Modeling and simulation of moving contact line problem for two-phase complex fluids flow

Zhang Zhen

Southern University of Science and Technology (SUSTech)

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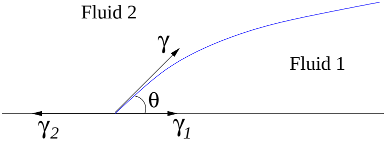
Outline

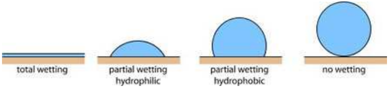
1. Backgroung
2. Moving contact lines in polymeric fluids (with W. Ren)
3. Asymptotic analysis in MCL (with W. Ren)
4. Thin-film Movement on Heterogeneous Surface
5. Concluding remarks and future work

Contact Lines (CL)

- Two immiscible fluids
- contact line: intersection of the interface and the solid

- Equilibrium, Young's equation (Young, 1805): $\gamma \cos\theta_Y = \gamma_2 - \gamma_1$





Non-integrable Singularity and Remedies

Non-integrable singularity at MCL for corner flows with no slip boundary condition (Huh and Scriven, 71; Dussan and Davis, 74):

$$F_{shear} = \int_{r=0}^{R} \mathbf{t} \cdot \tau_d(r) \cdot \mathbf{n} \mathrm{d}r \sim \int_{r=0}^{R} \eta \frac{U}{r} \mathrm{d}r = \infty$$

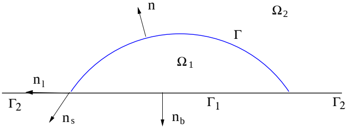
Remedies:

- Introduce slip $\mathbf{u}_s$: $\frac{\partial \mathbf{u}_s}{\partial \mathbf{n}} = -\beta \mathbf{u}_s, \quad \beta > 0$
- Alter the equivalent slip length scale (Ruckenstein and Dunn, 77; Huh and Mason, 77; Hocking and Rivers, 82; Zhou and Sheng, 90; ...)
- Molecular dynamics (Koplik et al, 88; De Coninck and Blake, 08; ...)
- Kinetic models (Blake and Haynes, 69; Blake, 93; ...)
- Diffuse interface models (Jacqmin, 00; Qian, Wang and Sheng, 03; Yue, Zhou, and Feng, 10; ...)
- Sharp interface models with contact angle conditions (Eggers and Stone, 04; Ren, Hu and E, 10; ...)
- ......

Energy Dissipations for a Sharp Interface Model

Total free energy:

$$F = \sum_{i=1,2} \int_{\Omega_i} \frac{1}{2}\rho_i |\mathbf{u}|^2 \,\mathrm{d}\mathbf{x} + (\gamma_1 - \gamma_2)|\Gamma_1| + \int_{\Gamma(t)} e(c)\,\mathrm{d}A$$



$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\sum_{i=1,2} \int_{\Omega_i} \eta_i |\nabla \mathbf{u}|^2 \,\mathrm{d}\mathbf{x}, \text{(Bulk viscous dissipation)}$$

$$+ \sum_{i=1,2} \int_{\Gamma_i} \mathcal{P}\left(\tau_d \cdot \mathbf{n}_b\right) \cdot \mathbf{u}_s \,\mathrm{d}A, \text{(Dissipation on solid surface)}$$

$$+ \int_{\Gamma(t)} \mathbf{u} \cdot \left\{ [\tau_d - p\mathbf{I}] \cdot \mathbf{n} + \gamma(c)\kappa \mathbf{n} - \nabla_s \gamma(c) \right\} \mathrm{d}A, \text{(Interfacial dissipation)}$$

$$+ \int_{\Gamma(t)} e''(c) \nabla_s c \cdot \mathbf{J}_c \,\mathrm{d}A, \text{(Surfactant diffusion dissipation)}$$

$$+ \int_{\Lambda} u_{CL} \left\{ \gamma(c) \cos\theta_d + (\gamma_1 - \gamma_2) \right\} \mathrm{d}l. \text{(Dissipation on contact line)}$$

Constitutive Relations

- Interface jump condition:

$$[\tau_d - p\mathbf{I}] \cdot \mathbf{n} = -\gamma(c)\kappa\mathbf{n} + \underbrace{\nabla_s\gamma(c)}_{\text{Marangoni force}} \quad ,$$

