A non-isothermal model of liquid crystals

Eduard Feireisl

Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague

joint work with

E. Rocca (Milano), G. Schimperna (Pavia), A. Zarnescu (Oxford)
and
M. Frémond (Rome)

Complex Fluids
Darmstadt, July 10 - 13, 2012

"Standard" Leslie-Ericksen models

Incompressibility - mass conservation

$$\mathrm{div}_x \mathbf{u} = 0$$

Momentum equation

$$\partial_t \mathbf{u} + \mathrm{div}_x (\mathbf{u} \otimes \mathbf{u}) = \mathrm{div}_x \sigma^d + \mathrm{div}_x \sigma^{nd} + \mathbf{g}$$

$$\sigma^d = \frac{\mu}{2}\left(\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} \right) - p\mathbb{I}$$

$$\sigma^{nd} = -\lambda \nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + \lambda \boxed{\left(\mathbf{f}(\mathbf{d}) - \Delta \mathbf{d} \right) \otimes \mathbf{d}}, \ \mathbf{f}(\mathbf{d}) = \partial_{\mathbf{d}} \left(|\mathbf{d}|^2 - 1 \right)^2$$

Director vector evolution

$$\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} - \boxed{\mathbf{d} \cdot \nabla_x \mathbf{u}} = \Gamma \left(\Delta \mathbf{d} - \mathbf{f}(\mathbf{d}) \right)$$

Q-tensor description

Q-tensor

$$\mathbb{Q} = \int_{S^2} \left(\mathbf{s} \otimes \mathbf{s} - \frac{1}{3}\mathbb{I} \right) \mathrm{d}\mu(\mathbf{s})$$

$Q-$tensor is a symmetric traceless matrix with eigenvalues contained in the interval $\left(-\frac{1}{3}, \frac{2}{3}\right)$

Landau-DeGennes free energy

$$\mathcal{F} = \frac{1}{2}|\nabla_x \mathbb{Q}|^2 + \Psi_B(\vartheta, \mathcal{L}(\mathbb{Q})) - \vartheta \log(\vartheta), \ \mathbb{Q} \in R^{3\times 3}_{\rm sym}$$

$\mathcal{L}(\mathbb{Q}) = \mathbb{Q} - \frac{1}{3}\mathrm{tr}(Q)\mathbb{I}$

ϑ-the absolute temperature

$$\Psi_B = f(\mathbb{O}) - U(\vartheta)\mathbb{G}(\mathbb{O}) \text{ for any } \mathbb{O} \in R^{3\times 3}_{\mathrm{sym}}, \ \mathrm{tr}(\mathbb{O}) = 0$$

Ball-Majumdar bulk potential

$$f(\mathbb{O}) = \inf_{p \in \mathcal{A}(\mathbb{O})} \int_{S^2} p(\mathbf{s}) \log p(\mathbf{s}) \, \mathrm{d}s$$

$$\mathcal{A}(\mathbb{O}) = \left\{ p \in L^1(S^2) \mid p \geq 0, \ \int_{S^2} p(\mathbf{s}) \, \mathrm{d}s = 1, \right.$$

$$\left. \mathbb{O} = \int_{S^2} \left(\mathbf{s} \otimes \mathbf{s} - \frac{1}{3}\mathbf{s}\mathbb{I} \right) p(\mathbf{s}) \, \mathrm{d}s \right\}$$

$$f(\mathbb{O}) = \infty \text{ if } \mathcal{A}(\mathbb{O}) = \emptyset$$

Perturbation

$$G(\mathbb{O}) = G(S\mathbb{O}S^t) \text{ for any } S \in SO(3)$$

Basic properties of the bulk potential

Lower semi-continuity

$f : R^{3\times 3}_{\rm sym,0} \to [-K, \infty)$ is convex, lower semi-continuous

Coercivity

$$\mathcal{D}[f] = \left\{ \mathbb{O} \in R^{3\times 3}_{sym,0} \ | \ \lambda_i(\mathbb{O}) \in \left(-\frac{1}{3}, \frac{2}{3} \right), \ i = 1,2,3 \right\}$$

