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Theoretical and numerical calculations for the dynamics of nematic liquid crystals with consideration of flow

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Most of the studies about dynamics of liquid crystals rely on the approximation of zero flow. One of the reasons for this is that the dynamical equations are quite complicated and difficult to study due to the coupling between the orientation motion and the translation motion of molecules. The extra effort, the slow computation and the modelling equations with some approximations and ignorance of physical effects needed to solve them have not always seemed warranted for giving accurate calculation results. In this paper, we present the coupled director equations and flow equations for nematic liquid crystals, as well as the general theoretical and numerical calculation methods for solving these equations. These equations and calculation methods can be further simplified for some director configurations, such as homogeneous and homeotropic cells without twist. These described theoretical and numerical calculation methods show the generality of calculation for various director configurations. They are also computational efficient and easy to implement and can be widely used in studies of nematic liquid crystal dynamics including flow.

Keywords: director; flow; molecular field; integration constants; discrete form; linear system

1. Introduction

As we know, most modelling of liquid crystal dynamics relies on the approximation of zero flow. There are a number of reasons for this. First, the dynamical equations involve six Leslie coefficients. These coefficients are not easily measured and are available for only a few liquid crystal materials. The most recent, a method to estimate the Leslie coefficients of liquid crystals based on *N*-(4-methoxybenzylidene)-4-butylaniline (MBBA) data, was given in Wang *et al.* (*1*). Second, the equations are quite complicated and difficult to study due to the coupling between the orientation motion and the translation motion of molecules. The extra effort, the slow computation and the modelling equations with some approximations and ignorance of physical effects needed to solve them have not always seemed warranted for giving an accurate description on the dynamics of liquid crystals.

After Leslie (*2*, *3*) and Ericksen (*4*, *5*) gave the theoretical framework for the viscoelastic behaviour of nematic liquid crystals, this theory was applied in simplified form by Brochard (*6*) and Pieranski *et al.* (*7*) to describe the dynamics of liquid crystal layers in magnetic fields. The hydrodynamic equations were numerically solved with some approximations by Van Doorn (*8*), Van Doorn and Heldens (*9*) and Berreman (*10*) to explain the time-dependent optical transmission during switching of twisted nematic devices. Recently, Kelly *et al.* (*11*) gave the direct connection between simulation parameters and liquid crystal material properties. In their studies, the Ericksen-Leslie equations in the one-dimensional approximation of Berremen and van Doorn provide an excellent quantitative description of the dynamic response of twisted nematic devices including flow.

Following the convention of Kelly, we present the coupled director equations and flow equations for nematic liquid crystals and give the general theoretical and numerical calculation methods. With this approach, the one-dimensional approximation will not be valid if the dimensions of the liquid crystal cell (or pixel) are comparable to the thickness of the cell. These described equations and calculation methods show the generality of calculation for various director configurations. They are also computational efficient and easy to implement and can be widely used in the studies of nematic liquid crystal dynamics including flow.

2. Hydrodynamics of nematic liquid crystals

The flow mechanics of liquid crystals is complicated and difficult to study due to the coupling between the orientation motion and the translation motion of molecules. A local rotation of director may induce a flow and conversely, the velocity gradient of flow exerts a viscous torque on the director and leads to the rotation of the director. There are two approaches used to describe the coupling between the orientation and flow in nematic liquid crystals. One is the microscopic approach, which has been used by different

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research groups (*12–20*) to study the nematic hydrodynamics at the molecular level. Another is the macroscopic approach based on classical mechanics in which the fluid is regarded as a continuous medium. This approach was mainly developed by Ericksen (*21*, *22*), Leslie (*2*, *3*) and Parodi (*23*), therefore is usually referred to as the ELP theory. In this theory, six Leslie viscosity coefficients were introduced to describe the rheological properties of nematic liquid crystals. This theory has been tested in numerous experiments and proven to be the most successful theory on the hydrodynamics of nematic liquid crystals.

2.1 Hydrodynamic equations and ELP theory

In a continuous medium, various fluid properties such as velocity, density, director orientation and temperature, etc., are the continuous functions of position and time. Therefore, liquid crystal fluid can be described by the velocity field $\vec{V}(\vec{r},t)$, the director field $\hat{n}(\vec{r},t)$, and two thermodynamic quantities, pressure $\vec{p}(\vec{r},t)$ and density $\rho(\vec{r},t)$.

In a continuous fluid, the continuity equation can be written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0. \tag{1}$$

For an incompressible fluid, the density is a constant, therefore, we have:

$$\nabla \cdot \vec{V} = 0. \tag{2}$$

In fluid dynamics, the motion equation is given by the Navier–Stokes equation (*24*):

$$\rho\left[\frac{\partial \vec{V}}{\partial t} + (\vec{V}\cdot\nabla)\vec{V}\right] = \vec{f}_B + \nabla \cdot \sigma, \tag{3}$$

where f_B is the body force, and σ is a second-rank stress tensor whose component $\sigma_{\beta\alpha}$ gives the α-component of surface force exerted on a surface element normal to the β-axis. There are two categories of forces acting on the fluid. The first category comes from the presence of an external field such as a gravitational, electric or magnetic field, etc., and is called body force. The second is the force exerted on the surface of a fluid element, which is given by the second term on the right-hand side of Equation (3), and is called the surface force. The surface force consists of normal force and shearing force. There are normal and shearing forces exerted on the surface of a fluid element due to the resistance to dilation, compression and shearing. There is also a normal surface force $-\nabla p$ exerted on the surface of a fluid element due to the pressure p.

The viscous part of the stress tensor is a linear function of the velocity gradient to the lowest order and it should vanish when the velocity is uniform. The velocity gradient tensor $\nabla\vec{V}$ is not a symmetric tensor. We can use the symmetric part $A_{\alpha\beta}$of velocity gradient tensor $\nabla\vec{V}$ to construct the viscous tensor. $A_{\alpha\beta}$ is written as:

$$A_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial V_\beta}{\partial x_\alpha} + \frac{\partial V_\alpha}{\partial x_\beta}\right). \tag{4}$$

For an incompressible isotropic fluid, the viscous stress tensor is symmetric and there is only one viscosity. Therefore, the stress tensor can be written as:

$$\sigma = 2\eta\overline{\overline{A}} - p\overline{\overline{I}}, \tag{5}$$

where η is the viscosity of the isotropic fluid, and $\overline{\overline{I}}$ is the unit tensor.