- Boundary conditions:

$$\mathcal{P}\left(\tau_d \cdot \mathbf{n}_b\right) = \mathbf{f}_i(\mathbf{u}_s), \quad \text{on } \Gamma_i, \quad (\mathbf{v} \cdot \mathbf{f}_i(\mathbf{v}) \leqslant 0)$$

$$\gamma(c)\cos\theta_d + (\gamma_1 - \gamma_2) = f_{CL}(u_{CL}), \quad \text{on } \Lambda, \quad (vf_{CL}(v) \leqslant 0)$$

$$e''(c)\nabla_s c \cdot \mathbf{J}_c \leqslant 0 \Rightarrow \text{Fick's law: } \mathbf{J}_c = -D\nabla_s c$$

- Linearization:

$$\mathbf{f}_i(\mathbf{u}_s) = -\beta_i\mathbf{u}_s \quad \Rightarrow \quad \text{Navier slip BC}$$

$$f_{CL}(u_{CL}) = -\beta_{CL}u_{CL} \quad \Rightarrow \quad \text{Contact angle dynamics}$$

Dimensionless Equations

$$\rho_i \left(\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \frac{1}{Re}\nabla\cdot\tau_d, \qquad \text{in } \Omega_i,$$

$$\nabla\cdot\mathbf{u} = 0, \qquad \text{in } \Omega_i,$$

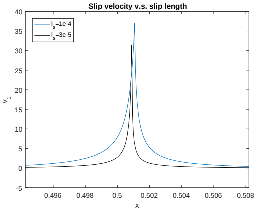
$$We\left[\frac{1}{Re}\tau_d - p\mathbf{I}\right]\cdot\mathbf{n} = -\gamma\kappa\mathbf{n}, \qquad \text{on } \Gamma(t),$$

$$-\beta_i \mathbf{u}_s = \eta_i l_s \partial_n \mathbf{u}_s, \qquad \text{on } \Gamma_i,$$

$$\mathbf{u}\cdot\mathbf{n}_b = 0, \qquad \text{on } \Gamma_i,$$

$$-\beta_{CL} u_{CL} = \frac{1}{Ca}\left(\gamma\cos\theta_d + (\gamma_1 - \gamma_2)\right), \qquad \text{on } \Lambda,$$

$$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t). \qquad \text{(kinematic condition)}$$



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Motivation and Related work

Experimental study:

- Change the effective viscosity (Min et al, J. Colloid Interface Sci., 2011)
- Bring in fluid memory effect (Ramé et al, Phys. Rev. E, 2004, Wei et al, J. Phys.: Condens. Matter, 2009)
- Bergeron et al (Nature, 2000) observed slow retraction during drop impact, energy dissipation by stretching of polymer near MCL
- Smith and Bertola (PRL, 2010) attributed the retraction to the deposition of polymer on the solid surface
- ...

Numerical study:

- Spaid and Homsy (J. Non-Newtonian Fluid Mech., 1994), spin coating
- Yue and Feng (J. Non-Newton. Fluid Mech., 2012), phase-field, Oldroyd-B, viscous bending
- ...

Models for Polymeric Fluids

Modify Navier-Stokes equation through stress tensor:

$$\mathbf{T} = \tau_d + \tau_p$$

where τ_p is the stress tensor due to the interaction between the polymer molecules and the fluids.

Some empirical constitutive relations for τ_p:

1. Generalized Newtonian models:

$$\tau_p = \eta(\mathbf{D})\mathbf{D}$$

2. Maxwell models (for visco-elastic fluids):

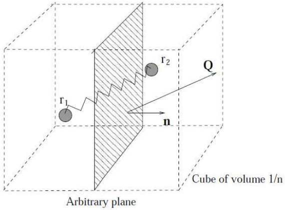
$$\tau_p(\mathbf{x}, t) = \int_{-\infty}^{t} \frac{\eta_s}{\lambda} e^{-\frac{t-s}{\lambda}} \mathbf{D}(\mathbf{x}, s)\mathrm{d}s$$

where $\frac{\eta_s}{\lambda} e^{-\frac{t-s}{\lambda}}$ is the relaxation modulus representing the memory effect.