$\mathcal{D}[f]$ is an open convex subset of $R^{3\times 3}_{\rm sym,0}$

Smoothness

f is smooth in $\mathcal{D}[f]$

Evolutionary system

Incompressibility - mass conservation

$$\mathrm{div}_x \mathbf{u} = 0$$

Momentum equation

$$\partial_t \mathbf{u} + \mathrm{div}_x (\mathbf{u} \otimes \mathbf{u}) = \mathrm{div}_x \sigma + \mathbf{g}$$

Q-tensor evolution

$$\partial_t \mathbb{Q} + \mathrm{div}_x (\mathbb{Q}\mathbf{u}) - \mathbb{S}(\nabla_x \mathbf{u}, \mathbb{Q})$$

$$= \Gamma(\vartheta) \left(\Delta \mathbb{Q} - \mathcal{L}\left[\frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} \right] + U(\vartheta) \mathcal{L} \left[\frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}} \right] \right)$$

Energy and entropy

Energy balance

$$\partial_t \left(\frac{1}{2}|\mathbf{u}|^2 + e \right) + \mathrm{div}_x \left((\frac{1}{2}|\mathbf{u}|^2 + e)\mathbf{u} \right) + \mathrm{div}_x \mathbf{q}$$

$$= \mathrm{div}_x(\sigma \mathbf{u})$$

$$+\mathrm{div}_x \left(\Gamma(\vartheta)\nabla_x \mathbb{Q} : \left(\Delta \mathbb{Q} - \mathcal{L}\left[\frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} \right] + U(\vartheta)\mathcal{L}\left[\frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}} \right] \right) \right) + \mathbf{g}\cdot\mathbf{u}.$$

Entropy inequality

$$\partial_t s + \mathrm{div}_x(s\mathbf{u}) - \mathrm{div}_x \left(\frac{\kappa(\vartheta)}{\vartheta} \nabla_x \vartheta \right)$$

$$\geq \frac{1}{\vartheta} \left(\frac{\mu(\vartheta)}{2} \left| \nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} \right|^2 + \Gamma(\vartheta) \left| \mathbb{H} \right|^2 + \frac{\kappa(\vartheta)}{\vartheta} |\nabla_x \vartheta|^2 \right).$$

Constitutive relations

Cauchy stress

$$\sigma = \sigma^d + \sigma^{nd}$$

$$\sigma^d = \frac{\mu(\vartheta)}{2}\left(\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u}\right) - p\mathbb{I}$$

$$\sigma^{nd} = \mathbb{Q}\mathbb{H} - \mathbb{H}\mathbb{Q} - (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q})$$

$$+2\xi\,[\mathbb{H} : \mathbb{Q}]\left(\mathbb{Q} + \frac{1}{3}\mathbb{I}\right) - \xi\left[\mathbb{H}\left(\mathbb{Q} + \frac{1}{3}\mathbb{I}\right) + \left(\mathbb{Q} + \frac{1}{3}\mathbb{I}\right)\mathbb{H}\right]$$

$$\mathbb{H} \equiv \Delta\mathbb{Q} - \mathcal{L}\left[\frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}}\right] + U(\vartheta)\mathcal{L}\left[\frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}}\right]$$

Q-tensor transport

Material derivative

$$\frac{D\mathbb{Q}}{Dt} \equiv \partial_t \mathbb{Q} + \mathbf{u} \cdot \nabla_x \mathbb{Q} - \mathbb{S}(\nabla_x \mathbf{u}, \mathbb{Q})$$

$$\mathbb{S}(\nabla_x \mathbf{u}, \mathbb{Q}) = (\xi \varepsilon(\mathbf{u}) + \omega(\mathbf{u})) \left(\mathbb{Q} + \frac{1}{3}\mathbb{I} \right)$$

$$+ \left(\mathbb{Q} + \frac{1}{3}\mathbb{I} \right) (\xi \varepsilon(\mathbf{u}) - \omega(\mathbf{u})) - 2\xi \left(\mathbb{Q} + \frac{1}{3}\mathbb{I} \right) (\mathbb{Q} : \nabla_x \mathbf{u})$$

$$\varepsilon(\mathbf{u}) \equiv \frac{1}{2} \left(\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} \right), \ \omega(\mathbf{u}) \equiv \frac{1}{2} \left(\nabla_x \mathbf{u} - \nabla_x^t \mathbf{u} \right)$$

