

Surface Tension Driven Thin Film Flow

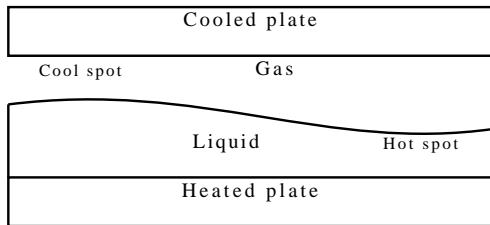
Roy Stogner

Computational Fluid Dynamics Lab
Institute for Computational Engineering and Sciences
University of Texas at Austin

October 30, 2008



Thin Film Flow



Two Layer Film

- Liquid heated from flat solid surface below
- Gas cooled from flat plate above
- Experiments + Theory from VanHook, Schatz, Swift, McCormick, Swinney
- Theory + Calculations from Wang, Carey, Stogner

Flow Instabilities

Buoyancy cells	Raleigh Number $\text{Ra} \equiv \frac{\alpha_T g \delta T d^3}{\nu k}$ Buoyancy / viscosity	d^3
Thermocapillary cells	Marangoni Number $\text{M} \equiv \frac{\sigma_T \delta T d}{\rho \nu k}$ Surface tension / viscosity	d
Thermocapillary deformation	Inverse dynamic Bond Number $\text{D} \equiv \frac{\sigma_T \delta T}{\rho g d^2}$ Surface tension / gravity	d^{-2}

Two-Dimensional Flow

- $d/L \ll 1$
- Flow is described by velocity $\vec{v}(x, y)$, pressure $P(x, y)$, temperature T
- Viscosity gives velocity profiles in z defined by $\vec{v}_{max}(x, y)$ or $\bar{v}(x, y)$
- Free surface flows determine pressure from surface height $u(x, y)$ + conditions
- Long wavelength thermocapillary flow describes \vec{v} , T in terms of u

Non-dimensionalization

Based on:

- representative thickness d
- density ρ
- thermal diffusivity
 $\kappa \equiv \frac{k}{\rho c_p}$
- viscosity ν

Length	u, \vec{x}	d
Time	t	$\frac{d^2}{\kappa}$
Velocity	\vec{v}	$\frac{\kappa}{d}$
Pressure	P	$\frac{\rho \nu \kappa}{d^2}$
Temperature	T	δT
Surface Tension	S	$\frac{d}{\rho \nu k}$

Non-dimensionalized Incompressible Flow

$$\begin{aligned} \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} &= \text{Pr} (-\nabla P + \Delta \vec{v} - G \hat{e}_z) \\ \nabla \cdot \vec{v} &= 0 \\ \frac{\partial T}{\partial t} + (\vec{v} \cdot \nabla) T &= \Delta T \end{aligned}$$

with Prandtl number $\text{Pr} \equiv \nu/\kappa$ and Galileo number $G \equiv \frac{gd^3}{\nu\kappa}$

Temperature Boundary Conditions

Lower: Fixed by hot plate

$$T(z = 0) = 0$$

Upper: $T(z = u)$ determined by conductivities in z

$$k \frac{T \delta T}{ud} = k_g \frac{(1 - T) \delta T}{d + d_g - ud}$$

$$H \equiv \frac{k_g d}{k d_g}$$

$$F \equiv \frac{d/d_g - H}{1 + H}$$

$$T = \frac{-u}{1 + F - Fu}$$

Velocity Boundary Conditions

Lower: No-slip

$$\vec{v}(z = 0) = \vec{0}$$

Upper: $P(z = u)$ and $\vec{v}(z = u)$ interact with surface tension

$$\begin{aligned} \nabla_{\perp} S &= \nabla_{\perp} \vec{v}_n + \nabla_n \vec{v}_{\perp} \\ P - S \left(\frac{1}{R_1} + \frac{1}{R_2} \right) &= 2 \frac{\partial \vec{v}_n}{\partial x_n} \end{aligned}$$

Long Wavelength Interior Equations

Expansion in d/L , low order terms dropped.

$$\frac{\partial^2 \vec{v}_\perp}{\partial z^2} = \nabla_\perp P$$

$$\frac{\partial P}{\partial z} = -G$$

$$\frac{\partial^2 T}{\partial z^2} = 0$$

$$\nabla_\perp \cdot \vec{v}_\perp + \frac{\partial \vec{v}_z}{\partial z} = 0$$

Long Wavelength Surface Equations

$$\frac{\partial u}{\partial t} + \vec{v}_\perp \cdot \nabla u = \vec{v}_z$$

$$\nabla u \cdot \nabla S - \nabla u \cdot \frac{\partial \vec{v}_\perp}{\partial z} = 0$$

$$\left(\nabla u \times \nabla S - \nabla u \times \frac{\partial \vec{v}_\perp}{\partial z} \right) \cdot \hat{e}_z = 0$$

$$P + S\Delta u = 0$$

Integrating Out Pressure

Surface tension + gravity determine pressure:

$$P = -S\Delta u + G(u - z)$$

Which forces horizontal momentum:

$$\frac{\partial^2 \vec{v}_\perp}{\partial z^2} = -\nabla S \Delta u + G \nabla u$$