For nematic liquid crystals, the viscous stress tensor is complicated due to the coupling between the director and the flow. The expression for the viscous stress tensor in an incompressible nematic fluid was given by Leslie (*2*, *3*) and Ericksen (*21*, *22*):

$$\begin{aligned}\sigma'_{\alpha\beta} = {} & \alpha_1 n_\alpha n_\beta n_\mu n_\rho A_{\mu\rho} + \alpha_2 n_\alpha N_\beta + \alpha_3 n_\beta N_\alpha \\ & + \alpha_4 A_{\alpha\beta} + \alpha_5 n_\alpha n_\mu A_{\mu\beta} + \alpha_6 n_\beta n_\mu A_{\mu\alpha},\end{aligned} \tag{6}$$

where α_i are Leslie viscosity coefficients, and $\vec{N}$ represents the change rate of director with respect to the background fluid. These Leslie coefficients are linked by the Parodi relation (*23*):

$$\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5. \tag{7}$$

Therefore, there are only five independent Leslie viscosity coefficients involved in the dynamics of incompressible nematic fluid. The rotation of fluid is defined as:

$$\vec{\omega} = \frac{1}{2}(\nabla \times \vec{V}), \tag{8}$$

and the local angular velocity of director is given by:

$$\vec{\Omega} = \hat{n} \times \frac{d\hat{n}}{dt}. \tag{9}$$

Therefore, the change rate of director is:

$$\vec{N} = (\vec{\Omega} - \vec{\omega}) \times \hat{n} = \frac{d\hat{n}}{dt} - \vec{\omega} \times \hat{n}. \tag{10}$$

In an isotropic fluid, the flow behaviour can be fully described by the motion Equation (3). For the

nematic fluid, the director rotation equation is needed in addition to the motion equation in order to describe the flow phenomena. At low rotation frequency, the rotation inertia is very small and can be neglected. The balance equation for the torques exerted on director is given by:

$$\Gamma_F + \Gamma_{visc} = 0, \tag{11}$$

where Γ_F is the body torque per unit volume exerted on the director, and Γ_{visc} is the torque per unit volume exerted on the director due to the frictional forces. The body torque is due to the elastic, electric, magnetic forces, etc. It can be written as:

$$\Gamma_F = \hat{n} \times \vec{h}, \tag{12}$$

where h is the molecular field. The molecular field generally consists of elastic, electric and magnetic field terms (*25*). The torque due to the frictional forces can be given by (*24*):

$$\Gamma_{visc} = -\gamma_1 \hat{n} \times \vec{N} - \gamma_2 \hat{n} \times \overline{\overline{A}} \cdot \hat{n}. \tag{13}$$

In Equation (13), γ_1 and γ_2 are two rotational viscosity coefficients and can be written in terms of Leslie viscosity coefficients (see Equations (28) and (29)).

The flow behaviour of nematic fluid can be fully determined by the motion equation of fluid (Equations (2) and (3)) and the director equation (Equation (11)). In the absence of flow, the viscous torque is reduced to:

$$\Gamma_{visc} = -\gamma_1 \hat{n} \times \frac{d\vec{n}}{dt}. \tag{14}$$

From Equations (11), (12) and (14), we can get the rotation equation of director, which has been widely used to calculate the director profile without consideration of flow.

2.2 *Leslie viscosities, shear viscosities and rotational viscosities*

Leslie viscosity coefficients are generally determined by the combinations of these coefficients and the aid of shear flow experiment. Corresponding to the shear flow experiment, there are three main effective viscosities for different orthogonal orientations of director with respect to the velocity and gradient of velocity as shown in Figure 1(a)–(c). These effective viscosities are often called Miesowicz viscosities.

In the description of shear flow, the flow is along the z-axis, the velocity gradient is along the x-axis and the director $\hat{n}$ is specified by the angles θ and ϕ (see Figure 2). With this coordinate system, the director field and velocity field can be written as:

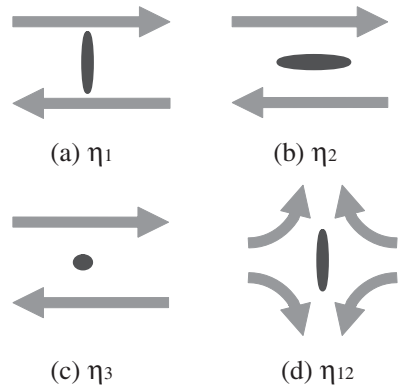

Figure 1. Effective viscosities for different geometries of shear flow.

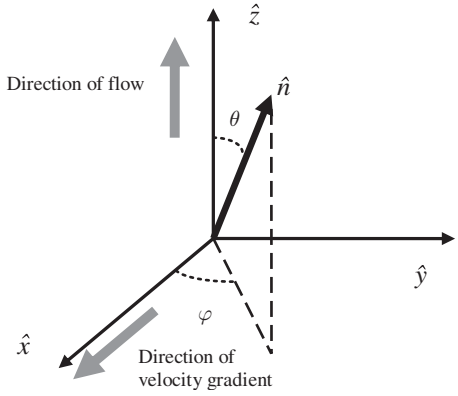

Figure 2. Director orientation, flow direction and velocity gradient.

$$\begin{aligned} \vec{V} &= (0, 0, u(x)), \text{and} \\ \hat{n} &= (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta). \end{aligned} \tag{15}$$

From Equation (6), we can get the xz and zx components of viscous stress tensor:

$$\begin{aligned} \sigma'_{xz} = &\frac{1}{2}\frac{du}{dx}\left[(2\alpha_1\cos^2\theta - \alpha_2 + \alpha_5)\sin^2\theta\cos^2\varphi \right. \\ &\left. + (\alpha_3 + \alpha_6)\cos^2\theta + \alpha_4\right], \end{aligned} \tag{16}$$

$$\begin{aligned} \sigma'_{zx} = &\frac{1}{2}\frac{du}{dx}\left[(2\alpha_1\cos^2\theta - \alpha_3 + \alpha_6)\sin^2\theta\cos^2\varphi \right. \\ &\left. + (\alpha_2 + \alpha_5)\cos^2\theta + \alpha_4\right]. \end{aligned} \tag{17}$$

For small velocity gradient, $\sigma'_{\alpha\beta}$ may be assumed to be a linear function of the spatial derivatives of the velocity, $\partial V_\beta / \partial x_\alpha$. In this case, the effective viscosity can be defined as:

$$\sigma'_{xz} = \eta\frac{du}{dx}. \tag{18}$$

Comparing Equation (16) with Equation (18), we have:

$$\eta = \frac{1}{2}\left[(2\alpha_1\cos^2\theta - \alpha_2 + \alpha_5)\sin^2\theta\cos^2\varphi + (\alpha_3 + \alpha_6)\cos^2\theta + \alpha_4\right]. \tag{19}$$

Therefore, the effective viscosities corresponding to the geometries shown in Figure 1(a)–(c) can be written in terms of Leslie viscosity coefficients as:

$$\eta_1 = \frac{1}{2}(-\alpha_2 + \alpha_4 + \alpha_5), \tag{20}$$

$$\eta_2 = \frac{1}{2}(\alpha_3 + \alpha_4 + \alpha_6), \tag{21}$$

$$\eta_3 = \frac{1}{2}\alpha_4. \tag{22}$$

In addition to the two antisymmetric shears in x and z, a symmetric stretch type of deformation in x and z is shown in Figure 1(d). For a fixed director at arbitrary angle θ and ϕ, the effective viscosity can also be given by (*24*):

$$\eta = (\eta_1 + \eta_{12}\cos^2\theta)\sin^2\theta\cos^2\varphi + \eta_2\cos^2\theta + \eta_3\sin^2\theta\sin^2\varphi. \tag{23}$$

From this equation, it is found that the largest contribution from the symmetric deformation (η_{12}) to the effective viscosity occurs when the director is in the shear plane at an angle of 45° to both the flow direction and the velocity gradient:

$$\eta_{45} = \frac{1}{2}(\eta_1 + \eta_2) + \frac{1}{4}\eta_{12}. \tag{24}$$

In addition, with

$$\eta_{12} = \alpha_1, \tag{25}$$

Equation (23) is equivalent to Equation (19). With these relations (Equations 19–25) and the Parodi relation, Leslie coefficients are completely related to the shear viscosities.

