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A Kinetic-Hydrodynamic Simulation of Liquid Crystalline Polymers Under Plane Shear Flow: 1+2 Dimensional Case†

Guanghua Ji[1], Haijun Yu[2] and Pingwen Zhang[3,*]

[1] *Laboratory of Mathematics and Complex Systems, Ministry of Education and School of Mathematical Sciences, Beijing Normal University, Beijing 100875, China.*
[2] *School of Mathematical Sciences and CCSE, Peking University, Beijing 100871, China.*
[3] *LMAM, School of Mathematical Sciences and CCSE, Peking University, Beijing 100871, China.*

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Abstract. We consider the extended Doi model for nematic liquid crystalline polymers in-planar shear flow, which is inhomogeneous in shear direction. We study the formation of microstructure and the dynamics of defects. We discretize the Fokker-Plank equation using the spherical harmonic spectral method. Five in-plane flow modes and eight out-of-plane flow modes are replicated in our simulations. In order to demonstrate the validity of our method in simulating liquid crystal dynamics, we replicated weak shear limit results and detected defects. We also demonstrate numerically that the Bingham closure model, which maintains energy dissipation, is a reliable closure model.

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Key words: Non-local potential, anchoring condition, spherical harmonic, kinetic-hydrodynamic, defects, Bingham closure.

1 Introduction

The nematic phase is one of the ”simplest” liquid crystal phases known, for which an orientational order exists [1]. Most of the hydrodynamic theories formulated for liquid crystalline polymers(LCPs) are based on rod-like molecules, including the well known Leslie-Eriksen (**LE**) theory [2], developed to describe low molecular weight nematic liquid crystals, the Doi kinetic theory [3] and a variety of tensor-based theories, such as

†Dedicated to Professor Xiantu He on the occasion of his 70th birthday.
*Corresponding author. *Email addresses:* `ghji@bnu.edu.cn` (G. Ji), `pzhang@pku.edu.cn` (P. Zhang)

Hand's theory [4], Beris and Edwards' theory formulated through Poisson brackets [5], and Tsuji and Rey's phenomenological theory [6]. The **LE** theory was popular in simulations of LCPs for its simplicity. However, the **LE** theory predicts flow aligning and tumbling, but fails to catch defects, where the director cannot be defined. The Doi kinetic theory for spatially homogeneous flows of rod-like molecules has been successfully used to describe the rheological behavior of liquid crystalline polymers [3]. Abundant phenomena, such as tumbling, wagging, flow-aligning and logrolling, were predicted using the Doi model (Marrucci and Maffettone [7], Larson [8], Larson and Öttinger [9] and Nayak [10]). Faraoni [11], Forest et al. [12,13] and others studied the Doi model in detail using spherical harmonic analysis, and generated the detailed phase diagram. Wang [14] extended the model to disc-shaped molecules by introducing a shape parameter $\alpha=\frac{r^2-1}{r^2+1}$, with the molecular aspect ratio r.

Liquid crystalline flows are characterized by the presence of three important effects: (1) short range order elasticity, (2) long range order elasticity, and (3) viscous flow. The **LE** theory addresses the long range order elasticity and viscous flow effects, while the Doi theory focuses on the short range order elasticity and the flow effect. Marrucci and Greco [15] extended the classical Maier-Saupe potential to the spatial inhomogeneous case, which accounts for spatial distortional elasticity. Wang [14] extended the Kuzuu and Doi theory to flowing systems of nonhomogeneous LCPs using an estimate of the Marrucci-Greco potential, and the shape parameter α. Fend et al. [16] adopted a one-constant Marrucci-Greco potential. Wang et al. [17] introduced a kernel type potential to describe the molecular interaction, and introduced an extra term in the form of an elastic body force. The Marrucci-Greco potential can be derived by local expansion, and the classical Ericksen-Leslie equations can be derived in the small Deborah number limit [18]. Rey and Tsuji [19] studied the complete tensor model [5] in detail, and showed the sketch of rheological phase diagram as a function of the ratio of short to long rang elasticity and the ratio of viscous flow to long rang elasticity effects, which is known as Ericksen number.

We apply the extended model to planar shear flow including kernel type potential and spatial diffusion term, which plays an important role in defect dynamics [20]. The paper is organized as follows. First, we present the extended kinetic-hydrodynamic model. In Section 3, we introduce the numerical scheme of LCPs imposed under shear flow. In Section 4, we show our numerical results including flow modes, dynamics of defects, weak shear limit results. A comparison among complete closure model, Bingham closure model, 1+1 kinetic model and our 1+2 kinetic model is given at the end of this section. Finally, we discuss the validity of this work.

2 The extended model

The extended Doi kinetic theory for inhomogeneous flow of rod-like LCPs can be specified by the following Smoluchowski equation: