Two-phase flow diffuse interface models for dynamic electrowetting

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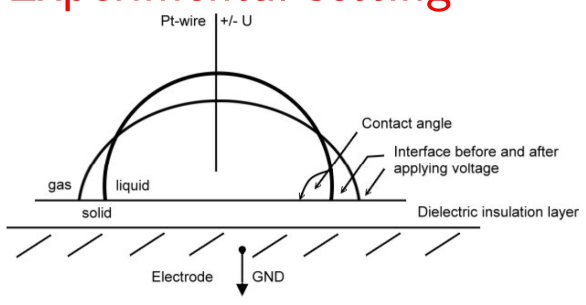
Experimental setting



Classical Lippmann formula (under scrutiny):
$\cos\Theta(V) = \cos\Theta(0) + \frac{\varepsilon_0\varepsilon}{2d\gamma}V^2$

- $\Theta(0)$ Young's contact angle,
- V voltage, ϵ_0, ϵ dielectric permittivities
- d thickness of the dielectric layer
- γ surface tension coefficient

General assumption: mass density of the two liquids identical!

Case 1: Conductive liquid surrounded by nonconductive ambient liquid

Model equations

$$\begin{aligned}
\mathbf{v}_t + (\mathbf{v}\cdot\nabla)\mathbf{v} - \nabla\cdot(\eta(\phi)\mathbf{T}(\mathbf{v})) + \nabla p - \mu\nabla\phi + \rho\nabla V &= 0 \quad \text{in } \Omega_T,\\
\nabla\cdot\mathbf{v} &= 0 \quad \text{in } \Omega_T,\\
\rho_t + \mathbf{v}\cdot\nabla\rho - \nabla\cdot(K(\phi)\nabla(V+\lambda\rho)) &= q \quad \text{in } \Omega_T,\\
\phi_t + \mathbf{v}\cdot\nabla\phi - \nabla\cdot(M(\phi)\nabla\mu) &= 0 \quad \text{in } \Omega_T,\\
-\nabla\cdot(\bar\varepsilon[\phi]\nabla V) &= \rho \quad \text{in } \Omega^* \quad \forall t\in(0,T).
\end{aligned} \tag{1}$$

with symmetric strain tensor and chemical potential

$$\begin{aligned}
\mathbf{T}(\mathbf{v}) &= \tfrac12\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^t\right),\\
\mu &= \gamma_0\left(-\delta\Delta\phi + \tfrac1\delta W'(\phi)\right) - \tfrac12\varepsilon'(\phi)\,|\nabla V|^2.
\end{aligned} \tag{2}$$

Formal energy estimate

$$\begin{aligned}
&\|\rho\|_{L^\infty(I;L^2(\Omega))} + \|\phi\|_{L^\infty(I;H^1(\Omega))} + \|W(\phi)\|_{L^\infty(I;L^1(\Omega))} + \|V\|_{L^\infty(I;H^1(\Omega^*))} + \|\mathbf{v}\|_{L^\infty(I;L^2(\Omega))}\\
&\quad + \|\mathbf{v}\|_{L^2(I;H^1(\Omega))} + \left\|K(\phi)^{1/2}\nabla\rho\right\|_{L^2(\Omega_T)} + \|\nabla\mu\|_{L^2(\Omega_T)} + \|\phi_t\|_{L^2(\partial\Omega\times I)} \le C
\end{aligned} \tag{3}$$

