Not even Hercules : the moving contact line problem

Carlos Chiquete
The Program

May 3, 2007

Term paper: Spring 2007

Introduction

- Fluid interface motion on solids is a natural occurrence.
  - Coffee.
  - Spreading of drops on surfaces or rising mercury in thermometers.
  - De-icing of planes, liquid is spread on plane to prevent formation of ice.
  - Important when placing thin protective coatings on solids, i.e. coating of microchips.
- The classical theory leads to a singularity: Why?
  - No clear continuum violation.
  - Exceptions are known at low density high speed flows.
  - Should we expect our theory to hold in all situations?

Static contact lines

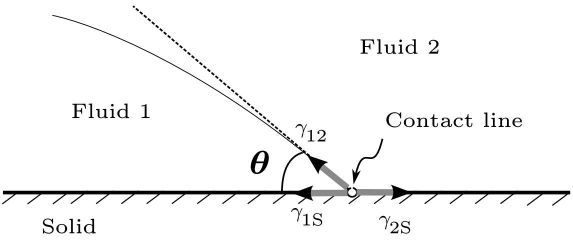


Figure: The contact angle arises out of a balance of interfacial energies

- The Young equation

$$\gamma_{2S} - \gamma_{1S} = \gamma \cos\theta$$

Incompressible Navier-Stokes equations

Based on the assumption that fluids are continuous and that both mass and momentum must be conserved. The following are the differential relations.

- Conservation of Mass

$$\nabla \cdot \mathbf{u} = 0$$

- Conservation of Momentum

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \rho \mathbf{f} + \mu \nabla^2 \mathbf{u}$$

The no-slip condition

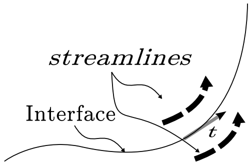


Figure: Velocity is continuous across the interface

- Based on molecular diffusion of momentum.
- The classical 'no-slip' condition,

$$(\mathbf{u}_- - \mathbf{u}_+) \cdot \mathbf{t} = 0$$

The moving contact line

Experimental observations:

- The motion is rolling.
- The static contact angle *grows* to a new *dynamic* contact angle. This angle may be related to the velocity of the CL.
- Instabilities occur when speed of propagation is increased.

The experiment

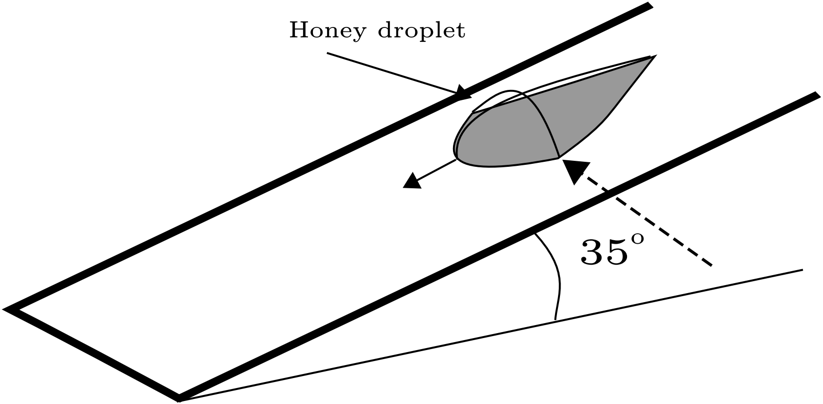
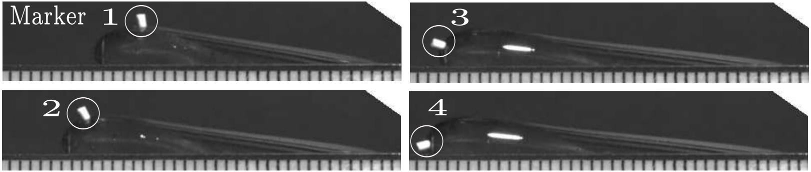


Figure: The camera was aligned sideways with the slope.

