# The Kinematic Effects of the Defects in Liquid Crystal Dynamics

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**Abstract.** Here we investigate the kinematic transports of the defects in the nematic liquid crystal system by numerical experiments. The model is a shear flow case of the viscoelastic continuum model simplified from the Ericksen-Leslie system. The numerical experiments are carried out by using a difference method. Based on these numerical experiments we find some interesting and important relationships between the kinematic transports and the characteristics of the flow. We present the development and interaction of the defects. These results are partly consistent with the observation from the experiments. Thus this scheme illustrates, to some extent, the kinematic effects of the defects.

**AMS subject classifications**: 65M70, 76A15

**Key words**: Nematic liquid crystals, kinematic effects, finite difference method, defects.

## 1 Introduction

The molecules of nematic liquid crystals have long-range orientational order and can be easily aligned by external forces. This will result in defects, textures and other important phenomena, e.g. disclination [4, 6, 10, 13, 32]. Many efforts have been made on theories to explore the liquid dynamics, such as Ericksen-Leslie (EL) theory [8, 10], tensor models [1, 24, 25], hard-rod models [6, 10, 12], capillary models [28, 30, 33, 34] and so on. Recently, many mathematicians are absorbed in investigating the solutions of these theoretical models, including the numerical simulations [7, 9, 17, 19, 20, 22, 23, 26, 36, 37, 39–41] and theoretical analysis [16, 18, 21] and references therein.

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Defects are classified in terms of strength (*S*) and dimensionality (*D*). The strength captures the degree of rotational discontinuity when encircling the defect, whereas the dimension refers to points (*D*=0), lines (*D*=1) and walls (*D*=2) [13,14,27]. Disclinations are line defects with *D*=1 and disclination ends cannot be found in the bulk. The strength of a disclination line is defined by a sign (+,−) and a magnitude (1/2,1,3/2,2,⋯). The sign indicates the direction of rotation and the magnitude is the amount of rotation. The defects with $s=\pm 1/2$ or $s=\pm 1$ has a singular core.

Toch et al. [35], showed that back-flow, the coupling between the order parameter and the velocity fields, has a significant effect on the motion of defects in nematic liquid crystals. In particular the defect speed can depend strongly on the topological strength in two dimensions and on the sense of rotation of the director about the core in three dimensions. They also considered that the annihilation of a pair of defects of strength $s=\pm 1/2$ and found that back-flow can change the speed of defects by up to $\sim 100\%$. Rey et al. [11,29,31] investigated the interaction of defects with different strength and compared them with the experiments. Here we study the interaction of defects immersing the fluids and find some interesting and important relationships between the kinematic transports and the characteristics of the flow.

In the Ericksen-Leslie (EL) theory, a vector field **d** is used to depict the alignment of the molecules and also to represent the direction of preferred orientation of the molecules in the neighbourhood of any point. The evolution of **d** expresses the kinematic motions. By the Ericksen and Leslie theory, the model is derived as the following nonlinear coupled system for nematic liquid crystals in fluid field [19,21]:

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mu\triangle\mathbf{u} + \lambda\nabla\cdot\sigma, \tag{1.1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{1.2}$$

$$\sigma = (\nabla\mathbf{d})^T\nabla\mathbf{d} + \beta(\triangle\mathbf{d} - \mathbf{f}(\mathbf{d}))\mathbf{d}^T + (\beta+1)\mathbf{d}(\triangle\mathbf{d} - \mathbf{f}(\mathbf{d}))^T, \tag{1.3}$$

$$\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d} = \gamma(\triangle\mathbf{d} - \mathbf{f}(\mathbf{d})). \tag{1.4}$$

Here **u** denotes the velocity of the nematic liquid crystals fluid, *p* the pressure, **d** the orientation of the molecules, $\mathbf{u},\mathbf{d}:\Omega\times\mathbb{R}^+\to\mathbb{R}^3, p:\Omega\times\mathbb{R}^+\to\mathbb{R}, \Omega\subset\mathbb{R}^2$. $\mathbf{x}\in\Omega$ is the Eulerian coordinate. $\mu,\lambda$ and $\gamma$ are positive constants. In Eq.(1.4) $\mathbf{f}(\mathbf{d})=(4/\varepsilon^2)(|\mathbf{d}|^2-1)\mathbf{d}$ can be treated as a penalty function to approximate the constraint $|\mathbf{d}|=1$ which is due to the molecules being of similar size for small $\varepsilon$. The corresponding energy density is $F(\mathbf{d})=(1/\varepsilon^2)(|\mathbf{d}|^2-1)^2$ and it is obvious $\mathbf{f}(\mathbf{d})$ is the gradient of $\nabla F(\mathbf{d})$. We define $D_\beta(\mathbf{u})=\beta\nabla\mathbf{u}+(1+\beta)(\nabla\mathbf{u})^T$ for $\beta\in\mathbb{R}$. Hence, it can be rewritten as

$$D_\beta(\mathbf{u}) = -\frac{\nabla\mathbf{u}-(\nabla\mathbf{u})^T}{2} - (-2\beta-1)\frac{\nabla\mathbf{u}+(\nabla\mathbf{u})^T}{2}. \tag{1.5}$$

The parameter $\beta$ depends on the shape of the molecules. In Eq. (1.4), the kinematic transport of **d** is $\frac{D}{Dt}\mathbf{d} = \mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d}$. When the size of the molecules is small compared with the scale of the macroscopic fluid, **d** is just transported by the flow trajectory. Then the kinematic transport of **d** is $\frac{D}{Dt}\mathbf{d} = \mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d}$ without the effect term $D_\beta(\mathbf{u})\mathbf{d}$ of