Integrating Out Velocity

Integrating momentum twice in z between boundary conditions:

$$\vec{v}_\perp = (-\nabla (S\Delta u) + \mathbf{G}\nabla u) \frac{z^2}{2} + (u\nabla S\Delta u - u\mathbf{G}\nabla u + \nabla S) z$$

And once more for $\partial_z \vec{v}_z = \nabla_\perp \cdot \vec{v}_\perp$:

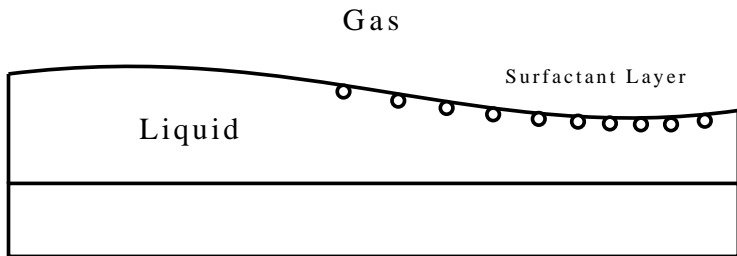
$$\vec{v}_z = (-\Delta (S\Delta u) + \mathbf{G}\Delta u) \frac{z^3}{6} + (\nabla \cdot (u\nabla S\Delta u) - \mathbf{G}\nabla \cdot (u\nabla u) + \Delta S)$$

Thin Film Flow Equation

\vec{v}_z and \vec{v}_\perp fully define $\frac{\partial u}{\partial t}$ in terms of u :

$$\begin{aligned}
 \frac{\partial u}{\partial t} &= \vec{v}_z(u) - \vec{v}_\perp(u) \cdot \nabla u \\
 &= \vec{v}_z(u) - \nabla \cdot (u\vec{v}_\perp(u)) + \nabla \cdot \vec{v}_\perp(u) \\
 &= \vec{v}_z(u) - \nabla \cdot (u\vec{v}_\perp(u)) - \left. \frac{\partial \vec{v}_z}{\partial z} \right|_{z=h} \\
 &= \nabla \cdot \left(\frac{u^3}{3} \nabla (S\Delta u) - \frac{u^2}{2} \nabla S + \frac{Gu^3}{3} \nabla u \right)
 \end{aligned}$$

Surfactant Transport



Flow Characteristics

- Temperature, surfactant concentration c_s determine surface tension
- Temperature destabilizes, surfactant stabilizes

Surface Transport Equation

$$\frac{\partial c_s}{\partial t} + \nabla \cdot (c_s \vec{v}_\perp) = 0$$

Expands based on \vec{v}_\perp to:

$$\frac{\partial c_s}{\partial t} + \nabla \cdot \left(c_s \frac{u^2}{2} \left(-\nabla (S \Delta u) + \mathbf{G} \nabla u \right) + \left(u^2 \nabla S \Delta u - u^2 \mathbf{G} \nabla u + u \nabla S \right) \right) = 0$$

Surfactant-dependent Surface Tension

Dilute surfactant model: linear dependencies on temperature, concentration

$$\begin{aligned}
 S &= S_0 - M(T - T_0) - \alpha ES_0 c_s \\
 S &= S_0 + \frac{Mu}{1 + F - Fu} - \alpha ES_0 c_s \\
 \nabla S &= \frac{M(1 + F)}{(1 + F - Fu)^2} \nabla u - \alpha ES_0 \nabla c_s
 \end{aligned}$$

Thin Film Flow and Transport Equations

Substituting in constitutive equations for S , ∇S completes the equation system:

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(\frac{u^3}{3} \nabla \left(\left(S_0 + \frac{Mu}{1+F-Fu} - \alpha ES_0 c_s \right) \Delta u \right) - \frac{u^2}{2} \frac{M(1+F)}{(1+F-Fu)^2} \nabla u + \frac{u^2}{2} \nabla c_s + \frac{Gu^3}{3} \nabla u \right)$$

$$\frac{\partial c_s}{\partial t} = \nabla \cdot \left(\left(\frac{u^2}{2} \nabla \left(\left(S_0 + \frac{Mu}{1+F-Fu} - \alpha ES_0 c_s \right) \Delta u \right) + \frac{M(1+F)u}{(1+F-Fu)^2} \nabla u - \alpha ES_0 u \nabla c_s \right) c_s \right)$$

