thus, the force $\mathbf{F}(\mathbf{p}L)$ reads:

$$\mathbf{F}(\mathbf{p}L) = \xi(\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L - \mathbf{v}_G - \dot{\mathbf{p}}L), \quad (2.2)$$

where ξ is the friction coefficient, $\mathbf{v}_0$ the fluid velocity at the rod center of gravity, and $\mathbf{v}_G$ the velocity of the center of gravity.

If $\mathbf{F}$ applies on the bead at $\mathbf{p}L$, then the force on the opposite bead at $-\mathbf{p}L$ reads

$$\mathbf{F}(-\mathbf{p}L) = \xi(\mathbf{v}_0 - \nabla \mathbf{v} \cdot \mathbf{p}L - \mathbf{v}_G + \dot{\mathbf{p}}L). \quad (2.3)$$

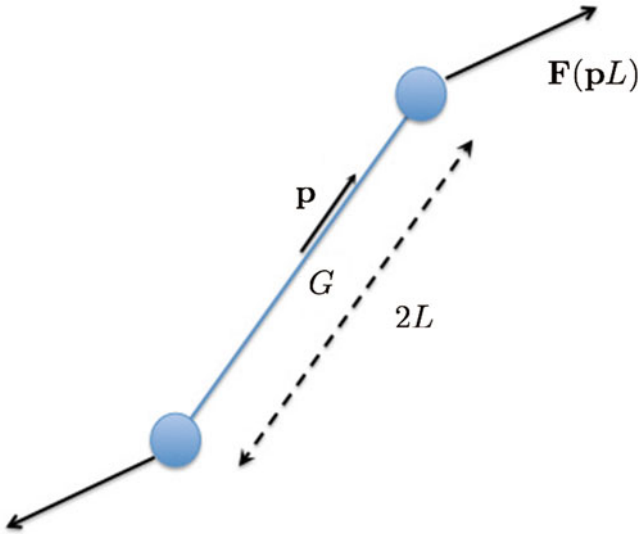


Fig. 2.1 Hydrodynamic forces applied on a rod immersed in a Newtonian fluid

By adding Eqs. (2.2) and (2.3), and neglecting inertial effects, we obtain the force balance

$$\mathbf{F}(\mathbf{p}L) + \mathbf{F}(-\mathbf{p}L) = 2\xi(\mathbf{v}_0 - \mathbf{v}_G) = \mathbf{0}, \quad (2.4)$$

which implies $\mathbf{v}_0 = \mathbf{v}_G$, that is, the rod center of gravity is moving with the fluid velocity. For simplicity of notation, we shall write $\mathbf{F} = \mathbf{F}(\mathbf{p}L)$ and $\mathbf{F}(-\mathbf{p}L) = -\mathbf{F}$.

As the resulting torque must also vanish, the only possibility is that the force $\mathbf{F}$ acts along $\mathbf{p}$, that is $\mathbf{F} = \lambda\mathbf{p}$, with $\lambda \in \mathbb{R}$. Thus, we can write

$$\lambda\mathbf{p} = \xi L(\nabla\mathbf{v} \cdot \mathbf{p} - \dot{\mathbf{p}}). \quad (2.5)$$

Premultiplying Eq. (2.5) by $\mathbf{p}$ and taking into account that $\mathbf{p} \cdot \mathbf{p} = 1$ and consequently $\mathbf{p} \cdot \dot{\mathbf{p}} = 0$, we have

$$\lambda = \xi L(\nabla\mathbf{v} : (\mathbf{p} \otimes \mathbf{p})), \quad (2.6)$$

which gives

$$\xi L(\nabla\mathbf{v} : (\mathbf{p} \otimes \mathbf{p}))\mathbf{p} = \xi L(\nabla\mathbf{v} \cdot \mathbf{p} - \dot{\mathbf{p}}). \quad (2.7)$$

We have thus obtained Jeffery's equation

$$\dot{\mathbf{p}} = \nabla\mathbf{v} \cdot \mathbf{p} - (\nabla\mathbf{v} : (\mathbf{p} \otimes \mathbf{p}))\mathbf{p}. \quad (2.8)$$

Remark 2 As the factor ξL appears in both sides of Eq. (2.7), the rod kinematics does not contain size effects.

2.2.1.3 Particle Contribution to the Stress

The forces applied at the rod ends $\mathbf{p}L$ and $-\mathbf{p}L$ are respectively $\lambda\mathbf{p}$ and $-\lambda\mathbf{p}$, i.e. directed along the rod and in equilibrium by construction.

With λ given by Eq. (2.6), we have

$$\mathbf{F}(\mathbf{p}L) = \xi L(\nabla\mathbf{v} : (\mathbf{p} \otimes \mathbf{p}))\mathbf{p}. \quad (2.9)$$

By applying Kramers' formula, the corresponding contribution to the stress is given by

$$\tau^p = \mathbf{p}L \otimes \mathbf{F} = \xi L^2(\nabla\mathbf{v} : (\mathbf{p} \otimes \mathbf{p}))\mathbf{p} \otimes \mathbf{p}, \quad (2.10)$$

which can be rewritten as

$$\tau^p = \xi L^2 \nabla\mathbf{v} : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p}). \quad (2.11)$$

2.2.1.4 Population Description

There are two natural descriptions of a population of $\mathcal{N}$ rods:

- The first one consists in specifying each rod orientation by considering the unit vector aligned along its axis, that is, by considering $\mathbf{p}_i$, $i = 1, \dots, \mathcal{N}$. As discussed in the next section, the main drawback of this approach lies in the necessity of tracking the evolution of each “computational” rod by solving the corresponding Jeffery equation, and even if conceptually there is no major difficulty, the computing cost could be excessive in most practical applications.
- The second approach is the introduction of the PFD $\psi(\mathbf{x}, t, \mathbf{p})$ that gives the fraction of rods that a position $\mathbf{x}$ and time t are oriented along direction $\mathbf{p}$.

Despite the fact that both mesoscopic models involve the same physics and richness of description, the main advantage of the second one is the manipulation of a scalar continuous function instead of the discrete description involved in the first approach. The price to be paid when using the description based on the use of the pdf is its inherent multidimensionality, because in that framework the pdf depends on the standard space and time coordinates and also on the conformation coordinates that the microstructural description involves, i.e. $\mathbf{p}$ in the present case.

2.2.1.5 Description of the Population Evolution

- When the population is described from the individuals describing it, whose conformation is given by vectors $\mathbf{p}_i$, $i = 1, \dots, \mathcal{N}$, the evolution of each one is given by Jeffery’s equation:

$$\dot{\mathbf{p}}_i = \nabla \mathbf{v} \cdot \mathbf{p}_i + (\nabla \mathbf{v} : (\mathbf{p}_i \otimes \mathbf{p}_i)) \mathbf{p}_i, \quad \forall i = 1, \dots, \mathcal{N}. \quad (2.12)$$

- The alternative description consists in using the pdf $\psi(\mathbf{x}, t, \mathbf{p})$ that satisfies the normalisation condition:

$$\int_{\mathcal{S}} \psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p} = 1, \quad \forall \mathbf{x}, \quad \forall t. \quad (2.13)$$

with $\mathcal{S}$ the surface of the unit sphere, where vector $\mathbf{p}$ is defined.

Conservation of probability yields

$$\frac{\partial \psi}{\partial t} + \nabla_x \cdot (\dot{\mathbf{x}} \psi) + \nabla_p \cdot (\dot{\mathbf{p}} \psi) = 0, \quad (2.14)$$

where, for inertialess rods, $\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t)$, and the rod rotary velocity is given by Jeffery’s equation:

$$\dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}. \quad (2.15)$$

The price to pay is the increase of the model dimensionality, as the orientation distribution is defined in a 6-dimensional domain, i.e. $\psi : (\mathbf{x}, t, \mathbf{p}) \rightarrow \mathbb{R}^+$ where $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, $d = 3$; $t \in \mathcal{T} \subset \mathbb{R}^+$, $\mathbf{p} \in \mathcal{S}$.

2.2.1.6 Contribution of the Particle Population to the Stress

Again, we consider the two alternative descriptions:

- When the population is described in a discrete manner by means of the $\mathbf{p}_i$ vectors, the contribution of rods to the suspension stress is calculated by adding their individual effects, that is:

$$\tau(\mathbf{x}, t) = \sum_{i=1}^{\mathcal{N}(\mathbf{x}, t)} \tau^i = \sum_{i=1}^{\mathcal{N}(\mathbf{x}, t)} \xi L^2 \nabla \mathbf{v} : (\mathbf{p}_i \otimes \mathbf{p}_i \otimes \mathbf{p}_i \otimes \mathbf{p}_i), \quad (2.16)$$

where $\mathcal{N}(\mathbf{x}, t)$ refers to the number of computational rods located at time t in the neighborhood of $\mathbf{x}$.

- When the population is described from the pdf, the sum in Eq. (2.16) is replaced by an integral in the conformation space $\mathcal{S}$:

$$\begin{aligned} \tau(\mathbf{x}, t) &= \int_{\mathcal{S}} \tau^p \psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p} \\ &= 2\eta N_p \int_{\mathcal{S}} \nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p}) \psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p}. \end{aligned} \quad (2.17)$$

Here, the particle number N_p accounts for the particle concentration and the viscosity is used instead of the friction coefficient to be consistent with the usual notation.

In terms of the fourth-order orientation tensor

$$\mathbf{A} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p}, \quad (2.18)$$

we obtain:

$$\tau = 2\eta N_p (\mathbf{A} : \nabla \mathbf{v}), \quad (2.19)$$

which in view of the symmetry of $\mathbf{A}$ can be rewritten as

$$\tau = 2\eta N_p (\mathbf{A} : \mathbf{D}). \quad (2.20)$$

2.2.1.7 Macroscopic Description

As just discussed, discrete descriptions are computationally expensive because of the large number of rods that must be considered in order to derive accurate-enough

model outputs. On the other hand, Fokker-Planck descriptions are rarely considered in view of the curse of dimensionality that introduction of conformation coordinates implies. Thus, standard mesh-based discretization techniques, as finite differences, finite elements or finite volumes, fail when addressing models defined in high-dimensional spaces.

For these reasons, mesoscopic models were coarsened to derive macroscopic models defined in standard physical domains, involving space and time. At the macroscopic scale, the orientation distribution function is substituted by its moments for describing the microstructure [46]. Usually, macroscopic descriptions of rod suspensions are based on the use of the first two non-zero moments, i.e. the second and the fourth-order moments, $\mathbf{a}$ and $\mathbf{A}$, defined by

$$\mathbf{a} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p}, \quad (2.21)$$

and

$$\mathbf{A} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p}, \quad (2.22)$$

respectively.

2.2.1.8 Microstructural Macroscopic Evolution

The microstructural evolution described at the macroscopic scale considers the time evolution of the pdf moments. The time evolution of the second-order orientation tensor is given by:

$$\begin{aligned} \dot{\mathbf{a}} &= \int_{\mathcal{S}} (\dot{\mathbf{p}} \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}}) \psi d\mathbf{p} \\ &= \int_{\mathcal{S}} (\nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}) \otimes \mathbf{p} \psi d\mathbf{p} \\ &\quad + \int_{\mathcal{S}} \mathbf{p} \otimes (\nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}) \psi d\mathbf{p} \\ &= \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 \mathbf{A} : \nabla \mathbf{v}. \end{aligned} \quad (2.23)$$

This equation involves the fourth-order moment $\mathbf{A}$. The time derivative of the fourth-order moment, using the same rationale, involves the sixth-order moment $\mathcal{A}$, and so on.

Thus, an approximate closure relation is needed in order to express the fourth-order moment $\mathbf{A}$ as a function of the lower-order moment $\mathbf{a}$. Different closure relations have been introduced and widely used [47–50]. With the quadratic closure relation (that is only exact when all rods are locally aligned in the same direction), the fourth-order moment is approximated as follows:

$$\mathbf{A} \approx \mathbf{a} \otimes \mathbf{a}. \quad (2.24)$$

This gives

$$\dot{\mathbf{a}} \approx \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 (\nabla \mathbf{v} : \mathbf{a}) \mathbf{a}, \quad (2.25)$$

and invoking again symmetry considerations,

$$\dot{\mathbf{a}} \approx \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 (\mathbf{D} : \mathbf{a}) \mathbf{a}. \quad (2.26)$$

2.2.1.9 Moment-Based Stress

We obtained previously the expression of the rod population contribution to the stress:

$$\tau = 2\eta N_p (\mathbf{A} : \nabla \mathbf{v}), \quad (2.27)$$

which involves the fourth-order moment $\mathbf{A}$. There is no closure issues when $\mathbf{A}$ is calculated from the pdf ψ by using (2.22). When one proceeds at the macroscopic scale, however, wherein the pdf is not available, a closure relation must be considered for either

- writing $\mathbf{A}$ from the knowledge of $\mathbf{a}$, itself being calculated by integrating (2.23) with an appropriate closure relation (e.g. Eq. (2.25) when considering the quadratic closure),

or

- calculating $\mathbf{A}$ by solving the equation that governs its time evolution in which, as just commented, the sixth-order moment appears requiring again an appropriate closure.

The first route is the simplest one and the most used in practice. It leads to

$$\tau = 2\eta N_p (\mathbf{A}^{cr}(\mathbf{a}) : \nabla \mathbf{v}), \quad (2.28)$$

where the superscript “*cr*” refers to the use of an appropriate closure relation.

With the quadratic closure, the stress reads:

$$\tau = 2\eta N_p (\mathbf{a} : \nabla \mathbf{v}) \mathbf{a} \equiv 2\eta N_p (\mathbf{a} : \mathbf{D}) \mathbf{a}. \quad (2.29)$$

2.2.2 Multi-scale Description of Brownian Rods Suspensions

Until now Brownian effects were neglected as well as hydrodynamical interactions between rods. The Brownian effects are due to the fluid’s molecular bombardment acting on the beads. These effects were widely analyzed in [10, 51, 52] when focusing on a microscopic description.

2.2.2.1 Microscopic Description

In this case the rod beads are subjected to the hydrodynamical forces and the ones coming from such bombardment. The first one was introduced previously

$$\mathbf{F}^H = \xi(\nabla \mathbf{v} \cdot \mathbf{p}L - \dot{\mathbf{p}}L), \quad (2.30)$$

where the superscript “ H ” refers to its hydrodynamic nature. Now the Brownian force $\mathbf{F}^B$ is assumed to apply during a short time interval δt following a certain statistical distribution concerning its magnitude and its orientation. The first one is assumed described by a Gaussian distribution of zero mean and a certain standard deviation and the one related to the orientation by a uniform distribution on the unit circle (2D) or on the unit sphere (3D).

Brownian forces applying in the rod direction are assumed equilibrated. However, the components of those forces perpendicular to the rod axis contribute to the rod rotation, and then they affect the rod rotary velocity. In what follows, for the sake of clarity, we restrict our analysis to the 2D case. Because the rod inertia is neglected, the resultant torque vanishes, implying:

$$\mathbf{F}^H \cdot \mathbf{t} + \mathbf{F}^B \cdot \mathbf{t} = 0, \quad (2.31)$$

where $\mathbf{t}$ is the unit vector tangent to the unit circle. By introducing in this balance the expression of the hydrodynamic force, we obtain

$$\mathbf{t}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p} - \|\dot{\mathbf{p}}\| = -\frac{\mathbf{F}^B \cdot \mathbf{t}}{\xi L}, \quad (2.32)$$

where the fact that $\dot{\mathbf{p}} = \|\dot{\mathbf{p}}\|\mathbf{t}$ was taken into account. The previous equation can be rewritten in the form:

$$\dot{\mathbf{p}} = (\mathbf{t}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{t} + \frac{\mathbf{F}^B \cdot \mathbf{t}}{\xi L} \mathbf{t}, \quad (2.33)$$

that, using the vectorial equivalence

$$(\mathbf{t}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{t} = \nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p}, \quad (2.34)$$

results in

$$\begin{aligned} \dot{\mathbf{p}} &= \nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p} + \frac{\mathbf{F}^B \cdot \mathbf{t}}{\xi L} \mathbf{t} \\ &= \nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p} + \frac{\mathbf{F}^B - (\mathbf{F}^B \cdot \mathbf{p}) \mathbf{p}}{\xi L}, \end{aligned} \quad (2.35)$$

where we can notice that the rotary velocity is given by the Jeffery expression $\dot{\mathbf{p}}^J$ complemented with a term describing the Brownian effects $\dot{\mathbf{p}}^B$:

$$\dot{\mathbf{p}}^J = \nabla \mathbf{v} \cdot \mathbf{p} - \left(\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p} \right) \mathbf{p}, \quad (2.36)$$

and

$$\dot{\mathbf{p}}^B = \frac{\mathbf{F}^B - (\mathbf{F}^B \cdot \mathbf{p})\mathbf{p}}{\xi L}, \quad (2.37)$$

from which

$$\dot{\mathbf{p}} = \dot{\mathbf{p}}^J + \dot{\mathbf{p}}^B. \quad (2.38)$$

Finally, we should discuss the effects of such Brownian contribution to the extra-stress tensor.

Consider a rod aligned along the x -axis, such that $\mathbf{p}^T = (1, 0)$ and the fluid at rest. This rod is subjected to a continuous bombardment from the solvent molecules (remember that the regime is dilute enough for neglecting the rod-rod interactions). The components of forces aligned with the rod axis do not participate to the rod rotation and by averaging on a time $\Delta t \gg \delta t$ the contributions of the components of those forces along the rod direction vanish. On the contrary, the ones perpendicular to the rod will participate to the stress. To derive the expression of this Brownian contribution we consider that due to a Brownian force the rod rotates a small angle $\delta\theta > 0$, with the rod orientation being defined by $\mathbf{p}_{\delta\theta}$. Considering the Brownian force applying at that position [51, 52], i.e. $\|\mathbf{F}^B\| \cdot \mathbf{t}_{\delta\theta}$, we obtain the contribution to the virial stress given by:

$$-\mathbf{p}_{\delta\theta} \otimes \|\mathbf{F}^B\| \mathbf{t}_{\delta\theta} = \|\mathbf{F}^B\| \begin{pmatrix} \sin(\delta\theta) \cdot \cos(\delta\theta) & -\cos^2(\delta\theta) \\ \sin^2(\delta\theta) & -\sin(\delta\theta) \cdot \cos(\delta\theta) \end{pmatrix}, \quad (2.39)$$

where the negative sign accounts for the fact that the hydrodynamic force considered in the virial stress applies in the opposite direction of the Brownian force.

We can notice in that expression two facts: (i) the trace is zero, and (ii) the contribution is non-symmetric. However, we can imagine that in other rod, the same Brownian force applies in the opposite direction, leading to an angle $-\delta\theta$, from which

$$\mathbf{p}_{-\delta\theta} \otimes \|\mathbf{F}^B\| \mathbf{t}_{-\delta\theta} = \|\mathbf{F}^B\| \begin{pmatrix} \sin(\delta\theta) \cdot \cos(\delta\theta) & \cos^2(\delta\theta) \\ -\sin^2(\delta\theta) & -\sin(\delta\theta) \cdot \cos(\delta\theta) \end{pmatrix}, \quad (2.40)$$

and then, after averaging, we obtain a Brownian contribution to the extra-stress due to rods aligned on the x -direction (i.e. $\varphi = 0$)

$$\tau_{\varphi=0}^B \approx \begin{pmatrix} \beta & 0 \\ 0 & -\beta \end{pmatrix} = \beta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \beta \mathbf{U}, \quad (2.41)$$

that becomes almost symmetric and traceless. Here we considered a population average, that, invoking ergodicity, is equivalent to averaging in Δt .

Now, for rods aligned in any other direction φ , it suffices to apply a rotation of angle φ to tensor $\tau_{\varphi=0}^B$:

$$\tau_{\varphi}^B = \beta \mathbf{R}_{\varphi}^T \cdot \mathbf{U} \cdot \mathbf{R}_{\varphi}, \quad (2.42)$$

with

$$R_{\varphi} = \begin{pmatrix} \cos(\varphi) & \sin(\varphi) \\ -\sin(\varphi) & \cos(\varphi) \end{pmatrix}, \quad (2.43)$$

that leads to:

$$\tau_{\varphi}^B = 2\beta \left(\begin{pmatrix} \cos^2(\varphi) & \sin(\varphi) \cdot \cos(\varphi) \\ \sin(\varphi) \cdot \cos(\varphi) & \sin^2(\varphi) \end{pmatrix} - \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \right). \quad (2.44)$$

This can be written as

$$\tau_{\mathbf{p}}^B = 2\beta \left(\mathbf{p} \otimes \mathbf{p} - \frac{\mathbf{I}}{2} \right), \quad (2.45)$$

where $\mathbf{I}$ is the identity tensor.

