Physica D 337 (2016) 18–29

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

A comparison of macroscopic models describing the collective response of sedimenting rod-like particles in shear flows

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HIGHLIGHTS

- Presentation of a kinetic multi-scale model, describing the sedimentation of rod-like particles.
- Derivation of macroscopic models, which describe the collective behavior of the system.
- A linear stability analysis, which predicts instability and a wavelength selection mechanism.
- Numerical simulations, which compare the macroscopic models with the kinetic model.

ARTICLE INFO

Article history:
Received 12 October 2015
Received in revised form
13 June 2016
Accepted 11 July 2016
Available online 22 July 2016

Keywords:
Rod-like particles
Sedimentation
Linear stability
Moment closure
Quasi-dynamic approximation
Diffusive scaling

ABSTRACT

We consider a kinetic model, which describes the sedimentation of rod-like particles in dilute suspensions under the influence of gravity, presented in Helzel and Tzavaras (submitted for publication). Here we restrict our considerations to shear flow and consider a simplified situation, where the particle orientation is restricted to the plane spanned by the direction of shear and the direction of gravity. For this simplified kinetic model we carry out a linear stability analysis and we derive two different nonlinear macroscopic models which describe the formation of clusters of higher particle density. One of these macroscopic models is based on a diffusive scaling, the other one is based on a so-called quasi-dynamic approximation. Numerical computations, which compare the predictions of the macroscopic models with the kinetic model, complete our presentation.

1. Introduction

We discuss different mathematical models which describe the sedimentation process for dilute suspensions of rod-like particles under the influence of gravity. The sedimentation of rod-like particles has been studied by several authors in theoretical as well as experimental and numerical works, see Guazzelli and Hinch [1] for a recent review paper. Experimental studies of Guazzelli and coworkers [2–4] start with a well stirred suspension. Under the influence of gravity, a well stirred initial configuration is unstable and it is observed that clusters with higher particles concentration form. These clusters have a mesoscopic equilibrium width. Within a cluster, individual particles tend to align in the direction of gravity.

The basic mechanism of instability and cluster formation was described in a fundamental paper of Koch and Shaqfeh [5]. In Helzel and Tzavaras [6], we recently derived a kinetic model which describes the sedimentation process for dilute suspensions of rod-like particles. By applying moment closure hypotheses and other approximations to an associated moment system, we derived macroscopic models for the evolution of the rod density and compared the prediction of such macroscopic models to the original kinetic model using numerical experiments. This is done in [6] for rectilinear flows with the particles taking values on the sphere.

In the present work, in order to explain our approach, we restrict our analysis to the simpler case of shear flows for particles with orientations restricted to take values on the plane. While the derivations in [6] are often quite technical, the restriction to this simpler situation provides a useful and technically simple setting in order to understand the underlying ideas. In addition, it turns out that the form of the derived macroscopic equations is identical in both cases apart from the values of numerical constants

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http://dx.doi.org/10.1016/j.physd.2016.07.004
0167-2789/

that capture the effect of dimensionality in the microstructure. Therefore, we hope that this paper will make our results accessible and useful to a wider community interested in the modeling of complex fluids. Moreover, we also consider an alternative route to closure at the density level via diffusive scaling. The closure via diffusive scaling leads to the classical Keller–Segel system while the quasi-dynamic approximation leads to a variant of a flux-limited Keller–Segel system. The different effective equations are numerically compared among each other and also compared with a computation of the full nonlinear kinetic model.

The article is organized as follows: In Section 2, we present the kinetic model from [6] and the non-dimensionalization of the problem. For vertical shear flows we derive a simplified one-space dimensional model, obtained by restricting the orientation of particles to move in a plane. In Section 3 a nonlinear moment closure system is derived (see (38)–(41)) which forms the basis for all further considerations. Effective equations for the evolution of the macroscopic density are obtained via two approaches: Starting from the moment system (38)–(41) in Section 4, we employ a quasi-dynamic approximation and derive an effective equation for the evolution of the macroscopic density. The approximation amounts to replacing the dynamical behavior of the second order moments by enslaving the second-order moments to their respective local equilibria. An alternative approach is presented in Section 5 and Appendix A, where the effective equation for the density is obtained directly from the kinetic equation via a diffusive limit. The diffusive approximation leads to the well known Keller–Segel model (52), while the quasi-dynamic approximation leads to a flux-limited Keller–Segel type model (46).