If the director is in the shear plane ($\varphi = 0$), the torque is along the $\hat{y}$ axis. From Equation (13), the torque can be given by:

$$\Gamma_{visc} = \frac{1}{2}\frac{du}{dx}[-\gamma_1 + \gamma_2(\sin^2\theta - \cos^2\theta)]. \tag{26}$$

This shear torque can also be expressed in terms of the antisymmetric part of the viscous stress tensor. From Equations (16) and (17), we have:

$$\Gamma_{visc} = \sigma'_{zx} - \sigma'_{xz} = \frac{du}{dx}(\alpha_2\sin^2\theta - \alpha_3\cos^2\theta). \tag{27}$$

Comparing Equation (26) with Equation (27), we have

$$\gamma_1 = \alpha_3 - \alpha_2, \tag{28}$$

$$\gamma_2 = \alpha_2 + \alpha_3. \tag{29}$$

In the middle region of the liquid crystal cell, the elastic torque is negligible. In the absence of an external field, the director will align in a direction where the shear torque vanishes. This angle is called the flow alignment angle. From Equations (26) and (27), the alignment angle θ_o can be given by:

$$\tan^2\theta_o = \frac{\alpha_3}{\alpha_2} = \frac{\gamma_1 + \gamma_2}{\gamma_2 - \gamma_1}. \tag{30}$$

3. The calculations with consideration of flow

3.1 Director equations and flow equations of nematic liquid crystals

Without consideration of flow, the rotation equation of the director can be obtained from Equations (11), (12) and (14). When the rotation inertia can be ignored, the rotation equation of the director can be written as:

$$\gamma_1\frac{\partial\hat{n}}{\partial t} = \vec{h} - (\vec{h}\cdot\hat{n})\hat{n}. \tag{31}$$

With consideration of flow, the rotation equation of the director can be written as:

$$\gamma_1\frac{\partial\hat{n}}{\partial t} = \vec{h} - \lambda\hat{n} + \gamma_1\vec{\omega}\times\hat{n} - \gamma_2\overline{\overline{A}}\cdot\hat{n} - \gamma_1(\vec{V}\cdot\nabla)\hat{n}, \tag{32}$$

where the Lagrange multiplier λ is defined as:

$$\lambda = (\vec{h}\cdot\hat{n}) - \gamma_2(\overline{\overline{A}}\cdot\hat{n})\cdot\hat{n}. \tag{33}$$

In the motion equation of liquid crystal fluid dynamics, the body force due to the external field can be ignored for the moment, and the stress tensor in Equation (3) can be defined as:

$$\sigma_{\alpha\beta} = -p\delta_{\alpha\beta} - \frac{\partial f_d}{\partial(\partial n_\gamma/\partial x_\alpha)}\frac{\partial n_\gamma}{\partial x_\beta} + \sigma'_{\alpha\beta}, \tag{34}$$

where p is the pressure, $\delta_{\alpha\beta}$ is the Kronecker delta, $\sigma'_{\alpha\beta}$ is the viscous stress tensor, and the second term is connected with the distortion free energy density. For small deformations, this term can be disregarded. The important differences generally come with the

viscous stress tensor. Therefore, the flow equation can be written as:

$$\rho\left(\frac{\partial V_\beta}{\partial t}+V_\alpha\frac{\partial V_\beta}{\partial x_\alpha}\right)=\frac{\partial \sigma'_{\alpha\beta}}{\partial x_\alpha}. \tag{35}$$

In the one-dimensional approximation of Berreman (*10*) and van Doorn (*8*), the flow is restricted to the plane of the cell. On the assumption that the anchoring of the director at the interface is rigid, we can neglect the surface director reorientation and the complication at the interface. With these approximations, we can get the three director equations from Equation (32) and the two flow equations from Equations (6) and (35). In one Cartesian dimension normal to the cell, here taken to be z, the coupled director equations and flow equations can be written as:

$$\gamma_1\frac{\partial n_x}{\partial t}=h_x-\lambda n_x-\alpha_2 n_z\frac{\partial V_x}{\partial z}, \tag{36}$$

$$\gamma_1\frac{\partial n_y}{\partial t}=h_y-\lambda n_y-\alpha_2 n_z\frac{\partial V_y}{\partial z}, \tag{37}$$

$$\gamma_1\frac{\partial n_z}{\partial t}=h_z-\lambda n_z-\alpha_3\left(n_x\frac{\partial V_x}{\partial z}+n_y\frac{\partial V_y}{\partial z}\right), \tag{38}$$

and

$$\begin{aligned}&\alpha_2 n_z\frac{\partial n_x}{\partial t}+\alpha_3 n_x\frac{\partial n_z}{\partial t}+\frac{1}{2}\left[2\alpha_1 n_x^2 n_z^2+(\alpha_5-\alpha_2)n_z^2\right.\\&\left.+\alpha_4+(\alpha_3+\alpha_6)n_x^2\right]\frac{\partial V_x}{\partial z}\\&+\left[\frac{1}{2}(\alpha_3+\alpha_6)+\alpha_1 n_z^2\right]n_x n_y\frac{\partial V_y}{\partial z}=c_1(t),\end{aligned} \tag{39}$$

$$\begin{aligned}&\alpha_2 n_z\frac{\partial n_y}{\partial t}+\alpha_3 n_y\frac{\partial n_z}{\partial t}+\frac{1}{2}\left[2\alpha_1 n_y^2 n_z^2+(\alpha_5-\alpha_2)n_z^2\right.\\&\left.+\alpha_4+(\alpha_3+\alpha_6)n_y^2\right]\frac{\partial V_y}{\partial z}+\left[\frac{1}{2}(\alpha_3+\alpha_6)+\alpha_1 n_z^2\right]\\&\times n_x n_y\frac{\partial V_x}{\partial z}=c_2(t),\end{aligned} \tag{40}$$

where $c_1(t)$ and $c_2(t)$ are two time-dependent integration constants and Lagrange multiplier λ equals:

$$\lambda=(\vec{h}\cdot\hat{n})-(\alpha_2+\alpha_3)n_z\left(n_x\frac{\partial V_x}{\partial z}+n_y\frac{\partial V_y}{\partial z}\right). \tag{41}$$