For a population of rods $\mathbf{p}_i$, $i = 1, \dots, \mathcal{N}$, the contribution of Brownian effects is finally:

$$\tau^B = 2\beta \sum_{i=1}^{\mathcal{N}} \left(\mathbf{p}_i \otimes \mathbf{p}_i - \frac{\mathbf{I}}{2} \right). \quad (2.46)$$

2.2.2.2 Mesoscopic Description

At the mesoscopic scale, we postulate that Brownian effects try to randomize the rod orientation distribution, i.e. a mechanism that can be modeled by assuming a diffusion term in the Fokker-Planck equation:

$$\frac{\partial \psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \psi) + \nabla_p \cdot (\dot{\mathbf{p}} \psi) = \nabla_p \cdot (D_r \nabla_p \psi), \quad (2.47)$$

with the flow-induced orientation term given by Jeffery's equation:

$$\dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - \left(\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p} \right) \mathbf{p}, \quad (2.48)$$

where D_r is the rotary diffusion. We can notice that in absence of flow, i.e. $\mathbf{v}(\mathbf{x}, t) = \mathbf{0}$ the Fokker-Planck equation reduces to

$$\frac{\partial \psi}{\partial t} = \nabla_p \cdot (D_r \nabla_p \psi), \quad (2.49)$$

which ensures a steady-state isotropic orientation distribution: $\psi(\mathbf{x}, t \rightarrow \infty, \mathbf{p}) = \frac{1}{2\pi}$ in 2D and $\psi(\mathbf{x}, t \rightarrow \infty, \mathbf{p}) = \frac{1}{4\pi}$ in 3D. The higher is the rotational diffusion the faster the isotropic orientation distribution is reached.

Thus, at the mesoscopic level, introduction of Brownian effects seems quite simple. The question is what are the microscopic and macroscopic counterparts of this diffusion term?

The Fokker-Planck equation can be rewritten in the form:

$$\begin{aligned} \frac{\partial \psi}{\partial t} + \nabla_x \cdot (\mathbf{v}\psi) + \nabla_p \cdot (\dot{\mathbf{p}}\psi) - \nabla_p \cdot (D_r \nabla_p \psi) \\ = \frac{\partial \psi}{\partial t} + \nabla_x \cdot (\mathbf{v}\psi) + \nabla_p \cdot (\dot{\mathbf{p}}\psi) = 0, \end{aligned} \quad (2.50)$$

where the effective rotary velocity $\dot{\mathbf{p}}$ is given by

$$\dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - \left(\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p} \right) \mathbf{p} - D_r \frac{\nabla_p \psi}{\psi}, \quad (2.51)$$

which contains the flow-induced Jeffery contribution $\dot{\mathbf{p}}^J$ plus the Brownian one $\dot{\mathbf{p}}^B$, i.e. $\dot{\mathbf{p}} = \dot{\mathbf{p}}^J + \dot{\mathbf{p}}^B$, with

$$\dot{\mathbf{p}}^B = -D_r \frac{\nabla_p \psi}{\psi}. \quad (2.52)$$

The Fokker-Planck multidimensionality issue was usually circumvented by using stochastic strategies for solving the Ito equation related to its Fokker-Planck counterpart. It is important to mention that any Fokker-Planck equation has an Ito counterpart, however the reciprocal is not true [53].

At the mesoscopic scale, the Brownian contribution to the extra-stress tensor results from the generalization of Eq. (2.46):

$$\tau^B = 2\gamma D_r \int_{\mathcal{S}} \left(\mathbf{p} \otimes \mathbf{p} - \frac{\mathbf{I}}{2} \right) \psi(\mathbf{p}) d\mathbf{p} = 2\gamma D_r \left(\mathbf{a} - \frac{\mathbf{I}}{2} \right). \quad (2.53)$$

2.2.2.3 Macroscopic Description

When moving towards the macroscopic scale, the Brownian contribution to the extra-stress is defined by Eq. (2.53). However, at the macroscopic scale the microstructure is defined by the different moments of the orientation distribution. In what follows, we derive the contribution of Brownian effects to the equation governing the evolution of the second-order moment.

We start from the definition of the second-order moment

$$\mathbf{a} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \psi d\mathbf{p}, \quad (2.54)$$

whose time derivative involves now the effective rotational velocity $\dot{\mathbf{p}}$

$$\dot{\mathbf{a}} = \int_{\mathcal{S}} \left(\dot{\mathbf{p}} \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}} \right) \psi \, d\mathbf{p}, \quad (2.55)$$

or

$$\begin{aligned} \dot{\mathbf{a}} &= \int_{\mathcal{S}} \left((\dot{\mathbf{p}}^J + \dot{\mathbf{p}}^B) \otimes \mathbf{p} + \mathbf{p} \otimes (\dot{\mathbf{p}}^J + \dot{\mathbf{p}}^B) \right) \psi \, d\mathbf{p} \\ &= \int_{\mathcal{S}} \left(\dot{\mathbf{p}}^J \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}}^J \right) \psi \, d\mathbf{p} \\ &\quad + \int_{\mathcal{S}} \left(\dot{\mathbf{p}}^B \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}}^B \right) \psi \, d\mathbf{p} = \dot{\mathbf{a}}^J + \dot{\mathbf{a}}^B, \end{aligned} \quad (2.56)$$

where, as proved before, the flow-induced microstructure evolution $\dot{\mathbf{a}}^J$ is given by

$$\dot{\mathbf{a}}^J = \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2\mathbf{A} : \mathbf{D}. \quad (2.57)$$

We now calculate the expression of the remaining contribution $\dot{\mathbf{a}}^B$:

$$\dot{\mathbf{a}}^B = \int_{\mathcal{S}} \left(\dot{\mathbf{p}}^B \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}}^B \right) \psi \, d\mathbf{p}, \quad (2.58)$$

with $\dot{\mathbf{p}}^B$ given by

$$\dot{\mathbf{p}}^B = -D_r \frac{\nabla_p \psi}{\psi}. \quad (2.59)$$

For the sake of clarity, we consider again the 2D case for which

$$\dot{\mathbf{p}}^B = -D_r \frac{\frac{\partial \psi}{\partial \theta}}{\psi} \mathbf{t}, \quad (2.60)$$

where $\mathbf{t}$ is the unit tangent vector to the unit circle. In this case, Eq. (2.58) reduces to

$$\dot{\mathbf{a}}^B = -D_r \int_{\mathcal{S}} (\mathbf{t} \otimes \mathbf{p} + \mathbf{p} \otimes \mathbf{t}) \frac{\partial \psi}{\partial \theta} \, d\theta. \quad (2.61)$$

Now, integrating Eq. (2.61) by parts and taking into account

$$\frac{d\mathbf{p}}{d\theta} = \mathbf{t}, \quad (2.62)$$

and

$$\frac{d\mathbf{t}}{d\theta} = -\mathbf{p}, \quad (2.63)$$

we obtain:

$$\dot{\mathbf{a}}^B = -2D_r \int_{\mathcal{S}} (\mathbf{p} \otimes \mathbf{p} - \mathbf{t} \otimes \mathbf{t}) \psi(\theta) d\theta. \quad (2.64)$$

It is easy to prove that

$$\mathbf{t} \otimes \mathbf{t} + \mathbf{p} \otimes \mathbf{p} = \mathbf{I} \rightarrow \mathbf{t} \otimes \mathbf{t} = \mathbf{I} - \mathbf{p} \otimes \mathbf{p}, \quad (2.65)$$

that allows us to write Eq. (2.64) in the form

$$\dot{\mathbf{a}}^B = -2D_r \int_{\mathcal{S}} (2\mathbf{p} \otimes \mathbf{p} - \mathbf{I}) \psi(\theta) d\theta = -2D_r (2\mathbf{a} - \mathbf{I}), \quad (2.66)$$

or

$$\dot{\mathbf{a}}^B = -4D_r \left(\mathbf{a} - \frac{\mathbf{I}}{2} \right). \quad (2.67)$$

We can notice that, in absence of flow, $\dot{\mathbf{a}}^J = \mathbf{0}$, and then $\dot{\mathbf{a}} = \dot{\mathbf{a}}^B$,

$$\dot{\mathbf{a}} = -4D_r \left(\mathbf{a} - \frac{\mathbf{I}}{2} \right), \quad (2.68)$$

thus ensuring an isotropic steady state, i.e. $\mathbf{a}(t \rightarrow \infty) = \frac{\mathbf{I}}{2}$ in the 2D case.

Thus, the macroscopic orientation equation reads:

$$\dot{\mathbf{a}} = \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 \cdot \mathbf{A} : \mathbf{D} - 2dD_r \left(\mathbf{a} - \frac{\mathbf{I}}{d} \right), \quad (2.69)$$

where d is the space dimension: $d = 2, 3$.

2.2.3 Semi-concentrated Regime

Semi-dilute and semi-concentrated regimes have been widely addressed, most of time by using phenomenological approaches. The most common approach consists in considering that rod-rod interactions tend to randomize the orientation distribution. Thus, a second diffusion coefficient is introduced for accounting for rod interactions. However, in the present case, that diffusion coefficient should scale with the flow intensity in order to ensure that in absence of flow the microstructure does not evolve artificially because of such a diffusion term. In general, the interaction diffusion coefficient D_I is assumed of the general form

$$D_I = C_I \cdot f(D^{eq}), \quad (2.70)$$

where D^{eq} is related to the second invariant of the rate of strain tensor, i.e. $D^{eq} = \sqrt{2\mathbf{D} : \mathbf{D}}$. The simplest choice consists in considering the dependence $f(D^{eq}) = D^{eq}$ [22].

Obviously, there are finer approaches based on the direct simulation where the rod-rod interactions are taken into account explicitly [40, 54]. A nice mesoscopic based macroscopic approach was proposed in [35] in which interactions are explicitly described from the introduction of some interaction tensors that can be obtained from the orientation moments [55].

2.3 Processing Flow Simulation

The flow model for short fibers suspensions is defined by the following equations:

- The balance of linear momentum, without inertia and mass terms,

$$\nabla \cdot \sigma = \mathbf{0}, \quad (2.71)$$

where σ is the stress tensor.

- The incompressibility condition,

$$\nabla \cdot \mathbf{v} = 0, \quad (2.72)$$

where $\mathbf{v}$ is the velocity field.

- The constitutive equation, with a quadratic closure relation for the fourth-order orientation tensor,

$$\sigma = -p\mathbf{I} + 2\eta\mathbf{D} + 2\eta N_p (\mathbf{a} : \mathbf{D}) \mathbf{a}. \quad (2.73)$$

The flow model is defined in the volume $\Omega_f(t)$ occupied by the fluid at time t . On its boundary, $\Gamma_f(t) \equiv \partial\Omega_f(t)$, either the velocity or the traction is imposed:

$$\mathbf{v}(\mathbf{x} \in \Gamma_1) = \mathbf{v}_g, \quad (2.74)$$

and

$$\sigma \cdot \mathbf{n}(\mathbf{x} \in \Gamma_2) = \mathbf{F}_g, \quad (2.75)$$

with $\Gamma_1 \cup \Gamma_2 = \Gamma_f(t)$, $\Gamma_1 \cap \Gamma_2 = \emptyset$, and where $\mathbf{n}(\mathbf{x})$ is the outward unit normal to the domain boundary.

The inflow boundary will be denoted by Γ^- :

$$\Gamma^- = \{\mathbf{x} \in \Gamma_1, \mathbf{v}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) < 0\}. \quad (2.76)$$

At the flow front Γ_{ff} , $\Gamma_{ff} \subset \Gamma_2$, a null traction is usually prescribed, i.e. $\mathbf{F}_g(\mathbf{x} \in \Gamma_{ff}) = \mathbf{0}$.

For calculating the orientation tensor involved in the constitutive equation, three routes are possible:

- Considering a population of computational particles $\mathbf{p}_i$ whose position $\mathbf{x}_i(t)$ results from the integration of

$$\frac{d\mathbf{x}_i(t)}{dt} = \mathbf{v}(\mathbf{x}_i, t), \quad (2.77)$$

and whose orientation $\mathbf{p}_i(t)$ is obtained from the integration of the Jeffery equation or its Brownian counterpart.

- Solving the Fokker-Planck equation and then evaluating the integral defining the orientation tensor $\mathbf{a}$.
- Integrating the equation governing the evolution $\dot{\mathbf{a}}$ of the second-order orientation tensor $\mathbf{a}$. Taking into account its hyperbolic character, this can be performed accurately by using the method of characteristics or a stabilized Eulerian integration.

2.3.1 Fixed Mesh Description of the Fluid Domain Evolution and Flow Front Tracking by Using a Volume of Fluid—VoF—Technique

As just indicated, the flow model is defined in the part $\Omega_f(t)$ of the whole domain Ω (of boundary Γ) occupied by the fluid at each time t . In order to update the fluid domain, we introduce the fluid presence function, $I(\mathbf{x}, t)$. This function takes a unit value in the fluid region and vanishes in the empty domain:

$$I(\mathbf{x}, t) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega_f(t) \\ 0 & \text{if } \mathbf{x} \in \Omega_e(t) \end{cases}, \quad (2.78)$$

with the empty domain $\Omega_e(t) = \Omega - \Omega_f(t)$.

The evolution of this function is given by the following scalar and linear advection equation

$$\frac{\partial I}{\partial t} + \mathbf{v} \cdot \nabla I = 0, \quad (2.79)$$

which is defined in the whole domain. The fluid presence function must verify a boundary condition on Γ^- (inflow boundary), which for simulating filling processes reads:

$$I(\mathbf{x} \in \Gamma^-, t) = 1, \quad (2.80)$$

as well as an initial condition. If we assume the domain empty at the initial time $t = 0$, the initial condition is

$$I(\mathbf{x}, t = 0) = 0. \quad (2.81)$$

The discretization of the equations of motion can be carried out by means of a standard mixed finite element technique, using for example an enriched P_1 ($P_1 + \text{"bubble"}$) $\mathcal{C}^0$ approximation of the velocity field and a linear $P_1 - \mathcal{C}^0$ approximation of the pressure field. This functional approximation verifies the inf-sup condition, also known as the LBB (Ladyzhenskaya-Babuska-Brezzi) condition. In order to extend the variational formulation of the flow equations defined in $\Omega_f(t)$ to the whole domain Ω , we enforce a pseudo-behavior in the empty volume, defined by $\mathbf{v} = \mathbf{0}$ and $p = 0$ [56]. Combining both the flow and the pseudo-behavior variational formulations, we obtain:

Find $\mathbf{v} \in (H^1(\Omega))^3$ and $p \in L^2(\Omega)$ verifying the essential boundary conditions $\mathbf{v}(\mathbf{x} \in \Gamma^-) = \mathbf{v}_g$ and $\mathbf{v}(\mathbf{x} \in \Gamma - \Gamma^-) = \mathbf{0}$, such that

$$\int_{\Omega} f(I) \sigma : \mathbf{D}^* d\Omega + \int_{\Omega} \alpha_v (1 - f(I)) \mathbf{v} \cdot \mathbf{v}^* d\Omega = 0, \quad (2.82)$$

$$\int_{\Omega} f(I) \nabla \cdot \mathbf{v} p^* d\Omega + \int_{\Omega} \alpha_p (1 - f(I)) p p^* d\Omega = 0, \quad (2.83)$$

$\forall \mathbf{v}^* \in (H_0^1(\Omega))^3$ and $\forall p^* \in L^2(\Omega)$, with $f(I = 1) = 1$ and $f(I = 0) = 0$ and where the expression of the stress tensor is given by the constitutive equation (2.73).

In this variational formulation, $H^1(\Omega)$ and $L^2(\Omega)$ denote the usual Sobolev and Lebesgue functional spaces and $H_0^1(\Omega)$ is the functional space of velocities vanishing on the domain boundary Γ . The choice of the functions $f(I)$, α_v and α_p is a key point for obtaining a numerical scheme without numerical dissipation and with a low diffusion of the flow front (required to locate accurately moving boundaries). The necessity of introducing functions α_v and α_p follows from the dimensional consistency requirements of Eqs. (2.82) and (2.83).

In [56] a linear combination of both variational formulations is considered, i.e. the fluid fraction was taken as weight function, i.e. $f(I) = I$, and both parameters α_v and α_p were considered constant.

To justify the required values of both parameters, we considered in [29] an element Ω^e which just starts its filling process. In this case the fluid fraction in this element I^e takes an intermediate value $0 < I^e < 1$. If parameters α_v and α_p are too high, the over-imposition of the zero velocity condition in the empty region or in the elements which start their filling process, tends to perturb the natural flow front movement. On the other hand, if those parameters are too small, the equation of motion as well as the fluid incompressibility will be over-imposed in the element Ω^e in spite of the little amount of fluid existing in this element which just starts its filling process. Thus, this pseudo-incompressibility, derived from the small values of both parameters, retards the filling process. In the same way, the resulting flow front thickness increases, and the localization of the flow front remains uncertain. In order to improve the flow front location (reducing its numerical thickness, i.e. the number of elements in the flow direction with a fluid fraction $0 < I < 1$), it was proposed in [56] to use small values of both parameters combined with a local mesh adaptation in the flow front neighbourhood.

Another choice able to reduce the flow front thickness was proposed in [29]:

$$f(I^e) = \begin{cases} 1 & \text{if } I^e \geq I_{\text{th}} \\ 0 & \text{if } I^e < I_{\text{th}} \end{cases}, \quad (2.84)$$

where I_{th} represents a threshold value, close to one. The first advantage of this choice is that no combinations of the fluid flow and the pseudo-behavior variational formulations are employed in the partially filled elements. Thus, only in the case that $I^e \geq I_{\text{th}}$ the flow model will be enforced in the element Ω^e . However, as proved below, a judicious choice of parameters α_v and α_p will be essential to enforce the mass conservation reducing the flow front thickness to one element.

To illustrate the parameters choice, we consider a one-dimensional domain. We denote by Ω^e a generic element where a linear approximation of the velocity field is considered. Thus, the velocity at each point of Ω^e can be expressed from their nodal values v^e and v^{e+1} , where the coordinates of both nodes are x^e and x^{e+1} ($x^{e+1} > x^e$) respectively. We assume the inlet located at $x = 0$, where the injection velocity is enforced to a value v_i . Now, let $I^e < I_{\text{th}}$ be the fluid fraction existing in the element Ω^e at time t . We will assume that the element located upstream of Ω^e , Ω^{e-1} , is fully filled, i.e. $I^{e-1} = 1$ and that the downstream element remains empty, i.e. $I^{e+1} = 0$.

At time t , with $I^{e-1} = 1$, the flow equations are imposed in the element Ω^{e-1} . Thus, the velocity at node x^e tends to be the injection velocity as a direct consequence of the fluid incompressibility and the one-dimensional flow regime. On the other hand, the node x^e also belongs to the element Ω^e where due to the fact that $I^e < I_{\text{th}}$ a null velocity is enforced, implying the annulation of both nodal velocities. An evident conflict appears because each element containing the node x^e enforces a different value of the velocity at this node. Due to the continuity assumed in the velocity interpolation the resulting velocity at this node will be an intermediate value between the injection velocity (required by the flow equations) and a null velocity (enforced by the pseudo-behavior). Therefore, the extended variational formulation to the whole domain, as has been presented until now, affects the natural flow front progression. To avoid these undesired effects one possibility consists in an adequate choice of parameters α_v and α_p . If we consider

$$\alpha_p(I^e) = \alpha_v(I^e) = \alpha(I^e) = \begin{cases} 1 & \text{if } I^e = 0 \\ \varepsilon & \text{if } I^e > 0 \end{cases}, \quad (2.85)$$

where ε is a constant small enough, the nodal velocity at node x^e is dominated by the flow equations enforced in the element Ω^{e-1} (the contribution of the pseudo-behaviour imposed in the element Ω^e , and consequently affected by the constant ε is negligible). Thus the velocity at node x^e approaches the exact value (the injection velocity v_i). The velocity at node x^{e+1} will be null due to the imposition of the pseudo-behavior (null velocity) in all the elements containing this node. Thus, the filling process of the element Ω^e will be accurately achieved and the flow front area is reduced to a single element improving significantly the flow front location.

Finally, we describe a first-order discontinuous finite element technique (higher-order discretization also exist) for solving the advection problems governing the evolution of fields $I(\mathbf{x}, t)$ and $\mathbf{a}(\mathbf{x}, t)$.

In order to alleviate the notation we consider the linear and scalar advection equation Eq. (2.79) governing the evolution of $I(\mathbf{x}, t)$.

Taking into account the fluid incompressibility, $\nabla \cdot \mathbf{v} = 0$, Eq. (2.79) can be rewritten in the form

$$\frac{\partial I}{\partial t} + \nabla \cdot (\mathbf{v} I) = 0, \quad (2.86)$$

whose integral conservation form in element Ω^e reads

$$\int_{\Omega^e} \frac{\partial I}{\partial t} d\Omega + \int_{\Omega^e} \nabla \cdot (\mathbf{v} I) d\Omega = 0. \quad (2.87)$$

Using the divergence theorem, the previous equation becomes

$$\int_{\Omega^e} \frac{\partial I}{\partial t} d\Omega + \int_{\partial\Omega^e} \mathbf{v} \cdot \mathbf{n} I dS = 0, \quad (2.88)$$

where $\partial\Omega^e$ denotes the boundary of Ω^e , and $\mathbf{n}$ is the outward unit normal to the element boundary. The element boundary can be divided in two parts: $\partial^+\Omega^e$ through which the flow leaves the element (i.e. the part of the boundary verifying the relation $\mathbf{v} \cdot \mathbf{n} > 0$); and the inflow boundary $\partial^-\Omega^e$, through which the fluid is coming to element Ω^e (verifying $\mathbf{v} \cdot \mathbf{n} < 0$). Thus, the mass balance yields

$$\int_{\Omega^e} \frac{\partial I}{\partial t} d\Omega + \int_{\partial^-\Omega^e} \mathbf{v} \cdot \mathbf{n} I dS + \int_{\partial^+\Omega^e} \mathbf{v} \cdot \mathbf{n} I dS = 0. \quad (2.89)$$

We now consider the simplest approximation choice, consisting of a constant value of function $I(\mathbf{x}, t)$ into each element. In this case function $I(\mathbf{x}, t)$ is not defined on the element boundary, and the flow coming to element Ω^e is approximated taking into account its value in the upstream neighbouring elements $\Omega^{e_i^-}$, $I^{e_i^-}$. In the same way, the outflow rate will depend on the fluid fraction existing in the element Ω^e , I^e . Thus, the previous equation can be written as

$$\frac{\partial I^e}{\partial t} |\Omega^e| = \sum_i q^{e_i^-} I^{e_i^-} - q^{e^+} I^e, \quad (2.90)$$

where $|\Omega^e|$ is the volume of Ω^e , q^{e^+} represents the flow rate leaving the element Ω^e , and $q^{e_i^-}$ denotes the flow coming to element Ω^e from the upstream neighbouring element $\Omega^{e_i^-}$.

Considering the time derivative, the Taylor's expansion of $I^e(t + \Delta t)$ reads

$$I^e(t + \Delta t) = I^e(t) + \left. \frac{\partial I^e}{\partial t} \right|_t \Delta t + \frac{1}{2} \left. \frac{\partial^2 I^e}{\partial t^2} \right|_t (\Delta t)^2 + \dots \quad (2.91)$$

With a first-order explicit scheme, the update reads:

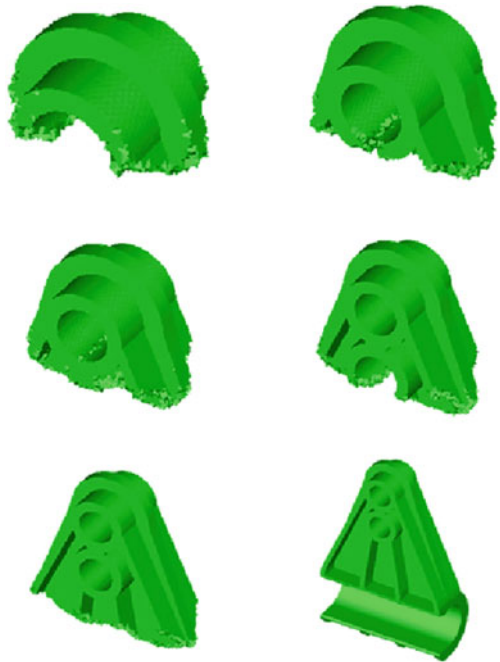
$$\begin{aligned} I^e(t + \Delta t) &= I^e(t) + \left. \frac{\partial I^e}{\partial t} \right|_t \Delta t \\ &= I^e(t) + \frac{\sum_i q_i^{e^-} I_i^{e^-} - q_i^{e^+} I_i^e}{|\Omega^e|} \Delta t. \end{aligned} \quad (2.92)$$

Figure 2.2 depicts different stages of the filling process of a complex 3D cavity. It represents the field $I(\mathbf{x}, t)$ at 6 different filling times. In addition to the evolution of the fluid domain $\Omega_f(t)$, the velocity field and the orientation state was calculated at each time step. The velocity field resulted from solving the weak form (2.82) and (2.83), whereas the orientation state was calculated by integrating the advection Eq. (2.69)

$$\dot{\mathbf{a}} = \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 \cdot \mathbf{A} : \mathbf{D} - 6D_r \left(\mathbf{a} - \frac{\mathbf{I}}{3} \right), \quad (2.93)$$

which, being purely advective, was integrated by applying exactly the same scheme as just described in the case of the fluid fraction $I(\mathbf{x}, t)$.

Fig. 2.2 Mould filling simulation: evolution of the presence of fluid field



2.3.2 Updated Lagrangian Meshless Simulation

Even if there are many variants of techniques operating on a fixed mesh, as the one just presented, all of them give similar results despite their apparent differences.

Another possibility consists in solving the flow problem in the fluid domain $\Omega_f(t)$ that must be updated at each time step. One could imagine that at time t a mesh $\mathcal{F}^t$ is associated to the fluid domain $\Omega_f(t)$. This mesh consists of a number of nodes N_n , with coordinates $\mathbf{x}_i(t)$, and a number of elements N_e . By solving the flow problem in $\Omega_f(t)$ we have access to the velocity field at each node of the mesh, from which it can be interpolated everywhere in $\Omega_f(t)$. Now, one could imagine updating the nodal positions with the material velocity, i.e. $\mathbf{x}_i(t + \Delta t) \approx \mathbf{x}_i(t) + \mathbf{v}(\mathbf{x}_i(t), t) \cdot \Delta t$. It is important to mention that during this Lagrangian update, purely advective equations, as the one governing the evolution of the orientation tensor $\mathbf{a}$, can be integrated accurately by using the method of characteristics.

Now, a tentative mesh $\mathcal{F}^{t+\Delta t}$ could be defined, for example from the Delaunay triangulation related to the updated nodal positions $\mathbf{x}_i(t + \Delta t)$. However, it is well known that such procedure entails the distortion of the elements involved in the updated meshes and thus it compromises the solution accuracy. For this reason, a remeshing step is compulsory. Nodes are redistributed within the fluid domain to ensure that the associated mesh $\mathcal{F}^{t+\Delta t}$ does not contain elements that are too distorted.

Thus, standard updated Lagrangian approaches involve frequent remeshing steps. In addition to their computational complexity (mainly in 3D), they require a projection of all the fields depending on the flow history (e.g. the orientation state) from the trial mesh $\tilde{\mathcal{F}}^{t+\Delta t}$ to the updated one $\mathcal{F}^{t+\Delta t}$, with the associated numerical diffusion.

To alleviate these drawbacks, meshless methods were introduced some years ago and intensively used in many engineering applications. Meshless methods can be defined as those discretization techniques able to construct field approximations whose quality does not depend on the geometrical quality of a subjacent mesh. That is, when using meshless approximations, one could expect to define the fields approximation at each time t from the nodal positions resulting of moving them with the material velocity all along the whole simulation. They constitute an appealing choice for simulating flows involving internal variables (e.g. orientation), because advective fields are integrated very accurately by using the method of characteristics and the description of free or moving boundaries is a trivial task [57].

The interested reader can refer to [58, 59] and the references therein. The main difficulty of most meshless methods concerns the enforcement of essential boundary conditions because most of them (the Natural Element Method being an exception) do not verify the Kroenecker's delta property when approximating a field $u(\mathbf{x})$ by $u^h(\mathbf{x})$, i.e. $u^h(\mathbf{x}_i) \neq u(\mathbf{x}_i)$, with $\mathbf{x}_i$ the coordinates of a generic node n_i .

The Natural Element Method—NEM—is a nice compromise because it allows for a robust interpolation despite the quality of the subjacent mesh and it allows for the enforcement of essential boundary condition like in the finite element method, among many other appealing properties [59].



Fig. 2.3 Delaunay triangulation and Voronoi diagram

The NEM is based on the application of two classes of Natural Neighbour interpolation (Sibson [60] and Belikov [61]) to the discretization of a variational formulation. In what follows, we will refer to the first one.

Sibson interpolation relies on the concepts of Delaunay triangulations and Dirichlet tessellations of a set of nodes to build the shape functions (see Fig. 2.3). A Delaunay triangulation (tetrahedrization in three-dimensions) is the unique triangulation for a given set of nodes that satisfies the empty circumcircle criterion, that is, given the three nodes of a triangle (four nodes on a tetrahedron) and the circle (sphere) that passes through them, no one of the other nodes lies inside this circle (sphere). A Voronoi diagram or a Dirichlet tessellation is the dual structure of a Delaunay triangulation. For a given node n_i , the associated Voronoi cell is composed by all of the points which are closer to the node n_i than to any other node. Formally,

$$T_i = \{\mathbf{x} \in \mathbb{R}^3 : d(\mathbf{x}, \mathbf{x}_i) < d(\mathbf{x}, \mathbf{x}_j) \forall j \neq i\}, \quad (2.94)$$

where T_i is the Voronoi cell and $d(\cdot, \cdot)$ represents the Euclidean distance. It is clear from Fig. 2.3 that the Delaunay triangulation is defined over the convex hull of the set of points.

In a similar way, the second-order Voronoi cell is defined as the locus of the points that have the node n_i as the closest node and the node n_j as the second closest node:

$$T_{ij} = \{\mathbf{x} \in \mathbb{R}^3 : d(\mathbf{x}, \mathbf{x}_i) < d(\mathbf{x}, \mathbf{x}_j) < d(\mathbf{x}, \mathbf{x}_k), \forall k \neq i, j; i \neq j\}. \quad (2.95)$$

Thus, if a new point is added to a given cloud of points, the natural neighbour coordinates of this point $\mathbf{x}$ with respect to one of his neighbours $\mathbf{x}_i$ is the ratio of the cell T_i that is transferred to T_x when adding $\mathbf{x}$ to the initial cloud of points, to the total area of T_x . In other words, with $\kappa(\mathbf{x})$ and $\kappa_i(\mathbf{x})$ being the Lebesgue measures of T_x and T_{xi} respectively, the natural neighbour coordinates of $\mathbf{x}$ with respect to the node n_i is defined as

$$\phi_i(\mathbf{x}) = \frac{\kappa_i(\mathbf{x})}{\kappa(\mathbf{x})}, \quad (2.96)$$

which, using the notation indicated in Fig. 2.4, with A the polygon area, gives

$$\phi_1(\mathbf{x}) = \frac{A_{abfe}}{A_{abcd}}. \quad (2.97)$$

It is straightforward to prove that natural element shape functions define a partition of unity. The resulting shape function is shown in Fig. 2.5.

A model variable $\mathbf{u}$ ($\mathbf{u}$ represents a scalar, a vector or a tensor) can be approximated in 1D, 2D or 3D in the form:

$$\mathbf{u}^h(\mathbf{x}) = \sum_{i=1}^{N_n} \phi_i(\mathbf{x}) \mathbf{u}_i, \quad (2.98)$$

with $\mathbf{u}_i = \mathbf{u}(\mathbf{x}_i)$.

Fig. 2.4 Natural neighbourhood coordinates

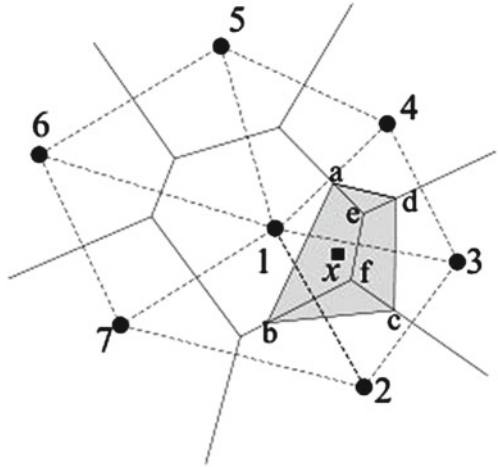
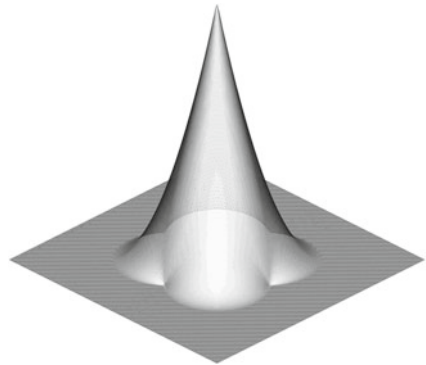


Fig. 2.5 Sibson's shape function



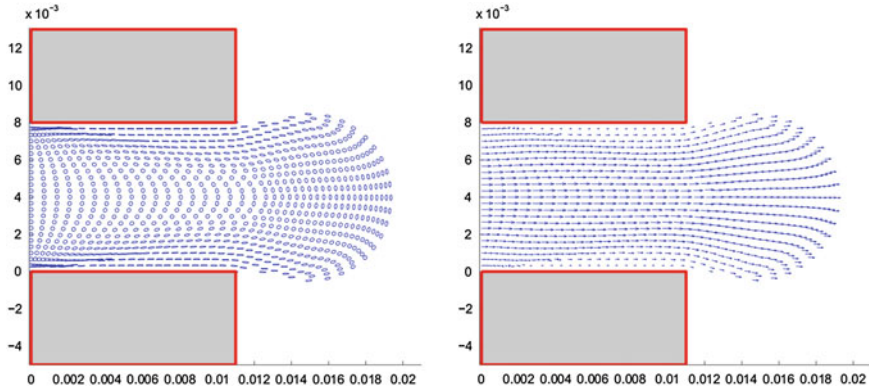


Fig. 2.6 NEM simulation of the flow leaving an extrusion die: orientation state (*left*) and velocity field (*right*)

The main issue related to the use of these interpolants is the treatment of non-convex domains, since, as indicated before, the Delaunay triangulation proceeds on the convex hull of the set of nodes. In that case, the simplest alternatives are the use of alpha-shapes [62] or the construction of the functional approximation on the so-called Constrained Voronoi Diagram—CVD—[63].

NEM-based discretization techniques are particularly appropriate for simulating very large thermomechanical transformations exhibiting possible free and moving boundaries [57, 64], and in particular those involving flow dependent internal variables, e.g. molecules conformation [65] or rod orientation [30, 66]. Figure 2.6 depicts the orientation and velocity fields in an extrusion simulation [31]. The orientation field is represented by an ellipse at each nodal position, whose semi axes are proportional to the orientation tensor eigenvalues and their orientation are given by the corresponding eigenvectors.

In this simulation, the nodal position is updated at each time step from the material velocity. Then, the fluid domain is extracted by using the alpha-shape constructor [62]. Next, the flow Eqs. (2.71), (2.72) and (2.73) are solved in the just updated fluid domain by using a Sibson approximation of the velocity field and considering the pressure field constant in each Voronoi cell. This approximation does not verify the LBB condition but generally works very well. It is much less expensive than using approximation fulfilling the LBB stability condition [67].

The solution of the flow problem at time $t + \Delta t$ in $\Omega_f(t + \Delta t)$ needs specifying the orientation state $\mathbf{a}(\mathbf{x} \in \Omega_f(t + \Delta t), t + \Delta t)$ that appears in the constitutive equation (2.73). Because of the meshless character of the discretization here employed, we can consider the cloud of nodes throughout the whole simulation. As we consider the orientation state attached to the nodes, and the orientation equation being purely advective, one could proceed to its integration along the nodal pathlines by using the method of characteristics, that is, proceeding from Eq. (2.69) in 2D:

$$\dot{\mathbf{a}} = \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 \cdot \mathbf{A} : \mathbf{D} - 4D_r \left(\mathbf{a} - \frac{\mathbf{I}}{2} \right). \quad (2.99)$$

We consider for each node $i = 1, \dots, N_n$ the simplest explicit first-order integration

$$\begin{aligned} & \frac{\mathbf{a}(\mathbf{x}_i(t + \Delta t), t + \Delta t) - \mathbf{a}(\mathbf{x}_i(t), t)}{\Delta t} \\ &= \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 \cdot \mathbf{A} : \mathbf{D} - 4D_r \left(\mathbf{a} - \frac{\mathbf{I}}{2} \right), \end{aligned} \quad (2.100)$$

where

$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \mathbf{v}(\mathbf{x}_i(t), t) \cdot \Delta t, \quad (2.101)$$

and in the right-hand side of Eq. (2.100), orientations and velocities are computed at positions $\mathbf{x}_i(t)$ and time t .

2.4 Concentrated Suspensions Involving Rod Clusters

Having considered rods immersed in a flow, we extend the approach to more complex configurations. Suspensions of industrial interest composed of rods (a limit case of an ellipsoid) aggregate, leading to clusters with particular shapes that exhibit, when immersed in a flow, an almost rigid motion. These situations are currently encountered when considering carbon nanotubes suspensions as discussed in [33, 39, 68]. In what follows, we address the modeling of both rigid and deformable clusters.

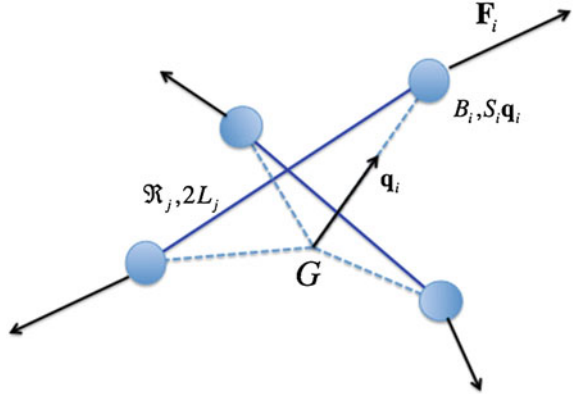
2.4.1 Rigid Clusters

We represent rigid clusters of general shape in both a discrete manner, assuming they are all composed of $N/2$ rods (N being an even integer) involving N beads, and in a continuous manner from the continuous pdf describing the configuration of those rod beads. In a rigid cluster, there is no relative motion between the rods composing it.

2.4.1.1 Discrete Description

First, we consider a 3D rigid cluster consisting of $N/2$ rods $\mathcal{R}_j$ of length $2L_j$. We assume that each rod $\mathcal{R}_j$ contains two beads at its ends on which hydrodynamic forces apply. Thus, the cluster contains N beads $\mathcal{B}_i$, $i = 1, \dots, N$. The location of each bead $\mathcal{B}_i$ with respect to the cluster center of gravity $\mathbf{G}$ is represented by $S_i \mathbf{q}_i$, where $\mathbf{q}_i$ is the unit vector pointing from $\mathbf{G}$ to $\mathcal{B}_i$. The cluster is sketched in Fig. 2.7.

Fig. 2.7 Rigid cluster composed of rods



Brownian effects are neglected and then only flow-induced hydrodynamic forces must be considered (hydrodynamic interactions are not considered in this work). Forces $\mathbf{F}_i$ apply on each bead located at position $S_i \mathbf{q}_i$ (Fig. 2.7) and are proportional to the difference of velocity between the one of the flow unperturbed by the presence of the cluster at the bead location and the one of the bead itself:

$$\mathbf{F}_i = \xi (\mathbf{V}_0 + \nabla \mathbf{v} \cdot \mathbf{q}_i S_i - \mathbf{V}_G - \dot{\mathbf{q}}_i S_i), \quad (2.102)$$

where ξ is the friction coefficient, $\mathbf{v}$ the flow velocity field, $\mathbf{V}_0$ the fluid velocity at the cluster centre of gravity $\mathbf{G}$ and $\mathbf{V}_G$ the velocity of the cluster center of gravity itself.

By adding all the forces we obtain

$$\mathbf{0} = \sum_{i=1}^{i=N} \mathbf{F}_i = N(\mathbf{V}_0 - \mathbf{V}_G) + \nabla \mathbf{v} \cdot \left(\sum_{i=1}^{i=N} S_i \mathbf{q}_i \right) - \left(\sum_{i=1}^{i=N} S_i \dot{\mathbf{q}}_i \right). \quad (2.103)$$

Both sums in Eq. (2.103) vanish, the first one as a direct consequence of the definition of the center of gravity, and the second because the cluster is assumed rigid. Thus, Eq. (2.103) becomes

$$\mathbf{V}_0 = \mathbf{V}_G, \quad (2.104)$$

implying that the cluster center of gravity is moving with the fluid velocity at that position.