In Section 6 we present numerical results comparing the diffusive approximation and the quasi-dynamic approximation to the full kinetic model. Although the idea of diffusive scalings to obtain macroscopic equations is commonplace in kinetic theory (see [7–9]), it has not been applied (to our knowledge) in the sedimentation problem. The derivation of the hyperbolic and diffusive scaling equations for general rectilinear flows is presented in Appendix A for the general case where the directions of the rod-like particles take values on the sphere. Finally, in Appendix B, we present a stability analysis for the linearized moment closure system to establish the linear instability of the rest state under a shear flow perturbation. It turns out that a nonzero Reynolds number provides a wavelength selection mechanism. An asymptotic analysis of the largest eigenvalue around $Re = 0$ explains this behavior.

2. A kinetic model for the sedimentation of rod-like particles

We describe a kinetic model for sedimentation in dilute suspensions of rod-like Brownian particles, following Doi and Edwards [10, Ch. 8]; see also [11,12]. The model accounts for the effects of gravity and hydrostatic interactions in a dilute suspension (see [6]).

Consider a suspension consisting of inflexible rod-like particles of thickness b and length l, with $b \ll l$, submerged in a solvent extending over the entire space. The rods are subjected to a gravity field $\boldsymbol{g} = -g\boldsymbol{e}_3$, with gravitational constant g and where $\boldsymbol{e}_3$ is the unit vector in the upward direction. If m_0 denotes the mass of an individual particle then $\boldsymbol{G} = -m_0 g\boldsymbol{e}_3$ is the force of gravity on a single particle. Some of our basic notation is depicted in Fig. 1.

The motion of the particles is friction dominated. If $\boldsymbol{u}(\boldsymbol{x}, t)$ stands for the velocity field of the solvent, then a rigid particle is described by the position $\boldsymbol{x} \in \mathbb{R}^d$ of the center of mass and the orientation $\boldsymbol{n} \in S^{d-1}$ of the rod. Kinematic considerations dictate that each rod obeys the equations

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{u} + \left(\frac{1}{\zeta_\parallel}\boldsymbol{n}\otimes\boldsymbol{n} + \frac{1}{\zeta_\perp}(I - \boldsymbol{n}\otimes\boldsymbol{n})\right)\boldsymbol{G}$$
$$\frac{d\boldsymbol{n}}{dt} = P_{\boldsymbol{n}^\perp}\nabla_{\boldsymbol{x}}\boldsymbol{u}\boldsymbol{n}$$

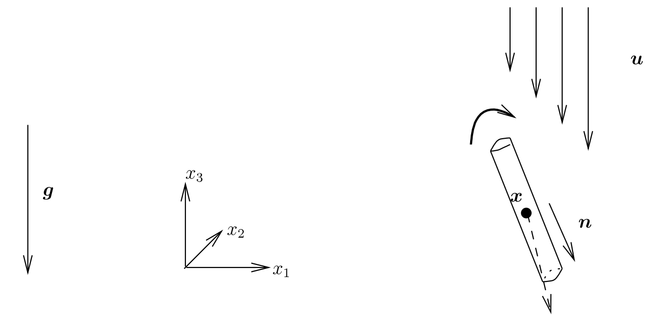

Fig. 1. Basic notation for rod-like molecule which is falling sidewards.

where

$$P_{\boldsymbol{n}^\perp}\nabla_{\boldsymbol{x}}\boldsymbol{u}\boldsymbol{n} = \big(I - \boldsymbol{n}\otimes\boldsymbol{n}\big)(\nabla_{\boldsymbol{x}}\boldsymbol{u})\boldsymbol{n}$$

is the projection of the vector $(\nabla_{\boldsymbol{x}}\boldsymbol{u})\boldsymbol{n}$ onto the tangent space at $\boldsymbol{n}$, while $\zeta_\parallel$ and $\zeta_\perp$ are the frictional coefficients in the tangential and the normal direction. Note that $\zeta_\perp = 2\zeta_\parallel$, see [10, App 8.I], implying that a particle with a vertical orientation sediments twice as fast as a particle with horizontal orientation while a particle of oblique orientation moves also sideways.

