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Theory and Simulation of Extensional Flow-Induced Biaxiality in Discotic Mesophases

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Abstract. — Flow-induced biaxiality is simulated for a uniaxial discotic nematic liquid crystal subjected to a constant uniaxial, isothermal, incompressible, irrotational, extensional, three dimensional flow, using a previously presented model [Singh A.P. and Rey A D., J Phys. II France 4 (1994) 645]. Numerical and analytical solutions of the director triad (n, m, l), and uniaxial (S) and biaxial (P) alignments are given. The unit sphere description of the director triad is used to discuss and analyze the sensitivity of the director triad trajectories and the coupled alignment (uniaxial and biaxial) relaxations to the initial orientation, nematic potential (U), and to the alignment Deborah number (dimensionless extension rate). The evolution of the director triad is given by the rotation of a moving triad (n, l) around a fixed director (m). When the poles of the orientation unit sphere are along the extension axis, and the equator lies in the compression plane of the flow, it is found that the director diad (n, l) dynamics follow geodesic flow and the trajectories belong to the same meridians (great circles through the poles). The space of stable steady state orientation of the uniaxial director n and the biaxial director m is the whole compression plane (the equator of the unit sphere), while that of the biaxial l is the extension direction (poles). A high degree extension flow-induced biaxiality is found when the uniaxial director is away from the extension axis and when S is relatively low. The scalar order parameter couplings are captured by analyzing the trajectories in the alignment triangle. Computed scientific visualizations of biaxial molecular orientation distributions are used to correlate the director triad dynamics and the alignment's dynamics. The tensor order parameter is used to calculate the main flow-birefringences, thus providing a direct way to verify the theoretical predictions of this paper.

1. Introduction

Carbonaceous mesophases are an important class of low cost precursors in the manufacture of high performance carbon fibers [1–3]. This mesophase precursor is a uniaxial discotic nematic liquid crystalline material. These mesophases are formed by the condensation of the aromatic molecules present in the coal or petroleum pitches [1, 2, 4] and tend to adopt a uniaxial discotic nematic phase Nd [5, 6], with unit normals to the disc-like molecules more or less aligned.

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Fig. 1. — Definition of director orientations of a discotic nematic liquid crystal undergoing flow induced biaxiality. The uniaxial director $\mathbf{n}$ in a discotic nematic phase is the average orientation of the unit normals to the disc-like molecules. The biaxial directors $\mathbf{m}$, $\mathbf{l}$ lie in a plane perpendicular to uniaxial director $\mathbf{n}$, and form a right hand triad. The biaxial director $\mathbf{m}$ is the average orientation of the projection of the unit normals to the disc-like molecules in a plane orthogonal to uniaxial director $\mathbf{n}$. The biaxial director $\mathbf{l}$ is given as $\mathbf{n} \times \mathbf{m}$. The lower 2D figure is the projection, of the upper 3D schematic, in $\mathbf{m} - \mathbf{l}$ plane. In this paper we consider the extension dynamics of a discotic nematic that is uniaxial prior to the imposition of flow.

along a common direction (see upper Fig. 1), represented by the uniaxial director $\mathbf{n}$; in what follows we use $\mathbf{n}$ and uniaxial orientation interchangeably. The degree of alignment of the unit normals along $\mathbf{n}$ is given by the scalar order parameter $S$ [7]; in what follows we use $S$ and uniaxial alignment interchangeably. Since spinning of discotic carbonaceous mesophases involves stretching and extension, a fundamental understanding of extensional flow-induced orientation and alignment is highly desirable. In this paper we use the extensional flow classification terminology of [8].

For flow of mesophase materials of relatively large molecular weights, the coupling between the director and the scalar order parameter should be retained [9]. This dynamic coupling introduces additional nonlinearities through the dependence of the generalized Leslie coefficients on the scalar order parameter, as shown in various works [9–13]. In previous works [14,15], the authors used variational principles to develop an approximate macroscopic model that allows for variable uniaxial orientation and alignment in discotic nematics, and applied it to various extensional flows. For uniaxial extensional flow, it was found that the uniaxial director trajec-
ories on the unit sphere \((\mathbf{n} \cdot \mathbf{n} = 1)\) follow, from the initial orientation to the compressional plane (normal plane to the extension direction), a geodesic meridian flow and that the uniaxial alignment relaxation was sensitive to the initial orientation, to the extension rate, and to the nematic potential that controls the magnitude of \(S\) in the absence of flow. The sensitivity to initial conditions, typical of geodesic flows, was shown to be the cause for the loss of predictability that occurs when the initial uniaxial director orientation lies along the extension axis of the flow. In addition, strong extension was found to produce large decreases in the uniaxial scalar order parameter when the uniaxial director was aligned near the extension axis. The previous works \([14,15]\) precluded flow-induced biaxiality because they are based on a uniaxial macroscopic model.

Field-induced biaxiality in nematic liquid crystals has been shown to occur under various conditions. Uniaxial nematic liquid crystals of negative dielectric anisotropy display biaxial ordering when subjected to an electric field normal to the uniaxial director axis \([16]\). Uniaxial nematics of negative magnetic susceptibility also display biaxial ordering when subjecting the material to a magnetic field oriented parallel to the initial director orientation \([17]\). Extensional flows are known \([14,15]\) to have orienting qualities similar to those of electromagnetic fields, and this forms the basis for the industrial manufacturing of organic fibers. The basic flow orienting phenomena of nematics in uniaxial extensional flows depends on the molecular geometry. In extensional flows the reactive parameter \(\lambda\) \([7]\) plays the analogous role as the diamagnetic susceptibility in the magnetic field-induced reorientations. For rod-like nematics \(\lambda > 0\) and extension aligns the director along the stretching direction, while for discotic nematics \(\lambda < 0\) and extension aligns the director anywhere in the compression plane. Given the stated field-orienting properties of the uniaxial discotic nematics and the analogy with magnetic reorientation phenomena, we expect that a uniaxial extensional flow will also induce biaxial ordering. The biaxial state is described by orthogonal director triad \((\mathbf{n}, \mathbf{m}, \mathbf{l})\) and two scalar order parameters \((S, P)\) \([18,19]\). Although no experimental measurements of the state of alignment of uniaxial discotic during extensional flows exist, significant flow-induced changes of the uniaxial scalar order parameter of rod-like mainchain nematic polymers are believed to dominate their rheology \([20]\). Thus we expect that flow-induced biaxiality may be accessible and significant for discotic mesophases subjected to uniaxial extensional flows.

The main objective of this work is to establish the relevant qualitative features that describe the relations between uniaxial extensional deformations inputs and orientation (uniaxial and biaxial) and alignment (uniaxial and biaxial) responses in an idealized, uniaxial discotic nematic liquid crystalline phase. Although the numerical predictions of this paper are not validated due to lack of available experimental data, a high degree of confidence can be expected since: i) the present model has been shown \([26]\) to capture the distinctive and experimentally observed shear-flow instability of discotic carbonaceous mesophases \([38]\); ii) the model used in this paper has been shown to capture all the complex nonlinear rheological phenomena actually exhibited by rod-like nematic polymers \([13]\); iii) the predictions of the present model were shown \([13]\) to be in full agreement with the predictions for the rheology of rod-like nematic polymers obtained by using the mesoscopic theory of Doi \([27]\); and iv) the present model reduces \([13]\) to the standard Leslie-Ericksen model of nematic liquid crystals \([9,35]\). The present paper is a continuation of our effort to increase the current understanding of the rheology of discotic nematic liquid crystals \([14,15,26,39]\). The particular objectives of this paper are:

1) To characterize the sensitivity of director triad \((\mathbf{n}, \mathbf{m}, \mathbf{l})\) trajectories and their stable steady states to the initial conditions, and to the extension rate, using analysis and numerical simulation.

2) To characterize the sensitivity of uniaxial \((S)\) and biaxial \((P)\) alignment relaxations,
along the corresponding director paths, to the initial conditions and to the extension rate, using numerical simulation.

In this paper we use the unit sphere description \([14,15]\) of nematics only to facilitate the discussion and classification of the numerical results that pertain to the above-mentioned objectives.

The organization of this paper is as follows. In Section 2 we define the coordinate system and the state variables, define the uniaxial extensional flow, briefly present the elements of the unit sphere description used to discuss and classify the analytical and numerical solutions, and present the governing equations. In this section we also present analytical orientation (uniaxial and biaxial) and alignment (uniaxial and biaxial) results, and the principles used to select the phenomenological parameters of the model. A brief description of the numerical method used to integrate the governing equations is also presented. In Section 3 we present, discuss, and classify the solution vector, consisting of the time dependent director and alignment fields, obtained from numerical integration and analytical solutions of the governing equations. Typical computations of the tensor order parameter relaxation and flow birefringence are presented.

