DYNAMIC EVOLUTION OF THE NEMATIC LIQUID CRYSTAL DIRECTOR IN MAGNETIC FIELD

Gabriela Eugenia IACOBESCU[1]

A comparative study of nematic liquid crystal relaxation times, in planar geometry, when subjected to a magnetic field, are presented using three different methods. Different approaches in calculating the temporal evolution of the nematic director deviation are considered for each method. The first method is the numerical solving of the equation which describes the temporal evolution of the liquid crystal director taking into account the backflow effect on the rotational viscosity coefficient. The second method consists in analytically solving an approximate equation for small angle deviations when neglecting the backflow. The third method is similar to the second but includes a correction on the rotational viscosity coefficient.

Keywords: relaxation time, nematic liquid crystal, magnetic field

1. Introduction

Technical applications of liquid crystals (LCs) in display industry research are concerned on obtaining faster devices working at low power. There are many ways to improve these parameters such as synthesizing new LC mixtures with higher performances or improving the existent ones by adding nanotubes [1-3], dyes [4,5] or nanoparticles [6,7]. On the other hand, deep understanding of dynamical processes appearing while subjected the LC to external stimuli, as electric, magnetic and/or optical fields, might be extremely useful for a proper device control and for obtaining high performances.

Thermotropic nematic liquid crystals (NLC) change their molecular orientation when an external field is applied. This reorientation process depends on many factors: material constants (anchoring forces and elastic constants), Freedericksz transition threshold [8-10], or the interactions with inserted particles [11-13]. The time needed by the molecular director to reach its final position is determined by the applied field and it is characterized by the relaxation time.

[1] Assoc. Prof., Faculty of Sciences, University of Craiova, Romania, e-mail: giacobescu@central.ucv.ro

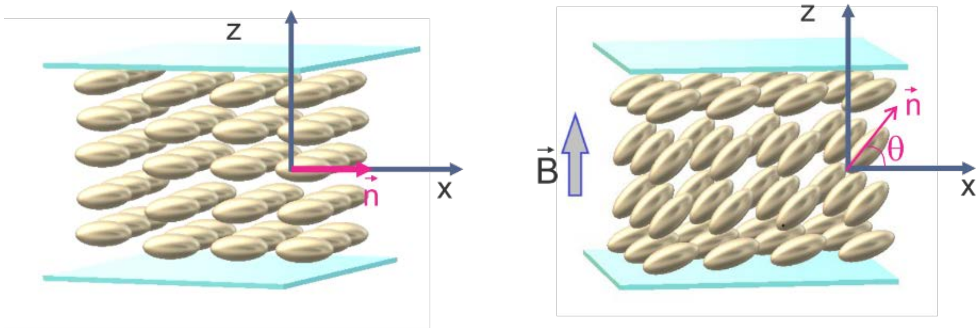


Fig. 1. Molecular orientation in planar LC-cell, subjected to an external magnetic field.

Pieranski [14] performed the first evaluation of the relaxation time. The simplest method to study the dynamical evolution of the nematic director consists in subjecting the LC simultaneously to a laser beam and a variable magnetic field. Due to the molecular reorientation induced by the applied field, the extraordinary refractive index varies, and we can observe changes in the laser beam intensity as an interference pattern between the ordinary and extraordinary rays.

Theoretical analysis of liquid crystal dynamic behavior is based on solving Euler-Lagrange equation of the distortion angle distribution between the glass plates. The most general case considers the Leslie viscosity coefficients [15] when backflow exists. However, the available data on these parameters for LCs are usually incomplete, in consequence, a simplified model, which neglects these parameters, is proposed.

In this work we compare the results obtained using a general model for the dynamic behavior of a nematic LC that considers the Leslie parameters and a simplified model, which neglects the backflow. We study the range, in the magnetic field relative variation, where the results of the simplified model are in very good agreement with those given by the complex model.

2. Theoretical considerations

In planar aligned LC cells with strong anchoring forces on the glass support, subjected to external magnetic field, it was found that, above a specific value of the magnetic field, named critical (threshold) field for the Freedericksz transition, the LC molecules reorient themselves. The reorientation of the LC director is characterized by the dependence of the tilting angle of the nematic director with the cell glasses (z coordinate) and on time, $\theta(z,t)$. When the transient regime stops, the tilting angle depends only on *z*. In this stationary case, the molecular director changes its orientation from ($\theta = 0$) on the edge of the cell to a maximum value ($\theta = \theta max$), in the middle of the cell (Fig. 1).