Case 2: Electrowetting with electrolyte solutions

Model equations

$$\begin{aligned}
\mathbf{v}_t + (\mathbf{v}\cdot\nabla)\mathbf{v} - \nabla\cdot(\eta(\phi)\mathbf{T}(\mathbf{v})) + \nabla p &= \mu\nabla\phi - (\rho_1-\rho_2)\nabla V \ \text{ in } \Omega_T,\\
\nabla\cdot\mathbf{v} &= 0 \text{ in } \Omega_T,\\
\tfrac{D}{Dt}\rho_0 - \nabla\cdot(K(\phi)\nabla\rho_0) &= R(\rho_1,\rho_2,\rho_0,\phi) \text{ in } \Omega_T,\\
\tfrac{D}{Dt}\rho_i - \nabla\cdot(K(\phi)\rho_i^+\nabla((-1)^{i+1}V + \log\rho_i)) &= -R(\rho_1,\rho_2,\rho_0,\phi) \ \text{ in } \Omega_T \text{ for } i\in\{1,2\},\\
\tfrac{D}{Dt}\phi - \nabla\cdot(M(\phi)\nabla\mu) &= 0 \ \text{ in } \Omega_T,\\
-\nabla\cdot(\bar\varepsilon[\phi]\nabla V) &= \rho_1-\rho_2 \ \text{ in } \Omega^* \text{ for all } t\in(0,T)
\end{aligned} \tag{4}$$

with no-slip boundary conditions for $\mathbf{v}$, Dirichlet b.c. for V, no-flux b.c. for the transported quantities and the additional non-standard b.c. for the phase-field

$$|\nabla\phi|^{s-2}\nabla\phi\cdot\mathbf{n} = -\gamma'_{fs}(\phi) - \alpha\phi_t \tag{5}$$

on $\partial\Omega\times(0,T)$. Here, $R(\rho_1,\rho_2,\rho_0,\phi)$ is an appropriate recombination term, e.g. $R(\rho_1,\rho_2,\rho_0,\phi) = K_1(\phi)\rho_1\rho_2 - K_0(\phi)\rho_0^\alpha$.

Formal energy estimate

$$\begin{aligned}
&\text{ess sup}_{t\in(0,T)}\left[\int_\Omega\left(\tfrac12|\mathbf{v}|^2 + \rho_1\log\rho_1 + \rho_2\log\rho_2 + \tfrac1s|\nabla\phi|^s + W(\phi)\right) + \int_{\partial\Omega}\gamma_{fs}(\phi) + \int_{\Omega^*}\tfrac12\bar\varepsilon[\phi]\,|\nabla V|^2\right](t)\\
&+\int_{\Omega_T}\left[\eta(\phi)\,|\mathbf{T}(\mathbf{v})|^2 + K(\phi)\,\rho_1\,|\nabla[V+\log\rho_1]|^2 + K(\phi)\,\rho_2\,|\nabla[-V+\log\rho_2]|^2 + M(\phi)\,|\nabla\mu|^2\right]\\
&\quad+\int_{\partial\Omega_T}\alpha\,|\phi_t|^2 + \int_{[\rho_1\ge1]}K_1(\phi)\rho_1^+\rho_2^+\log\rho_1 + \int_{[\rho_2\ge1]}K_1(\phi)\rho_1^+\rho_2^+\log\rho_2\\
&\qquad-\int_{[0<\rho_1<1]}K_0(\phi)\,(\rho_0)^\alpha\log\rho_1 - \int_{[0<\rho_2<1]}K_0(\phi)\,(\rho_0)^\alpha\log\rho_2\\
&\qquad\quad\le const.\text{(initial and boundary data)}
\end{aligned} \tag{6}$$

Sketch of model derivation

- total energy $\mathcal{E}$ = (kinetic + distributional + interfacial + adsorption + electrostatic) energy (cf. (3) and (6)),
- take general evolution equations as ansatz functions for ϕ, ρ etc, e.g. $\frac{D}{Dt}\phi + \nabla\cdot\mathbf{J}_\phi = 0$,
- consider dissipation functionals of the type

$$\Phi(\mathbf{J},\mathbf{J}) = \int_\Omega\frac{|\mathbf{J}_\phi|^2}{2M(\phi)} + \int_\Omega\frac{|\mathbf{J_D}|^2}{2K(\phi)} + \int_\Omega\frac{|\Pi|^2}{2\eta(\phi)} + \int_\Gamma\frac{\alpha}{2}\dot\phi^2 + \int_\Gamma\frac{\beta}{2}|\mathbf{v}_\tau|^2,$$

- apply Onsager's variational principle $\delta_{\mathbf{J}}(\dot{\mathcal{E}}(\mathbf{J}) + \Phi(\mathbf{J},\mathbf{J})) = 0$ to determine the unknown fluxes,
- use zero increase rate of total mechanical work to determine the force density in the hydrodynamic equation,
- inspired by the methods of [4] for pure two-phase flow with wall effects.