Macro-micro Models

Dumbbell model in the dilute limit of polymer solutions

$$\tau_p = \frac{\eta_p}{Wi} < \mathbf{F}(\mathbf{Q}) \otimes \mathbf{Q} >$$
$$= \int_{\mathbb{R}^3} \mathbf{F}(\mathbf{Q}) \otimes \mathbf{Q}\psi(\mathbf{x}, \mathbf{Q}, t)\mathrm{d}\mathbf{Q}$$
$$\frac{\partial \mathbf{Q}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{Q}$$
$$= \nabla \mathbf{u} \cdot \mathbf{Q} - \frac{1}{2Wi}\mathbf{F}(\mathbf{Q}) + \frac{1}{\sqrt{Wi}}\dot{\mathbf{W}}(t)$$

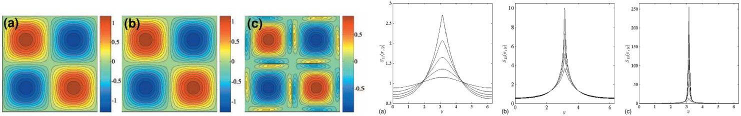


- Hookean spring: $\mathbf{F} = H\mathbf{Q}$, Oldroyd-B model (Bird et al, "Dynamics of Polymeric Fluids", 1987);
- FENE (Finitely Extensible Nonlinear Elastic) spring: $\mathbf{F} = \frac{H\mathbf{Q}}{1-(|\mathbf{Q}|/Q_0)^2}$, need closure approximation:
  - FENE-P (Keunings, J. Non-Newton Fluid Mech., 1997)
  - FENE-L (Lielens et al, J. Non-Newton Fluid Mech., 1999)
  - FENE-S (Du et al, Multiscale Model. Simul., 2005), etc.

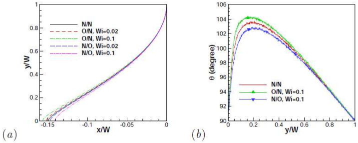
Oldroyd-B Model

$$\frac{\partial \tau_p}{\partial t} + \mathbf{u} \cdot \nabla \tau_p - (\nabla \mathbf{u})\tau_p - \tau_p(\nabla \mathbf{u})^\top + \frac{1}{Wi}\eta_p = \frac{\eta}{Wi}\mathbf{D}$$

- Singular structures for large *Wi* at the region with large deformation (Thomases and Shelley, Phys. Fluids, 2007);



- Bending effect of the two-phase interface near the contact line, (Yue and Feng, J. Non-Newton. Fluid Mech., 2012).



MCL coupled with FENE-P model

Immersed boundary formulation:

$$
\begin{aligned}
&\rho\left(\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \frac{1}{Re}(\eta\nabla^2\mathbf{u} + \nabla\cdot\tau_p) + \frac{1}{We}\mathbf{f},\\
&\nabla\cdot\mathbf{u} = 0,\\
&\mathbf{f}(\mathbf{x},t) = \int_D \mathbf{F}(s,t)\delta(\mathbf{x}-\mathbf{X}(s,t))\mathrm{d}s\\
&\mathbf{F}(s,t) = \frac{\partial(\gamma\mathbf{t}(s,t))}{\partial s} = \gamma\kappa(s,t)\mathbf{n}(s,t)|\partial_s\mathbf{X}(s,t)|\\
&\frac{\partial\mathbf{X}(s,t)}{\partial t} = \mathbf{U}(s,t) = \int_\Omega \mathbf{u}(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X}(s,t))\mathrm{d}\mathbf{x}
\end{aligned}
$$

with FENE-P model:

$$
\begin{aligned}
&\tau_p = \frac{\eta_p}{Wi}\left(\frac{1}{1-\mathrm{tr}\mathbf{A}/E_d}\mathbf{A} - \frac{1}{1-2/Q_0^2}\mathbf{I}\right),\\
&\frac{\partial\mathbf{A}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{A} - (\nabla\mathbf{u})\mathbf{A} - \mathbf{A}(\nabla\mathbf{u})^\top = \frac{1}{Wi}\left(\frac{1}{1-2/Q_0^2}\mathbf{I} - \frac{1}{1-\mathrm{tr}\mathbf{A}/Q_0^2}\mathbf{A}\right)
\end{aligned}
$$

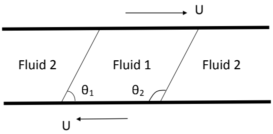
Wi: Weissenberg number, control relaxation time

η_p: polymer viscosity

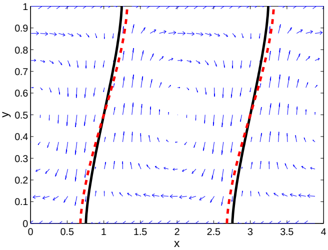
Numerical methods (Staggered Grid)