3.2 Molecular field

In order to solve these director and flow equations, we need to calculate the molecular field. Molecular field is defined as the functional derivative of free energy density f (*24*):

$$h_\alpha=-\frac{\partial f}{\partial n_\alpha}+\sum_\beta\frac{\partial}{\partial x_\beta}\left(\frac{\partial f}{\partial g_{\beta\alpha}}\right), \tag{42}$$

with $g_{\beta\alpha}=\dfrac{\partial n_\alpha}{\partial x_\beta}$. Therefore, we have:

$$h_\alpha=-\frac{\partial f_d}{\partial n_\alpha}+\sum_\beta\frac{\partial}{\partial x_\beta}\left(\frac{\partial f_d}{\partial g_{\beta\alpha}}\right)+\varepsilon_o\Delta\varepsilon(\vec{E}\cdot\hat{n})E_\alpha. \tag{43}$$

From Equation (43), the molecular field due to the distortion in the one-dimensional approximation can be obtained:

$$\begin{aligned}h_{d,x}=&K_{22}\left[n_y^2\frac{\partial^2 n_x}{\partial z^2}-n_x n_y\frac{\partial^2 n_y}{\partial z^2}+2n_y\frac{\partial n_x}{\partial z}\frac{\partial n_y}{\partial z}\right.\\&\left.-2n_x\left(\frac{\partial n_y}{\partial z}\right)^2\right]+K_{33}\left[n_z^2\frac{\partial^2 n_x}{\partial z^2}+2n_z\frac{\partial n_x}{\partial z}\frac{\partial n_z}{\partial z}\right],\end{aligned} \tag{44}$$

$$\begin{aligned}h_{d,y}=&K_{22}\left[n_x^2\frac{\partial^2 n_y}{\partial z^2}-n_x n_y\frac{\partial^2 n_x}{\partial z^2}+2n_x\frac{\partial n_x}{\partial z}\frac{\partial n_y}{\partial z}\right.\\&\left.-2n_y\left(\frac{\partial n_x}{\partial z}\right)^2\right]+K_{33}\left[n_z^2\frac{\partial^2 n_y}{\partial z^2}+2n_z\frac{\partial n_y}{\partial z}\frac{\partial n_z}{\partial z}\right],\end{aligned} \tag{45}$$

$$\begin{aligned}h_{d,z}=&K_{11}\frac{\partial^2 n_z}{\partial z^2}+K_{33}\left\{n_z^2\frac{\partial^2 n_z}{\partial z^2}\right.\\&\left.+n_z\left[\left(\frac{\partial n_z}{\partial z}\right)^2-\left(\frac{\partial n_x}{\partial z}\right)^2-\left(\frac{\partial n_y}{\partial z}\right)^2\right]\right\}.\end{aligned} \tag{46}$$

In one elastic constant approximation, the molecular field can be written as:

$$\vec{h}=K\nabla^2\hat{n}+u(\vec{r})\hat{n}+\varepsilon_o\Delta\varepsilon(\vec{E}\cdot\hat{n})\vec{E}, \tag{47}$$

where

$$u(\vec{r})=K\left[n_z\frac{\partial^2 n_z}{\partial z^2}+\left(\frac{\partial n_z}{\partial z}\right)^2-\left(\frac{\partial n_x}{\partial z}\right)^2-\left(\frac{\partial n_y}{\partial z}\right)^2\right]. \tag{48}$$

As one can always add to f_d a term of the form $\frac{1}{2}u(\vec{r})\hat{n}^2=\frac{1}{2}u(\vec{r})$ without change of the distortion energy, $\vec{h}$ and $\vec{h}+u(\vec{r})\hat{n}$ are equivalent (*25*). Thus we have:

$$\vec{h}=K\nabla^2\hat{n}+\varepsilon_o\Delta\varepsilon(\vec{E}\cdot\hat{n})\vec{E}. \tag{49}$$

The molecular field due to the distortion consists of three parts, splay, twist and bend, and can be written as (*25*):

$$\vec{h}_d=\vec{h}_s+\vec{h}_t+\vec{h}_b. \tag{50}$$

where

$$\vec{h}_s = K_{11}\nabla(\operatorname{div}\hat{n}), \tag{51}$$

$$\vec{h}_t = -K_{22}[A\ \operatorname{curl}\hat{n} + \operatorname{curl}(A\hat{n})], \tag{52}$$

$$\vec{h}_b = K_{33}[\vec{B}\times\operatorname{curl}\hat{n} + \operatorname{curl}(\hat{n}\times\vec{B})], \tag{53}$$

with

$$A = \hat{n}\cdot\operatorname{curl}\hat{n} \text{ and } \vec{B} = \hat{n}\times\operatorname{curl}\hat{n}. \tag{54}$$

In the one-dimensional approximation with one Cartesian dimension $\hat{z}$ normal to the cell, the equations for the splay, twist and bend components, which are given in Appendix A (see (A1)–(A3)), can be obtained from Equations 51–53. Thus, we can get the molecular field due to distortion as:

$$\begin{aligned} h_{d,x} = K_{22}\Bigg[&n_y^2\frac{\partial^2 n_x}{\partial z^2} - n_x n_y\frac{\partial^2 n_y}{\partial z^2} + 2n_y\frac{\partial n_x}{\partial z}\frac{\partial n_y}{\partial z} \\ &-2n_x\left(\frac{\partial n_y}{\partial z}\right)^2\Bigg] + K_{33}\Bigg[n_z^2\frac{\partial^2 n_x}{\partial z^2} \\ &+2n_z\frac{\partial n_x}{\partial z}\frac{\partial n_z}{\partial z}\Bigg] + un_x, \end{aligned} \tag{55}$$

$$\begin{aligned} h_{d,y} = K_{22}\Bigg[&n_x^2\frac{\partial^2 n_y}{\partial z^2} - n_x n_y\frac{\partial^2 n_x}{\partial z^2} + 2n_x\frac{\partial n_x}{\partial z}\frac{\partial n_y}{\partial z} \\ &-2n_y\left(\frac{\partial n_x}{\partial z}\right)^2\Bigg] + K_{33}\Bigg[n_z^2\frac{\partial^2 n_y}{\partial z^2} \\ &+2n_z\frac{\partial n_y}{\partial z}\frac{\partial n_z}{\partial z}\Bigg] + un_y, \end{aligned} \tag{56}$$

$$\begin{aligned} h_{d,z} = K_{11}\frac{\partial^2 n_z}{\partial z^2} + K_{33}\Bigg\{&n_z^2\frac{\partial^2 n_z}{\partial z^2} \\ &+n_z\left[\left(\frac{\partial n_z}{\partial z}\right)^2 - \left(\frac{\partial n_x}{\partial z}\right)^2 - \left(\frac{\partial n_y}{\partial z}\right)^2\right]\Bigg\} + un_z, \end{aligned} \tag{57}$$

where

$$u(\vec{r}) = -K_{33}\left[n_z\frac{\partial^2 n_z}{\partial z^2} + \left(\frac{\partial n_z}{\partial z}\right)^2\right]. \tag{58}$$

Comparing Equations 44–46 with Equations 55–57, these two calculation results for the molecular field differ only by $u(\vec{r})\hat{n}$. As we know, $\vec{h}$ and $\vec{h} + u(\vec{r})\hat{n}$ are equivalent, therefore, these two calculations coincide with each other.