Model features

A nonstandard boundary condition for the phase-field – consequences on contact angles

- boundary condition $\gamma_0\delta\frac{\partial}{\partial\mathbf{n}}\phi = -\gamma'_{fs}(\phi) - \alpha\phi_t$ entails for equilibrium contact angles ($\dot\phi = 0$) in first approximation (assuming ϕ to be linear inside the interface)

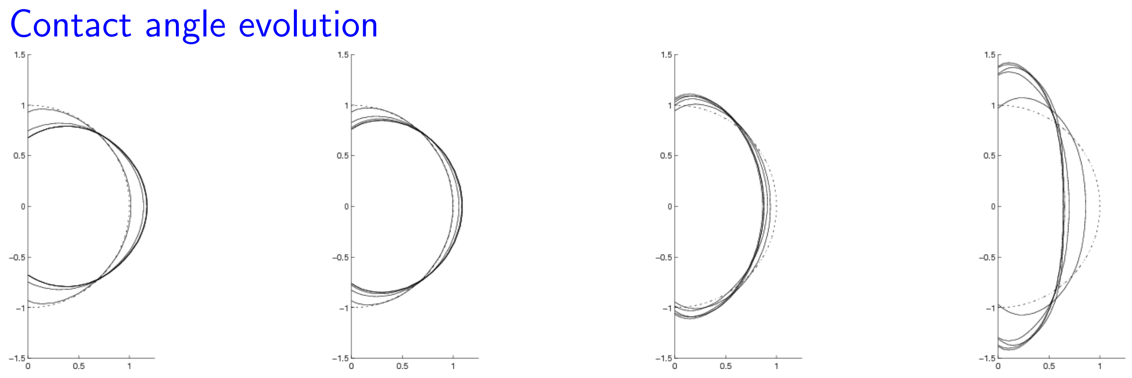
$$\cos\Theta_{static} = \frac{\gamma_{fs}(-1) - \gamma_{fs}(+1)}{\gamma_0}$$

  which is Young's law. HENCE: LIPPMANN FORMULA CAN HOLD AT MOST MACROSCOPICALLY! (see also [3] for another approach in the stationary case)

- taking a contact line movement to the left into account yields $\cos\Theta_{advancing} = \cos\Theta_{static} - \frac{\alpha}{\gamma_0}\int\dot\phi\phi_\tau < \cos\Theta_{static}$, hence contact angle hysteresis $\Theta_{advancing} > \Theta_{static}$ included in the model.

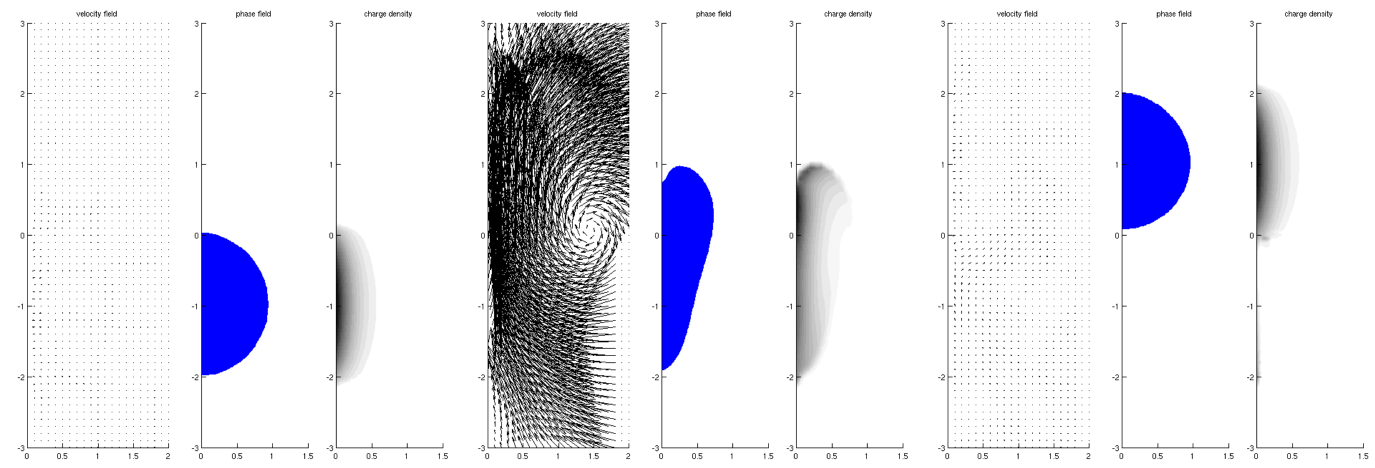
Numerical Simulations (Fabian Klingbeil)

