Commun. Comput. Phys.
doi: 10.4208/cicp.160110.290610a

Vol. **9**, No. 4, pp. 974-993
April 2011

Numerical Simulations of Hydrodynamics of Nematic Liquid Crystals: Effects of Kinematic Transports

Shupeng Zhang[1], Chun Liu[2] and Hui Zhang[1,*]

[1] *School of Mathematical Sciences, Beijing Normal University, Beijing 100875, China.*
[2] *Department of Mathematics, Pennsylvania State University, University Park, PA 18601, USA.*

Received 16 January 2010; Accepted (in revised version) 29 June 2010

Communicated by Pingwen Zhang

Available online 2 November 2010

Abstract. In this paper, we investigate the effects of kinematic transports on the nematic liquid crystal system numerically and theoretically. The model we used is a "1+2" elastic continuum model simplified from the Ericksen-Leslie system. The numerical experiments are carried out by using a Legendre-Galerkin spectral method which can preserve the energy law in the discrete form. Based on this highly accurate numerical approach we find some interesting and important relationships between the kinematic transports and the characteristics of the flow. We make some analysis to explain these results. Several significant scaling properties are also verified by our simulations.

AMS subject classifications: 65M70, 76A15

Key words: Nematic liquid crystals, kinematic transports, Legendre-Galerkin spectral method, tumbling, flow-aligning.

1 Introduction

When the liquid crystals (LCs) are in nematic phase the molecules have long-range orientational order and can be easily aligned by external forces. This property results in many interesting and important phenomena, such as defects and textures. Many efforts have been made on theories describing the behavior of nematic LCs, for example, Onsager hard-rod model, Ericksen-Leslie (EL) theory, Maier-Saupe mean field theory, Q tensor theory, etc. Each model developed through a theory has its own merits in studying some aspects of nematic LCs.

*Corresponding author. *Email addresses:* shupeng.zhang@gmail.com (S. Zhang), liu@math.psu.edu (C. Liu), hzhang@bnu.edu.cn (H. Zhang)

The kinematic motions of the molecules is a fundamental topic in the study of nematic LCs. These motions can transform the alignment of molecules and further induce the change of physical properties of nematic LCs. Based on a kinetic model extended from Doi theory, Yu and Zhang studied the microstructure formation and defects dynamics arising in LC polymers in plane shear flow in [1]. Taken the long-range order elasticity into account Tsuji and Rey used a Q tensor theory to make an extensive analysis of the flow orientation modes of sheared liquid crystalline materials [2]. In [3] Feng et al. simulated the roll cells and disclinations in sheared nematic polymers. All these works were carried out with fixed tumbling parameter. Wang extended the Kuzuu and Doi theory to get a model with different configurations of molecules [4].

In EL theory a vector field **d** is used to depict the alignment of the molecules. The evolution of **d** expresses the kinematic motions. When the size of the molecules is small compared with the scale of the macroscopic fluid, **d** is just transported by the flow trajectory. When the size of the molecules are big enough, the effect of stretch by the fluid on **d** must be taken into account. This difference is reflected by the kinematic transport term of **d**. In the big molecule case, the parameter related to the shape of the molecules is important. In the original EL theory this parameter is called tumbling parameter. Effect of different tumbling parameter and Ericksen number on spatial development of director orientation in pressure-driven channel flow was investigated by Chono et al. in [5].

Lin and Liu et al. simplified the EL system [6–9] and they used a penalty function to relax the nonlinear constraint. Based on this simplified elastic continuum theory, many numerical experiments have been carried out to study the kinematic behaviors of nematic LCs. For small molecule cases, in [10] Liu and Walkington used a C^1 finite element to make sure that the test function is in the right space and the energy law is kept in discrete form. A mixed finite element was applied in [11] to avoid the construction of the complicated C^1 element. But the mixed method introduces new variables and increase the complication of implementation. In [12] Lin and Liu proposed a simpler C^0 finite element method to improve the efficiency of the numerical simulations. Spectral method for the system on rectangle domains with periodic boundary conditions was studied in [13] by Du et al.. For big molecule cases, a numerical scheme was proposed in [8] in order to preserve the energy law. In [9] an efficient and accurate spectral method was carried out on an axi-symmetric domain and dynamics of defect motions was studied. The numerical simulations reveal the significant impact of molecule shape on the moving speed of defects. Finite difference scheme in "1+2" dimension case was designed in [14]. They observed many valuable tumbling phenomena using the energy law preserving scheme.

In this paper, high order spectral method is used to simulate the "1+2" model. This model is similar to that in [14]. Instead of observations of tumbling phenomena therein, we mainly focus on the effect of kinematic transports on the nematic LC system. The kinematic transport is mainly determined by the shape of molecules and shear rate. We want to show that even with this simple model, several flow modes can be predicted and some significant scaling properties can be verified. Meanwhile, we want to reveal the relationship between two important parameters and the flow behavior. Since the nonlin-