2. Theory and Governing Equations

2.1. Definition of Coordinates, Kinematics, Orientation and Alignment. — In this paper we study the temporal, spatially uniform microstructural response of a model uniaxial discotic nematic subjected at time \(t = 0\) to a constant uniaxial extension rate \(\dot{\varepsilon}\). The microstructure of the nematic is characterized by the tensor order parameter \(Q_{ij}(t)\) [19]:

\[
Q_{ij} = S \left( n_in_j - \frac{1}{3} \delta_{ij} \right) + \frac{1}{3} P \left( m_im_j - l_il_j \right),
\]

where the following restrictions apply:

\[
Q_{ij} = Q_{ji}; \quad Q_{ii} = 0; \quad \frac{1}{2} \leq S \leq 1; \quad \frac{3}{2} \leq P \leq \frac{3}{2};
\]

\[
n_in_i = m_im_i = l_il_i = 1;
\]

where \(i, j = x, y, z\). The uniaxial director \(n\) corresponds to the maximum eigenvalue \(\frac{2}{3}S\), the biaxial director \(m\) corresponds to the second largest eigenvalue \(-\frac{1}{3}(S - P)\), and the biaxial director \(l = n \times m\) corresponds to the smallest eigenvalue \(-\frac{1}{3}(S + P)\). The orientation is defined by the orthogonal director triad \((n, m, l)\). The magnitude of the uniaxial scalar order parameter \(S\) is a measure of the molecular alignment along the uniaxial director \(n\), and is given by \(S = 3(n_iQ_{ij}n_j)/2\). The magnitude of the biaxial scalar order parameter \(P\) is a measure of the molecular alignment along the biaxial director \(m\) in a plane perpendicular to uniaxial director \(n\), and is given as \(P = 3(m_iQ_{ij}m_j - l_iQ_{ij}l_j)/2\). On the principal axes, the tensor order parameter \(Q_{ij}(t)\) is given by:

\[
Q_{ij} = \begin{bmatrix}
-\frac{1}{3}(S - P) & 0 & 0 \\
0 & -\frac{1}{3}(S + P) & 0 \\
0 & 0 & \frac{2}{3}S
\end{bmatrix}.
\]

We next adopt this well known description to discotic nematic liquid crystals. Figure 1 shows an schematic side view (top) and top view (bottom) of a typical flow-induced biaxial ordering in a discotic nematic liquid crystal. The top figure shows that the uniaxial director \(n\)
describes the average orientation of the normals to the circular discs. The bottom figure shows a projection on a plane perpendicular to the uniaxial director, here given by the \( \mathbf{m} - \mathbf{l} \) plane. The bottom figure shows that \( \mathbf{m} \) is the average orientation of the projection of the normals to the circular discs onto the \( \mathbf{m} - \mathbf{l} \) plane. As explained in references [17,19], with the above given identification, both \( S \) and \( P \) are positive for both rod-like and disc-like uniaxial nematic liquid crystals, and no further distinction is required in this paper since rods are not considered here. Here \( S \) and \( P \) are the scalar order parameters in the direction of the directors \( \mathbf{n} \) and \( \mathbf{m} \), respectively.

Having established the ordering and orientation measures, we briefly discuss their restrictions and magnitudes in typical states. The correspondence between phase and alignment is: isotropic \( (S = 0, P = 0) \), uniaxial nematic \( (S \neq 0, P = 0) \), and biaxial nematic \( (S \neq 0, P \neq 0) \). Since the eigenvalues \( \mu_i \) \( (i = 1, 2, 3) \) of the tensor order parameter \( Q \) are restricted by:

\[
-\frac{1}{3} \leq \mu_i \leq \frac{2}{3};
\]

hence it follows that biaxial order parameter \( P \) obeys the following restrictions:

\[
S - 1 \leq P \leq 1 - S
\]

Equations (1d, 1e, 4) define the alignment triangle containing all the possible ordering states of discotic nematic liquid crystals. Figure 2 shows a schematic of the alignment triangle, whose sides are given by \( P = 1 - S(P \geq 0) \), \( P = S - 1(P \leq 0) \), and \( S = -0.5 \). The seven limiting alignment states are shown by an arrow originating from each corresponding unit sphere description [14] of the molecular orientation state. Wherever \( S = 0 \), the uniaxial director \( \mathbf{n} \) is undefined, and wherever \( P = 0 \), the biaxial directors \( \mathbf{m}, \mathbf{l} \) are undefined. The dark dot or the dark ring on the unit sphere indicates the orientation of the normals to the discs. For example, for \( (S = 1/4, P = 3/4) \), the uniaxial director \( \mathbf{n} \) is undefined, and the unit normals to the disc-like molecules lie along the meridian passing through the biaxial director \( \mathbf{m} \). The figure also shows that when \( P \to -P \), then \( \mathbf{m} \to \mathbf{l} \). The rings in the figure corresponding to \( (S = 1/4, P = 3/4) \), \( (S = -0.5, P = 0) \), and \( (S = 1/4, P = -3/4) \) correspond to planar orientation. The dark dots in the figures of \( (S = -0.5, P = 1.5) \), \( (S = 1, P = 0) \), and \( (S = -0.5, P = -1.5) \) correspond to various perfect perfect alignments. Since uniaxial extensional flow will not induce negative values of \( S \) and \( P \), in the present study the state of alignment lies within the triangle defined by \( S = 0 \), \( P = 0 \), and \( P = 1 - S \), whose vertices are the isotropic plane, the perfect uniaxial nematic phase, and the planar ordered phase. In what follows we refer to this restricted alignment space as the alignment triangle.

To enforce the unit length constraint on the orthogonal director triad \( (\mathbf{n} \mathbf{n} = \mathbf{m} \cdot \mathbf{m} = 1 \cdot 1 = 1) \) and to visualize and analyze the director triad orbits on the unit sphere, we parametrize director triad as follows.

\[
[n, m, l] : \begin{bmatrix} n_x, n_y, n_z \end{bmatrix} = (\cos \phi, \sin \phi \cos \theta, \sin \phi \sin \theta) \quad \begin{bmatrix} m_x, m_y, m_z \end{bmatrix} = (\cos \Psi, \sin \Psi \cos \alpha, \sin \Psi \sin \alpha) \quad l = n \times m
\]

(5a)

where \( \mathbf{n} \cdot \mathbf{m} \) implies

\[
\Psi = \tan^{-1} \left( \frac{\cot(-\phi)}{\cos(\theta - \alpha)} \right).
\]

(5b)

The parametrization is shown in Figure 3a, where \( \theta(0 \leq \theta \leq 2\pi) \) is the uniaxial azimuthal angle and \( \phi(0 \leq \phi \leq \pi) \) is the uniaxial polar angle defining the uniaxial director \( \mathbf{n} \). The biaxial director \( \mathbf{m} \) is completely defined by the biaxial polar angle \( \Psi(0 \leq \Psi \leq \pi) \) and biaxial
Fig. 2. — The alignment (uniaxial and biaxial) $P - S$ triangle. The unit sphere description of the director triad $(n, m, l)$ is used to explain the alignment characteristics at different limiting points on the alignment phase plane. The dark rings or dots represent the direction $m$ of which the unit normals to the disc-like molecules point. Seven limiting alignment states are shown by an arrow originating from each corresponding unit sphere. Wherever $S = 0$, the uniaxial director $n$ is undefined, and wherever $P = 0$, the biaxial directors $m$, $l$ are undefined. The figure shows that when $P ightarrow -P$, then $m ightarrow l$.

Azimuthal angle $\alpha (0 \leq \alpha \leq 2\pi)$. In terms of the uniaxial angles, the north pole of the sphere is located at $\phi = 0$, the south pole at $\phi = \pi$, and the equator at $(\theta, \phi) = ([0, 2\pi], \pm \pi/2)$. In this paper $x$ is along the extension direction of the imposed flow.

The unit sphere description of the director triad is used just to facilitate the analysis and discussion of the analytical and numerical results of director triad relaxation and alignment relaxation. In the unit sphere description [14, 15, 21–24] each director tip, in the presence of flow, defines a trajectory. As shown below, in uniaxial extensional flow, $m(t) \equiv m(0)$ and the trajectory of $m$ is just a point on the equator of the unit sphere. To characterize the moving director diad $(n(t), l(t))$ orbits we define geodesics and meridians. A geodesic is the shortest arc connecting two points on the surface of the sphere, and is given, in terms of the uniaxial
Fig 3. — Definition of a) coordinate system, b) uniaxial extensional flow deformation. a) Director angle and unit sphere $\theta$ ($0 \leq \theta \leq 2\pi$) is the azimuthal angle and $\phi$ ($0 \leq \phi \leq \pi$) is the polar angle which define completely the orientation of the uniaxial director $n$. The biaxial director $m$ is completely defined by the polar angle $\Psi$ ($0 \leq \Psi \leq \pi$) and azimuthal angle $\alpha$ ($0 \leq \alpha \leq 2\pi$). The north pole of the sphere is located at $\phi = 0$, the south pole at $\phi = \pi$, and the equator at $(\theta, \phi) = ([0, 2\pi], \pm \pi/2)$. b) deformation of a unit cube, subjected at time $t = 0$ to a uniaxial extensional flow. The $x$-axis is along the extension direction, and the $y-z$ plane contains the uniform compression, the flow is an irrotational 3D flow.
director angles, by [25]:
\[
\sin N_2 \cos \phi - \cos N_2 \sin \phi \cos \theta - \frac{\sin \phi \sin \theta}{\sqrt{N_1^{-2} - 1}} = 0,
\]
where \(N_1\) and \(N_2\) are constants that depend on the two points; the geodesic or great circle, is the intersection of the sphere with the plane containing the given points and the center of the sphere. When the two points are the poles \((N_2 = \pi)\) the degenerate geodesics are the meridians \(M\), which in terms of \((\theta, \phi)\) and the director components \((\hat{a}_i, i = x, y, z), \hat{a} = n, l)\), are given by [25]:
\[
\tan \theta = \frac{1}{b}; \quad b^2 = \frac{1}{(N_1^{-2} - 1)}; \quad 0 \leq \phi \leq \pi,
\]
where \(b (-\infty < b < \infty)\) is a constant whose numerical value defines a particular meridian. A family of meridians is shown by the solid lines passing through the poles in Figure 3a.