2.1 The stationary regime

In order to calculate the critical field for the magnetic Freedericksz transition, we use the Euler Lagrange equation resulting from the minimum condition of the system's free energy

$$\left(K_1\cos^2\theta+K_3\sin^2\theta\right)\theta_{zz}+(K_3-K_1)\sin\theta\cos\theta\cdot\theta_z^2+\mu_0^{-1}\chi_a B^2\sin\theta\cos\theta=0 \qquad (1)$$

where K_1 is the splay elastic constant, K_3 is the bend elastic constant, μ_0 is the vacuum magnetic permeability, χ_a is the liquid crystal's magnetic anisotropy, $\theta_z=\frac{\partial\theta}{\partial z}$ and $\theta_{zz}=\frac{\partial^2\theta}{\partial z^2}$.

For this cell geometry, the critical field is

$$B_c=\frac{\pi}{d}\sqrt{\frac{\mu_0 K_1}{\chi_a}} \qquad (2)$$

where d is the thickness of the LC cell.

In the stationary regime, $B>B_c$ we can obtain the dependence $\theta=\theta(z)$ from Eq. (1).

As seen from Fig. 1, with the same anchoring conditions on the both glass plates, the maximum value of the tilting angle is in the middle of the LC cell (where the influence of the glass plates anchoring forces is minimal).

The dependence of θ_m on the applied magnetic field, proposed by Vertogen and de Jeu [16] is an integral equation difficult to be solved:

$$\frac{B}{B_c}=\frac{2}{\pi}\int_0^{\pi/2}\sqrt{\frac{1+\beta\sin^2\psi\sin^2\theta_m}{1-\beta\sin^2\psi\sin^2\theta_m}}d\psi \qquad (3)$$

where $\beta=\frac{K_3}{K_1}-1$ and ψ is the azimuthal angle.

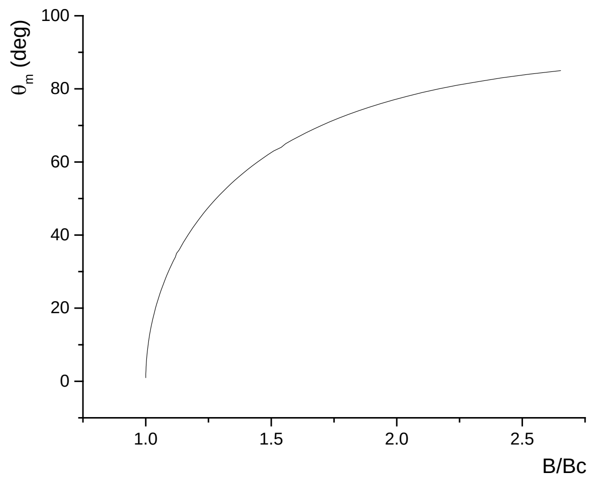


Fig.2. Maximum deviation angle versus the applied field for MBBA.

Another way to obtain θ_m, as a function of B (or B/B_c), is to provide numerical values for θ_m and to calculate, by integration, the B/B_c ratio. Following this procedure, we obtained the values of the maximum deviation angle in the middle of the cell for MBBA, considering the elastic constants $K_1 = 7.5\times10^{-12}$ N, and $K_3 = 6\times10^{-12}$ N as reported in [17]. Fig. 2 shows the results of our simulation.

In order to get the $\theta = \theta(z)$ dependence for a specific value of the maximum deviation angle, and consequently on the magnetic field, we can use the general formula [16]

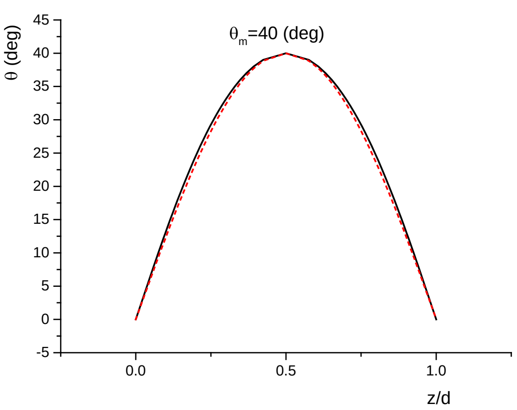
$$\frac{z}{d} = \left(\frac{B_c}{B}\right)\int_0^{\theta(z)} \sqrt{\frac{\cos^2\vartheta + \frac{K_3}{K_1}\sin^2\vartheta}{\sin^2\theta_m - \sin^2\vartheta}}\, d\vartheta \tag{4}$$

Similar with previous case, for different θ_m, we give numerical values to $\theta(z)$ and calculate z by integration.