3.3 Integration constants and matrix form of the equations

The director and flow equations can be expressed in matrix form as:

$$\gamma_1\begin{pmatrix}\dfrac{\partial n_x}{\partial t}\\ \dfrac{\partial n_y}{\partial t}\\ \dfrac{\partial n_z}{\partial t}\end{pmatrix} = \tilde{h} + D\begin{pmatrix}\dfrac{\partial V_x}{\partial z}\\ \dfrac{\partial V_y}{\partial z}\end{pmatrix}, \tag{59}$$

and

$$A\begin{pmatrix}\dfrac{\partial n_x}{\partial t}\\ \dfrac{\partial n_y}{\partial t}\\ \dfrac{\partial n_z}{\partial t}\end{pmatrix} + B\begin{pmatrix}\dfrac{\partial V_x}{\partial z}\\ \dfrac{\partial V_y}{\partial z}\end{pmatrix} = C, \tag{60}$$

where the matrices $\tilde{h}$, D, A, B and C are given in Appendix A (see (A4)–(A8)). From these two matrix equations, the flow can be expressed as:

$$\begin{pmatrix}\dfrac{\partial V_x}{\partial z}\\ \dfrac{\partial V_y}{\partial z}\end{pmatrix} = \left(B + \frac{1}{\gamma_1}AD\right)^{-1}\left(C - \frac{1}{\gamma_1}A\tilde{h}\right). \tag{61}$$

With the assumption of strong anchoring, the flow at the surfaces can be neglected, and thus the integral of Equation (61) over the cell along the Cartesian dimension normal to the cell is zero. Therefore, we have:

$$C = \frac{\frac{1}{\gamma_1}\int_0^d (B + \frac{1}{\gamma_1}AD)^{-1}A\tilde{h}\,dz}{\int_0^d (B + \frac{1}{\gamma_1}AD)^{-1}\,dz}. \tag{62}$$

After the time-dependent integration constant matrix C is known, we can calculate the gradient of flow at that moment from Equation (61), as well as the change rate of director from Equation (59). Thus, the flow and director at a time moment can be obtained from the following two equations:

$$\vec{V} = \int_0^z \frac{\partial\vec{V}}{\partial z}dz, \tag{63}$$

$$\hat{n} = \hat{n}_0 + \int_0^t \frac{\partial\hat{n}}{\partial t}dt. \tag{64}$$

3.4 Discrete form and linear system

Those equations in matrix form or integral form need to be written in discrete form in order to implement

them. We choose especially the implicit Crank–Nicolson scheme (*26*) to get the discrete forms for the two integral Equations (63) and (64). Corresponding to these two equations, the discrete forms can be written as:

$$\begin{pmatrix} V_x \\ V_y \end{pmatrix}_{i+1} = \begin{pmatrix} V_x \\ V_y \end{pmatrix}_i + \frac{1}{2}\left[\begin{pmatrix} \frac{\partial V_x}{\partial z} \\ \frac{\partial V_y}{\partial z} \end{pmatrix}_i + \begin{pmatrix} \frac{\partial V_x}{\partial z} \\ \frac{\partial V_y}{\partial z} \end{pmatrix}_{i+1}\right]\Delta z, \tag{65}$$

$$\hat{n}_{t+1} = \hat{n}_t + \frac{1}{2}\left[\left(\frac{\partial \hat{n}}{\partial t}\right)_t + \left(\frac{\partial \hat{n}}{\partial t}\right)_{t+\Delta t}\right]\Delta t. \tag{66}$$

At the interfaces, we do not assume that the gradient of flow is zero. With neglecting the surface director reorientation, Equation (60) shows that it is reasonable for choosing the gradient of flow at the interfaces as:

$$\begin{pmatrix} \frac{\partial V_x}{\partial z} \\ \frac{\partial V_y}{\partial z} \end{pmatrix}_{1,N} = \frac{C(t)}{B_{1,N}}. \tag{67}$$

Therefore, the discrete form of time-dependent integration constants can be written as:

$$C(t) = \frac{\frac{1}{\gamma_1}\sum_{i=2}^{N-1}\left(B_i + \frac{1}{\gamma_1}A_iD_i\right)^{-1}A_i\tilde{h}_i}{\frac{1}{2}\left(\frac{1}{B_1}+\frac{1}{B_N}\right) + \sum_{i=2}^{N-1}\left(B_i + \frac{1}{\gamma_1}A_iD_i\right)^{-1}}. \tag{68}$$

If we assume the gradient of flow is zero at the interfaces, then the discrete form can be written as:

$$C(t) = \frac{\frac{1}{\gamma_1}\sum_{i=2}^{N-1}\left(B_i + \frac{1}{\gamma_1}A_iD_i\right)^{-1}A_i\tilde{h}_i}{\sum_{i=2}^{N-1}\left(B_i + \frac{1}{\gamma_1}A_iD_i\right)^{-1}}. \tag{69}$$

Using Equation (66) to calculate the director can provide good accuracy and numerical stability with a relatively large time step compared with using the Euler method (*26*) with a small time step. From Equation (66), we can get a linear system (Equation (70)) by replacing the derivatives of the director in the molecular field by the central finite differences. The director at a time is mapped directly from the director at the previous time by this linear system equation:

$$\begin{bmatrix} A_x^{t+\Delta t} & B_x^{t+\Delta t} & C_x^{t+\Delta t} \\ A_y^{t+\Delta t} & B_y^{t+\Delta t} & C_y^{t+\Delta t} \\ A_z^{t+\Delta t} & B_z^{t+\Delta t} & C_z^{t+\Delta t} \end{bmatrix}\begin{pmatrix} n_x^{t+\Delta t} \\ n_y^{t+\Delta t} \\ n_z^{t+\Delta t} \end{pmatrix} = \begin{bmatrix} A_x^t & B_x^t & C_x^t \\ A_y^t & B_y^t & C_y^t \\ A_z^t & B_z^t & C_z^t \end{bmatrix}\begin{pmatrix} n_x^t \\ n_x^t \\ n_x^t \end{pmatrix} + \begin{pmatrix} D_x^t \\ D_y^t \\ D_z^t \end{pmatrix}, \tag{70}$$

where elements of matrices in this linear system are given in Appendix A (see (A9)–(A29)). In establishing this linear system, the Lagrange multiplier λ and the gradient of flow $\frac{\partial V}{\partial z}$ at time t are used in these elements of matrices.

