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# A Nonhomogeneous Kinetic Model of Liquid Crystal Polymers and Its Thermodynamic Closure Approximation

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**Abstract.** A general nonhomogeneous extension of the Doi's kinetic theory with translational diffusion and nonlocal potential is proposed to describe the microstructures and defect dynamics of Liquid Crystal Polymer (LCP) solutions. The long-range elasticity of polymer molecules is depicted by a kernel type potential, from which one can derive the well-known Marrucci-Greco potential with weak spatial distortion assumption. Applying quasi-equilibrium closure approximation, we get a second-order moment model for isotropic long-range elasticity, and this reduced moment model maintains the energy dissipation. Implemented by the invariant-based fitting method, the moment model is a decent tool for numerical simulations of defect dynamics and texture evolution in LCP solutions. The numerical results of in-plane rotational case show that the reduced second-order moment model qualitatively predicts complicated nonhomogeneous director dynamics under moderate nematic potential strength, and the translational diffusion plays an important role in defect dynamics.

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**Key words**: LCP, kinetic theory, energy dissipation, closure approximation, defect dynamics.

## 1 Introduction

The kinetic theory of LCPs, started from Hess [16] and developed by Doi etc. [4, 5], has been a popular topic for three decades. The Doi-Hess theory predicts plenty of director dynamics in homogeneous nematic LCP solutions, such as tumbling, wagging, flow-aligning and log-rolling [9, 10, 26] etc. The interaction between the inner bulk tumbling

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region and boundary anchoring layer introduces defects and complex microstructures in nonhomogeneous LCP solutions. Meanwhile, these defects and microstructures strongly influence the rheology of the solutions. Marrucci and Greco [27] first analyzed the long-range elasticity of LCPs by introducing a nonlocal intermolecular potential based on the Maier-Saupe potential. Some nonhomogeneous extensions of Doi's theory, differing in the intermolecular potential, have been presented. Feng, Sgarlari and Leal [8] adopted a one-constant Marrucci-Greco potential; Wang, E, Liu and Zhang [31] adopted an integral form potential; and Wang [30] extended the Marrucci-Greco potential to account for macromolecules with different shapes. Although these nonhomogeneous kinetic theories have appeared for several years, 2D and 3D numerical studies based on them are sparse, because of huge computational cost involved. However, reduced equations about the moments of configuration distribution function (CDF) can be obtained from the exact kinetic models. The problem is that the equations of lower-order moments of CDF obtained from kinetic theory are coupled with higher-order moments. To close these equations, one must express higher-order moments in terms of lower-order moments, which is the so-called closure approximation.

Closure approximations for complex materials have been under investigation for many years. Various closure approximations have been proposed, such as the Doi's quadratic closure [5], the HL closures [17], orthotropic closure [3] and the Bingham closure [1]. Feng et al. [7] provided detailed numerical comparisons among five commonly used closures and found that the Bingham closure gives better results than others, although it deviates from the solutions of the exact kinetic theory when both the shear rate and nematic potential strength are very big. In fact, the Bingham closure is a particular case of quasi-equilibrium closure approximation (QEA). The systemic depiction of QEA is given by Gorban and the coworkers [11–14]. Ilg, Karlin and Öttinger [21] applied QEA to flexible polymers in homogeneous systems, while Ilg, Karlin, Kröger and Öttinger [20] analyzed rod-like polymers. They proved that QEA maintains the energy dissipation for homogeneous systems when flow is absent.

In our opinion, there are four criteria to evaluate closure approximations. First of all, the reconstructed CDF should be positive; secondly, a good closure approximation should maintain thermodynamic properties, such as mass conservation and energy dissipation; thirdly, it should achieve good accuracy; the last but not the least, a low computational cost implementation can be established for nonhomogeneous simulations. Energy dissipation is a basic requirement in the modeling of dissipation systems. However, it was not considered in the closure approximations of LCP kinetic theory until the work of Ilg et al. [21] was published. From the thermodynamic point of view, QEA is the proper closure approximation, but the numerical integration scheme for QEA proposed by Ilg et al. [19] is too expensive for nonhomogeneous simulation.

We introduce a relatively simple but general nonhomogeneous kinetic model for LCPs, and develop an efficient reduced moment model by QEA, which maintains energy dissipation. The invariant-based fitting method [2,22,29] is adopted in the simulations to reduce the computational costs.