The torque created by forces applied on bead $\mathcal{B}_i$ is given by

$$\mathbf{M}_i = S_i \mathbf{q}_i \times \mathbf{F}_i. \quad (2.105)$$

Neglecting inertial effects, the resulting torque for the whole cluster must vanish:

$$\sum_{i=1}^{i=N} \mathbf{M}_i = \mathbf{0}. \quad (2.106)$$

Taking Eqs. (2.105) and (2.102) into account, we have

$$\sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times (\nabla \mathbf{v} \cdot \mathbf{q}_i) = \sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times \dot{\mathbf{q}}_i. \quad (2.107)$$

If we define the cluster angular velocity $\boldsymbol{\omega}$ such that

$$\dot{\mathbf{q}}_i = \boldsymbol{\omega} \times \mathbf{q}_i, \quad (2.108)$$

torque equilibrium reads

$$\sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times (\nabla \mathbf{v} \cdot \mathbf{q}_i) = \sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times (\boldsymbol{\omega} \times \mathbf{q}_i). \quad (2.109)$$

Now, by using the vector triple product relationship $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b} (\mathbf{a} \cdot \mathbf{c}) - \mathbf{c} (\mathbf{a} \cdot \mathbf{b})$, the right-hand side reads

$$\sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times (\boldsymbol{\omega} \times \mathbf{q}_i) = \sum_{i=1}^{i=N} S_i^2 (\boldsymbol{\omega} (\mathbf{q}_i \cdot \mathbf{q}_i) - \mathbf{q}_i (\mathbf{q}_i \cdot \boldsymbol{\omega})), \quad (2.110)$$

which, taking into account the normality of vectors $\mathbf{q}_i$ and the fact that $\mathbf{q}_i (\mathbf{q}_i \cdot \boldsymbol{\omega}) = (\mathbf{q}_i \otimes \mathbf{q}_i) \cdot \boldsymbol{\omega}$, becomes

$$\sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times (\boldsymbol{\omega} \times \mathbf{q}_i) = \sum_{i=1}^{i=N} S_i^2 (\mathbf{I} - (\mathbf{q}_i \otimes \mathbf{q}_i)) \cdot \boldsymbol{\omega}, \quad (2.111)$$

where $\mathbf{I}$ the unit matrix.

Now, the left-hand side of Eq. (2.109) can be rewritten by using the third-order Levi-Civita permutation tensor $\boldsymbol{\varepsilon}$ such that $(\mathbf{u} \times \mathbf{v}) = \boldsymbol{\varepsilon} : (\mathbf{v} \otimes \mathbf{u})$. We obtain

$$\sum_{i=1}^{i=N} S_i^2 \mathbf{q}_i \times (\nabla \mathbf{v} \cdot \mathbf{q}_i) = \sum_{i=1}^{i=N} S_i^2 \boldsymbol{\varepsilon} : (\nabla \mathbf{v} \cdot (\mathbf{q}_i \otimes \mathbf{q}_i)), \quad (2.112)$$

which finally yields

$$\sum_{i=1}^{i=N} S_i^2 \boldsymbol{\varepsilon} : (\nabla \mathbf{v} \cdot (\mathbf{q}_i \otimes \mathbf{q}_i)) = \sum_{i=1}^{i=N} S_i^2 (\mathbf{I} - (\mathbf{q}_i \otimes \mathbf{q}_i)) \cdot \boldsymbol{\omega}. \quad (2.113)$$

Expressed in a more compact form, we have

$$\begin{aligned} \boldsymbol{\varepsilon} : & \left(\nabla \mathbf{v} \cdot \left(\sum_{i=1}^{i=N} S_i^2 (\mathbf{q}_i \otimes \mathbf{q}_i) \right) \right) \\ & = \left(\left(\sum_{i=1}^{i=N} S_i^2 \right) \mathbf{I} - \left(\sum_{i=1}^{i=N} S_i^2 (\mathbf{q}_i \otimes \mathbf{q}_i) \right) \right) \cdot \boldsymbol{\omega}. \end{aligned} \quad (2.114)$$

2.4.1.2 Continuous Description

The continuous description considers the pdf $\Upsilon(\mathbf{q}, S)$ giving the fraction of rod beads located at position $\mathbf{q}S$, that can be expressed as

$$\Upsilon(\mathbf{q}, S) = \psi(\mathbf{q}; S) \Gamma(S), \quad (2.115)$$

where $\psi(\mathbf{q}; S)$ is the angular distribution of beads located at distance S from the cluster center of gravity $\mathbf{G}$, and $\Gamma(S)$ is the fraction of beads located at that distance S . The normality condition reads

$$\int_{\mathcal{S}} \psi(\mathbf{q}; S) d\mathbf{q} = 1, \quad \forall S. \quad (2.116)$$

By defining the conformation tensor $\mathbf{c}_S$ related to the population of beads located at distance S with respect to the cluster center of gravity $\mathbf{G}$ as

$$\mathbf{c}_S = \int_{\mathcal{S}} \mathbf{q} \otimes \mathbf{q} \psi(\mathbf{q}; S) d\mathbf{q}, \quad (2.117)$$

all sums in the previous expression (2.114) must be substituted by the corresponding integrals in the length and orientation domains, $\mathcal{L}$ and $\mathcal{S}$ respectively, weighted by the distribution function $\psi(\mathbf{q}; S) \Gamma(S)$.

In particular Eq. (2.114) becomes:

$$\begin{aligned} \boldsymbol{\varepsilon} : & \left(\nabla \mathbf{v} \cdot \left(\int_{\mathcal{L}} S^2 \left(\int_{\mathcal{S}} (\mathbf{q} \otimes \mathbf{q}) \psi(\mathbf{q}; S) d\mathbf{q} \right) \Gamma(S) dS \right) \right) \\ & = \left(\left(\int_{\mathcal{L}} S^2 \Gamma(S) dS \right) \mathbf{I} - \left(\int_{\mathcal{L}} S^2 \left(\int_{\mathcal{S}} (\mathbf{q} \otimes \mathbf{q}) \psi(\mathbf{q}; S) d\mathbf{q} \right) \Gamma(S) dS \right) \right) \cdot \boldsymbol{\omega}, \end{aligned} \quad (2.118)$$

which gives, using definition (2.117),

$$\begin{aligned} \boldsymbol{\varepsilon} : & \left(\nabla \mathbf{v} \cdot \left(\int_{\mathcal{L}} S^2 \mathbf{c}_S \Gamma(S) dS \right) \right) \\ & = \left(\left(\int_{\mathcal{L}} S^2 \Gamma(S) dS \right) \mathbf{I} - \left(\int_{\mathcal{L}} S^2 \mathbf{c}_S \Gamma(S) dS \right) \right) \cdot \boldsymbol{\omega}. \end{aligned} \quad (2.119)$$

By introducing the mean square length β and tensor $\tilde{\mathbf{c}}$ according to

$$\beta = \int_{\mathcal{L}} S^2 \Gamma(S) dS, \quad (2.120)$$

and

$$\tilde{\mathbf{c}} = \int_{\mathcal{L}} S^2 \mathbf{c}_S \Gamma(S) dS, \quad (2.121)$$

and due to the unit trace of $\mathbf{c}_S$, i.e. $Tr(\mathbf{c}_S) = 1$, we can infer that β is in fact the trace of $\tilde{\mathbf{c}}$, that is $\beta = Tr(\tilde{\mathbf{c}})$.

Thus, the particle kinematics finally results:

$$\boldsymbol{\varepsilon} : (\nabla \mathbf{v} \cdot \tilde{\mathbf{c}}) = (Tr(\tilde{\mathbf{c}})\mathbf{I} - \tilde{\mathbf{c}}) \cdot \boldsymbol{\omega}, \quad (2.122)$$

or dividing by $Tr(\tilde{\mathbf{c}})$,

$$\boldsymbol{\omega} = (\mathbf{I} - \mathbf{c})^{-1} \cdot (\boldsymbol{\varepsilon} : (\nabla \mathbf{v} \cdot \mathbf{c})), \quad (2.123)$$

where the conformation tensor $\mathbf{c}$ is given by

$$\mathbf{c} = \frac{\tilde{\mathbf{c}}}{Tr(\tilde{\mathbf{c}})}. \quad (2.124)$$

Remark 3 In the 2D case, $\mathbf{c} \cdot \boldsymbol{\omega} = \mathbf{0}$ and then $\boldsymbol{\omega} = (\boldsymbol{\varepsilon} : (\nabla \mathbf{v} \cdot \mathbf{c}))$. Moreover, if all beads are located at the same distance S , we recover the expression given in [44].

An extremely important consequence of this analysis is that rigid clusters composed of rods having the same conformation tensor $\mathbf{c}$ rotate at the same angular velocity.

As the conformation tensor $\mathbf{c}$ is symmetric and positive definite, it has real eigenvalues and eigenvectors. In 3D, the three mutually perpendicular eigenvectors will be denoted by $\mathbf{u}_1$, $\mathbf{u}_2$ and $\mathbf{u}_3$, with the associated eigenvalues τ_1 , τ_2 and τ_3 respectively.

Imagine a rigid cluster composed of three rods oriented in directions $\mathbf{u}_1$, $\mathbf{u}_2$ and $\mathbf{u}_3$ with respective lengths $\sqrt{\tau_1}$, $\sqrt{\tau_2}$ and $\sqrt{\tau_3}$. The conformation tensor of such a three-rod cluster coincides with $\mathbf{c}$ and then both tensors have the same rotary velocity. Thus in [45] we proved the link between a rigid cluster composed of three mutually orthogonal rods and the Jeffery triaxial-ellipsoid.

2.4.1.3 Multi-scale Description

In this chapter, we have only addressed the first brick of the proposed approach to the multi-scale modeling of suspensions involving rigid clusters composed of rigid rods. In way of perspectives for future work, we conclude with an overview of the complete nine-step approach to be followed:

1. The cluster conformation has been successfully described by tensor $\mathbf{c}$ given in Eq. (2.124). This choice was motivated by the fact that all clusters having the same conformation tensor $\mathbf{c}$ have the same kinematics as just proved.
2. Cluster conformation evolution. Knowing the cluster kinematics $\boldsymbol{\omega}$, we can obtain the expression of $\dot{\mathbf{q}}$ in order to define the conformation evolution from $\dot{\mathbf{c}}$.
3. Cluster contribution to the stress. The force acting on each rod bead involved in the rigid cluster must be taken into account by invoking Kramers' rule.
4. Population description. The population of rigid clusters at the mesoscopic scale can be represented by means of either a discrete or a continuous description. In the discrete framework, the population is described from different computational individuals, each one characterized by its conformation tensor $\mathbf{c}_i, i = 1, \dots, \mathcal{N}$. Within the continuous framework, the suspension is characterized by the pdf Ψ , which now depends on the physical coordinates (space $\mathbf{x}$ and time t) and the conformation coordinate $\mathbf{c}$. Thus, the pdf reads $\Psi(\mathbf{x}, t, \mathbf{c})$. It gives the fraction of clusters that at position $\mathbf{x}$ and time t have a conformation given by $\mathbf{c}$.
5. Description of the population evolution. Within the discrete framework, the population evolution is obtained by integrating the evolution equation for each cluster conformation $\dot{\mathbf{c}}_i$. Within the continuous framework, the pdf $\Psi(\mathbf{x}, t, \mathbf{c})$ evolves according to its associated Fokker-Planck equation, with the knowledge of $\dot{\mathbf{c}}$.
6. Contribution of cluster population to the stress requires adding the contribution of all computational clusters, within the discrete framework, or to integrate in conformation space when proceeding within the continuous framework.
7. The macroscopic description uses a coarser description based on the moments of the pdf. Here, the simplest choice consists of the first moment $\mathbf{C}(\mathbf{x}, t)$ defined as

$$\mathbf{C}(\mathbf{x}, t) = \int_{\mathcal{C}} \mathbf{c} \Psi(\mathbf{x}, t, \mathbf{c}) d\mathbf{c}. \quad (2.125)$$

8. Microstructural macroscopic evolution. In order to derive the time evolution of the first moment $\mathbf{C}$, we should consider its time derivative and propose adequate closure relations.
9. The moment-based stress requires consideration of the stress expression obtained in step (6) above. Here again, introduction of a suitable closure relation is required.

2.4.2 Deformable Clusters

In this section, we consider a more realistic scenario consisting of deformable clusters. We consider two types of forces applied on each bead of a generic rod $\mathcal{R}$ (of length $2L$), one due to the fluid-rod friction once more modeled as

$$\mathbf{F}_i^H = \xi (\mathbf{v}_0^i + \nabla \mathbf{v} \cdot \mathbf{p}_i L - \mathbf{v}_G^i - \dot{\mathbf{p}}_i L), \quad (2.126)$$

where the superscript “ H ” refers to its hydrodynamic nature. Here, $\mathbf{v}_0^i$ is the fluid velocity (assumed unperturbed by the presence of the cluster) at the rod $\mathcal{R}_i$ centre of gravity $\mathcal{G}_i$, and $\mathbf{v}_G^i$ the velocity of the rod $\mathcal{R}_i$ centre of gravity $\mathcal{G}_i$.

The other force $\mathbf{F}_i^C$ is due to the rod entanglements. This last force is assumed scaling with the difference between the rigid motion velocity (the one that the bead would have if the cluster would be rigid) $\mathbf{v}_{\mathcal{B}}^R$ and the real one $\mathbf{v}_G + \dot{\mathbf{p}}L$.

As proved in the previous section, the bead velocity when assuming the cluster rigid reads:

$$\mathbf{v}_{\mathcal{B}}^R = \mathbf{V}_0 + \mathbf{W} \cdot \mathbf{r} + \mathbf{W} \cdot \mathbf{p}L, \quad (2.127)$$

where tensor $\mathbf{W}$ derives from the rigid rotary velocity $\boldsymbol{\omega}$ given by Eq.(2.123) from

$$\mathbf{W} \cdot \mathbf{p} = \boldsymbol{\omega} \times \mathbf{p}, \quad \forall \mathbf{p}. \quad (2.128)$$

$\mathbf{V}_0$ is the unperturbed fluid velocity at the cluster centre of gravity $\mathbf{G}$ and $\mathbf{r}$ is the vector connecting the cluster centre of gravity $\mathbf{G}$ to the rod centre of gravity $\mathcal{G}$, i.e. $\mathbf{r} = \mathcal{G} - \mathbf{G}$.

Thus, the contribution to the bead force due to collective effects (a sort of mean field) when considering the generic rod $\mathcal{R}_i$ reads:

$$\mathbf{F}_i^C = \mu (\mathbf{V}_0 + \mathbf{W} \cdot \mathbf{r}_i + \mathbf{W} \cdot \mathbf{p}_i L - \mathbf{v}_G^i - \dot{\mathbf{p}}_i L). \quad (2.129)$$

This expresses that if the hypothetical rigid cluster is moving faster than the bead then this sort of mean field pushes the bead.

When μ is large enough, forces $\mathbf{F}_i^C$ dominate the momentum balances enforcing the cluster rotary velocity $\mathbf{W}$ to each rod composing it (rigid behaviour).

The resulting force at bead $\mathbf{p}_i L$ results $\mathbf{F}_i(\mathbf{p}_i L) = \mathbf{F}_i^H(\mathbf{p}_i L) + \mathbf{F}_i^C(\mathbf{p}_i L)$. The linear momentum balance, neglecting inertia effects, reads

$$\mathbf{F}_i(\mathbf{p}_i L) + \mathbf{F}_i(-\mathbf{p}_i L) = \mathbf{0}, \quad (2.130)$$

that implies

$$\xi \mathbf{v}_0^i - \xi \mathbf{v}_G^i + \mu \mathbf{V}_0 + \mu \mathbf{W} \cdot \mathbf{r}_i - \mu \mathbf{v}_G^i = \mathbf{0}, \quad (2.131)$$

or

$$\mathbf{v}_G^i = \frac{\xi \mathbf{v}_0^i + \mu \mathbf{V}_0}{\xi + \mu} + \frac{\mu}{\xi + \mu} \mathbf{W} \cdot \mathbf{r}_i. \quad (2.132)$$

When $\mu = 0$, this gives the standard non-interacting rod model (dilute suspension), with $\mathbf{v}_0^i = \mathbf{v}_G^i$, and when $\xi = 0$, we recover the solid motion $\mathbf{v}_G^i = \mathbf{V}_0 + \mathbf{W} \cdot \mathbf{r}_i$.

Now, taking into account the first gradient framework

$$\mathbf{v}_0^i = \mathbf{V}_0 + \nabla \mathbf{v} \cdot \mathbf{r}_i, \quad (2.133)$$

Eq. (2.132) reduces to:

$$\mathbf{v}_G^i = \mathbf{V}_0 + \frac{\xi}{\xi + \mu} \nabla \mathbf{v} \cdot \mathbf{r}_i + \frac{\mu}{\xi + \mu} \mathbf{W} \cdot \mathbf{r}_i. \quad (2.134)$$

This equation allows for the trajectory calculation of each rod centre of gravity. Now, we consider the equation governing the evolution of the rods orientations, that is $\dot{\mathbf{p}}$.

Coming back to the force applied on each rod bead,

$$\begin{aligned} \mathbf{F}_i = & \xi (\mathbf{v}_0^i + \nabla \mathbf{v} \cdot \mathbf{p}_i L - \mathbf{v}_G^i - \dot{\mathbf{p}}_i L) \\ & + \mu (\mathbf{V}_0 + \mathbf{W} \cdot \mathbf{r}_i + \mathbf{W} \cdot \mathbf{p}_i L - \mathbf{v}_G^i - \dot{\mathbf{p}}_i L), \end{aligned} \quad (2.135)$$

and taking (2.131) into account, we obtain

$$\mathbf{F}_i(\mathbf{p}_i L) = L (\xi (\nabla \mathbf{v} \cdot \mathbf{p}_i - \dot{\mathbf{p}}_i) + \mu (\mathbf{W} \cdot \mathbf{p}_i - \dot{\mathbf{p}}_i)). \quad (2.136)$$

Now, if we define the equivalent traceless gradient $\mathbb{G}$,

$$\mathbb{G} = \frac{\mu \mathbf{W} + \xi \nabla \mathbf{v}}{\xi + \mu}, \quad (2.137)$$

Eq. (2.136) can be rewritten as

$$\mathbf{F}_i(\mathbf{p}_i L) = L(\xi + \mu) (\mathbb{G} \cdot \mathbf{p}_i - \dot{\mathbf{p}}_i), \quad (2.138)$$

that allows for using all the rationale considered when developing the Jeffery model, by replacing the friction coefficient by $(\xi + \mu)$ and the gradient of velocity by $\mathbb{G}$.

Thus, the rod rotary velocity becomes:

$$\dot{\mathbf{p}}_i = \mathbb{G} \cdot \mathbf{p}_i - (\mathbb{G} : (\mathbf{p}_i \otimes \mathbf{p}_i)) \mathbf{p}_i. \quad (2.139)$$

The term $\mathbb{G} : (\mathbf{p}_i \otimes \mathbf{p}_i)$ deserves some additional comment. Since $\mathbf{W}$ and $\mathbf{\Omega}$ are both skew-symmetric, we obtain: $\mathbf{W} : (\mathbf{p}_i \otimes \mathbf{p}_i) = 0$, and the same in the case of considering $\mathbf{\Omega}$, implying $\mathbb{G} : (\mathbf{p}_i \otimes \mathbf{p}_i) = \frac{\xi}{\xi + \mu} \mathbf{D} : (\mathbf{p}_i \otimes \mathbf{p}_i)$ and then:

$$\dot{\mathbf{p}}_i = \mathbb{G} \cdot \mathbf{p}_i - \frac{\xi}{\xi + \mu} (\mathbf{D} : (\mathbf{p}_i \otimes \mathbf{p}_i)) \mathbf{p}_i \quad (2.140)$$

This can be rewritten as

$$\begin{aligned} \dot{\mathbf{p}}_i &= \frac{\mu}{\xi + \mu} \mathbf{W} \cdot \mathbf{p}_i + \frac{\xi}{\xi + \mu} \nabla \mathbf{v} \cdot \mathbf{p}_i - \frac{\xi}{\xi + \mu} (\mathbf{D} : (\mathbf{p}_i \otimes \mathbf{p}_i)) \mathbf{p}_i \\ &= \frac{\xi}{\xi + \mu} \dot{\mathbf{p}}_i^J + \frac{\mu}{\xi + \mu} \mathbf{W} \cdot \mathbf{p}_i = \frac{\xi}{\xi + \mu} \dot{\mathbf{p}}_i^J + \frac{\mu}{\xi + \mu} \dot{\mathbf{p}}_i^R, \end{aligned} \quad (2.141)$$

where $\dot{\mathbf{p}}_i^J$ represents the hydrodynamic contribution in absence of collective effects (dilute regime described by the Jeffery equation), and $\dot{\mathbf{p}}_i^R$ the one coming from the rod entanglements that results in a rigid-like cluster kinematics.