The experiment



- Note position and trajectory of marker.

Observations

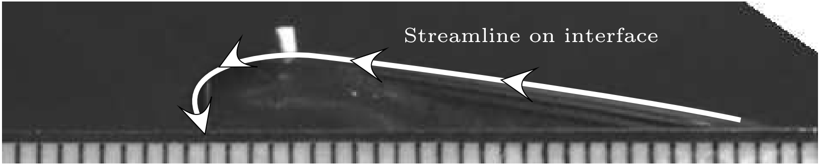
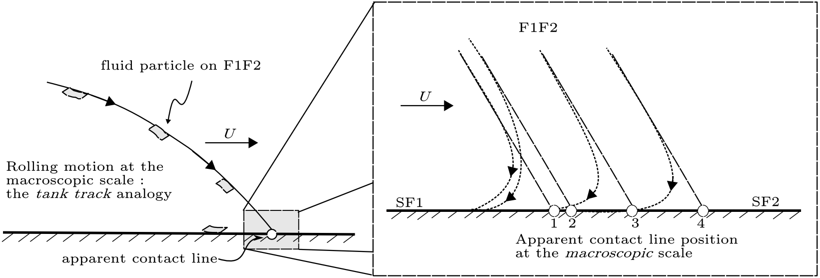


Figure: The inferred streamline at the surface. It means that different material points make up the surface at different times.

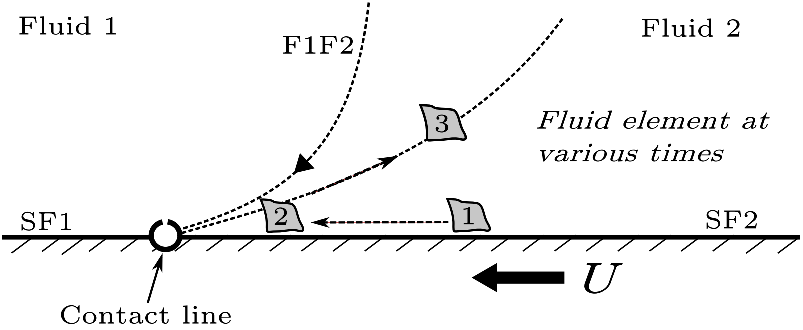
- The dynamic contact angle seems to be constant.
- Rolling assumption is confirmed.
- Material points on the interface reach the CL in finite time.

Application of the classic theory



- The tank track analogy.
- Microscopic picture.

Application of the classic theory



- What are the consequences of this motion if *no-slip* is applied?
  $\Rightarrow$ The velocity field is discontinuous at the contact line

Consequences

- The horizontal velocity u is discontinuous.
- Newtonian fluids have the following constuitive relation:

$$\tau = \mu \frac{\partial u}{\partial z}$$

  τ is the stress on the wall.
- The total force is $\int \tau dx$.
- At the contact line u is discontinuous $\Rightarrow \tau \to \infty$.
- An infinite force is thus predicted by the physical model at the CL.

The linear-slip shear relation (Navier slip)

When the singularity was explicitly formalized[1], it was hypothesized that perhaps no-slip does not apply at every point. It leads to a *slip* BC.

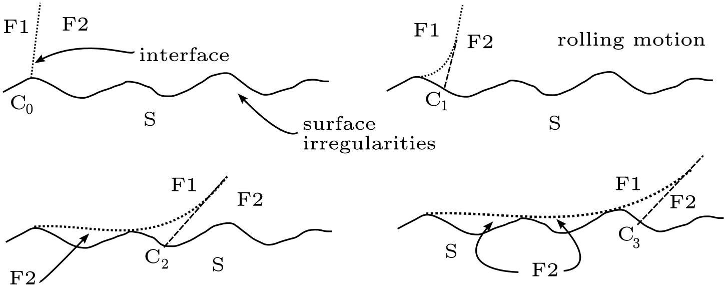
- The linear-slip shear relation is the simplest and most popular form of the slip BC,

$$(u_+ - u_-) \cdot \mathbf{t} = \beta \frac{\partial u}{\partial z}\bigg|_{interface}$$

  β has units of length, and is known as the slip coefficient.
- The singularity is removed at the contact line.