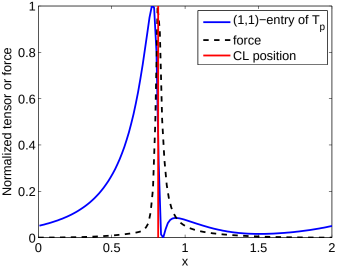
1. Interpolation of velocity: $\mathbf{U}_k^n = \sum_{\mathbf{x}} \mathbf{u}^n \delta_h(\mathbf{x} - \mathbf{X}_k^n)\Delta x \Delta y$
2. Update markers: $\mathbf{X}_k^{n+1} = \mathbf{X}_k^n + \Delta t \mathbf{U}_k^n$; contact line markers: $-\beta_{CL}\frac{\mathbf{X}_k^{n+1}-\mathbf{X}_k^n}{\Delta t} = \frac{1}{Ca}\big(\gamma \cos\theta_d^n + (\gamma_1 - \gamma_2)\big)$ with $k = 0, M$.
3. Equal-arclength redistribution of the interface markers;
4. Upper convective equation for $\mathbf{A}^{n+1}$: forward Euler in time, 3rd order WENO scheme in space (Jiang and Shu, J. Comput. Phys., 1996).
5. Spread the force: $\mathbf{f}^{n+1}(\mathbf{x}) = \sum_{k=1}^{M-1} \mathbf{F}_k^{n+1}\delta_h(\mathbf{x} - \mathbf{X}_k^{n+1})$ and $\mathbf{F}_k^{n+1} = \gamma(\mathbf{t}_{k+1}^{n+1} - \mathbf{t}_k^{n+1})$, with discrete delta δ_h (Peskin, 2002)
6. Projection method (Guermond et al, 2006) for Navier-Stokes

Two-phase Couette flow (static contact angle 90°)



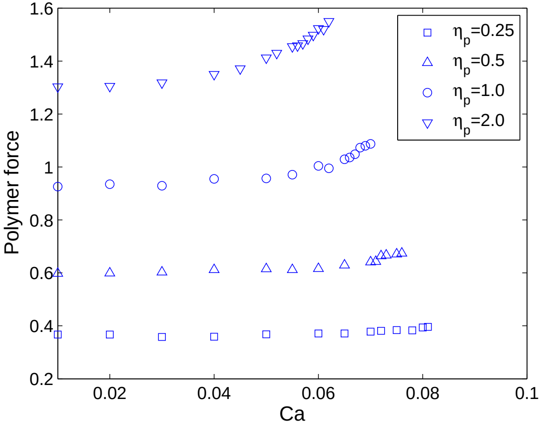
- Newtonian fluid interface (black), polymeric fluid (red) ($Ca = 0.07$, $Wi = 0.1$, $\eta_p = 0.5$);
- The polymer stress and force exert locally near the contact line.



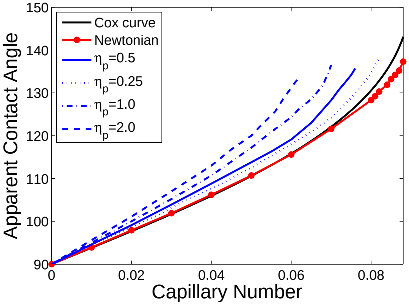


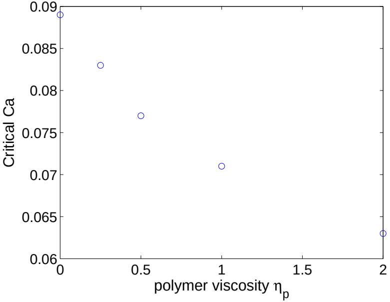
Capillary Force vs. Polymer Force

- $Ca \nearrow$, capillary force $\searrow$, polymer force $\nearrow$
- More evident for large η_p near critical Ca



Apparent Contact Angle vs. Capillary Number





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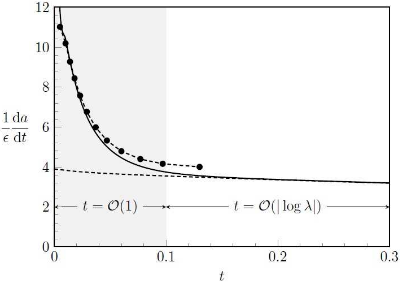
Slip Model