We can notice that, when $\xi \gg \mu$, hydrodynamic effects are preponderant and the rod kinematics are governed by the Jeffery equation, i.e. $\dot{\mathbf{p}}_i \approx \dot{\mathbf{p}}_i^J$. In the opposite case, $\mu \gg \xi$, the cluster is too rigid and the rods adopt the velocity dictated by the rigid cluster kinematics $\dot{\mathbf{p}}_i \approx \dot{\mathbf{p}}_i^R$.

Macroscopic description: cluster inertia and shape

From Eq. (2.134), the position of each rod composing the cluster can be integrated. It seems natural that knowing the location of the centre of gravity of each rod, the cluster inertia and shape could be obtained.

If we define the cluster inertia tensor $\mathbf{S}$ from:

$$\mathbf{S} = \int_{\mathcal{R}} \mathbf{r} \otimes \mathbf{r} \psi(\mathbf{r}) d\mathbf{r}, \quad (2.142)$$

its time evolution is given by

$$\dot{\mathbf{S}} = \int_{\mathcal{R}} (\dot{\mathbf{r}} \otimes \mathbf{r} + \mathbf{r} \otimes \dot{\mathbf{r}}) \psi(\mathbf{r}) d\mathbf{r}, \quad (2.143)$$

with $\dot{\mathbf{r}} = \mathbf{v}_G - \mathbf{V}_0$, where the fact that the (rigid) cluster centre of gravity is moving with the fluid velocity at that position was taken into account. Thus, we obtain

$$\dot{\mathbf{r}} = \frac{\xi}{\xi + \mu} \nabla \mathbf{v} \cdot \mathbf{r} + \frac{\mu}{\xi + \mu} \mathbf{W} \cdot \mathbf{r}. \quad (2.144)$$

Now, by introducing Eqs. (2.144) into (2.143) and making use of (2.142), we obtain

$$\dot{\mathbf{S}} = \frac{\xi}{\xi + \mu} \left(\nabla \mathbf{v} \cdot \mathbf{S} + \mathbf{S} \cdot (\nabla \mathbf{v})^T \right) + \frac{\mu}{\xi + \mu} (\mathbf{W} \cdot \mathbf{S} - \mathbf{S} \cdot \mathbf{W}), \quad (2.145)$$

where we used the fact that $\mathbf{W}^T = -\mathbf{W}$. The vorticity tensor appearing in both $\nabla \mathbf{v}$ and $\mathbf{W}$ ensures the objectivity of the cluster shape evolution.

In Eq. (2.145), the first term involving the velocity gradient $\nabla \mathbf{v}$ is responsible of the cluster deformation, whereas the second one involving $\mathbf{W}$ only rotates the cluster like a rigid solid because of collective effects. The standard flow-induced rotation (in absence of collective effects) is contained in the vorticity tensor. When $\mu = 0$, the cluster deforms and rotates according to the flow vorticity. When $\mu \neq 0$, there is an extra-rotation induced by collective effects. Finally, when $\xi = 0$ ($\mu \neq 0$), the cluster rotates without experiencing a deformation.

The trace of $\mathbf{S}$ gives information on the cluster size. Let us define the shape tensor $\mathbf{s}$ from the normalized inertia tensor

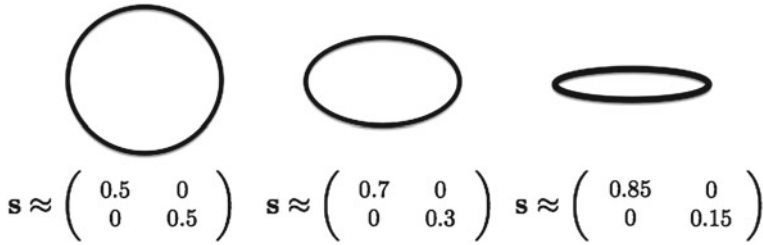


Fig. 2.8 Cluster shapes

$$\mathbf{s} = \frac{\mathbf{S}}{\text{Tr}(\mathbf{S})}. \quad (2.146)$$

The shape tensor being symmetric and positive definite, it can be diagonalized and represented by an ellipsoid (ellipse in 2D) whose eigenvalues describe the cluster orientation and its eigenvalues its shape. Figure 2.8 depicts different clusters and their associated shape tensors.

Macroscopic description: orientation

Now, concerning the orientation, if we assume the orientation of the rods of a deformable cluster given by the orientation distribution $\psi(\mathbf{p})$, the time derivative of its second order moment $\dot{\mathbf{a}}$ is given by

$$\dot{\mathbf{a}} = \int_{\mathcal{S}} (\dot{\mathbf{p}} \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}}) \psi(\mathbf{p}) d\mathbf{p}. \quad (2.147)$$

By considering the expression of the microscopic velocity $\dot{\mathbf{p}}$,

$$\dot{\mathbf{p}} = \frac{\xi}{\xi + \mu} \dot{\mathbf{p}}^J + \frac{\mu}{\xi + \mu} \dot{\mathbf{p}}^R, \quad (2.148)$$

we obtain:

$$\dot{\mathbf{a}} = \frac{\xi}{\xi + \mu} \dot{\mathbf{a}}^J + \frac{\mu}{\xi + \mu} \dot{\mathbf{a}}^R, \quad (2.149)$$

with $\dot{\mathbf{a}}^J$ and $\dot{\mathbf{a}}^R$ resulting once Eq. (2.148) is introduced into Eq. (2.147) by assuming $\mu = 0$ and $\xi = 0$, respectively:

$$\begin{cases} \dot{\mathbf{a}}^J = \nabla \mathbf{v} \cdot \mathbf{a} + \mathbf{a} \cdot (\nabla \mathbf{v})^T - 2 \mathbf{A} : \mathbf{D} \\ \dot{\mathbf{a}}^R = \mathbf{W} \cdot \mathbf{a} + \mathbf{a} \cdot \mathbf{W}^T \end{cases} \quad (2.150)$$

Here, $\mathbf{A}$ is the fourth-order moment defined by:

$$\mathbf{A} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \psi(\mathbf{p}) d\mathbf{p}. \quad (2.151)$$

The objectivity of the resulting evolution equation of $\dot{\mathbf{a}}$ was proved in [43]. Usually, the fourth-order moment $\mathbf{A}$ is expressed from the second-order one by considering any of the numerous closure relations proposed in the literature [47–50].

We just proved that the conformation of a deformable cluster is defined from both the orientation tensor $\mathbf{a}$ and the shape tensor $\mathbf{S}$. The evolution of both tensors makes use of tensor $\mathbf{W}$ that depends itself on the conformation tensor $\mathbf{c}$. Tensor $\mathbf{c}$ is very close to tensor $\mathbf{S}$; the first is defined from the vectors joining the cluster centre of gravity with each rod bead, whereas the second one involves vectors joining the cluster centre of gravity with the rods centre of gravity. The rod length being very small, both tensors are very close, and consequently tensor $\mathbf{W}$ can be evaluated by using $\mathbf{S}$ instead of $\mathbf{c}$.

To validate this approach, we come back to the definition of the conformation tensor $\mathbf{c}$ (2.124),

$$\mathbf{c} = \frac{\tilde{\mathbf{c}}}{Tr(\tilde{\mathbf{c}})}, \quad (2.152)$$

where the discrete form of $\tilde{\mathbf{c}}$ reads

$$\tilde{\mathbf{c}} = \sum_{i=1}^N (S_i \mathbf{q}_i) \otimes (S_i \mathbf{q}_i). \quad (2.153)$$

If we consider the contribution of the two beads of a generic rod $\mathcal{R}_j$, we obtain

$$\begin{aligned} \tilde{\mathbf{c}}^j &= (S_1^j \mathbf{q}_1^j) \otimes (S_1^j \mathbf{q}_1^j) + (S_2^j \mathbf{q}_2^j) \otimes (S_2^j \mathbf{q}_2^j) \\ &= (\mathbf{r}_j + L\mathbf{p}_j) \otimes (\mathbf{r}_j + L\mathbf{p}_j) + (\mathbf{r}_j - L\mathbf{p}_j) \otimes (\mathbf{r}_j - L\mathbf{p}_j) \\ &= 2\mathbf{r}_j \otimes \mathbf{r}_j + 2L^2 \mathbf{p}_j \otimes \mathbf{p}_j, \end{aligned} \quad (2.154)$$

which implies

$$\tilde{\mathbf{c}} = \sum_{j=1}^{\frac{N}{2}} \tilde{\mathbf{c}}^j = \sum_{j=1}^{\frac{N}{2}} (2\mathbf{r}_j \otimes \mathbf{r}_j + 2L^2 \mathbf{p}_j \otimes \mathbf{p}_j) = 2(\mathbf{S} + L^2 \mathbf{a}), \quad (2.155)$$

from which we obtain conformation tensor

$$\mathbf{c} = \frac{\mathbf{S} + L^2 \mathbf{a}}{Tr(\mathbf{S}) + L^2}. \quad (2.156)$$

Thus, as soon as $L^2 \ll Tr(\mathbf{S})$, we can assume $\mathbf{c} \approx \mathbf{S}$.

Cluster shape versus orientation

In the model just proposed, the cluster conformation is described from the orientation and shape tensors and the trace of the inertia tensor. In principle, orientation and shape are considered independent from one another, even if some correlation could

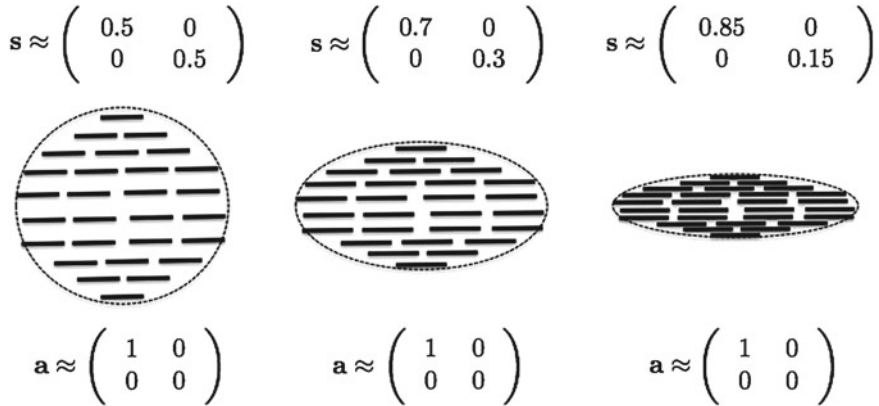


Fig. 2.9 Cluster shapes versus orientation: rods fully aligned

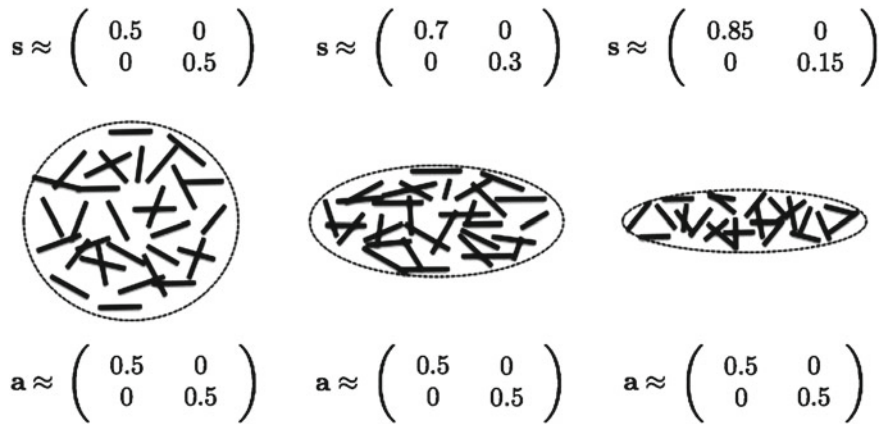


Fig. 2.10 Cluster shapes versus orientation: isotropic orientation

be expected from a physical point of view. Thus, we can define a spherical cluster with all its rods aligned or a very elongated cluster with all its rods isotropically oriented. Figures 2.9 and 2.10 depict different scenarios between these two limit cases.

2.5 Advanced Topics

2.5.1 On the Solution of the Fokker-Planck Equation

Since kinetic theory descriptions involve a probability distribution function depending on space, time and a number of conformational coordinates, the associated Fokker-Planck equations suffer the so-called curse of dimensionality typical of problems defined in highly dimensional spaces.

Thus, mesh-based discretization techniques fail for discretizing the problem because the number of degrees of freedom involved in a mesh or grid increases exponentially with the space dimension.

In what follows, we consider some alternatives to standard mesh-based discretization that are able to address the solution of Fokker-Planck equations associated with kinetic theory descriptions.

We consider, without loss of generality, a generic Fokker-Planck equation where diffusion terms are represented by fluxes $\mathbf{q}_x$ and $\mathbf{q}_a$ operating respectively in the physical and conformational spaces:

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \Psi) + \nabla_a \cdot (\dot{\mathbf{a}} \Psi) = -\nabla_x \cdot \mathbf{q}_x - \nabla_a \cdot \mathbf{q}_a. \quad (2.157)$$

2.5.1.1 Method of Particles for Solving Advection-Dominated Problems

This technique described in detail in [6, 8] consists in approximating the initial distribution $\Psi(\mathbf{x}, t = 0, \mathbf{a})$ from $\mathcal{M}$ Dirac's masses $\mathbf{a}_i^0$ at each one of the $\mathcal{Q}$ positions $\mathbf{x}_j^0$:

$$\Psi(\mathbf{x}, t = 0, \mathbf{a}) = \sum_{j=1}^{\mathcal{Q}} \sum_{i=1}^{\mathcal{M}} \alpha_i^j \delta(\mathbf{a} - \mathbf{a}_i^0) \delta(\mathbf{x} - \mathbf{x}_j^0). \quad (2.158)$$

This represents a sort of approximation based on $\mathcal{Q} \cdot \mathcal{M}$ computational particles $\mathcal{P}_{ij}$ with initial positions and conformations given by

$$\begin{cases} \mathbf{x}_{ij}^0 = \mathbf{x}_j^0, & i = 1, \dots, \mathcal{M}; \quad j = 1, \dots, \mathcal{Q} \\ \mathbf{a}_{ij}^0 = \mathbf{a}_i^0, & i = 1, \dots, \mathcal{M}; \quad j = 1, \dots, \mathcal{Q} \end{cases} \quad (2.159)$$

and whose position and conformation will be evaluated all along the flow simulation, from which the distribution will be reconstructed.

When considering the purely advective balance equation

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \Psi) + \nabla_a \cdot (\dot{\mathbf{a}} \Psi) = 0, \quad (2.160)$$

the time evolution of position and conformation of each particle $\mathcal{P}_{ij}$ is calculated by integrating

$$\begin{cases} \mathbf{x}_{ij}(t) = \mathbf{x}_{ij}^0 + \int_{\tau=0}^{\tau=t} \mathbf{v}(\mathbf{x}_{ij}(\tau)) d\tau \\ \mathbf{a}_{ij}(t) = \mathbf{a}_{ij}^0 + \int_{\tau=0}^{\tau=t} \dot{\mathbf{a}}_{ij}(\mathbf{a}_{ij}(\tau), \mathbf{x}_{ij}(\tau)) d\tau \end{cases} \quad (2.161)$$

As the position update only depends on the velocity field, that itself only depends on the position, it can be stressed that particles $\mathcal{P}_{ij}$, $i = 1, \dots, \mathcal{M}$ are following the same trajectory in the physical space, having $\mathbf{x}_j^0$ as departure point.

Now, the orientation distribution at time t can be reconstructed from

$$\Psi(\mathbf{x}, t, \mathbf{a}) = \sum_{j=1}^{\mathcal{Q}} \sum_{i=1}^{\mathcal{M}} \alpha_i^j \delta(\mathbf{a} - \mathbf{a}_{ij}(t)) \delta(\mathbf{x} - \mathbf{x}_{ij}(t)). \quad (2.162)$$

Obviously, smoother representations can be obtained by considering appropriate regularizations of the Dirac's distribution, as the one usually performed within the SPH (Smooth Particles Hydrodynamics) framework [5, 6].

When considering diffusion terms, there are two main routes based on the use of particles, one of stochastic nature, the other fully deterministic.

For illustrating the procedure when models involve diffusion terms, we consider the Fokker-Planck equation

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \Psi) + \nabla_a \cdot (\dot{\mathbf{a}} \Psi) = -\nabla_x \cdot \mathbf{q}_x - \nabla_a \cdot \mathbf{q}_a, \quad (2.163)$$

where $\mathbf{q}_x$ and $\mathbf{q}_a$ are two diffusive fluxes operating in the physical and conformational spaces respectively, both modeled from a Fick-type law:

$$\begin{cases} \mathbf{q}_x = -\mathbf{D}_x \cdot \nabla_x \Psi \\ \mathbf{q}_a = -\mathbf{D}_a \cdot \nabla_a \Psi \end{cases} \quad (2.164)$$

- Within the stochastic framework, diffusion terms can be modeled from appropriate random variables within a Lagrangian or a Eulerian description, the last one known as Brownian Configurations Fields (BCF). Both approaches were considered in our former works on the solution of Fokker-Planck equations [8, 69]. Within the Lagrangian stochastic framework and starting from the initial cloud of computational particles $\mathcal{P}_{ij}$ representing the initial distribution $\Psi(\mathbf{x}, t = 0, \mathbf{a})$, the simplest particles updating reads

$$\begin{cases} \mathbf{x}_{ij}(t_{n+1}) = \mathbf{x}_{ij}(t_n) + \mathbf{v}(\mathbf{x}_{ij}(t_n)) \Delta t + \mathcal{R}_x(\Delta t) \\ \mathbf{a}_{ij}(t_{n+1}) = \mathbf{a}_{ij}(t_n) + \dot{\mathbf{a}}_{ij}(\mathbf{a}_{ij}(t_n), \mathbf{x}_{ij}(t_n)) \Delta t + \mathcal{R}_a(\Delta t) \end{cases}, \quad (2.165)$$

where Δt is the time step and both random updates $\mathcal{R}_x$ and $\mathcal{R}_a$ depend on the chosen time step (see [53] for more details as well as for advanced stochastic integrations).

Obviously, because of the random effects operating in the physical space, the $\mathcal{M}$ particles initially located at each position $\mathbf{x}_j^0$, $j = 1, \dots, \mathcal{Q}$, will follow different trajectories in the physical space along the simulation. In order to obtain accurate enough results, we must consider a rich enough representation, that is, a large population of particles. For this purpose, we must consider large enough $\mathcal{M}$ and $\mathcal{Q}$. The large number of particles to be tracked seems a disadvantage of the approach at first sight, but it must be noticed that the integration of each particle is completely

independent of all the others, making possible the use of HPC on massively parallel computing platforms.

- The technique introduced for treating purely advective equations can be extended for considering diffusion contributions as was described in [5] and that we revisit in what follows, within a fully deterministic approach. Eq. (2.163) can be rewritten as:

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot \left(\left(\mathbf{v} + \frac{\mathbf{q}_x}{\Psi} \right) \Psi \right) + \nabla_a \cdot \left(\left(\dot{\mathbf{a}} + \frac{\mathbf{q}_a}{\Psi} \right) \Psi \right) = 0, \quad (2.166)$$

or

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\tilde{\mathbf{v}} \Psi) + \nabla_a \cdot (\dot{\tilde{\mathbf{a}}} \Psi) = 0, \quad (2.167)$$

where the effective velocities $\tilde{\mathbf{v}}$ and $\dot{\tilde{\mathbf{a}}}$ are given by:

$$\begin{cases} \tilde{\mathbf{v}} = \mathbf{v} - \frac{1}{\Psi} \mathbf{D}_x \cdot \nabla_x \Psi \\ \dot{\tilde{\mathbf{a}}} = \dot{\mathbf{a}} - \frac{1}{\Psi} \mathbf{D}_a \cdot \nabla_a \Psi \end{cases} \quad (2.168)$$

Now, the integration scheme (2.161) can be applied by replacing material and conformation velocities, $\mathbf{v}$ and $\dot{\mathbf{a}}$, by their effective counterparts $\tilde{\mathbf{v}}$ and $\dot{\tilde{\mathbf{a}}}$:

$$\begin{cases} \mathbf{x}_{ij}(t) = \mathbf{x}_{ij}^0 + \int_{\tau=0}^{\tau=t} \tilde{\mathbf{v}}(\mathbf{x}_{ij}(\tau)) d\tau \\ \mathbf{a}_{ij}(t) = \mathbf{a}_{ij}^0 + \int_{\tau=0}^{\tau=t} \dot{\tilde{\mathbf{a}}}(\mathbf{a}_{ij}(\tau), \mathbf{x}_{ij}(\tau)) d\tau \end{cases} \quad (2.169)$$

This fully deterministic particle description requires much less particles than its stochastic counterpart, but as noticed in Eq. (2.168), the calculation of the effective material and conformational velocities requires the derivative of the pdf Ψ with respect to both the physical and the conformational coordinates. To do so, the distribution must be reconstructed all along the simulation (at each time step), which constitutes a serious drawback for its implementation on massively parallel computing platforms. Moreover, to make possible the calculation of the distribution derivatives, the Dirac distribution must be regularized in order to ensure its derivability.