4. Untwisted nematic liquid crystal devices

For a liquid crystal cell without twist, there is no $\hat{y}$ component, and all of the equations can be simplified and the computation becomes relatively easy. In order to show the generality of calculation methods, we still use the x and z components of the director in the whole theoretical and numerical calculations for a liquid crystal cell without twist. With all terms related to the $\hat{y}$ component being zero in Equations 36–41, these equations can be simplified into two director equations and one flow equation:

$$\gamma_1\frac{\partial n_x}{\partial t} = h_x - \lambda n_x - \alpha_2 n_z\frac{\partial V_x}{\partial z}, \tag{71}$$

$$\gamma_1\frac{\partial n_z}{\partial t} = h_z - \lambda n_z - \alpha_3 n_x\frac{\partial V_x}{\partial z}, \tag{72}$$

and

$$\alpha_2 n_z\frac{\partial n_x}{\partial t} + \alpha_3 n_x\frac{\partial n_z}{\partial t} + \frac{1}{2}\left[2\alpha_1 n_x^2 n_z^2 + (\alpha_5 - \alpha_2)n_z^2 + \alpha_4 + (\alpha_3 + \alpha_6)n_x^2\right] \times \frac{\partial V_x}{\partial z} = c(t), \tag{73}$$

where

$$\lambda = (\vec{h}\cdot\hat{n}) - (\alpha_2 + \alpha_3)n_x n_z\frac{\partial V_x}{\partial z}. \tag{74}$$

From Equations 44–46, the molecular field has a simple form:

$$\vec{h}_d = K_{33}\left[n_z^2\frac{\partial^2 n_x}{\partial z^2} + 2n_z\frac{\partial n_x}{\partial z}\frac{\partial n_z}{\partial z}\right]\hat{x} + \left\{K_{11}\frac{\partial^2 n_z}{\partial z^2} + K_{33}\left[n_z^2\frac{\partial^2 n_z}{\partial z^2} + n_z\left(\frac{\partial n_z}{\partial z}\right)^2 - n_z\left(\frac{\partial n_x}{\partial z}\right)^2\right]\right\}\hat{z}. \tag{75}$$

In one elastic constant approximation, it can be written as:

$$\vec{h}_d = K(\nabla^2 n_x \hat{x} + \nabla^2 n_z \hat{z}). \tag{76}$$

The linear system Equation (70) can be simplified into a simple form as:

$$\begin{bmatrix} A_x^{t+\Delta t} & B_x^{t+\Delta t} \\ A_z^{t+\Delta t} & B_z^{t+\Delta t} \end{bmatrix} \begin{pmatrix} n_x^{t+\Delta t} \\ n_z^{t+\Delta t} \end{pmatrix} = \begin{bmatrix} A_x^t & B_x^t \\ A_z^t & B_z^t \end{bmatrix} \begin{pmatrix} n_x^t \\ n_z^t \end{pmatrix} + \begin{pmatrix} D_x^t \\ D_z^t \end{pmatrix}, \tag{77}$$

where the elements of the matrices are given in Appendix A (see (A33)–(A44)).

As we know, we assume that the cell length is much larger than its thickness and consider the region far from the cell edges. In this region the hydrodynamic flow has only the x component $\vec{v} = \{v(z,t), 0, 0\}$ and the director remains in the OXZ plane, and we can use the tilt angle to express the director $\hat{n} = \{\cos\theta(z,t), 0, \sin\theta(z,t)\}$in the whole theoretical and numerical calculations. Thus we have only two equations:

$$\gamma_1 \frac{\partial \theta}{\partial t} = (h_z \cos\theta - h_x \sin\theta) - (\alpha_3 \cos^2\theta - \alpha_2 \sin^2\theta)\frac{\partial v}{\partial z}, \tag{78}$$

$$(\alpha_3 \cos^2\theta - \alpha_2 \sin^2\theta)\frac{\partial \theta}{\partial t} + \frac{1}{2}\left[\frac{1}{2}\alpha_1 \sin^2 2\theta + (\alpha_5 - \alpha_2)\sin^2\theta + \alpha_4 + (\alpha_3 + \alpha_6)\cos^2\theta\right]\frac{\partial v}{\partial z} = c(t). \tag{79}$$

With using the tilt angle to express the director in the theoretical and numerical calculations for a liquid crystal cell without twist, the calculation is simplified further and the numerical stability can be relatively easy to achieve.

5. Summary

We have given the coupled director equations and flow equations of nematic liquid crystals, together with the general theoretical and numerical calculation methods. These equations and calculation methods can be further simplified for some director configurations, such as homogeneous and homeotropic cells without twist. In the numerical calculation, we use the Crank–Nicolson scheme instead of the Euler method to get a relatively accurate and numerically stable solution. With the standard Euler method, a small time step in the computation is needed, and the numerical stability is also a challenge, especially for complicated switching schemes such as the modulated electric field.

Our theoretical and numerical methods for solving these coupled director equations and flow equations have the generality for cases where the dimensions of a liquid crystal cell (or pixel) are far larger than the thickness of the cell. They are also computational efficient and easy to implement and can be widely used in studies of liquid crystal dynamics including flow. One should be aware that this one-dimensional approximation is not valid if the dimensions of the liquid crystal cell (or pixel) are comparable to the thickness of the cell.

References

(1) Wang, H.; Wu, T.X.; Gauza, S.; Wu, J.R.; Wu, S.-T. *Liquid Crystals* **2006**, *33*, 91–98.
(2) Leslie, F.M. *Quart. J. Mech. Appl. Math.* **1966**, *19*, 357–370.
(3) Leslie, F.M. *Arch. Rational Mech. Analysis* **1968**, *28*, 265–283.
(4) Ericksen, J.L. *Trans. Soc. Rheol.* **1961**, *5*, 23–24.
(5) Ericksen, J.L. *Mol. Cryst. Liq. Cryst.* **1969**, *7*, 153–161.
(6) Brochard, F. *J. Phys. (Paris)* **1972**, *33*, 607–615.
(7) Pieranski, P.; Brochard, F.; Guyon, E. *J. Phys. (Paris)* **1973**, *34*, 35–48.
(8) van Doorn, C.Z. *Phys. Lett.* **1973**, *A42*, 537–546.
(9) van Doorn, C.Z.; Heldens, J.L.A.M. *Phys. Lett.* **1974**, *A47*, 135–143.
(10) Berreman, D.W. *J. Opt. Soc. Am.* **1973**, *63*, 1374–1380.
(11) Kelly, J.; Jamal, S.; Cui, M. *J. Appl. Phys.* **1999**, *86*, 4091–4095.
(12) Forster, D.; Lubensky, T.C.; Martin, P.C.; Swift, J.; Pershan, P.S. *Phys. Rev. Lett.* **1971**, *26*, 1016–1019.
(13) Martin, P.C.; Parodi, O.; Pershan, P.S. *J. Phys. Rev.* **1972**, *A6*, 2401–2420.
(14) Diogo, A.C.; Martins, A.F. *Mol. Cryst. Liq. Cryst.* **1981**, *66*, 133–146.
(15) Doi, M. *J. Polym. Sci. Polym. Phys. Ed.* **1981**, *19*, 229–243.
(16) Kuzuu, N.; Doi, M. *J. Phys. Soc. Jpn* **1983**, *52*, 3486–3494.
(17) Osipov, M.A.; Terentjev, E.M. *Z. Naturforsch.* **1989**, *44a*, 785–791.
(18) Osipov, M.A.; Terentjev, E.M. *Phys. Lett. A* **1989**, *134*, 301–312.
(19) Archer, L.A.; Larson, R.G. *J. Chem. Phys.* **1995**, *103*, 3108–3111.
(20) Kroger, M.; Sellers, S. *J. Chem. Phys.* **1995**, *103*, 807–816.
(21) Ericksen, J.L. *Arch. Rational Mech. Analysis* **1960**, *4*, 231–237.
(22) Ericksen, J.L. *Phys. Fluids* **1966**, *9*, 1205–1207.
(23) Parodi, O. *J. Phys. (Paris)* **1970**, *31*, 581–584.
(24) De Jeu, W.H. *Physical Properties of Liquid Crystalline Materials*; Gordon and Breach Science Publishers: New York, 1980.
(25) De Gennes, P.G.; Prost, J. *The Physics of Liquid Crystals*, 2nd edition; Oxford University Press: New York, 1993.
(26) Heath, M.T. *Scientific Computing: An Introductory Survey*, 2nd edition; McGraw-Hill: New York, 2005.