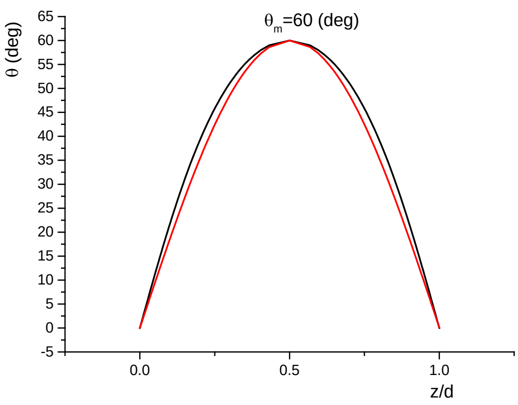
Some authors suggest that the effect of the magnetic field on the LC director can be approximated by the following simple equation:

$$\theta(z) = \theta_m \sin\frac{\pi z}{d} \tag{5}$$

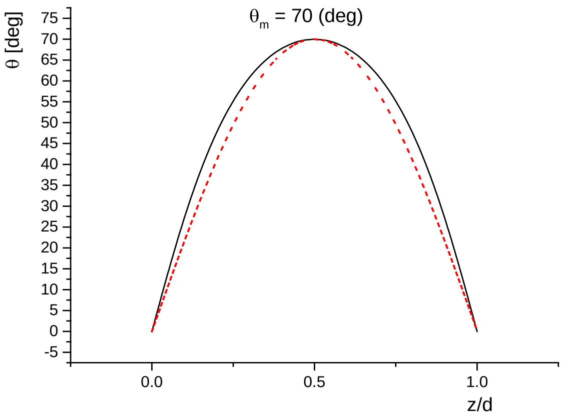
Simulations made for different maximum deviation angle, revealed negligible differences for angles range below $40°$ when considering the formula given in Eq. 5 compared to the results obtained from Eq. 4. For larger angles, up to $70°$ the difference begins to be significant but still small (Fig 3). Then, Eq. 5 is quite suitable to represent the deviation angle in the cell.



(a)



(b)



(c)

Fig.3. The deviation angle dependence on *z* coordinate for: (a) $\theta_m = 40°$, (b) $\theta_m = 60°$ and (c) $\theta_m = 70°$. Red (dashed) lines were obtained from Eq. 5, and the black (solid) ones from Eq (4).

2.2 The transient regime

To determine the LC’s dynamic behavior in magnetic field, the relaxation time τ_{on1}, we use three methods:

The first method is the most general case based on the Erickson-Leslie equations [15, 18]. In this case, considering the backflow effect, the deviation angle, as a function of time and *z*, coordinate satisfies the equation proposed in [19], adapted for the magnetic field:

$$I\frac{\partial^2\theta}{\partial t^2}+\gamma_1\frac{\partial\theta}{\partial t}=\left(K_1\cos^2\theta+K_3\sin^2\theta\right)\frac{\partial^2\theta}{\partial z^2}+\left(K_1-K_3\right)\sin\theta\cos\theta\left(\frac{\partial\theta}{\partial z}\right)+ \\ \mu_0^{-1}\chi_a B^2\sin\theta\cos\theta+\left(\alpha_2\sin^2\theta-\alpha_3\cos^2\theta\right)\left(\frac{\partial v}{\partial t}\right) \tag{6}$$

where α_i are the Leslie coefficients, *I* is the rotational inertia of nematic molecule and *v* is the flowing velocity.

Inertial effects in liquid crystals are very weak so we can neglect the first term in Eq. (6). Thus, as demonstrated in [19], the flow velocity satisfies the equation

$$\frac{\partial}{\partial z}\left(-A_1\frac{\partial\theta}{\partial t}+\frac{A_2}{2}\frac{\partial v}{\partial z}\right)=0 \tag{7}$$

with

$$A_1=-\alpha_3\cos^2\theta+\alpha_2\sin^2\theta \tag{9}$$

$$A_2=2\alpha_1\sin^2\theta\cos^2\theta+\left(\alpha_5-\alpha_2\right)\sin^2\theta+\left(\alpha_3+\alpha_6\right)\cos^2\theta+\alpha_4$$

We get

$$\frac{\partial v}{\partial z}=\frac{2A_1}{A_2}\frac{\partial\theta}{\partial t}+C \tag{10}$$

where *C* is a constant. But for $t=0$ we have $v=0$ and $\frac{\partial v}{\partial z}=0$, so $C=0$.

