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Microscopic modelling of orientation kinematics of non-spherical particles suspended in confined flows using unilateral mechanics

Adrien Scheuer [a,b], Emmanuelle Abisset-Chavanne [a], Francisco Chinesta [c,*], Roland Keunings [b]

[a] ICI – Institut de calcul intensif & ESI GROUP Chair, École centrale de Nantes, 1, rue de la Noe, 44300 Nantes, France
[b] ICTEAM, Université catholique de Louvain, avenue Georges-Lemaître 4, B-1348 Louvain-la-Neuve, Belgium
[c] PIMM & ESI GROUP Chair, ENSAM ParisTech, 151, boulevard de l'Hôpital, 75013 Paris, France

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ABSTRACT

The properties of reinforced polymers strongly depend on the microstructural state, that is, the orientation state of the fibres suspended in the polymeric matrix, induced by the forming process. Understanding flow-induced anisotropy is thus a key element to optimize both materials and process. Despite the important progresses accomplished in the modelling and simulation of suspensions, few works addressed the fact that usual processing flows evolve in confined configurations, where particles characteristic lengths may be greater than the thickness of the narrow gaps in which the flow takes place. In those circumstances, orientation kinematics models proposed for unconfined flows must be extended to the confined case. In this short communication, we propose an alternative modelling framework based on the use of unilateral mechanics, consequently exhibiting a clear analogy with plasticity and contact mechanics. This framework allows us to revisit the motion of confined particles in Newtonian and non-Newtonian matrices. We also prove that the confined kinematics provided by this model are identical to those derived from microstructural approaches (Perez et al. (2016) [1]).

1. Introduction

Over the last decades, composite materials, made of a suspending matrix and a reinforcement composed of fibres used to fortify the matrix in terms of strength and stiffness, were successfully introduced in the aerospace and automotive industries and proved to be a lightweight alternative to produce structural and functional parts. The mechanical properties of such reinforced polymers, however, strongly depend on the orientation state of their microstructure, which is established during the forming process [2]. Predicting the evolution of this orientation state is thus a key yet complex task, since the motion of the reinforcing fibres is impacted by the flowing matrix and the interactions with the neighbouring fibres and cavity walls. Thus, flow-induced anisotropy must be understood and modelled in order to optimize both materials and processes.

* Corresponding author.
E-mail addresses: Adrien.Scheuer@ec-nantes.fr, Adrien.Scheuer@uclouvain.be (A. Scheuer), Emmanuelle.Abisset-chavanne@ec-nantes.fr (E. Abisset-Chavanne), Francisco.Chinesta@ensam.edu (F. Chinesta), Roland.Keunings@uclouvain.be (R. Keunings).

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There is a long history of studies of the motion of slender bodies suspended in a viscous fluid, starting from the seminal work of Jeffery back in 1922 [3]. A vast literature dedicated to fibre and non-spherical particle suspensions is available, studying extensively different modelling scales and exploring the impact of the concentration regime and the nature of the suspending matrix. Schematically, the three main modelling scales involved when addressing the orientation kinematics of suspended particles can be summarized as follows: (i) the *microscopic* scale, the scale of a single particle; (ii) the *mesoscopic* scale, the scale of a population of particle, whose conformation is usually represented by a probability density function (pdf) of orientation, giving an unambiguous and complete description of the orientation state; and (iii) the *macroscopic* scale, the scale of the part, whose conformation is often given by the first moments of the aforementioned pdf, providing a coarse yet concise description of the orientation state in the part. Depending on the level of detail and accuracy required for a given application, a specific scale, or a combination of them might be chosen. For further detail on that subject, including the so-called multiscale approach, we refer the reader to the review [4] and the monograph [5], as well as to the references therein. Only a succinct overview of the microscopic modelling is proposed thereafter.

