Backflow-mediated domain switching in nematics – experiment-ready

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Outline

• a CFD study: OpenFOAM, adapted for nematodynamics
• nematic director switching in external electric field
• intricate switching behaviour due to hydrodynamic flow (backflow)
• robust and realistic (3D geometry, irregular domains)
• the effect is verified by 3D calculations in the LC cell geometry
• prediction and motivation for an interesting experiment

Kick-back effect

- upon removing the vertical electric field: reverse director rotation due to backflow

Basic idea: amplification

- amplifying the reverse director rotation by a horizontal electric field
- results in a reverse domain

only a weak effect!
... but this is quite artificial:

- 2D only
- monodomain
- rectangular shape with boundaries
- proper director anchoring at the boundaries
- no slip boundary condition for the velocity

Most of these seem to be key ingredients of the kickback. Not readily achievable in real life.

We aim to check to what extent these conditions may be relaxed.
The set of equations \((n, v)\)

\[
f = \frac{1}{2} K_{11} (\nabla \cdot n)^2 + \frac{1}{2} K_{22} \left[ n \cdot (\nabla \times n) \right]^2 + \frac{1}{2} K_{33} \left[ n \times (\nabla \times n) \right]^2 - \frac{1}{2} \varepsilon_a \varepsilon_0 (E \cdot n)^2
\]

\[
h_i = -\frac{\partial f}{\partial n_i} + \partial_j \left( \frac{\partial f}{\partial (\partial_j n_i)} \right)
\]

\[
\sigma_{ij}^e = -\frac{\partial f}{\partial (\partial_i n_k)} \partial_j n_k
\]

\[
\frac{\partial n}{\partial t} = \left[ \frac{1}{\gamma_1} h - \frac{\gamma_2}{\gamma_1} A \cdot n - W \cdot n - (v \cdot \nabla) n \right] \perp n
\]

\[
\rho \left[ \frac{\partial v}{\partial t} + (v \cdot \nabla) v \right] = -\nabla p + \nabla \cdot (\sigma^v + \sigma^e)
\]

\[
\nabla \cdot v = 0
\]

\[
N = \dot{n} + W \cdot n
\]

\[
\dot{n} = \frac{dn}{dt}
\]

\[
\sigma^v = \alpha_1 n \otimes n(n \cdot A \cdot n) + \alpha_2 n \otimes N + \alpha_3 N \otimes n + \alpha_4 A + \alpha_5 n \otimes (A \cdot n) + \alpha_6 (A \cdot n) \otimes n
\]

\[
A_{ij} = \frac{1}{2} (\partial_i v_j + \partial_j v_i)
\]

\[
W_{ij} = \frac{1}{2} (\partial_i v_j - \partial_j v_i)
\]

coupled equations for director and flow + incompressibility
Solving

- the open-source CFD package OpenFOAM
- augmented for nematodynamics
- material parameters of typical thermotropic liquid crystals (5CB)
- low Re, low Sr (Strouhal, unsteadiness), except transients (important!) in very strong fields
- full solver: time-dependent, with advection
- big discrepancy between time scales of the director and the velocity
- we did not combine transient (director) and stationary (flow) solvers; adaptive time step does a good job (and also captures all transients)
Required electric field strength

- for reverse domain creation, both electric fields must be strong enough

- holds also conversely (due to scalability of the systems with respect to length): given the fields, the domain must be large enough to be switched into the reverse configuration

electric field unit: the coherence length of the unit field equals the relevant system size

(the critical Fredericksz field in the square geometry is $\sqrt{2\pi} \approx 4.44$)
2D random domains

- multiple random Freedericksz domains of irregular shape
- can they be switched? (no boundary, no perfect square …)
- strong fields are required for nice reverse domains
- but strong electric field gives lots of small domains, to small for switching
- therefore one waits for the coarsening dynamics to do the job
- now we have big domains in a strong electric field
- let’s try to switch them!

\[ t = 5 \times 10^{-5} \quad t = 0.0001 \quad t = 0.0005 \]
Switching of the 2D random domains actually works!

(rather surprising!)

Why it works:

- in the domain walls, the director is immobilized by the secondary electric field and the neighbouring domains (replaces the anchoring at the square boundaries)

The kickback amplification takes place in each domain individually, regardless of the irregularity of domain shapes and positions – this is surprisingly robust!
**2D multiple irregular domains are still not realistic:**

- 2D samples are “not common”
- in 3D samples, 2D domains do not exist
- in 3D, the flow changes crucially
3D is trickier than simply 2D+1

- first check a monodomain in a cube
- new: twist domain wall, does not generate backflow
- the $xz$ cross section is similar to the 2D monodomain example
- BUT: the flow is screened due to $y$ gradients
Thus, in-plane switching not useful:

- 2D switching sandwiched between a pair of glass plates at a finite separation (in-plane switching in a LC cell)
- degenerate planar anchoring at the glass plates
- kickback does not work because of the flow screening
- when making the cell slightly thicker to reduce screening, domains are formed along this direction as well (twist – no backflow)

Well, only a slight change in perspective is needed: no one said in-plane geometry was a good idea ...

Make these two boundaries be the glass plates of the LC cell and make them extensive as usual.
Real life: LC cell geometry

- planar or homeotropic cell, both should work

Planar cell:
- primary field: normal to the cell (standard plate electrodes)
- secondary field: in the plane, requires in-plane electrodes
- the coherence length of the fields should be max. 1/30 of the cell thickness

- coalescence of Freedericksz domains before the switching

\[ t = 0.005 \quad t = 0.04 \quad t = 0.1 \]
Real life: amplified kickback switching in the LC cell

- planar

flow streamlines in the domain shrinking stage

multiple domains across cell thickness should also work!

screening again!
Connection with experimental scales

Assuming a LC cell thickness of 20 micron:

- characteristic switching time 5 ms
- max. velocities 35 microns/s
- width of domain walls 0.2 micron (relevant for the anchoring extrapolation length)

Assuming $\Delta \varepsilon \sim 10$, the required electric field strengths $\sim 2$ V/micron

- this is 40 V between the plate electrodes
- 2 kV across 1 mm wide array of in-plane electrodes (should be readily doable)
- the required voltage at the in-plane electrodes scales as $1$/cell thickness
Summary

• a clean monodomain geometry with precisely controlled boundaries is not required
• the kickback amplification and the resulting domain switching is very robust and generic
• works in 3D, i.e., in the real LC cell

The actual key ingredients are:
• sufficiently strong electric fields
• sufficiently big Freedericksz domains (through coalescence)
• near-perfect perpendicularity of the primary and secondary electric fields

• OpenFOAM: in the field of complex fluids, the support of higher rank tensors would be valuable ... (e.g. in nematodynamics, gradient of symmetric (traceless) tensor = 18 (15) components)