- No-slip model: $\frac{1}{r}$ singularity in both p and τ_d, no convergent numerical results (Moriarty and Schwartz, 1992)
- Quisi-static ($t \to \infty$) asymptotics, Hocking and Rivers 1982, Hocking 1983, Cox 1986, Sibley et al. 2015, ...
- $t = O(1)$, lubrication modell, effective macroscopic model as $l_s \to 0$, numerically consistent with full slip model (Ren, Trinh and E, 15)

1. $\theta_a^3(t) - \theta_Y^3 \sim 3\epsilon^{-1}\frac{\mathrm{d}a}{\mathrm{d}t}$, when $\epsilon = 1/|\ln l_s| \to 0$, $t = O(1)$;
2. $\theta_a^3(a(t)) - \theta_Y^3 \sim 3\epsilon^{-1}\frac{\mathrm{d}a}{\mathrm{d}t}$, when $\epsilon = 1/|\ln l_s| \to 0$, $t = O(\epsilon^{-1})$.

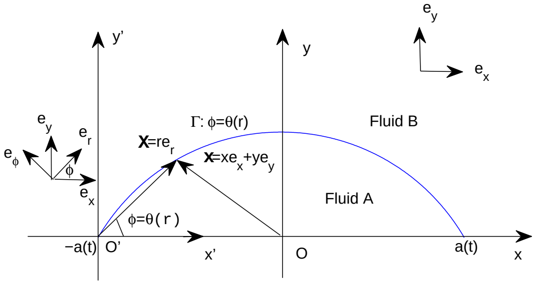


Polar representation of CL model with Stokes flow

Finite time: $t = O(1)$, $Ca = \frac{\mu_A U_{bulk}}{\gamma} = O(1)$, $\eta = \mu_B/\mu_A$

$$\begin{cases} \nabla^4 \psi^i = 0, & \mathbf{u}^i = \nabla^\perp \psi^i = \dfrac{1}{r}\dfrac{\partial \psi^i}{\partial \phi}\mathbf{e}_r - \dfrac{\partial \psi^i}{\partial r}\mathbf{e}_\phi, \\ Ca\mu_i \nabla^\perp \nabla^2 \psi^i = \nabla p^i & i = A, B \end{cases}$$

CL locates at $x = -a(t)$, $u_{CL} = a'(t)$ is the contact line speed



Small Parameter Limit

- Small slip length $l_s \to 0$
- Small contact line speed $a'(t) \sim \epsilon \to 0$
- Relation: $\epsilon = \frac{1}{|\log l_s|}$,as $l_s \to 0$, $\epsilon \gg l_s$
- Asymptotic expansion:

$$\begin{aligned} a(t) &= a_0 + \epsilon a_1(t) + \epsilon^2 a_2(t) + O(\epsilon^3) \\ \psi^i &= \psi_0^i + \epsilon\psi_1^i + O(\epsilon^2, l_s) \\ p^i &= p_0^i + \epsilon p_1^i + O(\epsilon^2, l_s) \\ \theta &= \theta_0 + \epsilon\theta_1 + O(\epsilon^2, l_s) \end{aligned}$$

Outer Solutions

- The correct order of behavior near CL:

$$\kappa_0 \sim \frac{\partial \theta_0}{\partial r} \sim \ln r, \qquad p_0 \sim \ln r, \qquad \psi_0 \sim r^2$$

- Find the solution ψ_0 in the form of separate variable $r^2 Q(\phi)$, leading order solutions close to CL:

$$\theta_0(r,t) \sim \theta_a(t) + \alpha_{0,1}(t) r \ln r.$$

- First order solutions close to CL:

$$\theta_1(r,t) \sim \alpha_{1,0}(t) \ln r.$$

where $\alpha_{1,0}(t) = a_1'(t) CaF(\theta_a, \eta)$, and

$$F(\theta,\eta) = \frac{2\sin\theta[\eta^2(\theta^2 - \sin^2\theta) + 2\eta(\theta(\pi-\theta) + \sin^2\theta) + ((\pi-\theta)^2 - \sin^2\theta)]}{\eta(\theta^2 - \sin^2\theta)((\pi-\theta) + \sin\theta\cos\theta) + ((\pi-\theta)^2 - \sin^2\theta)(\theta - \sin\theta\cos\theta)}$$