Appendix A. Equations, matrices and element of matrices

The equations for the splay, twist and bend components of the molecular field due to distortion in the one-dimensional approximation with one Cartesian dimension $\hat{z}$ normal to the cell can be written as:

$$\vec{h}_s = K_{11}\frac{\partial^2 n_z}{\partial z^2}\hat{z}, \tag{A1}$$

$$\begin{aligned}\vec{h}_t = K_{22}&\left[n_y^2\frac{\partial^2 n_x}{\partial z^2} - n_x n_y\frac{\partial^2 n_y}{\partial z^2} + 2n_y\frac{\partial n_x}{\partial z}\frac{\partial n_y}{\partial z}\right.\\ &\left. - 2n_x\left(\frac{\partial n_y}{\partial z}\right)^2\right]\hat{x} + K_{22}\left[n_x^2\frac{\partial^2 n_y}{\partial z^2} - n_x n_y\frac{\partial^2 n_x}{\partial z^2}\right.\\ &\left. + 2n_x\frac{\partial n_x}{\partial z}\frac{\partial n_y}{\partial z} - 2n_y\left(\frac{\partial n_x}{\partial z}\right)^2\right]\hat{y},\end{aligned} \tag{A2}$$

$$\begin{aligned}h_b =& K_{33}\left[n_z^2\frac{\partial^2 n_x}{\partial z^2} + 2n_z\frac{\partial n_x}{\partial z}\frac{\partial n_z}{\partial z}\right]\hat{x}\\ &+ K_{33}\left[n_z^2\frac{\partial^2 n_y}{\partial z^2} + 2n_z\frac{\partial n_y}{\partial z}\frac{\partial n_z}{\partial z}\right]\hat{y}\\ &+ K_{33}\left\{n_z^2\frac{\partial^2 n_z}{\partial z^2} + n_z\left[\left(\frac{\partial n_z}{\partial z}\right)^2 - \left(\frac{\partial n_x}{\partial z}\right)^2\right.\right.\\ &\left.\left. - \left(\frac{\partial n_y}{\partial z}\right)^2\right]\right\}\hat{z} - K_{33}\left[n_z\frac{\partial^2 n_z}{\partial z^2} + \left(\frac{\partial n_z}{\partial z}\right)^2\right]\hat{n}.\end{aligned} \tag{A3}$$

The matrices $\tilde{h}$, D, A, B and C in Equations (59) and (60) are given as:

$$\tilde{h} = \begin{pmatrix} h_x - (\hat{n}\cdot\hat{h})n_x \\ h_y - (\hat{n}\cdot\hat{h})n_y \\ h_z - (\hat{n}\cdot\hat{h})n_z \end{pmatrix} \tag{A4}$$

$$D = \begin{bmatrix} n_x^2 n_z(\alpha_2+\alpha_3) - \alpha_2 n_z & n_x n_y n_z(\alpha_2+\alpha_3) \\ n_x n_y n_z(\alpha_2+\alpha_3) & n_y^2 n_z(\alpha_2+\alpha_3) - \alpha_2 n_z \\ n_x n_z^2(\alpha_2+\alpha_3) - \alpha_3 n_x & n_y n_z^2(\alpha_2+\alpha_3) - \alpha_3 n_y \end{bmatrix} \tag{A5}$$

$$A = \begin{bmatrix} \alpha_2 n_z & 0 & \alpha_3 n_x \\ 0 & \alpha_2 n_z & \alpha_3 n_y \end{bmatrix} \tag{A6}$$

$$B = \begin{bmatrix} \frac{1}{2}\left[2\alpha_1 n_x^2 n_z^2 + (\alpha_5-\alpha_2)n_z^2 + \alpha_4 + (\alpha_3+\alpha_6)n_x^2\right] & \left[\frac{1}{2}(\alpha_3+\alpha_6) + \alpha_1 n_z^2\right] n_x n_y \\ \left[\frac{1}{2}(\alpha_3+\alpha_6) + \alpha_1 n_z^2\right] n_x n_y & \frac{1}{2}\left[2\alpha_1 n_y^2 n_z^2 + (\alpha_5-\alpha_2)n_z^2 + \alpha_4 + (\alpha_3+\alpha_6)n_y^2\right] \end{bmatrix} \tag{A7}$$

$$C = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}. \tag{A8}$$

The elements of matrices in the linear system Equation (70) are given as (A9) to (A29):

$$A_x^{t+\Delta t} = \frac{2\gamma_1}{\Delta t} + \frac{2(K_{22}+K_{33})}{\Delta z^2} + \lambda \tag{A9}$$

$$B_x^{t+\Delta t} = 0 \tag{A10}$$

$$C_x^{t+\Delta t} = \alpha_2\frac{\partial V_x}{\partial z} \tag{A11}$$

$$A_y^{t+\Delta t} = 0 \tag{A12}$$

$$B_y^{t+\Delta t} = \frac{2\gamma_1}{\Delta t} + \frac{2(K_{22}+K_{33})}{\Delta z^2} + \lambda \tag{A13}$$

$$C_y^{t+\Delta t} = \alpha_2\frac{\partial V_y}{\partial z} \tag{A14}$$

$$A_z^{t+\Delta t} = \alpha_3\frac{\partial V_x}{\partial z} \tag{A15}$$

$$B_z^{t+\Delta t} = \alpha_3\frac{\partial V_y}{\partial z} \tag{A16}$$

$$C_z^{t+\Delta t} = \frac{2\gamma_1}{\Delta t} + \frac{2(K_{22}+K_{33})}{\Delta z^2} + \lambda - \varepsilon_o\Delta\varepsilon E_z^2 \tag{A17}$$