Figure 3b shows the deformations of a unit cube of discotic nematic subjected at time \(t = 0\) to a uniaxial extensional flow; as shown below, the applied extension direction along the \(x\)-axis (polar axis), is parallel to the steady state biaxial director \(l_{ss} = (l_{ssx}, 0,0) = (\pm 1,0,0)\).

The uniform compression along the \((y - z)\) plane contains the equator of the unit sphere, and as shown below represents the degenerate geodesic circle of stable uniaxial and biaxial director orientations: \(n_{ss} = (0, n_{yss}, n_{zss}) = (0, \cos \theta_{ss}, \sin \theta_{ss})\); and \(m_{ss} = (0, m_{yss}, m_{zss}) = (0, \cos \alpha_{ss}, \sin \alpha_{ss})\), respectively; where the subscript “ss” denotes steady state.

To characterize the relaxation of the uniaxial and biaxial alignments as the directors traverse the surface of the sphere, we divide the sphere into three characteristic regions, denoted by \(R^-\) and \(R^+\), and shown in the schematic of Figure 4. The two equivalent \(R^-\) regions are given by \(|\hat{a}_x| > 1/\sqrt{3}\), and the \(R^+\) region is given by \(|\hat{a}_x| < 1/\sqrt{3}\), where \(\hat{a}\) is a unit vector. In an irrotational uniaxial extensional flow, the only flow effect on the orientation and alignment is due to the symmetric part of the velocity gradient tensor \((v_{ij})\), usually known as the rate of strain tensor or rate of deformation tensor and denoted by \(A\), and whose \(ij\) and \(ji\) components are given by \(A_{ij} = A_{ji} = (v_{ij} + v_{ji})/2\). An important observation, used below to classify the numerical results of alignment relaxations, is that a director whose tip lies in the \(R^-\) region samples extensional strains \((A : \hat{a} \hat{a} > 0, \hat{a} = n, l)\), while a director whose tip lies in the \(R^+\) region samples compressional strains \((A : \hat{a} \hat{a} < 0, \hat{a} = n, l)\).

2.2. GOVERNING EQUATIONS FOR UNIAXIAL EXTENSIONAL START-UP FLOW. — The macroscopic model used in this paper is described in detail in [14,15]. Here we just present the governing equations for the temporal evolution of the tensor order parameter and refer the reader to the above mentioned references for further details. The dimensional governing equations for the microstructure response of the model discotic nematics, subjected to isothermal, incompressible, irrotational extensional flow are approximated by:
\[
(1 - \frac{U}{3}) Q_{ij} - U \left(Q_{ik} Q_{kj} - \frac{1}{3} Q_{ik} Q_{kl} \delta_{ij}\right) + U \left(Q_{ik} Q_{kl} \right) Q_{ij} + \sigma_4 A_{ij} + \tau_4 \dot{Q}_{ij} + \sigma_6 \left(\dot{Q}_{ik} A_{kj} + A_{ik} \dot{Q}_{kj} - \frac{2}{3} Q_{ik} \dot{Q}_{kl} \delta_{ij}\right) + \tau_6 \left(\dot{Q}_{ik} \dot{Q}_{kj} + \dot{Q}_{ik} Q_{kj} - \frac{2}{3} Q_{ik} \dot{Q}_{kl} \delta_{ij}\right) = 0_{ij}
\]
where \((i, j = x, y, z); U\) is the nematic potential, \(A_{ij}\) is the rate of deformation tensor, \(\dot{Q}_{ij}\) is the time rate of change of the \(ij\) component of the symmetric traceless tensor order parameter \(Q_{ij}\), and \(\sigma_6, \sigma_4, \tau_6, \tau_4\) are the dimensional phenomenological parameters. The simplifying
assumptions and approximations made in deriving the model that describe the flow-induced tensor order parameter of an ideal discotic nematic liquid crystal, as given by equation (9) can be found in [14,26]; note that $\tau_4$ and $\tau_6$ in the present paper where denoted $\tau_1$ and $\tau_2$ in [14], respectively. Furthermore, in contrast to [14], the uniaxial assumption has now been removed in the present paper because flow-induced biaxiality affects the director dynamics and steady state morphological features. The numerically integrated set of dimensionless governing equations in component form and the dimensionless variables are given in Appendix A. The corresponding eigenvector-eigenvalue versions, governing the evolution of the director triad and alignment’s extension dynamics, are given by:

$$
\frac{d\mathbf{n}}{d\epsilon} = \lambda_n^0 \mathbf{A} \cdot \mathbf{n} - (\mathbf{A} \cdot \mathbf{n}) \mathbf{n} + \lambda_n^0 (\mathbf{A} : \mathbf{nn}) \mathbf{m} \tag{10}
$$

$$
\frac{d\mathbf{m}}{d\epsilon} = 0 \tag{11}
$$

$$
\frac{d\mathbf{l}}{d\epsilon} = \lambda_1^0 \mathbf{A} \cdot \mathbf{1} - (\mathbf{A} : \mathbf{ll}) \mathbf{1} + \lambda_1^0 (\mathbf{A} : \mathbf{ml}) \mathbf{m} \tag{12}
$$

$$
\frac{dS}{de} = \beta_1^0 S \mathbf{A} : \mathbf{nn} + \beta_1^m S \mathbf{A} : \mathbf{mm} + De^{-1} \beta_{2,S} \tag{13}
$$

$$
\frac{dP}{d\epsilon} = \beta_1^0 P \mathbf{A} : \mathbf{nn} + \beta_1^m P \mathbf{A} : \mathbf{mm} + De^{-1} \beta_{2,P} \tag{14}
$$

where $\mathbf{A} = A / \epsilon$ is the dimensionless rate of strain tensor, $De = \dot{\epsilon} \tau_4$, is the alignment Deborah number (dimensionless strain rate), and $\epsilon = \dot{\epsilon} t$ is the strain (dimensionless time). Equations (10-14) are only used to obtain analytical results and to develop a selection procedure for
Fig. 5. — a) Computed director triad \( (\mathbf{n}, \mathbf{m}, \mathbf{l}) \) trajectories on the surface of the unit sphere with representative meridians and equator; b) Corresponding computed director trajectories on the \( \phi - \theta \) plane for initial uniaxial director orientation \((\theta_0, \phi_0) = (45, 2.56)\). There is indeterminacy in the \( \mathbf{m}, \mathbf{l} \) trajectories, for each uniaxial director \( \mathbf{n} \) trajectory there are two different biaxial director \( \mathbf{m}, \mathbf{l} \) trajectories. The arrows indicate the direction of the director paths. The steady states for the uniaxial director \( \mathbf{n} \) and the biaxial director \( \mathbf{m} \) lie on the equator, the plane of uniform compression, whereas for the biaxial director \( \mathbf{l} \) the poles (extension direction) of the unit sphere are the stable states. The uniaxial director \( \mathbf{n} \) and biaxial director \( \mathbf{l} \) follow geodesic meridian flow, whereas the constant biaxial director \( \mathbf{m} \) remains at all the times on the equator.

The parameters of the model, all numerical results of this paper were obtained by numerical integration of equations (A.1-A.5). Equation (11) shows that \( \mathbf{m} \equiv \) constant for uniaxial extensional flow, as we prove below (see Fig. 5); this analytical result is not used in the numerical integration of equations (A.1-A.5). The director diad \( (\mathbf{n}, \mathbf{l}) \) evolution equations (10, 12) contain uncoupled and mixed flow terms. The parametric functions introducing these terms are the four reactive parameters \( (\lambda^*_i; i = \mathbf{n}, \mathbf{l}; j = \mathbf{n}, \mathbf{l}, \text{mix}) \), where the subscript "mix" denotes...
the cross coupling reactive parameters. In this paper the following terminology is used for the set of reactive parameters: uniaxial reactive parameter \( \lambda^n \), mixed-uniaxial reactive parameter \( \lambda^{mix}_n \), biaxial reactive parameter \( \lambda^b_1 \), and mixed-biaxial reactive parameter \( \lambda^{mix}_b \). The alignment relaxation equations (13,14) contain only uncoupled flow terms and the parametric functions introducing these terms are the four ordering functions \( (\beta^{\#}, j = n, m; j = S, P) \), and the two elastic functions \( (\beta^{n, P}, j = S, P) \). The following terminology is used for the set of ordering functions: \( n - S \) ordering function \( \beta_n^{n, S} \), \( m - S \) ordering function \( \beta_m^{m, S} \), \( n - P \) ordering function \( \beta_n^{b, P} \), and \( m - P \) ordering function \( \beta_m^{b, P} \). The elastic functions are called uniaxial elastic function \( \beta_n^{S} \) and biaxial elastic function \( \beta_n^{b, P} \) and contain the thermodynamic contribution. The expressions for the set of reactive parameters \( (\lambda^n, \lambda^{mix}, \lambda^b_n, \lambda^{mix}_b) \), the ordering set \( (\beta_n^{n, S}, \beta_m^{m, S}, \beta_n^{b, P}, \beta_m^{b, P}) \), and the elastic functions \( (\beta_n^{S}, \beta_n^{b, P}) \) are given in Appendix B. When \( De \to 0 \) the alignments dynamics are purely elastic, when \( De \to \infty \) purely viscous, and for the intermediate \( De \) values viscoelastic. At intermediate \( De \) the moving director diad \( (n, l) \) is also viscoelastic, as it is coupled to alignments \( (S, P) \) through the set of reactive parameters \( (\lambda^n, \lambda^{mix}, \lambda^b_n, \lambda^{mix}_b) \).