Eq. (10) is simplified to:

$$\frac{\partial v}{\partial z}=\frac{2A_1}{A_2}\frac{\partial\theta}{\partial t} \tag{11}$$

and equation (6) becomes

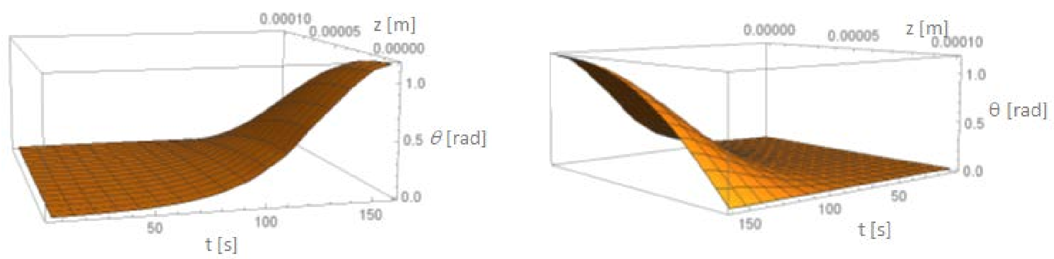
$$\left(K_1\cos^2\theta+K_3\sin^2\theta\right)\frac{\partial^2\theta}{\partial z^2}+\left(K_1-K_3\right)\sin\theta\cos\theta\left(\frac{\partial\theta}{\partial z}\right)+$$
$$\mu_0^{-1}\chi_a B^2\sin\theta\cos\theta+\left(\alpha_2\sin^2\theta-\alpha_3\cos^2\theta\right)\left(\frac{\partial v}{\partial t}\right)=\gamma^*\frac{\partial\theta}{\partial t} \tag{12}$$

Where $\gamma^*=\gamma-\frac{2A_1^2}{A_2}$ is the effective rotational viscosity.

Since A_1 and A_2 depend on θ, and θ is a function of t and z, Eq. (12) can be solved only numerically. Shoarinejed and Shahzamanian presented a numerically solving method in [20].

Using Mathematica software, we solved the Eq. (12) and obtained the deviation angle as a function of time and coordinate z. In Fig 4 we present the results of the simulation for MBBA, encapsulated in a LC cell with 200 µm thickness, for a given ratio B/B_c. We considered $z=0$ in the middle of the cell because, for similar anchoring conditions on the both glass plates, the inner geometry of the cell is symmetric.

The values of Leslie coefficients were given in [18] at room temperature of 25 ^{o}C: $\alpha_1=-0.0181$ Pa·s, $\alpha_2=-0.1104$ Pa·s, $\alpha_3=-0.00110$ Pa·s, $\alpha_4=0.0826$ Pa·s, $\alpha_5=0.0779$ Pa·s, $\alpha_6=-0.00336$ Pa·s. For the rotational viscosity, we used the value $\gamma=$ 0.1093 Pa·s as given in [21], very close to the value reported in [10].



a) b)

Fig.4. The deviation angle dependence as a function of time and position for $B/B_c=1.8$, which corresponds to $\theta_m=73°$; a) perspective to point the dependence of θ versus time and b) perspective to point the deviation angle θ versus position coordinate z.

Fig. 4a) shows the time evolution of the maximum tilting angle (the tilting angle in the middle of the LC cell (z = 0)).

From Fig. 4b) we can notice the dependence of the tilting angle θ on the coordinate z at $t = 150$ s, when the molecules aligned by the magnetic field.

In order to calculate the relaxation time τ_{on1}, we considered the dynamic evolution of the deviation angle $\theta_m^2(t)$, and proposed the following sigmoide shape:

$$\theta_m^2(t) = \frac{\theta_m^2(\infty)}{1 + C\exp\left(-\frac{t}{\tau_{on1}}\right)} \tag{13}$$

where C is a constant, and $\theta_m^2(\infty)$, is the maximum deviation angles in the middle of the cell at $t \to \infty$.

The second method for the relaxation time, τ_{on2}, neglects the backflow effect and considers the following approximation for small deviation angles:

$$\sin\theta = \theta - \frac{\theta^3}{6} \quad ; \quad \cos\theta = 1 - \frac{\theta^2}{2} \tag{14}$$

which are enough accurate for tilting angles smaller than 60-65 degrees.

