INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 6, Number 3, Pages 440–454

A THREE-STAGE OPERATOR-SPLITTING/FINITE ELEMENT METHOD FOR THE NUMERICAL SIMULATION OF LIQUID CRYSTAL FLOW

ROLAND GLOWINSKI, PING LIN, AND XING-BIN PAN

Abstract. In this article, we investigate the application of an operator-splitting/finite element method to the numerical simulation of a liquid crystal flow. The operator-splitting is achieved through three stages, so that each stage is simpler and easier to deal with than the step of any un-split implicit scheme. The first stage deals with the system coupling a Stokes equation for velocity with an equation modeling the diffusion of the liquid crystal director field. The second stage deals with the convection of both the velocity and director field; a wave-like equation approach is used to treat this advection part and proves being quite efficient. Finally, the third stage deals with the nonlinear terms; a (quasi) closed form solution can be derived for this stage. Overall, with this type of splitting, the nonlinear terms in the liquid crystal model can be treated quite easily. The results of several numerical experiments show the good performances of the three-stage splitting method discussed in this article.

Key Words. liquid crystal, incompressible flow, finite element method, operator-splitting method.

1. Introduction

The last two decades have been witnessing a strong interest among physicists, engineers and mathematicians for the theory and numerical modeling of liquid crystal related phenomena, including the flow of such materials. Liquid crystals do not show a single transition from solid to liquid, but rather a cascade of transitions involving new phases. The classical Oseen-Frank theory suggests that the nematic phase of liquid crystals can be described by a director field $\mathbf{d}$, which minimizes the so-called Oseen-Frank energy. The mathematical analysis and computational results for some special cases of the Oseen-Frank model can be found in [1, 4, 5, 11, 20, 12, 2, 3, 9, 17]. In order to describe liquid crystal flows we need not only the orientation, as represented by the director field $\mathbf{d}$, but also the velocity field $\mathbf{u}$. Ericksen and Leslie were able to derive a hydrodynamic model for nematic liquid crystals: a nematic flow behaves like a regular liquid with molecules of similar size. However, such a liquid displays anisotropic properties due to the molecule alignment described by the local director field $\mathbf{d}$. In order to facilitate the mathematical understanding of the Ericksen-Leslie theory, F. H. Lin and Liu proposed in [13] to consider a simplified model retaining most of mathematical and physical significance of the original model, but simple enough to make possible a rigorous mathematical

Received by the editors October 30, 2008 and, in revised form, January 5, 2009.
2000 *Mathematics Subject Classification.* 65M60, 76A15.

discussion. The model reads as follows:

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\nabla\cdot D(\mathbf{u}) + \nabla p + \lambda\nabla\cdot\left((\nabla\mathbf{d})^T\nabla\mathbf{d}\right) = \mathbf{0} \text{ in } \Omega\times(0,T), \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0 \text{ in } \Omega\times(0,T), \tag{2}$$

$$\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} - \gamma\left(\Delta\mathbf{d} - f(\mathbf{d})\right) = \mathbf{0} \text{ in } \Omega\times(0,T) \tag{3}$$

where in (1)-(3): (i) Ω ($\subset \mathbf{R}^d$) denotes the flow region and $(0,T)$ the time interval during which the flow is taking place. (ii) $\mathbf{u}$ represents the flow velocity and p the associated pressure. (iii) $\mathbf{d}$ represents the orientation of the liquid crystal molecules. (iv) $D(\mathbf{u}) = (1/2)\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)$ and $(\nabla\mathbf{d})_{ij} = \frac{\partial d_i}{\partial x_j}$. (v) $f(\mathbf{d}) = (1/\epsilon^2)(|\mathbf{d}|^2 - 1)\mathbf{d}$. The vector-valued functions $\mathbf{u}$ and $\mathbf{d}$ (resp., the real valued function p) are defined over $\Omega\times(0,T)$ and take their values in $\mathbf{R}^d$ (resp., $\mathbf{R}$). For our computations we will consider only test problems with $d = 2$. Concerning $f(\cdot)$, it is a *penalty operator*, used to enforce (approximately) the condition $|\mathbf{d}| = 1$ (where $|\mathbf{d}|$ denotes the canonical Euclidian norm of $\mathbf{d}$; actually, $f(\mathbf{d})$ is the differential at $\mathbf{d}$ of the *penalty functional* F defined by

$$F(\mathbf{d}) = (1/4\epsilon^2)(|\mathbf{d}|^2 - 1)^2.$$

The condition $|\mathbf{d}| = 1$ follows from the fact that the liquid crystal molecules are of similar size. Equation (1) describes the conservation of the linear momentum; it combines terms describing the flow of an isotropic fluid with an additional nonlinear term which is anisotropic. The second equation models the incompressibility of the liquid crystal material. The third equation is associated with the conservation of the angular momentum.

Of course, (1)-(3) have to be completed by initial and boundary conditions, such as:

$$\mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \mathbf{d}|_{t=0} = \mathbf{d}_0, \quad \mathbf{u}|_{\partial\Omega} = \mathbf{u}_0|_{\partial\Omega} = \mathbf{g}_\mathbf{u}, \quad \mathbf{d}|_{\partial\Omega} = \mathbf{g}_\mathbf{d}. \tag{4}$$

Even if the initial velocity is zero, the evolution of the director field may induce a velocity, which in turn will affect the evolution of the director field. Since the mathematical study of these interactions (between $\mathbf{u}$ and $\mathbf{d}$) is difficult, their numerical study is a most natural alternative. In [18] (resp., [19]), Liu & Walkington used an energy preserving C^1-conforming finite element method (resp., mixed finite element method) for the solution of problem (1)-(4). In [16], Lin & Liu further simplified the space approximations discussed in [18, 19] by deriving an energy preserving C^0-conforming finite element method. Some other methods have been used for the space approximation of (1)-(4); for example, the spectral method discussed in [6] appear to be efficient on rectangular domains when $\mathbf{u}$ and $\mathbf{d}$ verify periodic boundary conditions.

Considering the good results presented in [9], by the authors of the present article, for a simplified Oseen-Frank liquid crystal model, we would like to apply to the solution of problem (1)-(4) a variation of the operator-splitting scheme we employed in the above reference. As shown in, e.g., [8], the operator-splitting methodology provides quite often simple and efficient methods for the solution of complicated partial differential equations. In the particular case of problems such as (1)-(4), an appropriate operator-splitting time discretization scheme will allow us to treat rather easily the contribution of the nonlinear operator $f(\cdot)$, through the solution of simple cubic equations in one variable, reducing thus considerably the associated computational time compared to an implicit un-split time discretization scheme. In this article we are going to discuss a three-stage time-splitting scheme for the solution of problem (1)-(4); this scheme will have the 'nice' properties mentioned