The velocity field \( v(x, y, z) \) corresponding to the uniform uniaxial, irrotational, 3D extensional start-up flow of the discotic nematic crystals, is given by [8]:

\[
\begin{align*}
 v_x &= \dot{\epsilon} x H(t); \\
 v_y &= -\frac{\dot{\epsilon}}{2} y H(t); \\
 v_z &= -\frac{\dot{\epsilon}}{2} z H(t); \\
 H(t) &= \begin{cases} 
 0 & t < 0 \\
 1 & t \geq 0
\end{cases}
\end{align*}
\]

(15a, b, c, d)

where \( \dot{\epsilon} \) is the constant uniaxial extension rate. The non-zero components of the corresponding rate of deformation tensor \( A \) are: \( A_{11} = \dot{\epsilon}; \ A_{22} = A_{33} = -\dot{\epsilon}/2 \); this flow is irrotational and the vorticity tensor is zero, \( \mathbf{W} = 0 \).

The initial conditions used to solve equations (A.1-A.5), in eigenvalue-eigenvector form, are:

\[
\begin{align*}
 &at \ t = 0: \quad n = n_0; \quad m_0 = (0, m_{y0}, m_{z0}); \quad l_0 = n_0 \times m_0; \\
 &\quad n_0 \cdot n_0 = m_0 \cdot m_0 = l_0 \cdot l_0 = 1; \\
 &\quad S_0 = S_{eq}; \quad P_0 = 0;
\end{align*}
\]

(16)

where \( S_{eq}(U) \) is the equilibrium scalar order parameter of the normal \( (S > 0) \) uniaxial nematic phase, given by [27]:

\[
S_{eq} = \frac{1}{4} + \frac{3}{4} \sqrt{\left(1 - \frac{8}{3U}\right)}
\]

(17)

For \( U < 8/3 \) the stable phase is isotropic, for \( 8/3 \leq U \leq 3 \) there is biphasic equilibrium, and for higher values of uniaxial nematic potential \( U \) the phase is uniaxial nematic. High values of \( U \) correspond to stronger uniaxial alignment. In this paper we use two representative nematic potential \( U = 3 \) and \( U = 5 \), and the corresponding initial condition values for uniaxial scalar order parameter are: \( S_{eq}(U = 3) = 0.5 \) and \( S_{eq}(U = 5) = 0.76 \). In this paper, all angles are reported in degrees.

Equations (A.1-A.5) are integrated using an implicit corrector-predictor first order Euler integration method with an adaptable time step [28]. Application of the implicit corrector-predictor method transforms the set of coupled nonlinear ordinary differential equations (A.1-A.5) into a set of coupled nonlinear algebraic equations. For each time step the algebraic equations are solved using the Newton-Raphson iteration scheme [28]; the predictor step generates a first guess for the iteration loop and the corrector step is the iteration loop itself. The adopted convergence criteria is that the length of the difference vector between the calculated solution vectors corresponding to two successive iterations is less than \( 10^{-6} \). The transient solution
vector obtained from the numerical solutions consists of the five independent components of the tensor order parameter \( Q(\epsilon) \) as a function of the strain (dimensionless time) \( \epsilon = \epsilon t \). In addition to the uniaxial nematic potential \( U \), the other dimensionless parameter investigated in this paper is alignment Deborah number \( D_e \). The numerically obtained tensor order parameter \( Q(\epsilon) \) is subsequently transformed into principal form to find its eigenvectors or director triad \((n, m, l)\) and its eigenvalues, given by equation (2).

2.3. Analytical Results

2.3.1. Director Triad Dynamics. — Assuming that the biaxial director \( m \) always lies on the equator, or the plane of uniform compression, then it can be written as \( m = (0, m_y, m_z) \). Using this restriction \( (m_x = 0) \) and the symmetry of the flow type \( (A_{yy} = A_{zz}) \) the mixed terms, \( A : mn \) and \( A : ml \), in the director diad \((n, l)\) relaxation equations \((10, 12)\) take the following form:

\[
A : mn = A_{yy} (m_y n_y + m_z n_z); \tag{18}
\]

and

\[
A : ml = A_{yy} (m_y l_y + m_z l_z). \tag{19}
\]

The orthogonality of the directors \((m \perp n \text{ and } m \perp l)\) now gives:

\[
m_y n_y + m_z n_z = 0; \quad m_y l_y + m_z l_z = 0 \tag{20a, b}
\]

Use of equations (20) in equations \((18, 19)\) shows that the mixed terms \( A : mn \) and \( A : ml \) appearing in the director diad relaxation equations \((10, 12)\) are zero. Hence the uniaxial director relaxation \( n(\epsilon) \) and biaxial director relaxation \( l(\epsilon) \) are affected only by the uniaxial reactive parameter \( \lambda_n^u \) and the biaxial reactive parameter \( \lambda_l^b \), respectively. Integration of equations \((10)\) and \((12)\) yields the following expressions for the moving director diad \((n, l)\) relaxation in the uniaxial start-up extensional flow:

\[
\dot{a}_i(\epsilon) = \frac{E_{ij} \hat{a}_j(\epsilon)}{|E \cdot \hat{a}_0|}; \quad \dot{a}_i(0) = a_{i0}; \tag{21a, b, c, d}
\]

\[
E_{ij}(\epsilon) = \exp \left\{ \hat{A}_{ij} \int_0^\epsilon \lambda_n^u d\epsilon' \right\}; \quad \hat{A}_{ij} = \frac{A_{ij}}{e};
\]

and in the component form:

\[
\dot{a}_x = \frac{E_{xx} \hat{a}_{x0}}{|E \cdot \hat{a}_0|}; \quad \dot{a}_y = \frac{E_{yy} \hat{a}_{y0}}{|E \cdot \hat{a}_0|}; \quad \dot{a}_z = \frac{E_{zz} \hat{a}_{z0}}{|E \cdot \hat{a}_0|}; \tag{22a, b, c}
\]

\[
E_{xx} = \exp \left( \int_0^\epsilon \lambda_n^u d\epsilon' \right); \quad E_{yy} = E_{zz} = \exp \left( -\frac{1}{2} \int_0^\epsilon \lambda_n^u d\epsilon' \right); \tag{23a, b, c}
\]

where \( \hat{a} = n, l \); and \( a_{j0} \) is the \( j \)th component of the initial director orientation \( (\hat{a}(0) = n(0), l(0)) \). The direction of the director trajectory and steady state is governed by the sign of the corresponding director reactive parameter. The uniaxial reactive parameter \( \lambda_n^u \) is negative for discotic nematics \([14]\) (see Fig. 7). For the present case \((m_x = 0)\), it can be shown that the biaxial reactive parameter \( \lambda_l^b \) is related to the uniaxial reactive parameter by the following relation:

\[
\lambda_l^b = -\lambda_n^u; \tag{24}
\]

which, since \( \lambda_n^u < 0 \) \([14]\), implies that \( \lambda_l^b > 0 \) for discotic nematics (this relation follows from equations \((B.1, B.3)\)). The equations \((22, 23, 24)\) show that the \( y \) and \( z \) components of the
uniaxial director $\mathbf{n}$ will increase, whereas the corresponding components of the biaxial director $\mathbf{I}$ will decrease; hence $\mathbf{n}$ rotates towards the equator, and $\mathbf{I}$ towards the closest pole. From equations (22, 23) it also follows that $y$ and $z$ components of the moving director triad $(\mathbf{n}, \mathbf{I})$ are related by: $n_y = bn_z (b = n_{y0}/n_{z0})$, and $l_y = bl_z (b = l_{y0}/l_{z0})$. Using the last result and equations (7, 8), we conclude that the uniaxial director $\mathbf{n}$ and biaxial director $\mathbf{I}$ orbits belong to the meridians, and the director diad $(\mathbf{n}, \mathbf{I})$ dynamics belong to the class of geodesic flows. Comparison of equations (22, 23, 24) with equations (7, 8) also shows that the director diad $(\mathbf{n}, \mathbf{I})$ belong to the same meridian of the unit sphere. From the meridian flow of the director diad $(\mathbf{n}, \mathbf{I})$ it follows that the biaxial director $\mathbf{m}$ should lie somewhere on the equator of the unit sphere. The computed numerical simulations for the director triad relaxation, shown below, confirm the above analysis.