Contact angle evolution



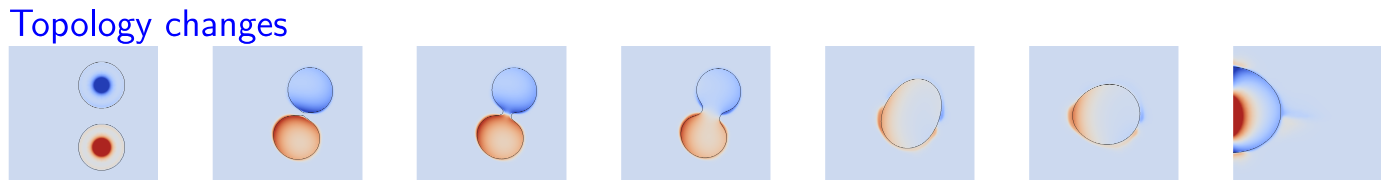
Charged droplet on a surface ($\Delta\gamma_{fs} = \gamma_0$, $\Theta(0) = \frac{2\pi}{3}$). The plots show the zero-level of ϕ at times $t = 0$ (dashed), 0.001, 0.0025, 0.005, 0.0075, 0.01. Each plot shows a different choice of $\rho_0 = 0$, 200, 400, 600 (from left to right). Here, ρ_0 is the total charge inside the drop. Note also the temporary increase in the microscopic contact angle.

Droplet motion



Snapshots of a charged droplet set in motion by switching-off/switching-on of two different electrodes. Depicted are velocity field, phase field and charge density

Topology changes



Two non-equally charged droplets (red: positive charge, dark blue: negative charge) are attracting each other – on the left, a negative electrode is switched on additionally – droplets merge and move towards the electrode

Mathematical analysis

Model (1) – see [1]

- 2D case: global existence of weak solutions for degenerate and for non-degenerate mobilities $K(\phi)$,
- 3D case: global existence in the degenerate case only under the additional assumption $\bar\varepsilon$ independent of ϕ.

Model (4) – see [2]

- 3D case: global existence established without further side conditions,
- species densities ρ_0, ρ_1, ρ_2 globally non-negative,
- novel iteration method suggested to establish $L^\infty(L^2)\cap L^2(H^1)$ regularity for the species densities.

References

[1] C. Eck, M. A. Fontelos, G. Grün, F. Klingbeil, and O. Vantzos. On a phase-field model for electrowetting. *Interfaces and Free Boundaries*, 11:259–290, 2009.

[2] M. A. Fontelos, G. Grün, and S. Jörres. On a phase-field model for electrowetting and other electrokinetic phenomena, Preprint 329, University of Erlangen-Nuremberg, Institute of Applied Mathematics, 2009, submitted for publication.

[3] F. Mugele and J. Bührle. Equilibrium drop surface profiles in electric fields. *Journal of Physics: Condensed Matter*, 19:375112 (20pp), 2007.

[4] Qian, T., Wang, X.P., and Sheng, P. A variational approach to moving contact line hydrodynamics, *J.Fluid Mech.*, 564:333–360, 2006.