

Numerical Investigation of Tumbling Phenomena Based on a Macroscopic Model for Hydrodynamic Nematic Liquid Crystals

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Abstract. This paper is concerned with the numerical investigation of a macroscopic model for complex fluids in “1+2” dimension case. We consider the planar pressure driven flow where the direction of the molecules is constrained in the shear plane. The modified Crank-Nicolson finite difference scheme satisfying a discrete energy law will be developed. By using this scheme, it is observed numerically that the direction of the molecules will tumble from the boundary layer and later on the inner layer with a much longer time period. This is consistent with the theoretical prediction. Moreover, we find some complex phenomena, where the tumbling rises from boundary layer and is then embedded into the interior area more clearly when the viscosity coefficient μ of the macro flow has a larger value. The norm of the molecular director \mathbf{d} will endure greater change as well. This implies that the viscosity of flow plays the role of an accelerator in the whole complex fluids. Comparing these results with the theoretical analysis, we can find that the gradient of the velocity has direct impact on the tumbling phenomena. These results show that the proposed scheme is capable of exploring some physical phenomena embedded in the macro-micro model.

AMS subject classifications: 76T99, 76D05, 65M06

Key words: Complex fluids, energy law, anchoring condition, modified Crank-Nicolson scheme, tumbling.

1 Introduction

The special hydrodynamical properties of complex fluids have attracted many researchers to build up mathematical models and to provide appropriate explanations, see, e.g., [1, 2, 5, 7, 8, 20] and references therein. Doi [2] introduced the Fokker-Plack equation [9]

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coupled with the Navier-Stokes equations, which is a well-known multi-scale model. This model assumed that the fluid is homogeneous in space and excluded volume effect by adopting either Onsager potential [23] or Maier-Saupe potential [2, 6, 21]. Later, Doi et al. [3] extended the theory to model flows of nonhomogeneous liquid crystal polymers by introducing a long-range intermolecular potential through a mean field calculation. Marrucci and Greco [22] further improved the extended Doi theory and obtained an approximate potential depending on gradients of the second moments of the possibility density function (PDF). Moreover, Wang et al. [24, 25] extended the Doi kinetic model from the rodlike molecule at large aspect ratio to the discotic one at small aspect ratios. Although these models are found useful, the computational cost is large since there are seven variables in the kinetic model (or Fokker-Plack equation of PDF) and the Navier-Stokes-like equations. Therefore, there have been attempts from the macroscopic point of view.

For the macroscopic continuum description of the hydrodynamics of complex fluids, such as the nematic liquid crystals, Ericksen and Leslie derived the following nonlinear coupled system [5, 6, 14] for those materials with isotropic elastic energies:

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \mu \Delta \mathbf{u} - \lambda \nabla \cdot \boldsymbol{\tau}, \quad \text{in } \Omega, \quad (1.1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega, \quad (1.2)$$

$$\mathbf{d}_t + (\mathbf{u} \cdot \nabla) \mathbf{d} - \alpha \boldsymbol{\kappa} \cdot \mathbf{d} - (\alpha - 1) \boldsymbol{\kappa}^T \cdot \mathbf{d} = \gamma (\Delta \mathbf{d} - \mathbf{f}(\mathbf{d})), \quad \text{in } \Omega, \quad (1.3)$$

$$\boldsymbol{\tau} = \nabla \mathbf{d} \odot \nabla \mathbf{d} + \alpha (\mathbf{d} \otimes \Delta \mathbf{d} - \mathbf{d} \otimes \mathbf{f}) + (\alpha - 1) (\Delta \mathbf{d} \otimes \mathbf{d} - \mathbf{f} \otimes \mathbf{d}), \quad (1.4)$$

where \mathbf{u} represents the velocity of the liquid crystal flow, p the pressure, $\boldsymbol{\kappa} = (\nabla \mathbf{u})^T$, and \mathbf{d} the orientation of the liquid crystal molecules. The domain $\Omega \subset \mathbb{R}^n$ is a bounded domain. The induced tensor $\boldsymbol{\tau}$ shows the impact of the microstructure on the macro fluid while the coupled term of velocity and director in (1.3) shows impact of the fluid on the microstructure. In Eq. (1.4), the term $\nabla \mathbf{d} \odot \nabla \mathbf{d}$ denotes a 3×3 matrix whose (i, j) -th entry is given by $\mathbf{d}_{x_i} \cdot \mathbf{d}_{x_j}$, for $1 \leq i, j \leq 3$, while the term $\mathbf{d} \otimes \Delta \mathbf{d}$ also denotes a 3×3 matrix whose (i, j) -th entry is given by $d_i \Delta d_j$. Here, μ is the viscosity coefficient of the macro fluid and γ is the diffusive parameter for the molecular direction \mathbf{d} . Moreover, λ is the competition ratio of the kinetic energy and the elastic energy, $\alpha \in [0, 1]$ is a shape parameter of the molecule, and $\mathbf{f}(\mathbf{d})$ may be seen as a penalty function to approximate the constraint $|\mathbf{d}| = 1$. In this paper, we choose

$$\mathbf{f}(\mathbf{d}) = \nabla \mathbf{F}(\mathbf{d}), \quad (1.5a)$$

where

$$\mathbf{F}(\mathbf{d}) = \frac{1}{\epsilon^2} (|\mathbf{d}|^2 - 1)^2, \quad (1.5b)$$

where the parameter ϵ is the penalty parameter. The transport of the director, $\mathbf{d}_t + (\mathbf{u} \cdot \nabla) \mathbf{d} - \alpha \boldsymbol{\kappa} \cdot \mathbf{d} - (\alpha - 1) \boldsymbol{\kappa}^T \cdot \mathbf{d}$ reflects the microscopic picture of those ellipsoid shaped molecules moving in Stokes fluids with no slip boundary conditions on the particle surface [10, 11]. It presents an effective stretching effect on the director \mathbf{d} , the reader may refer to [17] for the detail.