2.5.1.2 Separated Representations for Solving Diffusion-Dominated Problems

When the diffusion effects are dominant, the techniques presented in the previous section become inefficient because they require an excessive number of particles to produce accurate enough results, in particular for reconstructing the distribution. In this case, standard mesh-based discretizations seem a better choice. However, as discussed before, mesh-based discretizations fail when addressing highly dimensional models as it is the case when addressing the solution of the previous introduced Fokker-Planck equation. Separated representations seem the most appealing choice.

Considering the Fokker-Planck equation

$$\begin{aligned} \frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \Psi) + \nabla_a \cdot (\dot{\mathbf{a}} \Psi) \\ = \nabla_x \cdot (\mathbf{D}_x \cdot \nabla_x \Psi) + \nabla_a \cdot (\mathbf{D}_a \cdot \nabla_a \Psi), \end{aligned} \quad (2.170)$$

there are many separated representation choices. The most natural one consists in separating time, physical and conformational spaces, i.e.

$$\Psi(\mathbf{x}, t, \mathbf{a}) \approx \sum_{i=1}^N X_i(\mathbf{x}) \cdot T_i(t) \cdot A_i(\mathbf{a}). \quad (2.171)$$

Thus, when proceeding with the Proper Generalized Decomposition—PGD—constructor [43], we must solve of the order of N 2D or 3D (depending on the dimension of the physical space) boundary value problems—BVP—for calculating functions $X_i(\mathbf{x})$, the same number of 1D initial value problems—IVP—for calculating functions $T_i(t)$, and finally the same number of 2D or 5D (the number of components of tensor $\mathbf{a}$ in the 2D or 3D case, where the symmetry and its unit trace has been taking into account) BVP for calculating functions $A_i(\mathbf{a})$. A discussion of the difficulties related to the solution of the former multidimensional problems involving the conformational coordinates was addressed in [44].

2.5.2 Descriptions Based on Higher-Order Kinematics

The models proposed until now consider a first-order kinematics, that is, a constant velocity gradient at the particle scale. However, when the kinematics become rich enough or the particle size becomes large with respect to the characteristic flow dimension, first-order modeling must be enriched. In what follows, we address its extension to second and third-gradient flow kinematics.

2.5.2.1 Second-Gradient Description with Concentrated Forces at the Rod Beads

We now consider a rod $\mathcal{R}$ but with a higher-order description of the fluid velocity field at the rod scale. Again, forces applied on each bead $\mathbf{F}$ depend on the difference of velocities between the fluid and the bead, the first one now including the second-order velocity gradient $\mathbf{H}$ according to $\mathbf{v}(\mathbf{p}L) = \mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) L^2$ and the second one given by $\mathbf{v}_G + \dot{\mathbf{p}}L$. Thus, the force $\mathbf{F}(\mathbf{p}L)$ reads:

$$\mathbf{F}(\mathbf{p}L) = \xi (\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) L^2 - \mathbf{v}_G - \dot{\mathbf{p}}L), \quad (2.172)$$

where the third-order tensor $\mathbf{H}$ is defined by $\mathbf{H}_{ijk} = \frac{1}{2} \frac{\partial^2 \mathbf{v}_i}{\partial x_j \partial x_k}$.

Obviously, if $\mathbf{F}$ applies on the bead $\mathbf{p}L$, then at the opposite bead $-\mathbf{p}L$ the resulting force reads

$$\mathbf{F}(-\mathbf{p}L) = \xi (\mathbf{v}_0 - \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) L^2 - \mathbf{v}_G + \dot{\mathbf{p}}L). \quad (2.173)$$

By adding Eqs. (2.172) and (2.173) and enforcing the force balance, neglecting again inertial effects, we obtain

$$\mathbf{F}(\mathbf{p}L) + \mathbf{F}(-\mathbf{p}L) = \mathbf{0}, \quad (2.174)$$

than implies $\mathbf{v}_0 - \mathbf{v}_G = -(\mathbf{H} : (\mathbf{p} \otimes \mathbf{p}))L^2$, that is, the rod center of gravity has a relative velocity with respect to the fluid at this position.

Remark 4 The fact of having obtained a non-zero relative velocity $\mathbf{v}_0 - \mathbf{v}_G \neq \mathbf{0}$ does not imply the existence of a migration mechanism, as proved in [45, 70] and [71].

Since the resulting torque must also vanish, the only possibility is that force $\mathbf{F}$ acts along $\mathbf{p}$, that is $\mathbf{F} = \lambda \mathbf{p}$, with $\lambda \in \mathbb{R}$. Thus we can write

$$\lambda \mathbf{p} = \xi (\nabla \mathbf{v} \cdot \mathbf{p}L - \dot{\mathbf{p}}L), \quad (2.175)$$

which yields the same Jeffery equation that was obtained when considering the first-order velocity gradient:

$$\dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}. \quad (2.176)$$

The forces being again aligned in the rod direction, one could infer that the second gradient does not suffice for activating bending mechanisms.

Until now, forces were assumed applied at the rod ends (beads). However, we can distribute them all along the rod length as commonly considered when calculating particles motion by using DPD (dissipative particle dynamics) methods.

In the next section, we consider forces applied all along the rod length as was considered in [70]. We prove that as soon as a second-gradient description is retained, bending mechanism appears naturally.

2.5.2.2 Second-Gradient Description of Rods with Distributed Forces

We consider now the system illustrated in Fig. 2.11 consisting of a rod $\mathcal{R}$ and the hydrodynamical forces applied all along its length. With the same reasoning and notation as above, the applied distributed force $\mathbf{f}(s)$ at position $s\mathbf{p}$, $s \in [-L, L]$ reads

$$\mathbf{f}(s) = \bar{\xi} (\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}s + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p}))s^2 - \mathbf{v}_G - \dot{\mathbf{p}}s). \quad (2.177)$$

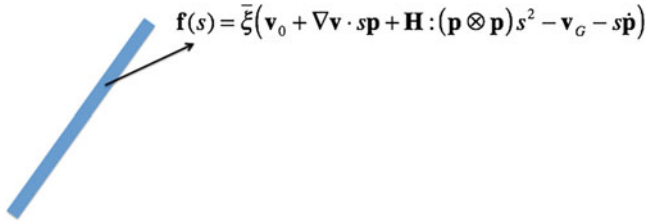


Fig. 2.11 Distributed hydrodynamic forces applied on a rod immersed in a Newtonian fluid, considering the second-order velocity gradient

The resultant force $\mathbf{F}$ must vanish, that is

$$\mathbf{F} = \int_{-L}^{+L} \mathbf{f}(s) ds = \mathbf{0}, \quad (2.178)$$

that leads to the following expression for the sliding velocity (rod-fluid relative velocity at the rod center of gravity):

$$\mathbf{v}_0 - \mathbf{v}_G = -\frac{L^2}{3} (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})). \quad (2.179)$$

Thus, the distributed force reads:

$$\mathbf{f}(s) = \bar{\xi} \left(\nabla \mathbf{v} \cdot \mathbf{p}s + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) \left(s^2 - \frac{L^2}{3} \right) - \dot{\mathbf{p}}s \right), \quad (2.180)$$

which leads to the moment $\mathbf{m}(s)$

$$\mathbf{m}(s) = s\mathbf{p} \times \bar{\xi} \left(\nabla \mathbf{v} \cdot \mathbf{p}s + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) \left(s^2 - \frac{L^2}{3} \right) - \dot{\mathbf{p}}s \right), \quad (2.181)$$

from which we can evaluate the resultant moment $\mathbf{M}$

$$\mathbf{M} = \int_{-L}^{+L} \mathbf{m}(s) ds = \mathbf{p} \times \bar{\xi} \alpha (\nabla \mathbf{v} \cdot \mathbf{p} - \dot{\mathbf{p}}) = \mathbf{0}, \quad (2.182)$$

with $\alpha = \int_{-L}^{+L} s^2 ds = \frac{2}{3}L^3$. This again yields Jeffery's equation

$$\dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \quad (2.183)$$

i.e. the same equation as that obtained by assuming forces applied at the rod beads.

Introducing Jeffery's equation (2.183) into the distributed force expression (2.180), we obtain

$$\mathbf{f}(s) = \bar{\xi} \left((\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) \left(s^2 - \frac{L^2}{3} \right) + (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p} s \right). \quad (2.184)$$

This force can be decomposed into two components, i.e. one, $\mathbf{f}^{\parallel}(s)$, aligned with the rod and the other, $\mathbf{f}^{\perp}(s)$, perpendicular to it:

$$\mathbf{f}^{\parallel}(s) = \bar{\xi} \left((\mathbf{H} \cdot : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) \mathbf{p} \left(s^2 - \frac{L^2}{3} \right) + (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p} s \right), \quad (2.185)$$

and

$$\mathbf{f}^{\perp}(s) = \bar{\xi} \left((\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) - (\mathbf{H} \cdot : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) \mathbf{p} \right) \left(s^2 - \frac{L^2}{3} \right). \quad (2.186)$$

Remark 5 We can notice from Eq. (2.186) that, when considering distributed forces within a first-gradient description ($\mathbf{H} = \mathbf{0}$), the perpendicular component of the resulting distributed forces vanishes, i.e. $\mathbf{f}^{\perp}(s) = \mathbf{0}$ and bending mechanisms are once again absent. However, bending seems possible as soon as second-gradient descriptions implying $\mathbf{H} \neq \mathbf{0}$ are retained.

The resultant axial force $\mathbf{F}^{\parallel}$ reads

$$\mathbf{F}^{\parallel} = \int_0^L \mathbf{f}^{\parallel}(s) ds = \bar{\xi} \frac{L^2}{2} (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \quad (2.187)$$

expression that corresponds to the one obtained in the case of concentrated forces if we consider the following relation between the distributed and concentrated friction coefficients:

$$\xi = \frac{L}{2} \bar{\xi}. \quad (2.188)$$

The main difference with respect to the situation in which forces were assumed applied at the rod beads, occurs when considering the distributed force perpendicular to the rod. In this case

$$\mathbf{F}^{\perp} = \int_0^L \mathbf{f}^{\perp}(s) ds = \mathbf{0}, \quad (2.189)$$

in agreement with the results found when considering concentrated forces, but the distributed force implies the existence of a bending moment $\mathcal{M}(s)\mathbf{k}$ (acting in the out-of-plane direction defined by the unit vector $\mathbf{k}$)

$$\mathcal{M}(s)\mathbf{k} = \int_s^L (r-s)\mathbf{p} \times \mathbf{f}^\perp(r) dr. \quad (2.190)$$

When the rod is rigid there are no major consequences, but in the case of flexible rods this force creates rod bending with the associated elastic effects.

Remark 6 In the case of elastic rods, the bending moment implies rod curvature. Within the small strain and displacement hypotheses, the curvature is given by

$$\frac{d^2 u}{ds^2} = \frac{\mathcal{M}(s)}{EI}, \quad (2.191)$$

where $u(s)$ is the rod deflection with respect to its undeformed configuration, E the elastic modulus and I the moment of area of the rod cross section with respect to the out-of-plane direction. By integrating this equation twice, we can obtain the rod bent configuration that, as expected, is symmetric with respect to the rod center of gravity.

2.5.2.3 Third-Gradient Description

Now, we assume that the forces $\mathbf{F}$ that act on each bead depend again on the difference of velocities between the fluid and the bead, but the former now including the third-order velocity gradient $\mathbf{J}$, i.e. that implies the fluid velocity at the bead position given by $\mathbf{v}(\mathbf{p}L) = \mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) L^2 + (\mathbf{J} \cdot : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) L^3$ and the second one by $\mathbf{v}_G + \dot{\mathbf{p}}L$. Thus, the force $\mathbf{F}(\mathbf{p}L)$ reads (see Fig. 2.12):

$$\begin{aligned} \mathbf{F}(\mathbf{p}L) = & \xi (\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) L^2 \\ & + (\mathbf{J} \cdot : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) L^3 - \mathbf{v}_G - \dot{\mathbf{p}}L), \end{aligned} \quad (2.192)$$

where the third-order velocity gradient $\mathbf{J}$ is the fourth-rank tensor with components $\mathbf{J}_{ijklm} = \frac{1}{6} \frac{\partial^3 \mathbf{v}_i}{\partial x_j \partial x_k \partial x_m}$.

Obviously, if $\mathbf{F}$ acts on the bead $\mathbf{p}L$, then for the opposite bead at $-\mathbf{p}L$ the resulting force reads

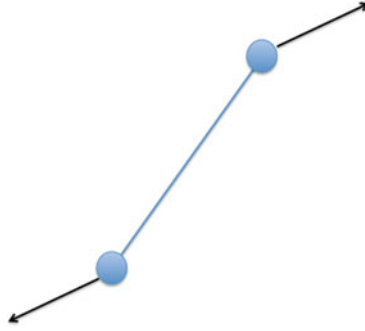
$$\begin{aligned} \mathbf{F}(-\mathbf{p}L) = & \xi (\mathbf{v}_0 - \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})) L^2 \\ & - (\mathbf{J} \cdot : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) L^3 - \mathbf{v}_G + \dot{\mathbf{p}}L). \end{aligned} \quad (2.193)$$

By adding Eqs. (2.192) and (2.193) and enforcing the force balance

$$\mathbf{F}(\mathbf{p}L) + \mathbf{F}(-\mathbf{p}L) = \mathbf{0}, \quad (2.194)$$

Fig. 2.12 Hydrodynamic forces acting on a rod immersed in a Newtonian fluid, considering the third-order velocity gradient

$$\mathbf{F} = \xi \left(\mathbf{v}_0 + \nabla \mathbf{v} \cdot L\mathbf{p} + \mathbf{H} : (\mathbf{p} \otimes \mathbf{p}) L^2 + \mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p}) L^3 - L\dot{\mathbf{p}} \right)$$



we obtain again $\mathbf{v}_0 - \mathbf{v}_G = -\left(\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})\right) L^2$.

As the resulting torque must also vanish, the only possibility is that the force $\mathbf{F}$ acts along $\mathbf{p}$, that is $\mathbf{F} = \lambda \mathbf{p}$, with $\lambda \in \mathbb{R}$. Thus, we can write

$$\lambda \mathbf{p} = \xi \left(\nabla \mathbf{v} \cdot \mathbf{p} L + (\mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) L^3 - \dot{\mathbf{p}} L \right), \quad (2.195)$$

which multiplied by $\mathbf{p}$ yields an expression of λ :

$$\lambda = \xi L \left(\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p}) + L^2 (\mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) \right). \quad (2.196)$$

We thus have

$$\begin{aligned} \mathbf{F} = \lambda \mathbf{p} = \xi L & \left(\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p}) \mathbf{p} \right. \\ & \left. + L^2 (\mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) \mathbf{p} \right), \end{aligned} \quad (2.197)$$

which yield the rotary velocity

$$\begin{aligned} \dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p} & + L^2 (\mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) \\ - (\mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \end{aligned} \quad (2.198)$$

where we can identify Jeffery's contribution $\dot{\mathbf{p}}^J$ and a third-order correction $\dot{\mathbf{p}}^{Th}$ that is affected by L^2 :

$$\dot{\mathbf{p}}^J = \nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \quad (2.199)$$

and

$$\dot{\mathbf{p}}^{Th} = \mathbf{J} \cdot : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p}) - (\mathbf{J} :: (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p}))\mathbf{p}, \quad (2.200)$$

with the total rotary velocity given by:

$$\dot{\mathbf{p}} = \dot{\mathbf{p}}^J + L^2 \dot{\mathbf{p}}^{Th}. \quad (2.201)$$

2.5.3 Accounting for Rod Bending

In this section, inspired from second-order fluids, we extend this higher-order framework to higher-order rod suspensions.

2.5.3.1 Second-Gradient Fluid Description

Within the first-gradient formulation, the internal power for a Newtonian fluid $\mathcal{W}_{int}$ reads

$$\mathcal{W}_{int} = \int_{\Omega} \mathbf{T} : \nabla \mathbf{v} \, d\mathbf{x}, \quad (2.202)$$

where $\mathbf{T} = -p\mathbf{I} + \tau$ with $\tau = 2\eta\mathbf{D}$. The associated balance of momentum reads:

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T}. \quad (2.203)$$

Fried and Gurtin [72] proposed a second-gradient formulation involving the vorticity gradient. They proposed a non-standard form of the principle of virtual power with the internal power given by

$$\mathcal{W}_{int} = \int_{\Omega} \mathbf{T} : \nabla \mathbf{v} \, d\mathbf{x} + \int_{\Omega} \mathbf{G} : \nabla \boldsymbol{\omega} \, d\mathbf{x}, \quad (2.204)$$

where $\boldsymbol{\omega}$ is the vorticity vector

$$\boldsymbol{\omega} = \nabla \times \mathbf{v}, \quad (2.205)$$

and $\mathbf{G}$ is the so-called hyper-stress. The associated generalized momentum balance reads:

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \nabla \times (\nabla \cdot \mathbf{G}). \quad (2.206)$$

The following constitutive equation was assumed in [73] for the fluid hyper-stress:

$$\mathbf{G} = \eta \mathcal{L}_f^2 \left(\nabla \boldsymbol{\omega} + \iota (\nabla \boldsymbol{\omega})^T \right), \quad (2.207)$$

where the parameter $\iota \in [-1, 1]$ controls the asymmetry of the hyper-stress and ensures a non-negative dissipation. In the previous equation $\mathcal{L}_f^2 > 0$ is known as the fluid gradient length.

In the case of an incompressible fluid, the introduction of both the stress and the hyper-stress constitutive equations into the generalized momentum balance leads to:

$$\rho \dot{\mathbf{v}} = -\nabla p + \eta \Delta \left(\mathbf{v} - \mathcal{L}_f^2 \Delta \mathbf{v} \right). \quad (2.208)$$

where $\eta \mathcal{L}_f^2$ represents the so-called hyper-viscosity [73].

See [73] for a discussion on the associated boundary conditions. The higher-order velocity derivatives involved in Eq. (2.208) require the enforcement of a larger number of boundary conditions compared to the standard first-gradient formulation.

2.5.3.2 Second-Gradient Description of a Dilute Suspension of Flexible Rods

Inspired by the use of the vorticity $\boldsymbol{\omega}$ in the above second-gradient fluid flow description, we consider now the rod beads being subjected to two actions, as depicted in Fig. 2.13:

- A hydrodynamic force $\mathbf{F}$ that depends on the difference of velocities between the fluid and the bead. The fluid velocity at the bead position $\mathbf{v}(\mathbf{p}L)$ taking into account second-gradient effects reads

$$\mathbf{v}(\mathbf{p}L) = \mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + \mathbf{H} : (\mathbf{p} \otimes \mathbf{p})L^2. \quad (2.209)$$

The bead velocity is again given by $\mathbf{v}_G + \dot{\mathbf{p}}L$. Thus, the resulting hydrodynamic force reads

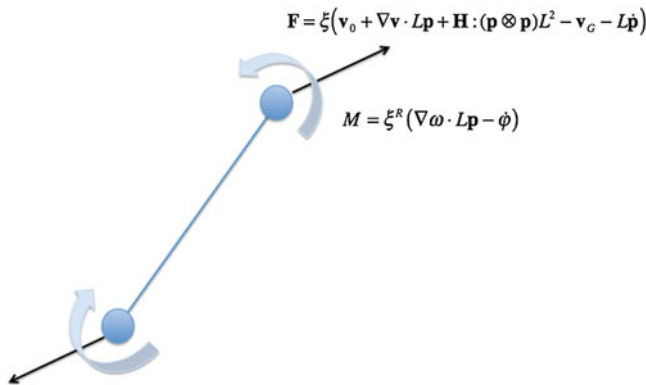


Fig. 2.13 Hydrodynamic forces applied on a flexible rod immersed in a Newtonian fluid

$$\mathbf{F}(\mathbf{p}L) = \xi (\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + \mathbf{H} : (\mathbf{p} \otimes \mathbf{p})L^2 - \mathbf{v}_G - \dot{\mathbf{p}}L). \quad (2.210)$$

- A hydrodynamic torque $\mathbf{M}$ that depends on the difference between the differential vorticity at the bead position and the bead rotary velocity $\dot{\boldsymbol{\phi}}$. The differential vorticity is the difference between the vorticity existing at the bead position minus the one existing at the rod center of gravity. This torque could have its origin in the distributed forces applied along the rod length as illustrated in Sect. 2.5.2.2.

