Advection of nematic liquid crystals by chaotic flow

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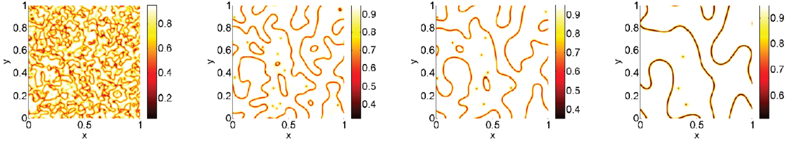
The Landau–de Gennes Equation

In the absence of flow, the Landau–de Gennes equation governs the orientation dynamics of an ensemble of liquid-crystal molecules:

$$\zeta_1 \frac{\partial \mathbf{Q}}{\partial t} = -\left[\frac{\delta F}{\delta \mathbf{Q}} - \tfrac{1}{3}\mathrm{tr}\left(\frac{\delta F}{\delta \mathbf{Q}} \right) \mathbb{I} \right]$$

where $\mathbf{Q}$ is the (symmetric, traceless) Q-tensor encoding information about the orientation of the molecules and F is the Landau free energy functional.



(a) $t = 100$ (b) $t = 1000$ (c) $t = 2000$ (d) $t = 5000$

Shown are snapshots of the scalar order parameter $\mathcal{S} = \sqrt{6\mathrm{tr}(\mathbf{Q}^2)}$. The system forms domains – coherent regions where the system relaxes locally to a single (stable) fixed point. The domains grow in time – **coarsening**.

Liquid-crystal dynamics with flow

An appropriate (materially frame-indifferent) model coupling the Q-tensor dynamics to hydrodynamics leads to a model with a highly non-Newtonian form for the stress tensor:

Q-tensor:

$$\zeta_1 \left(\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{Q} - \mathbf{\Omega} \mathbf{Q} - \mathbf{Q} \mathbf{\Omega} \right) + \underbrace{\zeta_2 \mathbf{D}}_{\text{Note inhomogeneity!}} =$$

$$k \nabla^2 \mathbf{Q} - \left(\alpha_F \mathbf{Q} - 3\beta_F \mathbf{Q}^2 + 4\gamma_F \mathrm{tr}(\mathbf{Q}^2) \mathbf{Q} \right) + \tfrac{1}{3} \mathbb{I} \left[\zeta_2 \mathrm{tr}(\mathbf{D}) - 3\beta_F \mathrm{tr}(\mathbf{Q}^2) \right],$$

Hydrodynamics:

$$\rho_0 \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \nabla \cdot \mathbf{T},$$

$$\mathbf{T} = -p \mathbb{I} - k \nabla \mathbf{Q} \odot \nabla \mathbf{Q} + \zeta_2 \overset{\circ}{\mathbf{Q}} + \zeta_3 \mathbf{D} + \zeta_{31} (\mathbf{D}\mathbf{Q} + \mathbf{Q}\mathbf{D}) + \zeta_{32} (\mathbf{D} \cdot \mathbf{Q}) \mathbf{Q},$$

Incompressibility: $\nabla \cdot \mathbf{v} = 0.$

Non-dimensional equations – dimensionless groups

Length scale ℓ and timescale $t_0 = \zeta_1/(8\gamma_F)$ – hence dimensionless Q-tensor equation

$$\frac{\partial \mathbf{Q}}{\partial \widetilde{t}} + \widetilde{\mathbf{v}} \cdot \widetilde{\nabla}\mathbf{Q} - \widetilde{\mathbf{\Omega}}\mathbf{Q} - \mathbf{Q}\widetilde{\mathbf{\Omega}} + \underbrace{\mathrm{Tu}}_{=(\zeta_2/\zeta_1)} \widetilde{\mathbf{D}}$$
$$= \epsilon^2 \widetilde{\nabla}^2 \mathbf{Q} + g_1(1-\theta)\mathbf{Q} + 3g_2\mathbf{Q}^2 - \tfrac{1}{2}\mathrm{tr}(\mathbf{Q}^2)\mathbf{Q} + \tfrac{1}{3}\mathbb{I}\left[\mathrm{Tu}\,\mathrm{tr}(\widetilde{\mathbf{D}}) - 3g_2\mathrm{tr}(\mathbf{Q}^2)\right],$$

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where

$$\alpha_F/(8\gamma_F) = -g_1[1-(T/T_*)] \equiv -g_1(1-\theta),\ \beta_F/(8\gamma_F) = g_2,\ \epsilon^2 = k/(8\ell^2\gamma_F).$$