In [3], Jeffery derived the expression of the hydrodynamic torque exerted on an ellipsoidal particle immersed in an unbounded creeping flow of a Newtonian fluid. He then obtained an equation of motion by assuming that the particle rotates so as to achieve instantaneous zero torque, resulting in the so-called Jeffery equation. Considering a spheroid (axisymetric ellipsoid) and defining the orientation of a particle by the unit vector $\mathbf{p}$ along its principal axis, Jeffery's equation reads

$$\dot{\mathbf{p}}^J = \boldsymbol{\Omega} \cdot \mathbf{p} + \kappa(\mathbf{D} \cdot \mathbf{p} - (\mathbf{D} : (\mathbf{p} \otimes \mathbf{p})\mathbf{p})) \tag{1}$$

where $\boldsymbol{\Omega}$ and $\mathbf{D}$ are, respectively, the skew-symmetric and symmetric parts of the unperturbed velocity gradient $\nabla \mathbf{v}$ of the flow, and κ is the shape factor of the spheroid, given by $\kappa = \frac{r^2-1}{r^2+1}$ with r the aspect ratio of the particle. Slender bodies like fibres and rods can be assimilated as infinite aspect ratio ellipsoids ($\kappa \approx 1$).

Jeffery's equation was experimentally verified by Taylor [6] and Mason [7]. Bretherton [8] showed that the equation is also valid for any axisymmetric particle provided that an effective aspect ratio is determined. Hinch and Leal [9–12] also studied Jeffery's model, addressing the impact of Brownian motion and proposing constitutive equations for the behaviour of suspensions. However, only a few works, either experimental [13,14] or numerical and theoretical [15,16], address the fact that flows of industrial interest take place in narrow gaps, whose thickness is of the same order of magnitude or smaller than the length of the reinforcing fibres, thus constraining the space of possible orientation, and as a consequence the kinematics.

In [1], we proposed a multiscale model to describe the orientation development of a dilute suspension of fibres confined in a narrow gap. The microscopic model was based on a dumbbell representation [17] of the confined rod, with hydrodynamic and contact forces (normal to the gap wall) acting on it. This confinement model was later extended in [18] to include unilateral contacts and non-uniform strain rates at the scale of the rod. In any case, the resulting kinematics are a combination of the unconfined Jeffery kinematics and a correction term that prevents the fibre from leaving the flow domain, that is,

$$\dot{\mathbf{p}} = \dot{\mathbf{p}}^J + \dot{\mathbf{p}}^C \tag{2}$$

The equation of motion of such a confined rod, derived in [1] and summarized in Eq. (2), presents thus significant similarities with equations of elastoplaticity. Indeed, we could draw a parallel between, on the one hand, the classical unconfined kinematics and the elastic deformation, and, on the other hand, the confined motion of the particle and elastoplatic deformation.

Hence, the purpose of this short communication is to explore the alternative modelling framework based on unilateral mechanics to revisit the motion of confined particles in Newtonian and non-Newtonian matrices.

The paper is organised as follows. In Section 2, we derive the model for the confined kinematics of suspended particles using unilateral mechanics. Then, in Section 3, we discuss how this general framework allows us to build the confined kinematics of fibres and spheroids immersed in a Newtonian (based on Jeffery's model [3]) or second-order (based on Brunn's model [19]) viscoelastic fluid. Finally, in Section 4, we draw the main conclusions and present some perspectives of this approach.

Remark. In this paper, we consider the following tensor products, assuming Einstein's summation convention:

- if $\mathbf{a}$ and $\mathbf{b}$ are first-order tensors, then the single contraction "$\cdot$" reads $(\mathbf{a} \cdot \mathbf{b}) = a_j\, b_j$;
- if $\mathbf{a}$ and $\mathbf{b}$ are first-order tensors, then the dyadic product "$\otimes$" reads $(\mathbf{a} \otimes \mathbf{b})_{jk} = a_j\, b_k$;
- if $\mathbf{a}$ and $\mathbf{b}$ are respectively second and first-order tensors, then the single contraction "$\cdot$" reads $(\mathbf{a} \cdot \mathbf{b})_j = a_{jk}\, b_k$;
- if $\mathbf{a}$ and $\mathbf{b}$ are second-order tensors, then the double contraction ":" reads $(\mathbf{a} : \mathbf{b}) = a_{jk}\, b_{kj}$.

2. Confined orientation kinematics using unilateral mechanics

In this section, we derive step by step the kinematics of a confined suspended particle using the framework of unilateral mechanics.