In this case, by replacing ($\gamma^* = \gamma$), Eq. (12) becomes:

$$\left[K_1\left(1-\theta^2\right) + K_2\theta^2\right]\frac{\partial^2\theta}{\partial z^2} + \left(K_3 - K_1\right)\left(\theta - \frac{2\theta^3}{3}\right)\left(\frac{\partial\theta}{\partial z}\right)^2 + \mu_0^{-1}\chi_a B^2\left(\theta - \frac{2\theta^3}{3}\right) = \gamma\frac{\partial\theta}{\partial t} \tag{15}$$

By applying the same method used in [9,11], and assuming that $\theta(z) = \theta_m \cos\frac{\pi z}{d}$, $z \in [-d/2\,, d/2]$ we obtained:

$$\theta_m^2(t) = \frac{\theta_m^2(\infty)}{1 + \left(\frac{\theta_m^2(\infty)}{\theta_m^2(0)} - 1\right)\exp\left(-\frac{t}{\tau_{on2}}\right)} \tag{16}$$

where $\theta_m^2(0)$, is the maximum deviation angle in the middle of the cell at $t = 0$.

In the third method, we keep the small angle approximation as in the second one, but we will take into consideration the backflow effect. This means that, $\gamma^* = \gamma_1 - \frac{2A_1^2}{A_2}$ should be considered instead of γ .

The equations for A_1 and A_2 might be simplified by developing them in power series and neglecting the terms containing the α_3 coefficients, which are very small for MBBA [19]. Unfortunately, this is not enough to solve the equation because we still have the term containing θ^2 at the nominator and denominator. Moreover, γ^* does not have the same value across the cell thickness and it is time dependent.

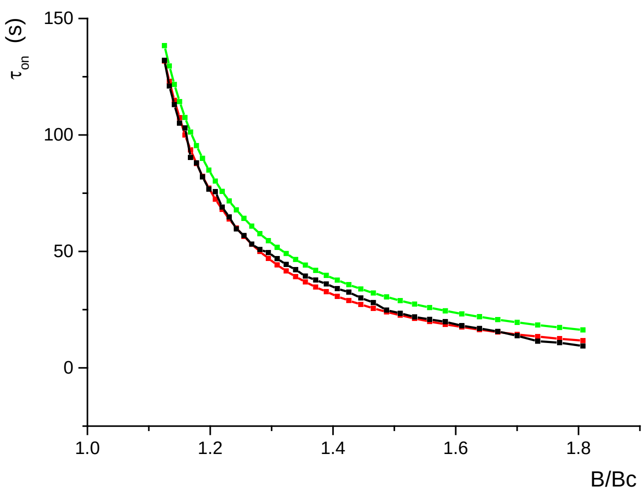


Fig. 5. The relaxation time versus the applied field: τ_{on1} - black dots, τ_{on2} - green dots, τ_{0n3} - red dots.

We can find an approximate solution considering an average value of γ^*, as $\langle \gamma^* \rangle = 1 - \left\langle \frac{2A_1^2}{A_2} \right\rangle = 1 - \frac{1}{\theta_m} \int_0^{\theta_m} \frac{2A_1^2}{A_2} d\theta$. In this way, we can obtain τ_{on3} by replacing γ with $\langle \gamma^* \rangle$ in Eq. (16).

3. Results and discussions

In order to describe the dynamic behavior of LCs when the magnetic field is switched on, we solved numerically the Eq. (12) and extracted the data for describing the temporal evolution of θ_m. With these data, we calculated the relaxation times for different B/B_c ratios using three methods with different level of approximation:

- τ_{on1} - obtained by the first method, the exact one;
- τ_{on2} - obtained by the second method, which considers the small angle deviation approximation and neglects the backflow;
- τ_{on3} - obtained with the third method, which considers both the small angle deviation approximation and the backflow.

The results are shown in Fig. 5.

The differences between the results obtained for each case are less than 5%.

For deviation angles smaller than 73° ($B/B_c < 1.8$), the results obtained with $\langle \gamma^* \rangle$ are the closest to the ones obtained for the exact case.

On the other side, because since at the initial moment the deviation angle $\theta_m^2(0)$ is very small the ratio $\theta_m^2(0)/\theta_m^2(\infty)$ in Eq. (16) is very large and we can neglect the unity inside the brackets, which drives us to the Eq. (13). Then, for magnetic fields not exceeding $1.8 \times B_c$, we can use Eq. (16) as a good approximation, which allows us to study the dynamics of the LC director when the Leslie coefficients are not available.

Because the order of magnitude for the elastic constants is similar for many LCs, we can assume the results obtained for MBBA are suitable for other nematic mixture, at room temperature.

4. Conclusions

We calculated the relaxation time for a nematic LC director subjected to a magnetic field, when the field is switched on, in the general case and in two simplified ways, which neglect and/or consider the backflow.

We found that, for deviation angles less than 70°, the results obtained using the rotational viscosity coefficient γ and the average rotational viscosity $\langle \gamma^* \rangle$ are quite precise being very close to the ones obtained by numerically solving the exact equation.

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