Thus, the resulting torque reads

$$\mathbf{M}(\mathbf{p}L) = \xi^R (\nabla \boldsymbol{\omega} \cdot \mathbf{p}L - \dot{\boldsymbol{\phi}}(\mathbf{p}L)), \quad (2.211)$$

where ξ^R is the rotary friction coefficient.

A forces balance yields

$$\mathbf{v}_0 - \mathbf{v}_G = -\mathbf{H} : (\mathbf{p} \otimes \mathbf{p})L^2, \quad (2.212)$$

implying a second-order relative velocity of the rod center of gravity with respect to the fluid velocity at this position. Again, for notational simplicity, we consider $\mathbf{F} = \mathbf{F}(\mathbf{p}L) = -\mathbf{F}(-pL)$.

As soon as we consider a first gradient of the vorticity-based bending mechanism $\nabla \boldsymbol{\omega} \cdot \mathbf{p}L$, it is easy to prove [74] that the rod kinematics remains unchanged relative to Jeffery's model, and that this term only affects rod bending. Thus, we obtain:

- The standard expression of the forces applying on the rod beads:

$$\mathbf{F} = \xi L (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \quad (2.213)$$

- Jeffery's rod kinematics:

$$\dot{\mathbf{p}} = \nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \quad (2.214)$$

- The bending mechanism. Being $\dot{\boldsymbol{\phi}} = \dot{\boldsymbol{\phi}}(\mathbf{p}L) = -\dot{\boldsymbol{\phi}}(-pL)$ [74] and assuming a linear elastic behavior of the rod, the relation between the applied torque $\mathbf{M}$ and the bending angle $\boldsymbol{\phi}$ at the rod bead is given by

$$\boldsymbol{\phi} = \frac{L}{EI} \mathbf{M}, \quad (2.215)$$

or

$$\mathbf{M} = \frac{EI}{L} \boldsymbol{\phi} = \kappa \boldsymbol{\phi}, \quad (2.216)$$

where E is the elastic modulus and I the moment of area of the rod cross section.

Introducing the expression of the moment $\mathbf{M}$ (2.211) into Eq. (2.216), we obtain

$$\xi^R (\nabla \boldsymbol{\omega} \cdot \mathbf{p} L - \dot{\boldsymbol{\varphi}}) = \kappa \boldsymbol{\varphi}, \quad (2.217)$$

whose integration allows calculating $\boldsymbol{\varphi}(t)$ and from it the moment $\mathbf{M}$.

Remark 7 It is noteworthy that:

- In first-gradient flows, rods orient according to Jeffery's equation without experiencing bending effects because the vorticity gradient vanishes.
- In second-order flows, rods orient according to Jeffery's equation experiencing a bending induced by the second gradient.
- In rigid kinematics, a rod moves with the fluid without experiencing any relative movement. Since the vorticity gradient vanishes, there are no bending effects, ensuring the formulation objectivity.

The rod kinematics are then fully described by $\mathbf{p}$ and $\boldsymbol{\varphi}$. Knowing $\mathbf{p}$, we can locate both rod beads. Then, knowing the bead bending angle $\boldsymbol{\varphi}$ and all the forces and moments being applied at both ends, the deformed rod configuration is parabolic and symmetric with respect to the center of gravity. Thus, from $(\mathbf{p}$ and $\boldsymbol{\varphi})$, we can predict the bent configuration.

The stress has two components, the standard one and the one related to the hyper-stress. The first one is related to forces applied at both opposite beads acting in the rod direction and includes the suspending medium contribution $\tau^f = 2\eta \mathbf{D}$:

$$\begin{aligned} \tau &= \tau^f + \tau^r = 2\eta \mathbf{D} + \sum_{i=1}^N \mathbf{p}_i \otimes \mathbf{F}_i \\ &= 2\eta \mathbf{D} + \beta \nabla \mathbf{v} : \left(\sum_{i=1}^N \mathbf{p}_i \otimes \mathbf{p}_i \otimes \mathbf{p}_i \otimes \mathbf{p}_i \right), \end{aligned} \quad (2.218)$$

with the total stress $\mathbf{T}$ given by

$$\mathbf{T} = -p \mathbf{I} + \tau, \quad (2.219)$$

which, as expected, is symmetric.

The second one is related to second-gradient fluid contribution and rod bending. We consider a partition of the total hyper-stress $\mathbf{G}$ consisting of the fluid $\mathbf{G}^f$ and the rods $\tilde{\mathbf{G}}^r$ contributions, with $\mathbf{G} = \mathbf{G}^f + \tilde{\mathbf{G}}^r$.

We consider a standard form of the second-gradient fluid contribution $\mathbf{G}^f$,

$$\mathbf{G}^f = \eta \mathcal{L}_f^2 \left(\nabla \boldsymbol{\omega} + \iota (\nabla \boldsymbol{\omega})^T \right), \quad (2.220)$$

where $\mathcal{L}_f^2$ is the fluid gradient length.

On the other hand, we compute the rod contribution to the hyper-stress $\mathbf{G}^r$ from

$$\mathbf{G}^r = \nu \sum_{i=1}^N \mathbf{p}_i \otimes \mathbf{M}_i, \quad (2.221)$$

from which we assume the more general form

$$\tilde{\mathbf{G}}^r = \mathbf{G}^r + \varsigma (\mathbf{G}^r)^T. \quad (2.222)$$

2.5.3.3 Mesoscopic Description

Making use of the orientation distribution function $\Psi(\mathbf{x}, t, \mathbf{p}, \boldsymbol{\varphi})$, we can proceed to the calculation of the stress within a continuous macroscopic description. Considering the stress expression (2.218) and the use of the quadratic closure relation $\mathbf{A} \approx \mathbf{a} \otimes \mathbf{a}$, we obtain:

$$\boldsymbol{\tau} = \boldsymbol{\tau}^f + \boldsymbol{\tau}^r = 2\eta \mathbf{D} + 2\eta N_p (\mathbf{D} : \mathbf{A}) \approx 2\eta \mathbf{D} + 2\eta N_p (\mathbf{D} : \mathbf{a}) \mathbf{a}, \quad (2.223)$$

with $\mathbf{T} = -p \mathbf{I} + \boldsymbol{\tau}$.

On the other hand, the hyper-stress is given by:

$$\mathbf{G}^r = \nu \int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \mathbf{M} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi}, \quad (2.224)$$

and, by using the expression of the moment,

$$\begin{aligned} \mathbf{G}^r &= \nu \kappa \int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \boldsymbol{\varphi} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi} \\ &= \tilde{\kappa} \int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \boldsymbol{\varphi} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi}. \end{aligned} \quad (2.225)$$

In the previous expressions, the distribution function $\Psi = \Psi(\mathbf{x}, t, \mathbf{p}, \boldsymbol{\varphi})$ (its dependence on the different coordinates is omitted for the sake of clarity) gives the fraction of rods that at position $\mathbf{x}$ and time t have a conformation given by $(\mathbf{p}, \boldsymbol{\varphi})$. The domains $\mathcal{S}$ and $\mathcal{C}$ refer respectively to the domains in which coordinates $\mathbf{p}$ and $\boldsymbol{\varphi}$ are defined.

Remark 8 One could expect that the moment (2.225) vanishes, however taking into account that $\Psi(\mathbf{p}, \boldsymbol{\varphi}) = \Psi(-\mathbf{p}, -\boldsymbol{\varphi})$, the integral does not vanish.

In order to close the formulation, we consider the second-order tensor $\mathbf{g}$ (such that $\mathbf{G}^r = \tilde{\kappa} \mathbf{g}$):

$$\mathbf{g} = \int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \boldsymbol{\varphi} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi}, \quad (2.226)$$

and compute its time derivative taking into account the expressions of $\dot{\mathbf{p}}$ (2.214) and $\dot{\boldsymbol{\varphi}}$ (2.217):

$$\begin{aligned}
 \dot{\mathbf{g}} &= \int_{\mathcal{S} \times \mathcal{C}} (\dot{\mathbf{p}} \otimes \boldsymbol{\varphi} + \mathbf{p} \otimes \dot{\boldsymbol{\varphi}}) \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi} \\
 &= \int_{\mathcal{S} \times \mathcal{C}} (\nabla \mathbf{v} \cdot \mathbf{p} - (\nabla \mathbf{v} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}) \otimes \boldsymbol{\varphi} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi} \\
 &\quad + \int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \left(\nabla \boldsymbol{\omega} \cdot \mathbf{p} L - \frac{\kappa}{\xi^R} \boldsymbol{\varphi} \right) \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi} \\
 &= \nabla \mathbf{v} \cdot \mathbf{g} - \nabla \mathbf{v} : \left(\int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \boldsymbol{\varphi} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi} \right) \\
 &\quad + L \mathbf{a} \cdot (\nabla \boldsymbol{\omega})^T - \frac{\kappa}{\xi^R} \mathbf{g}.
 \end{aligned} \tag{2.227}$$

If we adopt the following closure relation:

$$\int_{\mathcal{S} \times \mathcal{C}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \boldsymbol{\varphi} \Psi \, d\mathbf{p} \, d\boldsymbol{\varphi} \approx \mathbf{a} \otimes \mathbf{g}, \tag{2.228}$$

then we obtain a closed form for the evolution of $\mathbf{g}$:

$$\dot{\mathbf{g}} = \nabla \mathbf{v} \cdot \mathbf{g} - (\nabla \mathbf{v} : \mathbf{a}) \mathbf{g} + L \mathbf{a} \cdot (\nabla \boldsymbol{\omega})^T - \frac{\kappa}{\xi^R} \mathbf{g}. \tag{2.229}$$

Multiplying Eq. (2.229) by $\tilde{\kappa}$, we obtain the time evolution of the contribution of rods to the hyper-stress:

$$\dot{\mathbf{G}}^r = \nabla \mathbf{v} \cdot \mathbf{G}^r - (\nabla \mathbf{v} : \mathbf{a}) \mathbf{G}^r + L \tilde{\kappa} \mathbf{a} \cdot (\nabla \boldsymbol{\omega})^T - \frac{\kappa}{\xi^R} \mathbf{G}^r. \tag{2.230}$$

If we consider the coefficient affecting the vorticity gradient in Eq. (2.230) and take into account the relations $\tilde{\kappa} = \nu \kappa$ and $\kappa = EI/L$, we obtain

$$L \tilde{\kappa} = E(\nu I) = E \mathcal{L}_r^2, \tag{2.231}$$

where $\mathcal{L}_r^2$ represents the rod gradient length. The last term in equation (2.230) involves the coefficient κ/ξ^R with reciprocal time units, which, in absence of flow, controls the relaxation to the undeformed reference configuration. Thus, the inverse of this coefficient has the meaning of a relaxation time that we denote by $\mathcal{T}$. Moreover, taking into account the symmetry of tensor $\mathbf{a}$, we have $\nabla \mathbf{v} : \mathbf{a} = \mathbf{D} : \mathbf{a}$. Thus, Eq. (2.230) can be rewritten as

$$\dot{\mathbf{G}}^r = \nabla \mathbf{v} \cdot \mathbf{G}^r - (\mathbf{D} : \mathbf{a}) \mathbf{G}^r + E \mathcal{L}_r^2 \mathbf{a} \cdot (\nabla \boldsymbol{\omega})^T - \frac{1}{\mathcal{T}} \mathbf{G}^r. \tag{2.232}$$

It is important to notice that the above equation involves two closure relations, the one related to the fourth-order orientation tensor $\mathbf{A}$ and the one expressed in Eq. (2.228).

The macroscopic flow model can thus be summarized as follows:

- Generalized momentum balance:

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \nabla \times (\nabla \cdot \mathbf{G}), \quad (2.233)$$

- Mass balance

$$\nabla \cdot \mathbf{v} = 0, \quad (2.234)$$

- Constitutive equation:

$$\mathbf{T} = -p \mathbf{I} + \boldsymbol{\tau}, \quad (2.235)$$

with $\boldsymbol{\tau} = \boldsymbol{\tau}^f + \boldsymbol{\tau}^r$:

$$\boldsymbol{\tau}^f = 2\eta \mathbf{D}, \quad (2.236)$$

and

$$\boldsymbol{\tau}^r = 2\eta N_p (\nabla \mathbf{v} : \mathbf{a}) \mathbf{a} = 2\eta N_p (\mathbf{D} : \mathbf{a}) \mathbf{a}, \quad (2.237)$$

- Hyper-stress $\mathbf{G} = \mathbf{G}^f + \tilde{\mathbf{G}}^r$:

$$\mathbf{G}^f = \eta \mathcal{L}_f^2 \left(\nabla \boldsymbol{\omega} + \iota (\nabla \boldsymbol{\omega})^T \right), \quad (2.238)$$

and

$$\tilde{\mathbf{G}}^r = \mathbf{G}^r + \varsigma (\mathbf{G}^r)^T, \quad (2.239)$$

with

$$\dot{\mathbf{G}}^r = \nabla \mathbf{v} \cdot \mathbf{G}^r - (\mathbf{D} : \mathbf{a}) \mathbf{G}^r + E \mathcal{L}_r^2 \mathbf{a} \cdot (\nabla \boldsymbol{\omega})^T - \frac{1}{\mathcal{J}} \mathbf{G}^r. \quad (2.240)$$

2.5.4 Delaying Orientation Mechanisms

While the models proposed until now allowed the introduction of rod bending mechanisms, the rotary velocity remained unchanged however. In this section, we propose alternative models able to control the rod rotary velocity.

A simple proposals consists in considering rods subjected to three actions:

1. The hydrodynamic force, which reads as in previous sections

$$\mathbf{F}(\mathbf{p}L) = \xi (\mathbf{v}_0 + \nabla \mathbf{v} \cdot \mathbf{p}L + (\mathbf{H} : (\mathbf{p} \otimes \mathbf{p}))L^2 - \mathbf{v}_G - \dot{\mathbf{p}}L). \quad (2.241)$$

2. A torque acting at each bead involving the first gradient of potential $\mathcal{V}$. Thus, the resulting torque at bead $\mathbf{p}L$ reads

$$\mathbf{M}(\mathbf{p}L) = \xi^I (\nabla \mathcal{V} \cdot \mathbf{p}L - \dot{\boldsymbol{\phi}}(\mathbf{p}L)). \quad (2.242)$$

3. A torque $\mathcal{M}$ at the rod centre of gravity scaling with the difference between $\mathcal{V}$ and the objective rotary velocity $\dot{\boldsymbol{\theta}} - \boldsymbol{\omega}$,

$$\mathcal{M} = \xi^R (\mathcal{V} - (\dot{\boldsymbol{\theta}} - \boldsymbol{\omega})). \quad (2.243)$$

Here, $\boldsymbol{\omega}$ is the vorticity: $\boldsymbol{\omega} = \nabla \times \mathbf{v}$, such that $\boldsymbol{\omega} \times \mathbf{p} = \boldsymbol{\Omega} \cdot \mathbf{p}$, with $\boldsymbol{\Omega}$ the antisymmetric component of the velocity gradient.

A force balance yields again

$$\mathbf{v}_0 - \mathbf{v}_G = -\mathbf{H} : (\mathbf{p} \otimes \mathbf{p}) L^2. \quad (2.244)$$

By enforcing the moment balance, we obtain

$$2L\mathbf{p} \times \mathbf{F} + \mathcal{M} + \mathbf{M}(\mathbf{p}L) + \mathbf{M}(-\mathbf{p}L) = \mathbf{0}, \quad (2.245)$$

which reads

$$2\xi L^2 (\mathbf{p} \times \nabla \mathbf{v} \cdot \mathbf{p} - \dot{\boldsymbol{\theta}}) + \xi^R (\mathcal{V} - (\dot{\boldsymbol{\theta}} - \boldsymbol{\omega})) - \xi^I (\dot{\boldsymbol{\phi}}(\mathbf{p}L) + \dot{\boldsymbol{\phi}}(-\mathbf{p}L)) = \mathbf{0}. \quad (2.246)$$

Taking into account $\mathbf{p} \times \boldsymbol{\Omega} \cdot \mathbf{p} = \mathbf{p} \times \boldsymbol{\omega} \times \mathbf{p} = \boldsymbol{\omega}$, we obtain the rod rotary velocity

$$\begin{aligned} \dot{\boldsymbol{\theta}} = & \boldsymbol{\omega} + \frac{2\xi L^2}{2\xi L^2 + \xi^R} (\mathbf{p} \times \mathbf{D} \cdot \mathbf{p}) \\ & + \frac{\xi^R}{2\xi L^2 + \xi^R} \mathcal{V} - \frac{2\xi^I}{2\xi L^2 + \xi^R} \bar{\boldsymbol{\phi}}, \end{aligned} \quad (2.247)$$

with $\mathbf{D}$ being the symmetric component of the velocity gradient and $\bar{\boldsymbol{\phi}} = \frac{\dot{\boldsymbol{\phi}}(\mathbf{p}L) + \dot{\boldsymbol{\phi}}(-\mathbf{p}L)}{2}$.

The previous equation can be rewritten as:

$$\begin{aligned} \dot{\mathbf{p}} = & \boldsymbol{\Omega} \cdot \mathbf{p} + \frac{2\xi L^2}{2\xi L^2 + \xi^R} (\mathbf{D} \cdot \mathbf{p} - (\mathbf{D} : (\mathbf{p} \otimes \mathbf{p}))\mathbf{p}) \\ & + \frac{\xi^R}{2\xi L^2 + \xi^R} \mathcal{V} \times \mathbf{p} - \frac{2\xi^I}{2\xi L^2 + \xi^R} \bar{\boldsymbol{\phi}} \times \mathbf{p}, \end{aligned} \quad (2.248)$$

where it can be noticed that the objectivity is ensured, and for that, consideration of the relative velocity $(\dot{\boldsymbol{\theta}} - \boldsymbol{\omega})$ in the expression of $\mathcal{M}$ was a key choice.

Remark 9 With $\xi^R = \xi^I = 0$, we recover the Jeffery kinematics. With $\xi^I = 0$, we remove elastic effects but the Jeffery kinematics are affected when considering ξ^R large enough. In the case of $\xi^R \gg 2\xi L^2$ (or $\xi^R \rightarrow \infty$), we obtain

$$\dot{\mathbf{p}} \approx \boldsymbol{\Omega} \cdot \mathbf{p} + \boldsymbol{\Upsilon} \times \mathbf{p} = (\boldsymbol{\omega} + \boldsymbol{\Upsilon}) \times \mathbf{p}. \quad (2.249)$$

When $\boldsymbol{\Upsilon} = -\boldsymbol{\omega}$, rods can translate without rotating at all. On the other hand, if $\boldsymbol{\Upsilon} = \mathbf{0}$, we obtain rigid kinematics with $\dot{\mathbf{p}} = \boldsymbol{\Omega} \cdot \mathbf{p}$ governed by the flow vorticity.