Thin Film Flow and Transport Equations

Use static Bond number $B \equiv \frac{\rho g L^2}{S_{eq}}$, inverse dynamic Bond number $D \equiv \frac{M}{G}$, Wang number $D_s \equiv \frac{\alpha E S_0}{\rho g d^2}$, rescaling \vec{x} by L/d , t by $\frac{3L^2}{GD^2}$:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla \cdot \left(\frac{u^3}{B} \nabla \left(\left(1 + \frac{Dud^2}{(1+F-Fu)L^2} - D_s \frac{d^2}{L^2} c_s \right) \Delta u \right) - \right. \\ &\quad \left. \frac{3u^2}{2} \frac{D(1+F)}{(1+F-Fu)^2} \nabla u + \frac{u^2}{2} \nabla c_s + \frac{Gu^3}{3} \nabla u \right) \\ \frac{\partial c_s}{\partial t} &= \nabla \cdot \left(\left(\frac{3u^2}{2B} \nabla \left(\left(1 + \frac{Dud^2}{(1+F-Fu)L^2} - D_s \frac{d^2}{L^2} c_s \right) \Delta u \right) + \right. \right. \\ &\quad \left. \left. \frac{D(1+F)u}{(1+F-Fu)^2} \nabla u - D_s u \nabla c_s \right) c_s \right) \end{aligned}$$

Thin Film Flow and Transport Equations

Finally, dropping terms scaling with d^2/L^2 gives standard equations:

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(\left(u^3 - \frac{3D(1+F)u^2}{2(1+F-Fu)^2} \right) \nabla u - \frac{u^3}{B} \nabla \Delta u + \frac{3D_s u^2}{2} \nabla c_s \right)$$

$$\frac{\partial c_s}{\partial t} = \nabla \cdot \left(\left(\frac{u^2}{2} - \frac{3D(1+F)u}{(1+F-Fu)^2} \right) c_s \nabla u - \frac{c_s u^2}{2B} \nabla \Delta u + 3D_s c_s u \nabla c_s \right)$$

Weak Approximation

Taking weighted residuals of $\frac{\partial u}{\partial t}$, integrating each 2nd order term by parts once and each 4th order term twice,

$$\begin{aligned}
 \left(\frac{\partial u}{\partial t}, v \right) &= \left(\left(\frac{3D(1+F)u^2}{2(1+F-Fu)^2} - u^3 \right) \nabla u - \frac{3D_s u^2}{2} \nabla c_s, \nabla v \right)_{\Omega} + \\
 &\left(\left(u^3 - \frac{3D(1+F)u^2}{2(1+F-Fu)^2} \right) \partial_{\bar{n}} u + \frac{3D_s u^2}{2} \partial_{\bar{n}} c_s, v \right)_{\partial\Omega} - \\
 &\left(\frac{u^3}{B} \Delta u, \Delta v \right)_{\Omega} - \left(\frac{3u^2}{B} \Delta u \nabla u, \nabla v \right)_{\Omega} + \\
 &\left(\frac{u^3}{B} \partial_{\bar{n}} \Delta u, v \right)_{\partial\Omega} - \left(\frac{u^3}{B} \Delta u, \partial_{\bar{n}} v \right)_{\partial\Omega}
 \end{aligned}$$

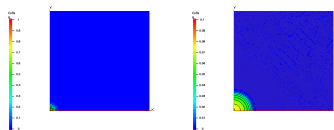
Weak Approximation

Taking weighted residuals of $\frac{\partial c_s}{\partial t}$, integrating each 2nd order term by parts once and each 4th order term twice,

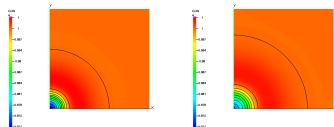
$$\begin{aligned}
 \left(\frac{\partial c_s}{\partial t}, w \right) &= \left(\left(\frac{3D(1+F)u}{(1+F-Fu)^2} - \frac{u^2}{2} \right) c_s \nabla u - 3D_s c_s u \nabla c_s, \nabla w \right)_{\Omega} + \\
 &\quad \left(\left(\frac{u^2}{2} - \frac{3D(1+F)u}{(1+F-Fu)^2} \right) c_s \partial_{\bar{n}} u + 3D_s c_s u \partial_{\bar{n}} c_s, w \right)_{\partial\Omega} - \\
 &\quad \left(\frac{c_s u^2}{2B} \Delta u, \Delta w \right)_{\Omega} - \left(\Delta u \frac{2c_s u \nabla u + u^2 \nabla c_s}{2B}, \nabla w \right)_{\Omega} + \\
 &\quad \left(\frac{c_s u^2}{2B} \partial_{\bar{n}} \Delta u, w \right)_{\partial\Omega} - \left(\frac{c_s u^2}{2B} \Delta u, \partial_{\bar{n}} w \right)_{\partial\Omega}
 \end{aligned}$$