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Hence also, a dimensionless momentum equation:

$$\frac{\partial \widetilde{\mathbf{v}}}{\partial \widetilde{t}} + \widetilde{\mathbf{v}} \cdot \widetilde{\nabla}\widetilde{\mathbf{v}} = -\widetilde{\nabla}\widetilde{p} + \frac{1}{\mathrm{Re}}\nabla \cdot \widetilde{\mathbf{D}} + \mathrm{Br}\nabla \cdot \left[-\epsilon^2 \widetilde{\nabla}\mathbf{Q} \odot \widetilde{\nabla}\mathbf{Q} + \cdots\right],$$

Non-dimensional equations – dimensionless groups

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where

$$\mathrm{Br} = \frac{\zeta_1}{\rho_0 \ell(\ell/t_0)}, \qquad \mathrm{Re} = \frac{\rho_0 \ell(\ell/t_0)}{\zeta_3}.$$

Limiting case

We work on the limit where $\mathrm{Br} = 0$ – no feedback of Q-tensor gradients into the flow – flow is independent of Q-tensor. We can therefore apply **standard chaotic flows** to the Q-tensor dynamics

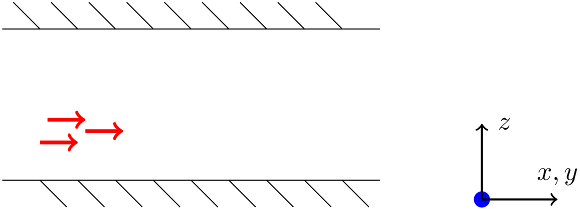
$$\frac{\partial \mathbf{Q}}{\partial \tilde{t}} + \tilde{\mathbf{v}} \cdot \tilde{\nabla} \mathbf{Q} - \tilde{\mathbf{\Omega}} \mathbf{Q} - \mathbf{Q} \tilde{\mathbf{\Omega}} + \underbrace{\mathrm{Tu}}_{=(\zeta_2/\zeta_1)} \tilde{\mathbf{D}}$$

$$= \epsilon^2 \tilde{\nabla}^2 \mathbf{Q} + g_1 (1-\theta) \mathbf{Q} + 3 g_2 \mathbf{Q}^2 - \tfrac{1}{2} \mathrm{tr}(\mathbf{Q}^2) \mathbf{Q} + \tfrac{1}{3} \mathbb{I} \left[\mathrm{Tu}\, \mathrm{tr}(\tilde{\mathbf{D}}) - 3 g_2 \mathrm{tr}(\mathbf{Q}^2) \right],$$

The **flow timescales** and the **tumbling parameter** Tu are the key parameters.

Two-dimensional geometry

We work with a sample confined between two narrowly separated parallel plates. **Anchoring conditions** are applied in the same fashion at the top and bottom walls such that the director is parallel to the plates.



As such, the Q-tensor simplifies:

$$\mathbf{Q} = \begin{pmatrix} q & r & 0 \\ r & s & 0 \\ 0 & 0 & -(q+s) \end{pmatrix}.$$

Fixed-point analysis

We look at fixed points for $\mathbf{v} = \nabla = \partial_t = 0$. Remarkably, all fixed points can be found in closed form (not shown) and classified:

- Case 1a ($r = 0$, $s = q$) gives stable and unstable states – **biaxial**
- Case 1b,c ($r = 0$, $s \neq q$) give neutral and unstable state – **uniaxial**
- Case 2 gives neutral and unstable state – **uniaxial**

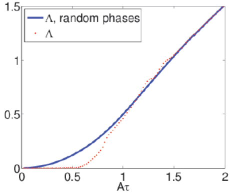
Model sine flow

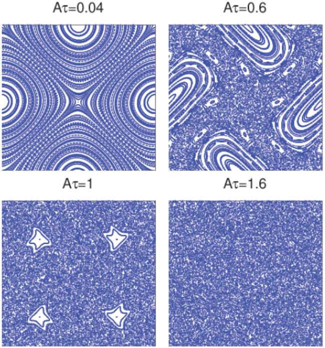
We use a model (quasi-) periodic velocity field,

$$\begin{aligned} u &= A\sin\left(k_0 y + \varphi_n\right), \qquad 0 \le \mathrm{mod}(t,\tau) < \tfrac{1}{2}\tau, \\ v &= A\sin\left(k_0 x + \psi_n\right), \qquad \tfrac{1}{2}\tau \le \mathrm{mod}(t,\tau) < \tau, \end{aligned}$$