$$A_x^t = \frac{2\gamma_1}{\Delta t} - \frac{2(K_{22}+K_{33})}{\Delta z^2} - \lambda \tag{A18}$$

$$B_x^t = 0 \tag{A19}$$

$$C_x^{t+\Delta t} = -\alpha_2\frac{\partial V_x}{\partial z} \tag{A20}$$

$$A_y^t = 0 \tag{A21}$$

$$B_y^t = \frac{2\gamma_1}{\Delta t} - \frac{2(K_{22}+K_{33})}{\Delta z^2} - \lambda \tag{A22}$$

$$C_y^t = -\alpha_2 \frac{\partial V_y}{\partial z} \tag{A23}$$

$$A_z^t = -\alpha_3 \frac{\partial V_x}{\partial z} \tag{A24}$$

$$B_z^t = -\alpha_3 \frac{\partial V_y}{\partial z} \tag{A25}$$

$$C_z^t = \frac{2\gamma_1}{\Delta t} - \frac{2(K_{22}+K_{33})}{\Delta z^2} - \lambda + \varepsilon_o \Delta\varepsilon E_z^2 \tag{A26}$$

$$D_x^t = \frac{2(K_{22}+K_{33})}{\Delta z^2}(n_{x,i+1}^t + n_{x,i-1}^t) + 2Q_x^t \tag{A27}$$

$$D_y^t = \frac{2(K_{22}+K_{33})}{\Delta z^2}(n_{y,i+1}^t + n_{y,i-1}^t) + 2Q_y^t \tag{A28}$$

$$D_z^t = \frac{2(K_{11}+K_{33})}{\Delta z^2}(n_{z,i+1}^t + n_{z,i-1}^t) + 2Q_z^t \tag{A29}$$

$$\begin{aligned} Q_x^t = K_{22}\Bigg\{ & 2n_y^t\left(\frac{\partial n_x^t}{\partial z}\right)\left(\frac{\partial n_y^t}{\partial z}\right) - 2n_x^t\left(\frac{\partial n_y^t}{\partial z}\right)^2 \\ & - n_x^t n_y^t\left(\frac{\partial^2 n_y^t}{\partial z^2}\right) - \left[(n_x^t)^2 + (n_z^t)^2\right]\left(\frac{\partial^2 n_x^t}{\partial z^2}\right)\Bigg\} \\ & + K_{33}\Bigg\{ 2n_z^t\left(\frac{\partial n_x^t}{\partial z}\right)\left(\frac{\partial n_z^t}{\partial z}\right) \\ & - \left[(n_x^t)^2 + \left(n_y^t\right)^2\right]\left(\frac{\partial^2 n_x^t}{\partial z^2}\right)\Bigg\} \end{aligned} \tag{A30}$$

$$\begin{aligned} Q_y^t = K_{22}\Bigg\{ & 2n_x^t\left(\frac{\partial n_x^t}{\partial z}\right)\left(\frac{\partial n_y^t}{\partial z}\right) - 2n_y^t\left(\frac{\partial n_x^t}{\partial z}\right)^2 \\ & - n_x^t n_y^t\left(\frac{\partial^2 n_x^t}{\partial z^2}\right) - \left[\left(n_y^t\right)^2 + (n_z^t)^2\right]\left(\frac{\partial^2 n_y^t}{\partial z^2}\right)\Bigg\} \\ & + K_{33}\Bigg\{ 2n_z^t\left(\frac{\partial n_y^t}{\partial z}\right)\left(\frac{\partial n_z^t}{\partial z}\right) \\ & - \left[(n_x^t)^2 + \left(n_y^t\right)^2\right]\left(\frac{\partial^2 n_y^t}{\partial z^2}\right)\Bigg\} \end{aligned} \tag{A31}$$

$$\begin{aligned} Q_z^t = & K_{33}\Bigg\{ n_z^t\left[\left(\frac{\partial n_z^t}{\partial z}\right)^2 - \left(\frac{\partial n_x^t}{\partial z}\right)^2 - \left(\frac{\partial n_y^t}{\partial z}\right)^2\right] \\ & - \left[(n_x^t)^2 + \left(n_y^t\right)^2\right]\left(\frac{\partial^2 n_z^t}{\partial z^2}\right)\Bigg\}. \end{aligned} \tag{A32}$$

The elements of matrices in the linear system Equation (77) are given as A33 to A44:

$$A_x^{t+\Delta t} = \frac{2\gamma_1}{\Delta t} + \frac{2K_{33}}{\Delta z^2} + \lambda \tag{A33}$$

$$B_x^{t+\Delta t} = \alpha_2 \frac{\partial V_x}{\partial z} \tag{A34}$$

$$A_z^{t+\Delta t} = \alpha_3 \frac{\partial V_x}{\partial z} \tag{A35}$$

$$B_z^{t+\Delta t} = \frac{2\gamma_1}{\Delta t} + \frac{2(K_{11}+K_{33})}{\Delta z^2} + \lambda - \varepsilon_o \Delta\varepsilon E_z^2 \tag{A36}$$

$$A_x^t = \frac{2\gamma_1}{\Delta t} - \frac{2K_{33}}{\Delta z^2} - \lambda \tag{A37}$$

$$B_x^{t+\Delta t} = -\alpha_2 \frac{\partial V_x}{\partial z} \tag{A38}$$

$$A_z^t = -\alpha_3 \frac{\partial V_x}{\partial z} \tag{A39}$$

$$B_z^t = \frac{2\gamma_1}{\Delta t} - \frac{2(K_{11}+K_{33})}{\Delta z^2} - \lambda + \varepsilon_o \Delta\varepsilon E_z^2 \tag{A40}$$

$$D_x^t = \frac{2K_{33}}{\Delta z^2}(n_{x,i+1}^t + n_{x,i-1}^t) + 2Q_x^t \tag{A41}$$

$$D_z^t = \frac{2(K_{11}+K_{33})}{\Delta z^2}(n_{z,i+1}^t + n_{z,i-1}^t) + 2Q_z^t \tag{A42}$$

$$Q_x^t = K_{33}\left[2n_z^t\left(\frac{\partial n_x^t}{\partial z}\right)\left(\frac{\partial n_z^t}{\partial z}\right) - (n_x^t)^2\left(\frac{\partial^2 n_x^t}{\partial z^2}\right)\right] \tag{A43}$$

$$Q_z^t = K_{33}\left\{ n_z^t\left[\left(\frac{\partial n_z^t}{\partial z}\right)^2 - \left(\frac{\partial n_x^t}{\partial z}\right)^2\right] - (n_x^t)^2\left(\frac{\partial^2 n_z^t}{\partial z^2}\right)\right\}. \tag{A44}$$