The selection criteria for the biaxial director $\mathbf{m}$ can be explained by the following argument. Biaxiality will be present in a plane normal to the extension direction, that is, in the $(y-z)$ plane. Since $\mathbf{m}$ is normal to $\mathbf{n}$ and must lie on the equator, hence $\mathbf{m}(0)$ is normal to $\mathbf{P} \cdot \mathbf{n}(0)$, where $\mathbf{P} = (\delta - \mathbf{n}\mathbf{n})$ is the projection operator. In addition, since $\mathbf{n}$ follows a geodesic meridian flow $(n_y = bn_z, b = n_{y0}/n_{z0})$, thus it follows that:

$$\hat{n}_\perp = \frac{\mathbf{P} \cdot \mathbf{n}(0)}{|\mathbf{P} \cdot \mathbf{n}(0)|} = \frac{1}{\sqrt{1 + b^2}} (\hat{y} + \hat{b} \hat{k}) \quad (25)$$

and from $\mathbf{m} \perp \hat{n}_\perp$ we finally get the following components for $\mathbf{m}$:

$$m_x = 0; \quad m_y = \pm \frac{1}{\sqrt{1 + b^2}}; \quad m_z = -bm_y \quad (26a, b, c)$$

Equations (26) show that for a given $b = n_{y0}/n_{z0}$, there is indeterminacy in the selection of the biaxial director $\mathbf{m}$, since there are two equivalent directions perpendicular to $\mathbf{n}_0$ and farthest away from the extension direction for each initial uniaxial orientation $\mathbf{n}_0$. As $\mathbf{I} = \mathbf{n} \times \mathbf{m}$, there are also two possible equivalent biaxial director $\mathbf{I}$ trajectories for each uniaxial director $\mathbf{n}$ trajectory. Equations (22, 23, 24, 26) show that the stable state director triad is given by:

$$[\mathbf{n}_{ss}, \mathbf{m}_{ss}, \mathbf{l}_{ss}]: \begin{bmatrix} \mathbf{n}_{ss} = (0, n_{yss}, n_{zss}) = \left(0, \frac{b}{\sqrt{1 + b^2}}, \frac{1}{\sqrt{1 + b^2}} \right) \\
\mathbf{m}_{ss} = (0, m_{yss}, m_{zss}) = \left(0, \pm \frac{1}{\sqrt{1 + b^2}}, \pm \frac{b}{\sqrt{1 + b^2}} \right) \\
\mathbf{l}_{ss} = (1, l_{yss}, l_{zss}) = (\pm 1, 0, 0) \end{bmatrix} \quad (27a, b, c)$$

where $b = n_{y0}/n_{z0}$.

Figure 5a shows the computed director triad $(\mathbf{n}, \mathbf{m}, \mathbf{I})$ trajectories on the surface of the unit sphere, and Figure 5b shows the corresponding computed director triad trajectories on the $\phi - \theta$ plane, for an initial uniaxial director orientation of $(\theta_0, \phi_0) = (45, 2.56)$. The figure shows that for the given uniaxial director $\mathbf{n}$ trajectory there are two different biaxial director $\mathbf{m}, \mathbf{I}$ trajectories, where the arrows indicate the direction of the director paths. The uniaxial director trajectory and the two corresponding equivalent biaxial director trajectories lie on the same meridian. The computed director triad steady states agree with equation (27): $\mathbf{l}_{ss}$ lies along the poles, $\mathbf{n}_{ss}$ lies on the equator, and $\mathbf{m}_{ss}$ lies on the equator and is normal to $\mathbf{n}_{ss}$.

The uniaxial director $\mathbf{n}$ and biaxial director $\mathbf{I}$ orbits follow geodesic flow due to the inherent symmetry in the uniaxial extensional flow. This result is also predicted by the TIF equations of [29], which are applicable to uniaxial nematics of constant order parameter, since as mentioned above, for irrotational flows the geometry of the director orbits are insensitive to variations in the magnitude of the alignment. The director trajectories should exhibit the characteristic
sensitive dependence on initial conditions which is typical of geodesic flows [30]. When the initial uniaxial orientation is \( n_x = \pm 1 \), along the poles, predictability is lost. Close to the poles there is high sensitivity to initial uniaxial orientation \( n_0 \). Figure 6 shows the director triad trajectories on the surface of the unit sphere when the initial uniaxial orientation is close to the north pole; for \((\theta_0, \phi_0) = (45, 2.56)\) (solid line, corresponding director triad trajectories are denoted with subscript "A") and \((\theta_0, \phi_0) = (315, 2.56)\) (dot-dash line, corresponding director triad trajectories are denoted with subscript "B"). The arrows indicate the direction of the director paths. The figure illustrates that there is a high sensitivity of the director triad trajectories and steady states, when the initial uniaxial orientation is close to the poles. The whole compression plane or equator contains the space of stable uniaxial \( n_{ss} \) and biaxial \( m_{ss} \) orientations, while the poles or the extension directions are the stable states for the biaxial director \( l \).

2.3.2. Uniaxial Alignment Dynamics. — The uniaxial alignment relaxation \( S(\varepsilon) \) and biaxial alignment relaxation \( P(\varepsilon) \) depend on \( \dot{A}_0(\dot{\alpha} = n, l) \) through the ambient strain rate \( A : \dot{\alpha} \dot{\alpha} \). Figure 4 shows different representative regions for \( A : \dot{\alpha} \dot{\alpha} \). In the \( R^- \) regions the ambient strain rate is positive \( (A : \dot{\alpha} \dot{\alpha} > 0) \), and in the \( R^+ \) regions the ambient strain rate is negative \( (A : \dot{\alpha} \dot{\alpha} < 0) \). The uniaxial alignment relaxation equation (13) can be written, using the right handed orthogonality of the director triad \( (\delta = nm + mm + ll) \), as:

\[
\frac{dS}{dc} = (\beta_{1,S}^n - \beta_{1,S}^m) \dot{A} : nn - \beta_{1,S}^m \dot{A} : ll + D_\varepsilon^{-1} \beta_{2,S}
\]

(28)

where \( (\beta_{1,S}^n - \beta_{1,S}^m) \) and \( \beta_{1,S}^m \) both are negative (see Fig. 7); hence the initial uniaxial alignment relaxation characteristics are given by:
Fig 7 — Parametric functions of the model. The uniaxial reactive parameter $\lambda_B^U$ and the set of ordering functions $\beta_1^U, \beta_2^U, \beta_3^U, \beta_4^U$ as a function of the uniaxial scalar order parameter $S$ and biaxial scalar order parameter $P$ for the chosen set of dimensionless phenomenological parameters $(\sigma^*_4, \sigma^*_6, \tau^*_6)$. For discotic nematic liquid crystals these all are negative (see text).

$$\begin{align*}
n_0 & \text{ in } R^- : \left( \frac{dS}{de} \right)_{\epsilon=0^+} < 0; \quad n_0 \text{ in } R^+ : \left( \frac{dS}{de} \right)_{\epsilon=0^+} > 0; \\
\text{n}_0 \text{ in } \partial R^- = \partial R^+ : \left( \frac{dS}{de} \right)_{\epsilon=0^+} = 0;
\end{align*}$$

It follows from the equations (29) that for any $De$, a sufficient condition for increasing uniaxial alignment $S$ is that $n_0$ is in $R^+$. For large $De$, discotic nematics, initially in $R^-$ undergo a temporary melting the uniaxial director is in the region $R^-$ [14].

2.4. SELECTION OF PHENOMENOLOGICAL PARAMETERS. — In this section we show and use the concepts used to construct a selection procedure for the three dimensionless phenomenological parameters $(\sigma^*_4, \sigma^*_6, \tau^*_6)$ of the present model. The non-dimensionalization of the three parameters is given in equation (A.41). To select the numerical values of the three dimensionless parameters $\sigma^*_4, \sigma^*_6, \tau^*_6$ we enforce the following constraints on the signs
of $\lambda_n^0, \gamma_{2,n}^0, \gamma_{1,n}^0$ [14, 15, 31–34] and on the values of $\lambda_n^0$ when $S = 0, S = 1$ [31]:

$$\lambda_n^0 = -\frac{\gamma_{2,n}^0}{\gamma_{1}^0} < 0; \quad \gamma_{2,n}^0 \geq 0; \quad \gamma_{1}^0 \geq 0;$$  \hspace{1cm} (30a, b, c)

$$\lim_{S \rightarrow 0} \lambda_n^0 = -\infty; \quad \lim_{S \rightarrow 1} \lambda_n^0 = -1; \quad P = 0 \quad P = 0$$  \hspace{1cm} (30d, e)

$$\lim_{P \rightarrow 0} \lambda_n^0 = -\infty; \quad \lim_{P \rightarrow 1} \lambda_n^0 = -1, \quad S = 0 \quad S = 0$$  \hspace{1cm} (30f, g)

where $\gamma_{1}^0$ is the rotational viscosity for $n$, and $\gamma_{2,n}^0$ is the irrotational viscosity for $n$, whose meaning is identical to that of uniaxial nematics [7].

In addition to the above-mentioned well-known constraints, additional restrictions imposed on the phenomenological parameters, appear for the physically meaningful alignment of the director triad at steady state ($n_{ss}$ and $m_{ss}$ lie perpendicular to the extension direction). This physically meaningful steady state director triad orientation is automatically selected by using equation (24).

The adopted values that satisfy the above mentioned constraints are: $\sigma_a^x = 0.55, \sigma_a^z = 0.30, \tau_a^a = 1.05$. The resulting uniaxial reactive parameter $\lambda_n^0$ ($\lambda_1^0 = -\lambda_n^0$) and the set of ordering functions $\beta_{1,S}^n, \beta_{1,S}^m, \beta_{1,P}^n, \beta_{1,P}^m$, given by equations (B.1, B.5, B.6, B.7, B.8), respectively, are shown in Figure 7. The values of the phenomenological parameters used in this paper are not fitted to any of the original existing discotic mesophases, but capture the essential phenomena of the problem. Other parameter values will only change the time scales for the various relaxations.

The appropriateness of the signs of the various ordering functions shown in Figure 7, for discotic nematics, can be justified by expected physical phenomena [14, 15]. When extension is applied normal to the uniaxial director $n$ of a discotic nematic, there is an increase in the alignment of the molecular normals along $n$. Hence when the uniaxial director $n$ lies on the equator (region $R^+$), the start-up uniaxial extensional flow should tend to increase the alignment along $n$. Moreover when $n$ lies in region $R^+$, the flow contributions in equation (13) are both negative ($A : nn < 0$, and $A : mm < 0$). Hence, for $S(e)$ to increase, equation (13) shows that the two ordering functions must be negative: $\beta_{1,S}^n < 0$, and $\beta_{1,S}^m < 0$.

