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Complex flows of micro/nano structured fluids: Reinforced polymer composites

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Résumé — The motion of an ellipsoidal particle immersed in a flow of a Newtonian fluid was obtained 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 work, 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.

Mots clés — Suspensions, Multi-scale description, Numerical simulation.

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 [28]. 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 [30] and the references therein for a review on multiscale 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 [21] [9]. 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 justifies 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 are exactly the same that

the ones 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 [37] [10] [43] [44] [13] [11] [4] [18] [19]. On the other hand, there are few works focusing on the solution of Fokker-Planck equations by using standard discretization techniques [33] [11]. 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 [5] [6]. The interested reader can refer to [36] [15] [17] 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 [29] [12]. 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, as soon as the concentration increases the difficulties appear. 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 [23]. There is a wide literature concerning dilute and semi-dilute suspensions, addressing modeling [24] [25] [26], flows [40] [3] [8] [20] and rheology [38] [35]. These models describe quite well the experimental observations. When the concentration increases rods interactions can not be neglected anymore and appropriate models addressing these intense interactions must be considered, as for example the one proposed in [22]. 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 [41]. For addressing this issue Wang et al. [41] 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 [42]. In [39] an anisotropic rotary diffusion is proposed for accounting 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 [34]. The first natural question is how describing such systems? At the macroscopic scale one could try to fit some power-law constitutive equation, however, this description does not allow to describe the microstructure. At the microscopic scale, direct numerical simulations describing complex fiber-fiber interactions can be carried out in small enough representative volumes [31] [32] [7]. A natural candidate to be a reasonable compromise between (fine) micro and (fast) macro descriptions consists of considering again a kinetic theory description.

The main issue of 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 [16] authors propose a first attempt to describe such clusters from a micromechanical model. Later in [1] 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 [2] in the case of rigid clusters.

In this talk, we summarize the various facets of our current studies on the multi-scale kinetic theory

modeling of fiber suspensions. For each of the topics outlined below, we propose a suitable theoretical approach, give recent results, and discuss open issues. Most available theories for fiber suspensions are based on the seminal Jeffery model and phenomenological modifications of it for the semi-dilute regime. Such models do not consider size effects and only first velocity gradient descriptions are retained. In the semi-dilute case, when percolation is attained, a mild elasticity is observed experimentally. We have shown recently that this elastic behaviour originates from an anomalous diffusion mechanism and that it is well described by means of a fractional modeling approach.

When the fiber concentration increases, many hypotheses fail and new approaches are needed for describing suspensions of industrial interest. First, the suspending medium, in general assumed a Newtonian fluid, must be substituted by the suspension itself in order to take into account possible collective effects. Moreover, migration can occur. How to properly take account of the non-Newtonian rheology of the suspending fluid remains an open issue that has to date only been addressed via direct numerical simulations. Mesoscopic and macroscopic models requires an extension of the Jeffery model to this situation. When the characteristic length of the suspended particles is of the same order than that of the flow, higher-order velocity gradient descriptions are needed that in general induce rod bending. When the concentration is large enough, rods can aggregate, and the suspension of rigid particles becomes a suspension of rigid or deformable rod clusters with a particular and rich kinematics. Finally, higher concentration induces the existence of an entangled network, as in a polymer melt, that requires appropriate macroscopic models able to take into account the interaction effects on the fiber kinematics.

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