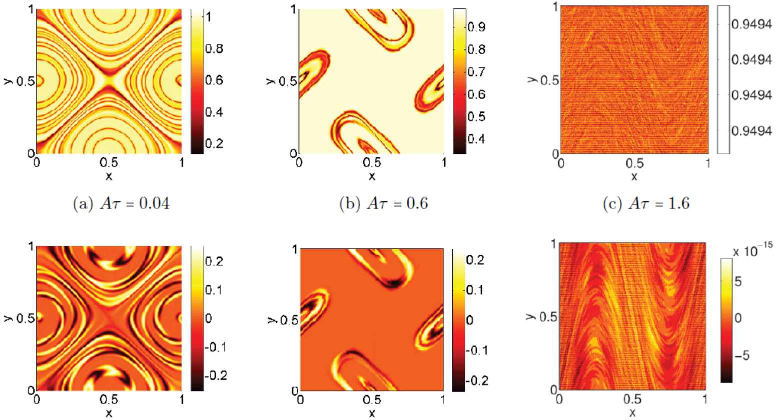
which mimics the effect of turbulence at high Prandtl number.

- The phases φ_n and ψ_n are held constant or are randomized periodically.
- The velocity field has a Lagrangian timescale given by the Lyapunov exponent Λ, which can be computed for the constant-phase and random-phase cases.





Results – no tumbling, constant-phase sine flow

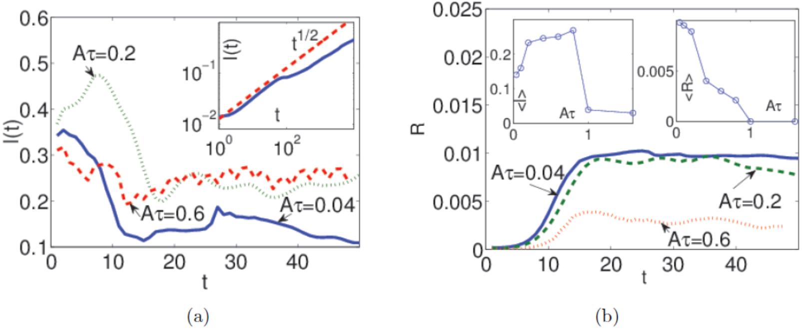


(a) $A\tau = 0.04$ (b) $A\tau = 0.6$ (c) $A\tau = 1.6$

(d) $A\tau = 0.04$ (e) $A\tau = 0.6$ (f) $A\tau = 1.6$

Across the top: snapshots of scalar order parameter at various times for various values of $A\tau$, with Tu = 0. Across the bottom: corresponding snapshots of r. Snapshots in the first two columns are taken at $t = 320$. The third column (figures (c) and (f)) concerns $A\tau = 1.6$, for which the snapshots are taken at $t = 320$; these are included here to demonstrate the relaxation to a uniform state for the large values of $A\tau$. The compressed colour bars in these figures is a consequence of the rapid relaxation to the uniform steady state.

Coarsening is arrested / overwhelmed



(a) Time evolution of the domain scale $L(t)$ for various values of $A\tau$. The inset shows the time-averaged values of $L(t)$ for a much larger range of $A\tau$-values, with angle brackets denoting a time average. The time-averages are taken over intervals where the Q-tensor dynamics are in a statistically steady state. (b) The same, for $R := L_x^{-1} L_y^{-1} \iint r^2 \, \mathrm{d}x \, \mathrm{d}y$

Discussion / Conclusions

Stirring by inhomogeneous shear affects orientation of liquid-crystal molecules:

- Low values of τ – domain structures 'frozen in' to flow structure.
- High values – domains overwhelmed and everything relaxes to biaxial state.
- Random-phase sine flow – everything is biaxial.
- Understanding depends on studying dynamics along Lagrangian trajectories:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q \\ r \\ s \end{pmatrix} = \begin{pmatrix} F_1(q,r,s) \\ F_2(q,r,s) \\ F_3(q,r,s) \end{pmatrix} + \begin{pmatrix} 2r\Omega_{12} \\ \Omega_{12}(s-q) \\ -2r\Omega_{12} \end{pmatrix}, \qquad \mathrm{Tu}=0,$$

(Diffusion negligible)

- Ongoing work – investigate robustness of results to different model flows
- Future work – Apply known techiques to the reduced planar model:
  - Bounds and *a priori* estimates
  - Lubrication theory
  - DNS of the fully coupled system – **the backreaction will be back!**