[1] Dussan V and Davis (1974), Huh and Scriven (1971)

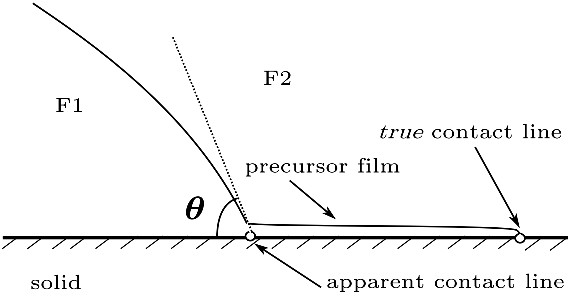
Physical justification



- Hocking[2] theorized that at the microscopic scale, surface roughness of the solid boundary produces the macroscopic slip condition.
- The fluid in the pocket would satisfy the no-slip condition.

[2]Hocking, (1977)

Precursor films



- Thin films have been observed in the spread of various fluid systems over solids. Thicknesses vary between 100 – 1000 angstroms.
- However, precursor films form because of molecular forces which are important at very small scales.

Other Methods

- Variational methods based on energy dissipation explicitly eliminate the singularity at the CL. This is an energy-based description, forces are not explicitly dealt with.
- The generalized Navier boundary condition (GNBC) is a generalization of the slip condition. It based on a force-based description at the contact line.
- Shear-thinning rheology tolerates the growth of the shear stress $\partial u / \partial z$ near the contact line but supposes that the viscosity μ is not constant but is decreasing at a rate such that $\mu \to 0$ ensures

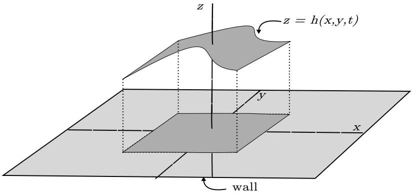
$$\int \tau dx = \int \mu \frac{\partial u}{\partial z} dx < \infty$$

This means that the stress is integrable and so the total force is finite.

Lubrication approximation

- Numerically and analytically, the full NS equations are hard to deal with. Many studies introduce the lubrication approximation to introduce slip, precursor films, etc..
- For very thin films (w.r.t. to longitudinal scale), the lubrication can be introduced to reduce the Navier Stokes equations to a highly non-linear PDE for the film height.

$$\frac{\partial h}{\partial t} + \frac{1}{\mu}\nabla \cdot \Big(f(h)(\gamma \nabla \nabla^2 h - \nabla \phi(h)) \Big) = 0$$



- $f(h) = h^3 + \beta(h)h$
- $\phi(h) = A_D h^{D-5}$, D is dimension of film, i.e. $D = 1, 2$.

Thin film equation

- The lubrication equation describes so-called degenerate diffusion. In contrast to regular diffusion, the equation can become negative even when the initial data is positive. Premature *rupture* can also occur.
- Numerically, the complex behavior exhibited by equation is hard to simulate. Positivity preserving schemes based on entropy dissipation are typically introduced[3].
- Weak solutions to the lubrication equation have been found in special circumstances.

[3] Zhorniskaya and Bertozzi (2000)

Conclusions

- This problem shows the normal hydrodynamic theory *is* fallible.
- The rolling assumption was demonstrated to be true.
- However, the *correct* method to resolve the singularity is not clear.
- Different methods exhibit good agreement with data.
- The GNBC can be derived from variational principles and is in good agreement with molecular dynamic (MD) simulations[4].
- Is the data not resolving key aspects of MCL that would resolved the issue?

[4] Qian, Wang and Sheng (2006)

Acknowledgments

Thanks to Dr. Venkataramani, Bob Reinking, the Applied Math Laboratory and also, the people who retrieve articles at the Science library (and JFM).