Three-region Expansion and Matching

- Two-term outer expansion:

$$\theta_{out} = \Big(\theta_a + \alpha_{0,1} r \ln r + O(r)\Big) + \epsilon\Big(a_1'(t) CaF(\theta_a, \eta) \ln r + O(1)\Big) + O(\epsilon^2, l_s), \quad r \to 0.$$

- Inner variables: $\tilde{r} = \frac{r}{l_s}$, two-term expansion far from CL ($\tilde{r} \to \infty$):

$$\theta_{in} = \theta_Y + \epsilon\Big(a_1'(t) CaF(\theta_Y, \eta) \ln \tilde{r} + O(1)\Big) + O(\epsilon^2, l_s), \quad \tilde{r} \to \infty.$$

- Intermediate variable: $z = \epsilon \ln \tilde{r} = \epsilon \ln r + 1$, two-term expansion:

$$\theta_{int} = G^{-1}(K_0 + a_1'(t) Caz) + O(\epsilon, l_s)$$

where $G(\theta, \eta) = \int_0^\theta \frac{\mathrm{d}\phi}{F(\phi, \eta)}$

- $G(\theta_a(t)) - G(\theta_Y) \sim \epsilon^{-1} a'(t) Ca$

Quasi-static State

- $t \to \infty$ and $\lambda, \epsilon \to 0$
- Time rescaling: $t = O(\frac{1}{\epsilon})$ and $\tau = \epsilon t = O(1)$
- Small quantities: $a'(t) = \epsilon a'(\tau) = \epsilon u_1 + \epsilon^2 u_2 + O(\epsilon^3)$, $\mathbf{u} = O(\epsilon)$
- Leading order is part of circle:
- Matching: $G(\theta_a(a)) - G(\theta_Y) = u_1 Ca \sim \epsilon^{-1} a'(t) Ca$ (Cox, J. Fluid Mech., 1986), solving this ODE yields the quasi-static contact line motion.

Numerical Validation

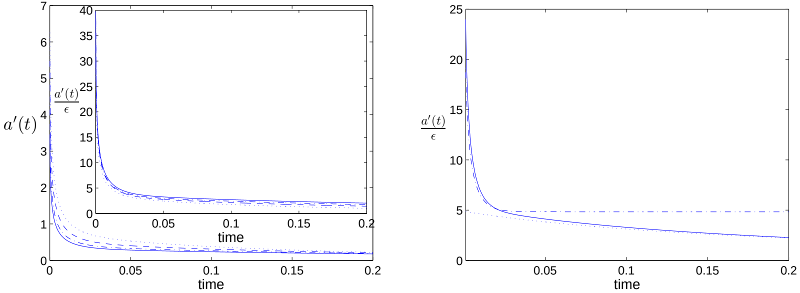


Figure: Left: Different curves correspond to different values of slip length: $l_s = 10^{-2}$ (dotted), 10^{-3} (dashed), 10^{-4} (dash-dotted), 10^{-5} (solid). The inset plot shows the re-scaled contact line speed $a'(t)/\epsilon$ versus time. Right: The contact line speed computed using the slip model with $l_s = 10^{-5}$ (solid) is compared with predictions by the angle-speed relation (dash-dotted) in the finite-time regime and that (dotted) in the quasi-static regime.

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Thin-film Model

- Symmetric spreading of a thin viscous droplet of height $z = h(x,t)$ with $0 \leqslant x \leqslant a(t)$, brought-in Navier slip law (Ren et al, Phys. Fluids, 2010), moving substrate with speed U:

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left[\frac{\partial^3 h}{\partial x^3} h^2 (h + l_s)\right] + U\frac{\partial h}{\partial x} = 0$$

- Boundary conditions at CL ($x = a(t)$):

$$h = 0, \qquad \frac{\mathrm{d}a}{\mathrm{d}t} - U = \frac{1}{2\beta}\left[\left(\frac{\partial h}{\partial x}\right)^2 - \theta_y^2\left(\frac{x}{\epsilon}\right)\right],$$

where $\theta_y = \theta_y(\frac{x}{\epsilon})$ is the equilibrium angle depending on location periodically with period ϵ ($\theta_m < \theta_M$):

1. $\theta_y(z) = \frac{\theta_m + \theta_M}{2} + \frac{\theta_M - \theta_m}{2}\sin(\frac{z}{2\pi})$;
2. $$\theta_y(z) = \begin{cases} \theta_m, & 0 \leqslant z < c, \\ \theta_M, & c \leqslant z < 1. \end{cases}$$

