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AN ENERGY-DISSIPATION FINITE ELEMENT PRESSURE-CORRECTION SCHEME FOR THE HYDRODYNAMICS OF SMECTIC-A LIQUID CRYSTALS

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Abstract. In this paper, we develop a new linear, fully-decoupled, unconditional energy-stable BDF2-SAV-FEM scheme for solving the smectic-A liquid crystals, based on the finite element method (FEM) for spatial discretization and two-step backward differentiation formula (BDF2) for temporal discretization. To decouple the computations of the layer function and velocity field, we introduce an additional stabilization term into the constitutive equation. The nonlinear energy potential and the Navier-Stokes equations are treated by the scalar auxiliary variable (SAV) method and the rotational pressure-correction method, respectively. The unique solvability, unconditional energy stability, and error estimations of the proposed numerical scheme have been demonstrated. Several numerical experiments are carried out to validate our theoretical analysis.

Key words. Liquid crystals flows, unconditional energy stability, second-order, finite element method.

1. Introduction

Liquid crystals (LCs) are a novel intermediate state that appears in nature. Some substances in a molten state or after being dissolved by solvents, although losing the rigidity of solid substances, gain the fluidity of liquids and retain the anisotropic ordered arrangement of some crystalline substance molecules, forming an intermediate state that combines the properties of both crystals and liquids. This oriented ordered fluid that exists during the transition from solid to liquid is called liquid crystals (see [5,11,22]). LCs are widely used in daily life for a variety of applications, such as using them to indicate temperature and alarm toxic gases based on its color-changing characteristics, and using the optical properties of liquid crystals to make liquid crystal displays. Divide liquid crystals into thermotropic liquid crystals and lyotropic liquid crystals due to different conditions of liquid crystals production. Thermotropic liquid crystals include two essential types: the nematic phase and the smectic phase. The molecular arrangement of the smectic phase is arranged in layers, and the long axes of molecules within the layer are parallel to each other and perpendicular to the layer. There are many different smectic phases, which are characterized by different types and degrees of positional and orientational order(see [11,48–50]). For example, in the smectic-A phase, the director of liquid crystals molecules is perpendicular to the smectic plane, which means that the direction is consistent with the layers' normal vector. But in the smectic-C phase, the arrangement of molecules deviates from the normal vector of the layer. This paper mainly studies the numerical approximation of the smectic-A phase.

Recently, there has been a lot of interest in liquid crystals with many of these works focused on studying the nematic phase, see [1,17,35,43,55,57] and references therein. One of the most famous continuum theories for nematic liquid crystals

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is the Ericksen-Leslie model, which is derived by Ericksen and Leslie using the variational method for the Oseen-Frank energy [14, 15, 24, 25, 29]. For smectic-A liquid crystals, de Gennes and Prost proposed the first mathematical model in [11] by coupling two order parameters that, respectively, characterize the layer structure and the average direction of molecular alignment. In [2], the authors modified the model of de Gennes and Prost by adding a second-order gradient term for the smectic order parameter and studied the transition of nematic to smectic-A and smectic-C phases. In [23], the authors investigated the smectic-A liquid crystals by using the de Gennes energy to simulate the chevron pattern formed under the effect of an external magnetic field. In [12], by assuming that the director field is completely equal to the layer's gradient, the author succeeded to derive the simplified model of the smectic-A phase while reducing the free energy to one order parameter.

The mathematical analysis and numerical methods for the smectic-A liquid crystals are available in the literature. There are a lot of works for the theoretical analysis [9, 10, 26, 31, 53, 54]. For examples, the energy dissipative relation for the density-dependent system of the smectic-A liquid crystals were obtained and the existence of global weak solutions in the system was demonstrated in [26]. The authors studied a hydrodynamic system of smectic-A liquid crystals and analyzed the well-posedness as well as asymptotic behavior of strong solutions in [53]. From the view of computation, in [22] an unconditionally energy stable numerical scheme for the model of smectic-A liquid crystals was developed, which was first-order, linear, and decoupled time-marching. In [20], an energy-stable and second-order time-accurate numerical scheme was proposed for the smectic-A liquid crystals model, and numerical simulations were presented for 2D domains. The authors in [5] developed two linear, second-order time marching schemes for the system, one is the Crank-Nicolson scheme, another is the BDF2 scheme with the Adam-Bashforth explicit interpolation, further proved the well-posedness and unconditionally energy stability of numerical methods rigorously and used numerical experiments to validate the stability and accuracy of the schemes, but the schemes are partially decoupled and the error estimates of two schemes are missing. As far as we know, there fails to be any investigation on the convergence analysis of numerical methods for the smectic-A liquid crystals in the literature.

The discussed smectic-A phase model above is a highly nonlinear system that couples a constitutive equation for the layer function and the incompressible Navier-Stokes equations. For this system, there are several numerical difficulties: (i) the coupling of layer function and fluid velocity field; (ii) the existence of nonlinear terms; (iii) the coupling of fluid velocity field and pressure. This study is primarily focused on developing a second-order time-accurate fully discrete finite element scheme that can provide unconditional energy stability, full decoupling, and linearity. To overcome the first difficulty, we add an artificial stabilization term into the constitutive equation, which plays a significant role in decoupling the computations of the velocity field $\boldsymbol{u}$ and layer function ϕ, and use the implicit-explicit (IMEX) approach to handle other nonlinear coupling terms [36, 42, 44, 58]. For the nonlinear term $f(\nabla\phi)$, which brings a lot of difficulties when proving unconditionally energy stable and error estimates of the numerical scheme, the SAV method is applied to linearize this term [45–47]. Moreover, We decouple the velocity and pressure in the Navier-Stokes equations by applying the rotational pressure-correction method. Compared with the projection method [5, 22], the rotational pressure-correction method removes the need for artificial pressure boundary conditions. Eventually,