Upon including the effects of rotational and translational Brownian motion the kinematics of the microstructure is described by the system of stochastic differential equations

$$\begin{aligned} d\boldsymbol{x} &= \left[\boldsymbol{u} + \left(\frac{1}{\zeta_\parallel}\boldsymbol{n}\otimes\boldsymbol{n} + \frac{1}{\zeta_\perp}(I - \boldsymbol{n}\otimes\boldsymbol{n})\right)\boldsymbol{G}\right]dt \\ &\quad + \sqrt{\frac{2k_B\theta}{\zeta_\parallel}\boldsymbol{n}\otimes\boldsymbol{n} + \frac{2k_B\theta}{\zeta_\perp}(I - \boldsymbol{n}\otimes\boldsymbol{n})}\, dW \\ d\boldsymbol{n} &= P_{\boldsymbol{n}^\perp}\nabla_{\boldsymbol{x}}\boldsymbol{u}\boldsymbol{n}\, dt + \sqrt{\frac{2k_B\theta}{\zeta_r}}\, dB \end{aligned} \tag{1}$$

where W is the translational Brownian motion and B the rotational Brownian motion, ζ_r the rotational friction coefficient, k_B the Boltzmann constant and θ the absolute temperature.

We consider a suspension of many such molecules in the dilute regime, characterized by the relation $\nu l^3 \ll 1$. In this regime the average distance of molecules is much larger than their length and the molecules remain nearly statistically independent. By the law of large numbers the empirical distribution of particles as a function of the center of mass $\boldsymbol{x}$ and orientation $\boldsymbol{n}$ is well approximated by a probability distribution $f(t, \boldsymbol{x}, \boldsymbol{n})\, d\boldsymbol{n}d\boldsymbol{x}$. By the equivalence of drift–diffusion equations and Fokker–Planck equations, the dynamics can be described by the Smoluchowski equation

$$\begin{aligned} &\partial_t f + \nabla_{\boldsymbol{x}}\cdot\left[\left(\boldsymbol{u} + \frac{1}{\zeta_\perp}(\boldsymbol{n}\otimes\boldsymbol{n} + I)\,\boldsymbol{G}\right)f\right] + \nabla_{\boldsymbol{n}}\cdot\big(P_{\boldsymbol{n}^\perp}\nabla_{\boldsymbol{x}}\boldsymbol{u}\boldsymbol{n}f\big) \\ &\quad = \frac{k_B\theta}{\zeta_r}\Delta_{\boldsymbol{n}} f + \frac{k_B\theta}{\zeta_\perp}\nabla_{\boldsymbol{x}}\cdot(\boldsymbol{n}\otimes\boldsymbol{n} + I)\,\nabla_{\boldsymbol{x}} f. \end{aligned} \tag{2}$$

Here, $\nabla_{\boldsymbol{x}}$ and $\nabla_{\boldsymbol{x}}\cdot$ denote the usual gradient and divergence in the macroscopic flow domain. On the other hand, $\nabla_{\boldsymbol{n}}$ stands for the surface gradient operator (on the sphere), acting on a scalar function $\varphi = \varphi(\boldsymbol{n})$ by the formula $\nabla_{\boldsymbol{n}}\varphi = \nabla\varphi - \boldsymbol{n}(\boldsymbol{n}\cdot\nabla\varphi)$ where ∇ stands for the usual gradient operator. The gradient, divergence and Laplacian on the sphere are denoted by $\nabla_{\boldsymbol{n}}$, $\nabla_{\boldsymbol{n}}\cdot$ and $\Delta_{\boldsymbol{n}}$, The second term on the left hand side of (2) models transport of the center of mass of the particles due to the macroscopic flow velocity and due to gravity. The last term on the left hand side models the rotation of the axis due to a macroscopic velocity gradient $\nabla_{\boldsymbol{x}}\boldsymbol{u}$. The