When $n$ lies on the pole the effect of biaxiality is zero, since both biaxial directors ($m, l$) lie on the compression $(y - z)$ plane. As $n$ moves towards the equator the biaxiality increases because of the preference of the projections of the molecular normals to align themselves along $m$ in a plane perpendicular to $n$. Thus when $n$ lies on the equator ($l$ lies on the pole, and $m$ lies on the equator) the application of the flow should increase biaxiality, and when $n$ lies along the poles flow will not induce any biaxiality. Consideration of equation (14) with $n$ on the equator indicates that the expected increase of $P$ is captured only if the two ordering functions are negative: $\beta_{1,P}^n < 0$, and $\beta_{1,P}^m < 0$.

3. Numerical Results

3.1. Uniaxial and Biaxial Orientation Relaxation. — Figure 8 shows the polar uniaxial angle $\phi$ as a function of strain (dimensionless time) $\epsilon = \epsilon t$, for $De = 0.6$ (a), 0.4 (b), 0.1 (c); $U = 3$ (dash-dot line), $U = 5$ (full line), and for the initial uniaxial director orientation $(\theta_0, \phi_0) = (45, 2.56)$. The figure shows that the uniaxial director $n$ relaxation is viscoelastic, and that it is faster at higher $De$ and lower $U$, since for these conditions the uniaxial reactive parameter $\lambda_n^0$ samples higher absolute values. The biaxial director $m$ is fixed at the equator.
Fig 8. — Polar uniaxial angle $\phi$ as a function of strain (dimensionless time) $\epsilon = \epsilon t$, for $De = 0.6$ (a); 0.4 (b), 0.1 (c), $U = 3$ (dash-dot line), $U = 5$ (full line), and initial uniaxial director orientation $(\theta_0, \phi_0) = (45, 2.56)$. The uniaxial director relaxation is viscoelastic, and it is faster at higher $De$ and at lower $U$. The biaxial director $m$ is fixed on the equator, and the biaxial director $l$ follows the viscoelastic relaxation of the uniaxial director $n$.

(see Fig. 5), and the biaxial director $l$ follows the viscoelastic relaxation of the uniaxial director $n$, since $l \perp n$.

3.2. UNIAXIAL AND BIAXIAL ALIGNMENT RELAXATION. — Figure 9 shows the uniaxial alignment relaxation $S(\epsilon)$, and the biaxial alignment relaxation $P(\epsilon)$, for $De = 0.6$ (full line), $De = 0.4$ (dash-dot line), and $De = 0.1$ (triple dot dash line) corresponding to the initial uniaxial director orientation of Figure 8, for (a, c) $U = 5$, (b, d) $U = 3$. The figure shows that the uniaxial and biaxial alignment relaxations are viscoelastic. For a high nematic potential ($U = 5$) the viscous mode dominates for higher $De$ ($De = 0.6$), while the elastic mode dominates the viscoelastic relaxation for lower $De$ ($De = 0.1$). For a low nematic potential ($U = 3$) the viscous mode dominates at higher $De$ ($De = 0.6$); at lower $De$ ($De = 0.1$) the viscous mode dominates the initial response but the elastic mode dominates the viscoelastic relaxation at the later stage. Since in this figure the initial orientation of the uniaxial director $n_0$ is in
Fig. 9 — Uniaxial alignment relaxation $S(\varepsilon)$ and biaxial alignment relaxation $P(\varepsilon)$, for $De = 0.6$ (full line), $De = 0.4$ (dash-dot line), and $De = 0.1$ (triple dot dash line) corresponding to initial uniaxial director orientation of Figure 8, for (a, c) $U = 5$, (b, d) $U = 3$. The figure shows that at higher $De$ the viscous mode dominates and the effect of relative magnitude of $U$ is small, while at lower $De$ the elastic mode dominates and the effect of relative magnitude of $U$ is large. The Deborah number $De$ is the dimensionless strain rate ($De = \varepsilon \tau_4$).

$R^-$, there is an initial decrease in the uniaxial alignment relaxation (Figs. 9a,b), and there is an initial lag in the biaxial alignment relaxation (Figs. 9c,d). A comparison of the computed steady state alignment shows that at higher $De$, the viscous mode dominates and the effect of the relative magnitude of the nematic potential $U$ is small, while at lower $De$, the elastic mode dominates and the effect of $U$ is large.

Figure 10 shows the alignment's evolution in the alignment triangle ($P - S$ triangle) for $De = 0.6$ (full line), $De = 0.4$ (dash-dot line), and $De = 0.1$ (triple dot dash line) corresponding to initial the uniaxial director orientation of Figure 8, for (a) $U = 5$ and (b) $U = 3$. The empty circles show the initial alignments condition ($S = S_{eq}, P = 0$), and the direction of arrows represents the relaxation with increasing strain $\varepsilon$ ($\varepsilon = \varepsilon t$). The figure shows an initial decrease in the magnitude of the uniaxial scalar order parameter $S$, from the equilibrium value $S_{eq}$, because the uniaxial orientation prior to flow was in region $R^-$. Figure 10 shows that the alignment trajectory is well approximated by a three-stage process. In the initial stage, $S$ decreases and $P$ remains close to zero, since the uniaxial orientation $n$ is close to the poles, and the flow will not induce biaxiality. In the intermediate stage, $S$ is relatively low, $n$ is
Fig. 10 — Alignment trajectories in the alignment triangle (P - S triangle) for $De = 0.6$ (full line), $De = 0.4$ (dash-dot line), and $De = 0.1$ (triple dot dash line), corresponding to initial uniaxial director orientation of Figure 8, for a) $U = 5$ and b) $U = 3$. The circles show the initial alignment condition ($S = S_{eq}, P = 0$), and the direction of arrows represent the relaxation with increasing strain $e (e = \dot{\varepsilon})$. Initially, the uniaxial scalar order parameter $S$ decreases significantly, and there is no significant increase in the small magnitude of $P$. Subsequently, $P$ increases considerably; finally, $S$ reaches a stable relatively high value that results in the relatively low value of the biaxial parameter. For the same dimensionless extension rate $De$, there is more biaxiality at low values of the nematic potential $U$ than at high $U$.

Initially, the uniaxial scalar order parameter $S$ decreases significantly, and there is no significant increase in the small magnitude of $P$. Subsequently, $P$ increases considerably; finally, $S$ reaches a stable relatively high value that results in the relatively low value of the biaxial parameter. For the same dimensionless extension rate $De$, there is more biaxiality at low values of the nematic potential $U$ than at high $U$.

Fig. 11 shows a trajectory in the alignment triangle and the corresponding computed scientific visualizations representing the density ($f(\omega_1, \omega_2)$) of the unit normals to the discs in $m - l$ plane ($n$ is out of the plane of paper), for $U = 3$, $De = 0.6$, and for the initial uniaxial director orientation of Figure 8. The density $f(\omega_1, \omega_2)$ is approximated by:

$$f(\omega_1, \omega_2) \approx \frac{1}{4\pi} + \frac{5}{8\pi} \left( (2\cos^2\omega_1 - \sin^2\omega_1) S + (\sin^2\omega_1 \cos^2\omega_2) P \right);$$

where $(\omega_1, \omega_2)$ are the polar and azimuthal angles, respectively, of the unit normal $u$ to a disc-like molecule with respect to the $(n, m, l)$ frame. Equation (31) was obtained by using the standard single molecule distribution function $f(u) \approx \frac{1}{4\pi} + \frac{15}{8\pi} uu : Q$, where $u$ is the unit normal to the disc-like molecule. In the figure we mapped the magnitude of $f(\omega_1, \omega_2)$ onto a gray scale; darker (lighter) regions correspond to higher (lower) value of $f(\omega_1, \omega_2)$. The four
Computed scientific visualizations representing the density of the unit normals to the molecular discs in $\mathbf{m} - \mathbf{l}$ plane ($\mathbf{n}$ is out of the plane of paper,) for $U = 3$, $D \varepsilon = 0.6$ corresponding to the initial uniaxial director orientation of Figure 8. The four insets correspond to the following alignment states: bottom right ($S = 0.5$, $P = 0$), bottom left ($S = 0.03$, $P = 0.03$), top left ($S = 0.25$, $P = 0.65$), top right ($S = 0.74$, $P = 0.2$). A darker area represents the higher density of unit normals to the disc-like molecules. For cases where $P \neq 0$, the figure shows a considerable higher distribution of unit normals along $\mathbf{m}$ than along $\mathbf{l}$ See text

insets correspond to the following alignment states: bottom right ($S = 0.5$, $P = 0$), bottom left ($S = 0.03$, $P = 0.03$), top left ($S = 0.25$, $P = 0.65$), and top right ($S = 0.74$, $P = 0.2$). A darker area represents the higher density of unit normals to the disc-like molecules. The bottom right visualization, representing the initial uniaxial state, shows that the $\mathbf{m} - \mathbf{l}$ plane is isotropic as $P = 0$; since $S \neq 0$ the density of the unit normals is high near the center ($\mathbf{n}$ is pointing out of the plane of paper at the center) but it decreases as we move away from the center. The bottom left visualization, representing a nearly isotropic state, shows a higher distribution of unit normals along $\mathbf{m}$ than $\mathbf{l}$; as $S$ is nearly zero there is almost a constant density of the unit normals. The top left visualization, representing a stronger biaxial state, shows a stronger anisotropy of the distribution than in the previous bottom left case, as $P$ is now higher. The top right visualization, representing the stable state, shows a weaker anisotropy of the distribution of the unit normals along $\mathbf{m}$ than previous visualizations, since an increase in $S$ has lowered $P$; also as the magnitude of $S$ is now significant there is a higher density of unit normals near the center than away from the center. Comparison of the top
Biaxial relaxation $P(\epsilon = \dot{\epsilon})$ for $De = 0.6$, $U = 3$, and for $n_0$ near the pole, $(\theta_0, \phi_0) = (45, 2.56)$, (full line), and $n_0$ on the equator, $(\theta_0, \phi_0) = (45, 90)$, (dot dash line). The figure shows an initial lag in the biaxial relaxation when initial uniaxial director orientation is along poles. The steady state biaxiality $P$ is the same for both of the initial orientations, however, the number of strains (dimensionless time) units required to achieve steady state biaxial alignment is considerably higher when the initial uniaxial director orientation is along the poles (region $R^-$) than when the initial uniaxial orientation is along the equator (region $R^+$). The intermediate strain stage displays the highest biaxiality.