The force acting on the bead reads

$$\begin{aligned} \mathbf{F}(\mathbf{p}L) = & \xi L \left(\mathbf{D} \cdot \mathbf{p} \left(1 - \frac{2\xi L^2}{2\xi L^2 + \xi^R} \right) + \frac{2\xi L^2}{2\xi L^2 + \xi^R} (\mathbf{D} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p} \right) \\ & - \frac{\xi^R \xi L}{2\xi L^2 + \xi^R} \boldsymbol{\Upsilon} \times \mathbf{p} + \frac{2\xi^I \xi L}{2\xi L^2 + \xi^R} \bar{\boldsymbol{\phi}} \times \mathbf{p}. \end{aligned} \quad (2.250)$$

The force applied on the beads has a component acting along the rod direction

$$\mathbf{F}^{\parallel}(\mathbf{p}L) = \xi L (\mathbf{D} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}, \quad (2.251)$$

and another perpendicular to it and contained in the plane in which the rod orientation is defined

$$\begin{aligned} \mathbf{F}^{\perp}(\mathbf{p}L) = & \frac{\xi^R \xi L}{2\xi L^2 + \xi^R} (\mathbf{D} \cdot \mathbf{p} - (\mathbf{D} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}) \\ & - \frac{\xi^R \xi L}{2\xi L^2 + \xi^R} \boldsymbol{\Upsilon} \times \mathbf{p} + \frac{2\xi^I \xi L}{2\xi L^2 + \xi^R} \bar{\boldsymbol{\phi}} \times \mathbf{p}. \end{aligned} \quad (2.252)$$

This implies that

$$\mathbf{F}^{\perp}(-\mathbf{p}L) = -\mathbf{F}^{\perp}(\mathbf{p}L). \quad (2.253)$$

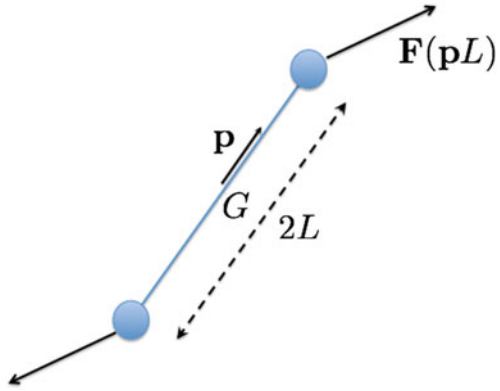
This modeling approach allows for modifying the Jeffery kinematics while keeping a first-gradient description of the induced torques able to activate rod bending.

The choice of the interaction potential $\boldsymbol{\Upsilon}$ is the key point of this modeling approach. A simple choice consists in assuming that at position $\mathbf{p}L$ the microstructure is described by the second-order moment $\mathbf{a}(\mathbf{x}, t)$ of the orientation distribution function $\psi(\mathbf{x}, t, \mathbf{p})$. The simplest choice for the interaction potential $\boldsymbol{\Upsilon}$ is the rotary velocity of the eigenvectors of tensor $\mathbf{a}$.

2.5.5 Collective Effects

We start by obtaining the Jeffery equation but now with the force $\mathbf{F}$ applied at the rod beads (see Fig. 2.14) calculated from the Cauchy stress $\boldsymbol{\tau}$.

Fig. 2.14 Forces applied on a rod immersed in a flowing fluid



Thus, we write

$$\mathbf{F}(\mathbf{p}L) = \boldsymbol{\tau} \cdot \mathbf{p} - \kappa(\dot{\mathbf{p}} - \boldsymbol{\Omega} \cdot \mathbf{p}), \quad (2.254)$$

where κ is a model parameter whose impact will be analyzed later. The fact of considering the term involving the vorticity tensor $\boldsymbol{\Omega}$ ensures the objectivity of the resulting rotary velocity.

We can notice that if $\mathbf{F}$ applies at bead located at $\mathbf{p}L$, then the force at the opposite bead at $-\mathbf{p}L$ reads

$$\mathbf{F}(-\mathbf{p}L) = -\mathbf{F}(\mathbf{p}L), \quad (2.255)$$

which ensures the equilibrium of forces. For the sake of notational simplicity, the force acting on bead $\mathbf{p}L$ will be noted simply by $\mathbf{F}$.

As the resulting torque must also vanish, the only possibility is that force $\mathbf{F}$ acts along $\mathbf{p}$, that is $\mathbf{F} = \lambda \mathbf{p}$, with $\lambda \in \mathbb{R}$. Thus, we can write

$$\lambda \mathbf{p} = \boldsymbol{\tau} \cdot \mathbf{p} - \kappa(\dot{\mathbf{p}} - \boldsymbol{\Omega} \cdot \mathbf{p}). \quad (2.256)$$

Premultiplying Eq. (2.256) by $\mathbf{p}$ and taking into account that $\mathbf{p} \cdot \mathbf{p} = 1$ and consequently $\mathbf{p} \cdot \dot{\mathbf{p}} = 0$, and that $\boldsymbol{\Omega} : (\mathbf{p} \otimes \mathbf{p}) = 0$ since $\boldsymbol{\Omega}$ is skew-symmetric, we have

$$\lambda = \boldsymbol{\tau} : (\mathbf{p} \otimes \mathbf{p}), \quad (2.257)$$

which leads to the extended Jeffery equation

$$\dot{\mathbf{p}} = \boldsymbol{\Omega} \cdot \mathbf{p} + \frac{1}{\kappa} (\boldsymbol{\tau} \cdot \mathbf{p} - (\boldsymbol{\tau} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}). \quad (2.258)$$

When considering $\boldsymbol{\tau} = 2\eta \mathbf{D}$ and $\kappa = 2\eta$, Eq. (2.258) reduces to the standard Jeffery equation.

The forces applied at the rod ends $\mathbf{p}L$ and $-\mathbf{p}L$ are respectively $\lambda\mathbf{p}$ and $-\lambda\mathbf{p}$, i.e. directed along the rod and in equilibrium by construction.

With λ given by Eq. (2.257), we have

$$\mathbf{F}(\mathbf{p}L) = (\boldsymbol{\tau} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}. \quad (2.259)$$

By applying Kramers' formula, the corresponding contribution to the stress is given by

$$\Sigma^p = (\boldsymbol{\tau} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p} \otimes \mathbf{p}, \quad (2.260)$$

which can be rewritten as

$$\Sigma^p = \boldsymbol{\tau} : (\mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p}). \quad (2.261)$$

For considering the effect of all rods in the suspensions, it suffices to consider the integral of each contribution averaged with the orientation distribution function, adding the Newtonian matrix contribution $2\eta\mathbf{D}$. The self-consistency implies:

$$\boldsymbol{\tau} = 2\eta\mathbf{D} + \mathbf{A} : \boldsymbol{\tau}. \quad (2.262)$$

We now consider the equation governing the evolution of the second-order moment $\mathbf{a}$. For this purpose, we take its time derivative

$$\dot{\mathbf{a}} = \int_{\mathcal{S}} (\dot{\mathbf{p}} \otimes \mathbf{p} + \mathbf{p} \otimes \dot{\mathbf{p}}) \psi \, d\mathbf{p}, \quad (2.263)$$

and consider the extended Jeffery expression (2.258) to express the rod rotary velocity $\dot{\mathbf{p}}$. Thus, we obtain

$$\dot{\mathbf{a}} = \boldsymbol{\Omega} \cdot \mathbf{a} - \mathbf{a} \cdot \boldsymbol{\Omega} + \frac{1}{\kappa} (\boldsymbol{\tau} \cdot \mathbf{a} + \mathbf{a} \cdot \boldsymbol{\tau}) - \frac{2}{\kappa} \mathbf{A} : \boldsymbol{\tau}. \quad (2.264)$$

Remark 10 When considering again $\boldsymbol{\tau} = 2\eta\mathbf{D}$ and $\kappa = 2\eta$, Eq. (2.264) reduces to the standard orientation evolution equation. However, by considering the same constitutive equation $\boldsymbol{\tau} = 2\eta\mathbf{D}$ but $\kappa \neq 2\eta$, we obtain a sort of sliding while ensuring the objectivity of the evolution equation that involves the so-called Johnson-Segalman objective derivative. Some authors introduced such sliding affecting the gradient of velocities, a choice that violates the objectivity of the resulting model.

2.5.5.1 Jeffery's Model with Feedback

We consider in the case of dilute rod suspensions the Cauchy stress

$$\boldsymbol{\tau} = 2\eta\mathbf{D} + 2\eta N_p \mathbf{A} : \mathbf{D}, \quad (2.265)$$

that was derived from the standard Jeffery model.

By considering the stress (2.265) in the extended Jeffery expression (2.258), we obtain

$$\begin{aligned} \dot{\mathbf{p}} = & \boldsymbol{\Omega} \cdot \mathbf{p} + \frac{2\eta}{\kappa} (\mathbf{D} \cdot \mathbf{p} - (\mathbf{D} : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}) \\ & - \frac{2\eta N_p}{\kappa} ((\mathbf{A} : \mathbf{D}) \cdot \mathbf{p} - ((\mathbf{A} : \mathbf{D}) : (\mathbf{p} \otimes \mathbf{p})) \mathbf{p}). \end{aligned} \quad (2.266)$$

The associated orientation equation governing the evolution of $\dot{\mathbf{a}}$ (2.264) reads

$$\begin{aligned} \dot{\mathbf{a}} = & \boldsymbol{\Omega} \cdot \mathbf{a} - \mathbf{a} \cdot \boldsymbol{\Omega} + \frac{2\eta}{\kappa} (\mathbf{D} \cdot \mathbf{a} + \mathbf{a} \cdot \mathbf{D} - 2\mathbf{A} : \mathbf{D}) \\ & - \frac{2\eta N_p}{\kappa} ((\mathbf{A} : \mathbf{D}) \cdot \mathbf{a} + \mathbf{a} \cdot (\mathbf{A} : \mathbf{D})^T - 2\mathbf{A} : (\mathbf{A} : \mathbf{D})). \end{aligned} \quad (2.267)$$

Remark 11 By considering $\kappa = 2\eta$ and $N_p = 0$ in Eqs. (2.266) and (2.267), we obtain the standard orientation equations. The extra-term, the one affected by the coefficient N_p , is related to the feedback.

2.5.6 Orientation Induced by an Electric Field

In this section, we propose first the equation governing the orientation of a rod immersed in a Newtonian fluid of viscosity η considering an electrical field $\boldsymbol{\varepsilon}(\mathbf{x}, t)$ and a velocity field $\mathbf{v}(\mathbf{x}, t)$. Then, this model will be introduced in coarser descriptions of the rod population within the kinetic theory framework.

We consider a suspending medium consisting of a Newtonian fluid in which there are suspended N rigid slender rods (e.g. CNTs) of length $2L$. As first approximation, it is assumed that the rod presence and orientation do not affect the flow kinematics that are defined by the velocity field $\mathbf{v}(\mathbf{x}, t)$, with $\mathbf{x} \in \Omega \in \mathbb{R}^d$.

The microstructure can be described at the microscopic scale by the unit vector defining the orientation of each rod, i.e. $\mathbf{p}_i$, $i = 1, \dots, N$. In absence of electrical field, one fiber can be defined by $\mathbf{p}$ or $-\mathbf{p}$ and a symmetry condition is retained in the orientation distribution. However, when considering the electrical field induced charges, that symmetry is broken and the orientation is defined univocally. We assume that $\mathbf{p}$ points from the negative bead to the positive one.

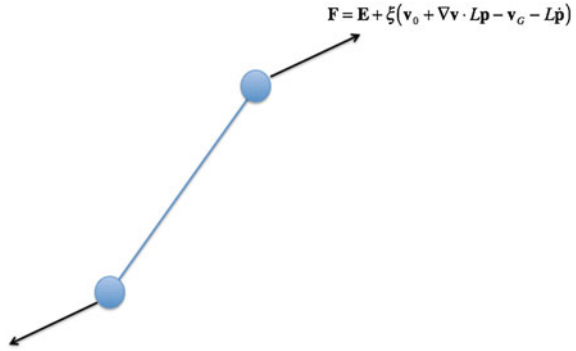
If the suspension is dilute enough, rod interaction can be neglected and then a micro-mechanical model can be derived by considering a single generic rod whose orientation is defined by the unit vector $\mathbf{p}$.

We consider the system illustrated in Fig. 2.15 consisting of a rod immersed in a fluid flow and experiencing the effects of an external electric field.

The resulting forces applied at the rod beads, again taking into account that $\mathbf{v}_0 = \mathbf{v}_G$, read:

$$\mathbf{F}(\mathbf{p}L) = \mathbf{E} + \xi L (\nabla \mathbf{v} \cdot \mathbf{p} - \dot{\mathbf{p}}). \quad (2.268)$$

Fig. 2.15 Hydrodynamic and electrostatic forces applied on a rod immersed in a Newtonian fluid



Obviously, if $\mathbf{F}$ applies on the bead $\mathbf{p}L$, then at the opposite bead $-\mathbf{p}L$, the resulting force reads

$$\mathbf{F}(-\mathbf{p}L) = -\mathbf{E} - \xi L (\nabla \mathbf{v} \cdot \mathbf{p} - \dot{\mathbf{p}}), \quad (2.269)$$

where both beads are assumed having an electrical charge of opposite sign. Thus, the linear momentum balance is ensured. As the resulting torque must also vanish, the only possibility is that force $\mathbf{F}$ acts along $\mathbf{p}$, that is $\mathbf{F} = \lambda \mathbf{p}$, with $\lambda \in \mathbb{R}$. Thus we can write

$$\lambda \mathbf{p} = \mathbf{E} + \xi L (\nabla \mathbf{v} \cdot \mathbf{p} - \dot{\mathbf{p}}). \quad (2.270)$$

Premultiplying Eq. (2.270) by $\mathbf{p}$ and taking into account that $\mathbf{p} \cdot \mathbf{p} = 1$ and consequently $\mathbf{p} \cdot \dot{\mathbf{p}} = 0$, we obtain:

$$\lambda = \mathbf{E} \cdot \mathbf{p} + \xi L (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}), \quad (2.271)$$

implying

$$\mathbf{F} = (\mathbf{E} \cdot \mathbf{p}) \mathbf{p} + \xi L (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p}, \quad (2.272)$$

and

$$\dot{\mathbf{p}} = \frac{1}{\xi L} (\mathbf{E} - (\mathbf{E} \cdot \mathbf{p}) \mathbf{p}) + (\nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p}). \quad (2.273)$$

This can be rewritten as:

$$\begin{aligned} \dot{\mathbf{p}} &= \frac{1}{\xi L} (\mathbf{I} - \mathbf{p} \otimes \mathbf{p}) \cdot \mathbf{E} + (\nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p}) \\ &= \dot{\mathbf{p}}^E + \dot{\mathbf{p}}^J, \end{aligned} \quad (2.274)$$

where $\dot{\mathbf{p}}^E$ stands for the rotary velocity due to the electrostatic forces and $\dot{\mathbf{p}}^J$ represents the hydrodynamic contribution (described by the Jeffery equation).

2.5.6.1 Mesoscopic Description

As the rod population is very large, the description that we just proposed, despite its conceptual simplicity, fails to address the situations usually encountered in practice. For this reason, coarser descriptions are preferred. The first plausible coarser description applies a zoom-out, in which the rod individuality is lost in favour of probability distribution function based descriptions.

In the case of rods, one could describe the microstructure at a certain point $\mathbf{x}$ and time t from the orientation distribution function $\Psi(\mathbf{x}, t, \mathbf{p})$ that gives the fraction of rods that at position $\mathbf{x}$ and time t are oriented in direction $\mathbf{p}$. Obviously, the function Ψ verifies the normality condition:

$$\int_{\mathcal{S}} \Psi(\mathbf{x}, t, \mathbf{p}) d\mathbf{p} = 1, \quad \forall \mathbf{x}, \quad \forall t, \quad (2.275)$$

where $\mathcal{S}$ is the surface of the unit ball that defines all possible rod orientations. The balance ensuring the probability conservation reads:

$$\frac{\partial \Psi}{\partial t} + \nabla_{\mathbf{x}} \cdot (\dot{\mathbf{x}} \Psi) + \nabla_{\mathbf{p}} \cdot (\dot{\mathbf{p}} \Psi) = 0, \quad (2.276)$$

wherein for inertialess rods $\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t)$ and the rod rotary velocity is given by Eq. (2.274),

$$\dot{\mathbf{p}} = \frac{1}{\xi L} (\mathbf{I} - \mathbf{p} \otimes \mathbf{p}) \cdot \mathbf{E} + \left(\nabla \mathbf{v} \cdot \mathbf{p} - \left(\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p} \right) \mathbf{p} \right). \quad (2.277)$$

2.5.6.2 Macroscopic Description

In this section, we illustrate the transition from the mesoscopic to the macroscopic scale. At the macroscopic scale, the orientation distribution function is substituted by its moments for describing the microstructure. We consider the first to fourth orientation moments $\mathbf{a}^{(1)}$, $\mathbf{a}^{(2)}$, $\mathbf{a}^{(3)}$ and $\mathbf{a}^{(4)}$, respectively defined from:

$$\mathbf{a}^{(1)} = \int_{\mathcal{S}} \mathbf{p} \Psi d\mathbf{p}, \quad (2.278)$$

$$\mathbf{a}^{(2)} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \Psi d\mathbf{p}, \quad (2.279)$$

$$\mathbf{a}^{(3)} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \Psi d\mathbf{p} \quad (2.280)$$

and

$$\mathbf{a}^{(4)} = \int_{\mathcal{S}} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \Psi \, d\mathbf{p}. \quad (2.281)$$

The time derivative of $\mathbf{a}^{(1)}$ reads

$$\begin{aligned} \dot{\mathbf{a}}^{(1)} &= \int_{\mathcal{S}} \dot{\mathbf{p}} \Psi \, d\mathbf{p} = \int_{\mathcal{S}} (\dot{\mathbf{p}}^E + \dot{\mathbf{p}}^J) \Psi \, d\mathbf{p} \\ &= \frac{1}{\xi L} \int_{\mathcal{S}} (\mathbf{I} - \mathbf{p} \otimes \mathbf{p}) \cdot \mathbf{E} \Psi \, d\mathbf{p} + \int_{\mathcal{S}} (\nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p}) \Psi \, d\mathbf{p} \\ &= \frac{1}{\xi L} (\mathbf{E} - \mathbf{a}^{(2)} \cdot \mathbf{E}) + \nabla \mathbf{v} \cdot \mathbf{a}^{(1)} - \nabla \mathbf{v} : \mathbf{a}^{(3)}. \end{aligned} \quad (2.282)$$

In the previous expression, a closure issue appears related to $\mathbf{a}^{(2)}$ and $\mathbf{a}^{(3)}$. We could evaluate the time derivative of the second moment, but again higher-order moments are involved and the closure issue persists.

2.5.6.3 Introducing Randomizing Mechanisms

The main issue of the modeling approach just presented is that it tends to fully align rods along a given direction, that is:

$$\mathbf{p}(t \rightarrow \infty) = \hat{\mathbf{p}}, \quad (2.283)$$

and

$$\mathbf{a}^{(1)}(t \rightarrow \infty) = \hat{\mathbf{p}}, \quad (2.284)$$

where $\hat{\mathbf{p}}$ is a given orientation that results as a compromise between the ones enforced by the flow and the electrical field.

In flowing systems, full alignment is prevented by rod-rod interactions that have a randomizing effect. This effect can be accurately modeled with a diffusion term in the Fokker-Planck equation, that moreover accounts for Brownian effects:

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \Psi) + \nabla_p \cdot (\dot{\mathbf{p}} \Psi) = \nabla_p \cdot (D_r \nabla_p \Psi), \quad (2.285)$$

where D_r quantifies the isotropic Brownian diffusion. The rotary velocity is given again by:

$$\dot{\mathbf{p}} = \frac{1}{\xi L} (\mathbf{I} - \mathbf{p} \otimes \mathbf{p}) \cdot \mathbf{E} + (\nabla \mathbf{v} \cdot \mathbf{p} - (\mathbf{p}^T \cdot \nabla \mathbf{v} \cdot \mathbf{p}) \mathbf{p}). \quad (2.286)$$

Equation (2.285) can be rewritten as:

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\mathbf{v} \Psi) + \nabla_p \cdot (\dot{\mathbf{p}} \Psi) = 0, \quad (2.287)$$

with the equivalent rotary velocity given by

$$\dot{\mathbf{p}} = \dot{\mathbf{p}} \Psi - D_r \frac{\nabla_p \Psi}{\Psi}. \quad (2.288)$$

Now, coming back to the macroscopic scale, the evolution of the first moment of the orientation distribution function, following the rationale considered in [43] (Sect. 3.3), is obtained:

$$\dot{\mathbf{a}}^{(1)} \approx \frac{1}{\xi L} \left(\mathbf{E} - \mathbf{a}^{(2)} \cdot \mathbf{E} \right) + \nabla \mathbf{v} \cdot \mathbf{a}^{(1)} - \nabla \mathbf{v} : \mathbf{a}^{(3)} - D_r \mathbf{a}^{(1)}, \quad (2.289)$$

which ensures, in absence of electrical field $\mathbf{E} = \mathbf{0}$ and absence of flow $\mathbf{v}(\mathbf{x}, t) = \mathbf{0}$, a fully random (isotropic) distribution, i.e. $\mathbf{a}^{(1)}(t \rightarrow \infty; \mathbf{E} = \mathbf{0}, \mathbf{v} = \mathbf{0}) = \mathbf{0}$.

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