Surfactant-Driven Flow Computation

- Initially flat film surface
- Symmetry BCs
- Surfactant droplet in corner
- Local surface tension reduction
- Fluid wave pushed through domain



Concentration at $t = 0, 0.2$



Depth at $t = 0.1, 0.2$

Stability: Analytic Linearization

Perturbing around steady state $u = 1$ and $c_s = 1$:

$$\begin{aligned}u(x, y, t) &= 1 + \delta u = 1 + \sum_p \eta_p e^{\gamma_p t} e^{i2\pi \mathbf{p} \cdot \mathbf{x}} \\c_s(x, y, t) &= 1 + \delta c_s = 1 + \sum_q \xi_q e^{\lambda_q t} e^{i2\pi \mathbf{q} \cdot \mathbf{x}}\end{aligned}$$

Stability: Analytic Linearization

For small δu and δc_s , linearizing gives:

$$\begin{aligned} \frac{\partial \delta u}{\partial t} &= \nabla \cdot \left(\left(1 - \frac{3D(1+F)}{2} \right) \nabla \delta u - \right. \\ &\quad \left. \frac{1}{B} \nabla \Delta \delta u + \frac{3D_s}{2} \nabla \delta c_s \right) \\ \frac{\partial \delta c_s}{\partial t} &= \nabla \cdot \left(\left(\frac{1}{2} - 3D(1+F) \right) \nabla \delta u - \right. \\ &\quad \left. \frac{1}{2B} \nabla \Delta \delta u + 3D_s \nabla \delta c_s \right) \end{aligned}$$

Stability: Analytic Linearization

Substituting in Fourier expansions allows analytic evaluation of derivatives, leads to algebraic equations for each mode:

$$\begin{aligned} \gamma_q &= \lambda_q \\ \gamma_q + 6\pi^2 q^2 D_s \left(\frac{\xi_q}{\eta_q} \right) + 4\pi^2 q^2 \left(-\frac{3}{2} D(1+F) + 1 + \frac{4\pi^2 q^2}{B} \right) &= 0 \\ \lambda_q + 6\pi^2 q^2 \left(-2D(1+F) + 1 + \frac{4\pi^2 q^2}{B} \right) \left(\frac{\xi_q}{\eta_q} \right)^{-1} + 12\pi^2 q^2 D_s &= 0 \end{aligned}$$

for all $\mathbf{q} = (1, 0), (0, 1), (1, 1), \dots$

Stability: Analytic Linearization

Solving for time growth rates γ_q and λ_q gives:

$$(\gamma_q)_{1,2} = (\lambda_q)_{1,2} = 2\pi^2 q^2 \left(\varepsilon_q - 3D_s \pm \sqrt{\Delta_q} \right)$$

Based on terms:

$$\Delta_q \equiv (\varepsilon_q - 3D_s)^2 - 3D_s \left(1 + \frac{4\pi^2 q^2}{B} \right)$$

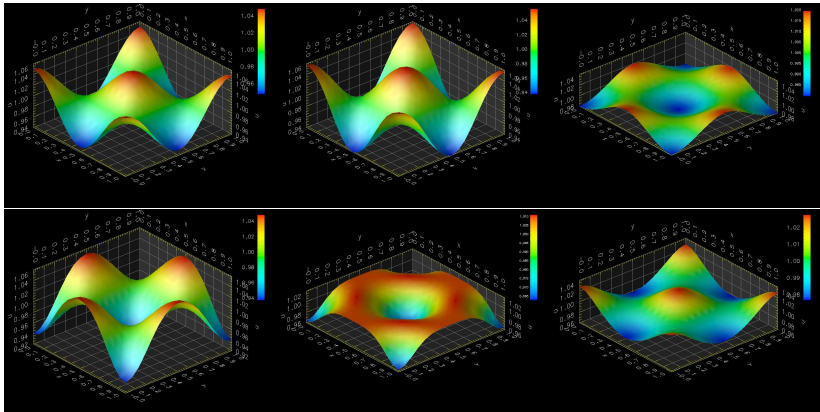
$$\varepsilon_q \equiv \frac{3D(1+F)}{2} - 1 - \frac{4\pi^2 q^2}{B}$$

$\varepsilon_q > 3D_s$: unstable time growth

$\Delta_q < 0$: surfactant-driven oscillation

Stability: Computation

$$u(t), t = 0 \rightarrow 0.4$$



Open Questions

- Proper 2D boundary conditions
- FEM Eigenproblem convergence
- Surfactant diffusion effects
- Nonlinear surfactant effects