Figure 12 shows the biaxial alignment relaxation $P(\epsilon = \dot{\epsilon})$ for $De = 0.6$, $U = 3$, and for $n_0$ near the pole, $(\theta_0, \phi_0) = (45, 2.56)$, (full line), and $n_0$ on the equator, $(\theta_0, \phi_0) = (45, 90)$, (dot dash line). The figure shows an initial lag in the biaxial relaxation when the initial uniaxial director orientation is near the poles (region $R^-$). The source of this is the competition between two effects: i) when the initial uniaxial director orientation is near the poles (region $R^-$) there is always a decrease in the initial uniaxial alignment response, which does not impede an increase in biaxiality; ii) when the uniaxial director is near the poles, the biaxial director $l(\mathbf{m})$ lies near (on) the equator and there is no significant competition of the unit normals to align along any one of the two biaxial directors, and hence there is no significant inducement for biaxiality. When the initial uniaxial director orientation is near the poles (region $R^-$) the combination of the two effects results in a lag in the initial biaxial alignment relaxation. When the initial uniaxial director orientation is in the region $R^+$, the biaxial director $l$ is in the region $R^-$, and there is preference of the molecular normals to lie along the director which lies in the compressional plane (biaxial director $\mathbf{m}$), and hence the biaxial alignment relaxation shows a monotonic increase. The steady state biaxiality $P$ is the same for both initial orientations. However, the relaxation time is considerably longer when the initial uniaxial director orientation is along the poles (region $R^-$) than when the initial uniaxial orientation is along the equator (region $R^+$).

Figure 13 shows the relaxation of the components of the tensor order parameter $Q(\epsilon = \dot{\epsilon})$, with the initial orientation $(\theta_0, \phi_0) = (45, 2.56)$ close to the north pole, for $U = 5$, and $De = 0.6$ (full line), 0.4 (dash-dot line), and 0.1 (triple dot-dash line). For the chosen initial orientation $n_{y0} = n_{z0}$, and from equation (1a) it follows that $Q_{yy} = Q_{zz}$ and $Q_{zz} = Q_{yy}$. For the shown
Fig. 13 — Relaxation of the components of the tensor order parameter $Q(ε)$ with the initial orientation $(θ₀, φ₀) = (45, 2.56)$ close to the pole, for $U = 5$, and $De = 0.6$ (full line), 0.4 (dash-dot line), and 0.1 (triple dot-dash line). The relaxation coordinate $ε = 6t$ is the strain or dimensionless time. For the chosen initial orientation $n_{y₀} = n_{z₀}$, and from equation (1a) it then follows that $Q_{xz} = Q_{yz}$ and $Q_{zz} = Q_{yy}$. See text for discussion.

parameters the relaxation is virtually complete after 4 strains units. At lower $De$ the relaxation of the components of the tensor order parameter is controlled by the orientation relaxation, as for $U = 5$ and lower $De$ the uniaxial alignment is nearly constant and there is not much increase in the biaxial alignment (see Fig. 9). At higher $De$ the relaxation of the trace components of the tensor order parameters is governed by the alignment because there is larger changes in the uniaxial and biaxial alignments as viscous mode dominates the viscoelastic relaxation. At lower $De$ the non-diagonal components of the tensor order parameter $Q$ are governed by the orientation relaxation, while at higher $De$, the viscous effects introduces an initial large decrease in uniaxial alignment and a lag in biaxial alignment. The latter case follows since the initial uniaxial orientation $n₀$ is in region $R^-$, and a subsequent increase in both uniaxial and
Fig. 14 — Magnitude of the difference of the steady state diagonal components a) \(|(Q_{xx} - Q_{yy})_{SS}|\), b) \(|(Q_{yy} - Q_{zz})_{SS}|\); and c) \(|(Q_{zz} - Q_{xx})_{SS}|\) of the tensor order parameter as a function of the dimensionless strain rate \(D_e\), for \(U = 3\). The initial uniaxial director orientations are: \((\theta_0, \phi_0) = (45, 256)\) or \(b = 1\) (full line), \((\theta_0, \phi_0) = (90, 256)\) or \(b = 0\) (dash-dot line), and \((\theta_0, \phi_0) = (0, 256)\) or \(b = \infty\) (triple dot-dash line). These differences are proportional to the steady flow birefringences \([34]\). Except for one case (Fig 14b, \(b = 1\)), the birefringences increase with the increasing \(D_e\).

Biaxial alignment (see Fig. 9), with the result that the only large component is \(Q_{yz}\), which follows a lag plus exponential growth relaxation.

At steady state, the magnitude of the differences of diagonal components of tensor order parameter are proportional to the steady flow birefringences \([35]\). Using equations (A.1-A.5) these differences are given by:

\[
\left|(Q_{xx} - Q_{yy})_{SS}\right| = \left|\frac{b^2 S_{SS} + \frac{1}{3} (2 + b^2) P_{SS}}{1 + b^2}\right|
\]

(32a)
\[ |(Q_{yy} - Q_{zz})_{SS}| = \left| \frac{1 - b^2}{1 + b^2} \left( S_{SS} - \frac{1}{3} P_{SS} \right) \right| \] (32b)

\[ |(Q_{zz} - Q_{xx})_{SS}| = \left| \frac{S_{SS} + \frac{1}{3} (2b^2 + 1) P_{SS}}{1 + b^2} \right| \] (32c)

where \( S_{ss} \) and \( P_{ss} \) are the steady state alignments. Figure 14 shows the absolute of the difference of the steady state diagonal components \(|(Q_{xx} - Q_{yy})_{SS}| \) (a), \(|(Q_{yy} - Q_{zz})_{SS}| \) (b), and \(|(Q_{zz} - Q_{xx})_{SS}| \) (c), of the tensor order parameter as a function of \( De \), for \( U = 3 \). The initial uniaxial director orientations are: \((\theta_0, \phi_0) = (45, 2.56)\) or \( b = 1 \) (full line), \((\theta_0, \phi_0) = (90, 2.56)\) or \( b = 0 \) (dash-dot line), and \((\theta_0, \phi_0) = (0, 2.56)\) or \( b = \infty \) (triple dot-dash line). In all cases there is a monotonic increase with increasing \( De \). The value of the \( y - z \) birefringence is identical for \( b = 0 \) and \( b = \infty \), hence the shown curves for these cases superpose. Comparison of Figures 14a and 14c show that: the \( x - y \) and the \( z - x \) birefringences are the same for \( b = 1 \); the \( x - y \) birefringence for \( b = 0 \) is equal to the \( z - x \) birefringence for \( b = \infty \) and vice versa. The figure shows that \( y - z \) birefringence is a weaker function of \( De \), whereas the \( x - y \) and the \( z - x \) birefringences are stronger functions of \( De \). The computed flow-birefringences provide a direct way to verify the predictions of the model.

4. Conclusions

In this initial investigation of the nematorheology of discotic nematics subjected to uniaxial extensional flows, we have performed a useful characterization of the sensitivity of the director triad \((n, m, l)\) trajectories, uniaxial and biaxial alignments \((S, P)\), and tensor order parameter relaxations with respect to the strength of the uniaxial nematic potential, the alignment Deborah number (dimensionless strain rate), and the initial director orientation. The use of unit sphere description identified the dynamics of the uniaxial director \( n \) and biaxial director \( l \) as geodesic meridian flows, whereas the constant orientation of the biaxial director \( m \) always lies on the equator. The stable steady state director triad is collinear with the axes of the strain rate ellipsoid. The uniaxial alignment undergoes an initial decrease, whereas the biaxial alignment shows an initial lag when the initial uniaxial orientation is close to the extension axis. Relatively large transient decreases of the uniaxial alignment and relatively large transient increases of the biaxial alignment are predicted to occur whenever the initial uniaxial director is along the extension direction. Computed predictions of the flow-birefringence offer a direct way to compare the theoretical predictions with experimental results, as successfully done for rod-like nematic polymers [13]. This comprehensive and unified view of microstructure relaxation under extension may be used in the future to explain the characteristic patterns found in the cross-section of melt spun fibers from carbonaceous mesophases [3, 36, 37].