ξ a scalar parameter

Internal energy flux

Energy flux

$$\mathbf{q} = \mathbf{q}^d + \mathbf{q}^{nd}$$

Fourier law

$$\mathbf{q}^d = -\kappa(\vartheta)\nabla_x \vartheta$$

$$\mathbf{q}^{\rm nd} = -\nabla_x \mathbb{Q} : \mathbb{S}(\nabla_x \mathbf{u}, \mathbb{Q})$$

Internal energy and entropy

$$e = \frac{1}{2}|\nabla_x \mathbb{Q}|^2 + f(\mathbb{Q}) - \Big(U(\vartheta) - \vartheta U'(\vartheta) \Big) G(\mathbb{Q}) + \vartheta$$

$$s = 1 + \log(\vartheta) + U'(\vartheta) G(\mathbb{Q})$$

A priori bounds

Energy bounds

$$\mathbf{u} \in L^\infty(0,T;L^2(\Omega;R^3))$$

$$f(\mathbb{Q}) \in L^\infty(0,T;L^1(\Omega))$$

in particular

$$\mathbb{Q} \in L^\infty((0,T)\times\Omega;R^3_{\rm sym,0}),\ \nabla_x\mathbb{Q} \in L^\infty(0,T;L^2(\Omega;R^{27}))$$

and

$$\vartheta \in L^\infty(0,T;L^1(\Omega)),$$

Entropy bound

$$\log(\vartheta) \in L^\infty(0,T;L^1(\Omega)) \cap L^2(0,T;W^{1,2}(\Omega))$$

Dissipation

$$\nabla_x \mathbf{u} \in L^2((0,T)\times\Omega;R^3),\ \mathbb{Q} \in L^2(0,T;W^{2,2}(\Omega;R^{3\times 3}_{\mathrm{sym},0}))$$

$$\mathcal{L}\left[\frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}}\right] \in L^2(0,T;L^2(\Omega;R^{3\times 3}_{\mathrm{sym},0}))$$

Temperature gradient

$$\nabla_x (1+\vartheta)^{\frac{1-\alpha}{2}} \in L^2((0,T)\times\Omega;R^3) \text{ for any } \alpha > 0$$

Pressure

$$p \in L^{5/3}((0,T)\times\Omega)$$

Main result

Initial data

$$\mathbf{u}_0 \in L^2(\Omega; R^3), \ \mathrm{div}_x \mathbf{u}_0 = 0$$

$$\left\{ \begin{array}{c} \mathbb{Q}_0 \in W^{1,2}(\Omega; R^{3\times 3}_{\mathrm{sym},0}), \\ \\ f(\mathbb{Q}_0) \in L^1(\Omega) \end{array} \right\}$$

$$\vartheta_0 \in L^\infty(\Omega), \ \mathrm{ess} \inf_\Omega \vartheta_0 = \underline{\vartheta} > 0$$

Function U

$$U \in C^0[0,+\infty) \cap C^2(0,+\infty), \ \ U(0) > 0, \ \ U' \leq 0$$

$$U \text{ convex in } [0,\infty), \ \ \limsup_{\vartheta \to \infty} U''(\vartheta)\vartheta^{3/2} < +\infty$$

Transport coefficients

$$\mu, \ \kappa, \ \Gamma \in C^2[0,\infty), \ \left\{ \begin{array}{c} 0 < \underline{\mu} \leq \mu(\vartheta) \leq \overline{\vartheta}, \\ \\ 0 < \underline{\kappa} \leq \kappa(\vartheta) \leq \overline{\kappa}, \\ \\ 0 < \underline{\Gamma} \leq \Gamma(\vartheta) \leq \overline{\Gamma} \end{array} \right\} \text{ for all } \vartheta \geq 0$$

Conclusion: Global existence

Global-in-time weak solutions for large data

The problem possesses at least one weak solution provided Ω is a periodic box and

$$\mathbf{g} \in L^\infty(0, T; L^2(\Omega; R^3))$$

Proof strategy

Difficulties

- Explicit presence of the pressure in the energy equation
- Highly non-linear parabolic system
- *A priori estimates* based on coercivity of the singular potential not available at the first level of approximation

- Faedo-Galerkin approximation
- Smoothing and cutting the singular potential
- Artificial viscosity of "power law" type
- Regularizing of non-smooth quanitities by convolution kernels