Quasi-static Asymptotics

- Assume $U \ll 1$, and $t = \tau / U$ with $\tau = O(1)$;
- Leading order solution: $h_0(x,\tau) = -\frac{1}{2a}\theta(\tau)(x-a)^2 + \theta(\tau)(a-x)$ is a hyperbola where $\theta(\tau) = -\frac{\partial h_0}{\partial x}|_{x=a}$ is apparent CL;
- Solubility condition on h_0 arises in first order equation (plugging in hyperbolic form):

$$\frac{\mathrm{d}\theta}{\mathrm{d}\tau} = \frac{2\theta}{a}\Big(- \frac{\mathrm{d}a}{\mathrm{d}\tau} + \frac{3}{4}\Big)$$

- Assume slow relaxation on the CL so that $\frac{1}{\beta} = \frac{U}{\tilde{\beta}} = O(U) \ll 1$, leading order in CL condition:

$$\frac{\mathrm{d}a}{\mathrm{d}\tau} - 1 = \frac{1}{2\tilde{\beta}}\Big[\theta(\tau)^2 - \theta_y^2(\frac{a}{\epsilon})\Big]$$

Simplified ODEs and Averaging

- Leading order approximations at original time scale:

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \frac{2\theta}{a}\Big(- \frac{\mathrm{d}a}{\mathrm{d}t} + \frac{3}{4}U\Big)$$
$$\frac{\mathrm{d}a}{\mathrm{d}t} = U + \frac{1}{2\beta}\Big[\theta^2 - \theta_y^2(\frac{a}{\epsilon})\Big]$$

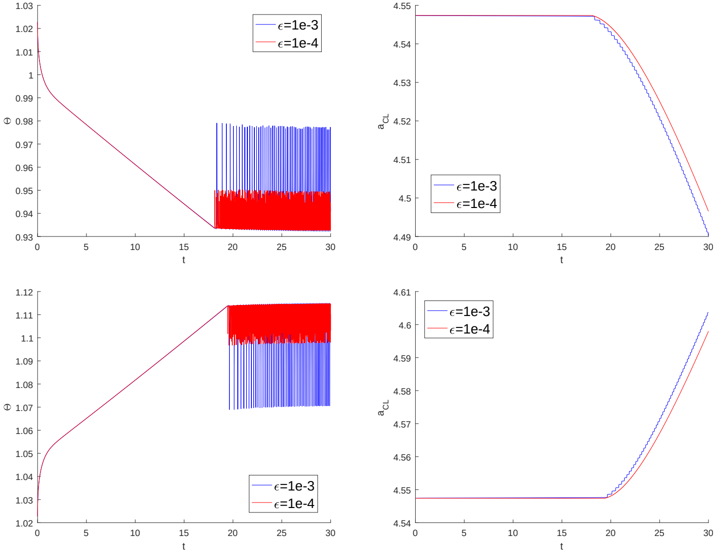
- Introduce fast variable $b = \frac{a}{\epsilon}$, fast dynamics:

$$\frac{\mathrm{d}b}{\mathrm{d}t} = \frac{1}{\epsilon}\Big\{U + \frac{1}{2\beta}\Big[\theta^2 - \theta_y^2(b)\Big]\Big\} = \frac{1}{\epsilon}g(\theta, a, b)$$

- Averaging out fast dynamics by its invariant measure (Pavliotis & Stuart, 2008), $\rho^\infty(b;\theta,a) =< g(\theta,a,b)^{-1} >_b^{-1} /g(\theta,a,b)$, gives effective dynamics:

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = \frac{2\Theta}{A}\Big(- < g(\Theta, A, b)^{-1} >_b^{-1} + \frac{3}{4}U\Big)$$
$$\frac{\mathrm{d}A}{\mathrm{d}t} =< g(\Theta, A, b)^{-1} >_b^{-1}$$

Contact Angle and CL Speed for Sine Structure



Outline

1. Backgroung
2. Moving contact lines in polymeric fluids (with W. Ren)
3. Asymptotic analysis in MCL (with W. Ren)
4. Thin-film Movement on Heterogeneous Surface
5. Concluding remarks and future work

Concluding Remarks

- An immersed boundary method is developed on the staggered grid to study the MCL model with FENE-P fluids;
- Asymptotic analysis on zero-slip limit of slip model, in particular, apparent contact angle vs. contact line speed;
- Study the effective dynamics of thin film on heterogeneous surfaces.
- Related work: extension to soluble surfactant

Thank you !