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Appendix A

The dimensionless coupled, nonlinear ordinary first-order differential equations governing the microstructure of a discotic nematic, subjected to uniaxial extensional flow, are:

\[
\eta_1 \frac{dQ_{xx}}{d\epsilon} + \eta_2 \frac{dQ_{xy}}{d\epsilon} + \eta_3 \frac{dQ_{xz}}{d\epsilon} + \eta_4 \frac{dQ_{yy}}{d\epsilon} + \eta_5 \frac{dQ_{yz}}{d\epsilon} + \kappa_1 De^{-1} + \zeta_1 = 0 \quad (A.1)
\]

\[
\eta_6 \frac{dQ_{xx}}{d\epsilon} + \eta_7 \frac{dQ_{xy}}{d\epsilon} + \eta_8 \frac{dQ_{xz}}{d\epsilon} + \eta_9 \frac{dQ_{yy}}{d\epsilon} + \eta_{10} \frac{dQ_{yz}}{d\epsilon} + \kappa_2 De^{-1} + \zeta_2 = 0 \quad (A.2)
\]

\[
\eta_{11} \frac{dQ_{xx}}{d\epsilon} + \eta_{12} \frac{dQ_{xy}}{d\epsilon} + \eta_{13} \frac{dQ_{xz}}{d\epsilon} + \eta_{14} \frac{dQ_{yy}}{d\epsilon} + \eta_{15} \frac{dQ_{yz}}{d\epsilon} + \kappa_3 De^{-1} + \zeta_3 = 0 \quad (A.3)
\]

\[
\eta_{16} \frac{dQ_{xx}}{d\epsilon} + \eta_{17} \frac{dQ_{xy}}{d\epsilon} + \eta_{18} \frac{dQ_{xz}}{d\epsilon} + \eta_{19} \frac{dQ_{yy}}{d\epsilon} + \eta_{20} \frac{dQ_{yz}}{d\epsilon} + \kappa_4 De^{-1} + \zeta_4 = 0 \quad (A.4)
\]

\[
\eta_{21} \frac{dQ_{xx}}{d\epsilon} + \eta_{22} \frac{dQ_{xy}}{d\epsilon} + \eta_{23} \frac{dQ_{xz}}{d\epsilon} + \eta_{24} \frac{dQ_{yy}}{d\epsilon} + \eta_{25} \frac{dQ_{yz}}{d\epsilon} + \kappa_5 De^{-1} + \zeta_5 = 0 \quad (A.5)
\]

where \( De = \dot{\epsilon} \tau_4 \), is the alignment Deborah number (dimensionless strain rate) and \( \epsilon = \dot{\epsilon} t \) is the strain. The coefficients \( \eta_i (i = 1, 2, ..., 25) \) and \( \kappa_i (i = 1, 2, ..., 11) \) are given by:

\[
\eta_1 = 1 + \frac{2}{3} \tau_6^* (Q_{xx} - Q_{yy}) \quad (A.6)
\]

\[
\eta_2 = \frac{2}{3} \tau_6^* Q_{xy} \quad (A.7)
\]

\[
\eta_3 = \frac{2}{3} \tau_6^* Q_{xz} \quad (A.8)
\]

\[
\eta_4 = -\frac{2}{3} \tau_6^* (Q_{xx} + 2Q_{yy}) \quad (A.9)
\]

\[
\eta_5 = -\frac{4}{3} \tau_6^* Q_{yz} \quad (A.10)
\]

\[
\eta_6 = \tau_6^* Q_{xy} \quad (A.11)
\]

\[
\eta_7 = 1 + \tau_6^* (Q_{xx} + Q_{yy}) \quad (A.12)
\]

\[
\eta_8 = \tau_6^* Q_{yz} \quad (A.13)
\]

\[
\eta_9 = \tau_6^* Q_{xy} \quad (A.14)
\]

\[
\eta_{10} = \tau_6^* Q_{xz} \quad (A.15)
\]

\[
\eta_{11} = 0 \quad (A.16)
\]

\[
\eta_{12} = \tau_6^* Q_{yz} \quad (A.17)
\]

\[
\eta_{13} = 1 - \tau_6^* Q_{yy} \quad (A.18)
\]

\[
\eta_{14} = -\tau_6^* Q_{xz} \quad (A.19)
\]

\[
\eta_{15} = \tau_6^* Q_{xy} \quad (A.20)
\]

\[
\eta_{16} = -\frac{2}{3} \tau_6^* (2Q_{xx} + Q_{yy}) \quad (A.21)
\]

\[
\eta_{17} = \frac{2}{3} \tau_6^* Q_{xy} \quad (A.22)
\]
The non-dimensional parameters \( \sigma_4^*, \sigma_6^*, \) and \( \tau_6^* \) are given by:

\[
\sigma_4^* = \frac{\sigma_4}{\tau_4}; \quad \sigma_6^* = \frac{\sigma_6}{\tau_4}; \quad \tau_6^* = \frac{\tau_6}{\tau_4}.
\]
Appendix B

The reactive parameter set \((\lambda_n^R, \lambda_{n,\max}^R, \lambda_1^R, \lambda_{\min}^R)\), the ordering function set \((\beta_1^m, \beta_1^S, \beta_1^n, \beta_1^m, \beta_1^n)\), and the elastic functions set \((\beta_2, \beta_2, \beta_2)\) are given by:

\[
\lambda_n^R = -\frac{\gamma_{n}^R}{\gamma_{n,\max}^R} = -\frac{9\sigma_4^* + 3\sigma_6^*(S - P)}{3S(3 + \tau_6^S) + 3P(3 - \tau_6^P) - 2\tau_6^SSP} \tag{B.1}
\]

\[
\lambda_{\min}^R = -\frac{\gamma_{\min,\max}^R}{\gamma_{1}^R} = -\frac{6\sigma_6^P}{3S(3 + \tau_6^S) + 3P(3 - \tau_6^P) - 2\tau_6^SSP} \tag{B.2}
\]

\[
\lambda_1^R = -\frac{\gamma_{1,\max}^R}{\gamma_{1}^R} = \frac{3\sigma_4^* + 3\sigma_6^*(S - P)}{3S(3 + \tau_6^S) + 3P(3 - \tau_6^P) - 2\tau_6^SSP} \tag{B.3}
\]

\[
\lambda_{\max}^R = -\frac{\gamma_{\max,\max}^R}{\gamma_{1}^R} = \frac{3\sigma_6^*(3P - S)}{3S(3 + \tau_6^S) + 3P(3 - \tau_6^P) - 2\tau_6^SSP} \tag{B.4}
\]

\[
\beta_{1,S}^m = -\frac{8\sigma_6^0\tau_6^S(3S + P)}{4\tau_6^S(3 + 2\tau_6^S(S + P))} - \frac{9(\sigma_4^* + 2\sigma_6^*(3S - P))(9 - 2\tau_6^*(3S - P))}{6 + 4\tau_6^S(S + P)} \tag{B.5}
\]

\[
\beta_{1,S} = \frac{4\tau_6^S(9\sigma_4^* - 2\sigma_6^*(3S - P))P - 4\sigma_6^*(9 - 2\tau_6^*(3S - P))P}{4\tau_6^S(3 + 2\tau_6^S(S + P))} - \frac{9\tau_6^*(3 + 2\tau_6^*(S + P))P - 2\tau_6^*(9\tau_6^S(S + P))}{6 + 4\tau_6^S(S + P)} \tag{B.6}
\]

\[
\beta_{1,P}^m = \frac{6\sigma_6^0(3S + P)(6 + 4\tau_6^S) - 3(9\sigma_4^* + 2\sigma_6^*(3S - P))(3 + 2\tau_6^*(S + P))}{4\tau_6^S(3 + 2\tau_6^S(S + P))} - \frac{6\sigma_6^0(3S + P)(6 + 4\tau_6^S) - 3(9\sigma_4^* + 2\sigma_6^*(3S - P))(3 + 2\tau_6^*(S + P))}{4\tau_6^S(3 + 2\tau_6^S(S + P))} \tag{B.7}
\]

\[
\beta_{1,P} = \frac{3(9\sigma_4^* - 2\sigma_6^*(3S - P))(6 + 4\tau_6^S) - 12\sigma_6^*(3 + 2\tau_6^*(S + P))P}{4\tau_6^S(3 + 2\tau_6^S(S + P))} - \frac{3(9\sigma_4^* - 2\sigma_6^*(3S - P))(6 + 4\tau_6^S) - 12\sigma_6^*(3 + 2\tau_6^*(S + P))P}{4\tau_6^S(3 + 2\tau_6^S(S + P))} \tag{B.8}
\]

\[
\beta_2 = \frac{\chi_1 + \chi_2}{\chi_5} \tag{B.9}
\]

\[
\beta_2 = \frac{\chi_3 + \chi_4}{\chi_5} \tag{B.10}
\]

\[
\chi_1 = \left(\frac{4\tau_6^*(S - P)}{S_1^*P}ight) \tag{B.11}
\]

\[
\chi_2 = \left(3 - \frac{2}{3}\tau_6^*(3S - P)\right) \tag{B.12}
\]

\[
\chi_3 = \left(\frac{4\tau_6^*(S - P)}{S_1^*P}\right) \tag{B.13}
\]

\[
\chi_4 = \left(\frac{3 + 2\tau_6^*(S + P)}{S_1^*P}\right) \tag{B.14}
\]

\[
\chi_5 = \left(\frac{(3 + 2\tau_6^*(S + P))P - (6 + 4\tau_6^S)(9 - 2\tau_6^*(3S - P))}{4\tau_6^S(S + P)}\right) \tag{B.15}
\]
References