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Dynamics of Defect Motion in Nematic Liquid Crystal Flow: Modeling and Numerical Simulation

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Abstract. The annihilation of a hedgehog-antihedgehog pair in hydrodynamics of (elastically isotropic) nematic liquid crystal materials is modeled using the Erickson-Leslie theory which results in a nonlinear system for the flow velocity field and liquid crystal director field coupled through the transport of the directional order parameter and the induced elastic stress. An efficient and accurate numerical scheme is presented and implemented for this coupled nonlinear system in an axi-symmetric domain. Numerical simulations of annihilation of a hedgehog-antihedgehog pair with different types of transport are presented. In particular, it is shown that the stretching parameter in the transport equation contributes to the symmetry breaking of the pair's moving speed during the dynamics of annihilation.

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Key words: Hedgehog-antihedgehog, liquid crystal, Navier-Stokes, spectral-Galerkin method, defect motion.

1 Introduction

Liquid crystal is often viewed as the fourth state of the matter besides the gas, liquid and solid, or as an intermediate state between liquid and solid. It possesses no or partial positional order, while at the same time, displays an orientational order. To illustrate this special orientational ordering, a (nematic) liquid crystal molecule is often pictured as a rod whose orientation is depicted by the director field $\boldsymbol{d}$. This nematic phase is the simplest of liquid crystal phases and is close to the liquid phase. The molecules float around as in a liquid phase, but have the tendency of aligning along a preferred direction due to their orientation.

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In order to capture the coupling between the flow field and the dynamics of the director field, we will start with the following simplified system modeling the motion of nematic phase of liquid crystal flows (cf. [1,2]):

$$\begin{cases} \dfrac{\partial \boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}-\mu\nabla\cdot D(\boldsymbol{u})+\nabla p+\lambda\nabla\cdot(\nabla\boldsymbol{d}\otimes\nabla\boldsymbol{d})=0, \\ \nabla\cdot\boldsymbol{u}=0, \\ \dfrac{\partial \boldsymbol{d}}{\partial t}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{d}-\gamma(\Delta\boldsymbol{d}-f(\boldsymbol{d}))=0, \end{cases} \tag{1.1}$$

in a domain $\Omega\in R^3$ filled with liquid crystals, along with initial conditions

$$\boldsymbol{u}(x,0)=u_0; \qquad \boldsymbol{d}(x,0)=\boldsymbol{d}_0, \tag{1.2}$$

and suitable boundary conditions for $\boldsymbol{u}$ and $\boldsymbol{d}$. In the above, $\boldsymbol{u}=(u,v,w)^T$ is the flow velocity and p is the pressure; $\boldsymbol{d}=(d_1,d_2,d_3)^T$ represents the director of the molecules; μ,λ,γ are positive constants representing, respectively, the viscosity of the flow, the coupling coefficient representing the competition parameter between the kinetic energy and the elastic energy, and the parameter of elastic relaxation time; $\nabla\boldsymbol{d}$ is the Jacobian matrix with the (j,k)-th entry to be $\partial\boldsymbol{d}^{(j)}/\partial x_k$, and $\nabla\boldsymbol{d}\otimes\nabla\boldsymbol{d}$ is the Erickson stress tensor whose (j,k)-th entry is $\partial\boldsymbol{d}/\partial x_j\cdot\partial\boldsymbol{d}/\partial x_k$; $D(\boldsymbol{u})=(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T)/2$ is the symmetric part of the strain rate tensor; $\sigma=-pI+2\mu D(\boldsymbol{u})$ is the Newtonian part of the stress tensor. Finally, $f(\boldsymbol{d})=F'(\boldsymbol{d})$ where $F(\boldsymbol{d})$ is the bulk part of the elastic energy. The choice of $F(\boldsymbol{d})$ holds the information on the extensibility of the molecules.

With a set of suitable boundary conditions, the solution $(\boldsymbol{u},\boldsymbol{d})$ of the above system satisfies the following energy identity:

$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\boldsymbol{u}|^2+\frac{\lambda}{2}|\nabla\boldsymbol{d}|^2+\lambda F(\boldsymbol{d})\,dx=\int_\Omega \mu|\nabla\boldsymbol{u}|^2+\lambda\gamma|\Delta\boldsymbol{d}-f(\boldsymbol{d})|^2\,dx. \tag{1.3}$$

The elastic energy in the above system can be viewed as the relaxation as the following Oseen-Franck energy functional for the equilibrium configuration of a unit director field $\boldsymbol{d}$:

$$E(\boldsymbol{d})=\frac{k_1}{2}(\nabla\cdot\boldsymbol{d})^2+\frac{k_2}{2}|\boldsymbol{d}\times(\nabla\times\boldsymbol{d})|^2+\frac{k_3}{2}(\boldsymbol{d}\cdot(\nabla\times\boldsymbol{d}))^2. \tag{1.4}$$

In the elastically isotropic situation, i.e., $k_1=k_2=k_3=k$, this energy can be reduced to the Dirichlet functional $\frac{k}{2}|\nabla\boldsymbol{d}|^2$ plus the null-Lagrangian term which is determined by the boundary anchoring of the director [3]. Furthermore, if we allow the director to stretch at the expense of the bulk energy $F(\boldsymbol{d})$, then we can take $F(\boldsymbol{d})$ to be of the Ginzburg-Landau type, i.e.,

$$F(\boldsymbol{d})=\frac{1}{4\epsilon^2}(|\boldsymbol{d}|^2-1)^2$$

where $\epsilon\ll 1$ is a penalization parameter.