Thin Liquid Films and Fluid Interfaces: Models, Experiments and Applications (12w5035)

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1 Overview of the Field

Broadly considered, fluid dynamics is one of the most longstanding and fundamental areas in the physical sciences. The very intricate and diverse phenomena observed in fluid systems have motivated a vast body of mathematical research seeking to analyze and predict these behaviors. Building on the classical Navier-Stokes equations, mathematical formulations of problems in fluid dynamics are comprised of statements for the conservation of mass and force balances on all of the components in the system. These mathematical models take the form of systems of coupled nonlinear partial differential equations. In problems where the masses of fluids being considered have a finite extent, appropriate boundary conditions must be imposed at the edges of the fluid volume. The primary focus of this workshop was problems where the fluid is free to move within the system and the domain occupied by the fluid must be determined as part of the solution of the problem. In such *free-surface* problems the governing system can often be reduced to equations for the evolution of the liquid-gas interface, as in the study of water waves on the surface of rivers or ponds described by the shallow water equations, in which slenderness of the fluid layer is employed to obtain an asymptotic model. For problems at small lengthscales, as in many naturally occurring phenomena (e.g. rain drops on lotus leaves) and the design of engineering materials and microfluidic devices, surface tension can play a strong role in determining the dynamics. The inclusion of surface tension (and related surface tension gradient effects) yields challenging models given by higher-order nonlinear partial differential equations.

This workshop brought together a broad array of researchers working on problems in fluids dynamics spanning experimental studies, materials science, basic physics, engineering design, biological applications, mathematical modeling and computations. The diverse and interdisciplinary participants of the workshop created a very open and interactive forum that addressed issues stemming from novel physical problems and engineering designs. These directions generally motivate improved mathematical formulations for the observed delicate fluid behaviors.

2 Recent Developments and Open Problems

While the foundations of lubrication theory for thin liquid films date back to the work of Reynolds in the late 1800's, the 1985 survey paper *"Wetting: statics and dynamics"* by P.G. de Gennes [26] was an important recent milestone in the study of the fluid dynamics of thin films. From a very physically oriented perspective, it reviewed the state of the experimental and theoretical understanding of the small-scale behaviors in spreading of liquid layers over solid substrates. De Gennes' paper highlighted results showing that the presence of capillary forces in simple models for advancing fluid fronts produced unphysical singularities in the stress at the moving contact line. Among the physical effects mentioned for consideration in resolving this open question were physical properties (topography and surface roughness) and chemical properties (van der Waals and other intermolecular forces) of the solid substrate, microscopic precursor fluid films, and slip effects. Among the further areas and open questions that de Gennes pointed to for further work were the spreading behaviors of complex fluids (mixtures and long-chain polymer melts) and the role of surfactant chemicals in dynamically modifying surface tension. Many questions in these directions are still open problems.

These fundamental physical questions regarding fluid dynamics have become even more pressing in recent times with the development of technologies that can precisely control surface properties of materials at micro- and nano-scales – these issues underpin problems like the design of water repellent materials, microfluidic devices for manipulating of tiny volumes of liquids, and better medical treatments for disorders involving physiological fluid layers (on the eye, or in the lung, for example). Careful mathematical analysis of these complicated systems has driven extensive studies of stability, dynamics, and asymptotics of partial differential equations, which in turn can identify important operating regimes for further experimental studies.

Following de Gennes, the next generation of research produced many advances on mathematical modeling and formulations of computationally tractable systems of equations. An extensive review was given in Oron [60] of models and results for lubrication models of flows of thin films of viscous fluids with special attention to van der Waals forces, surface tension, thermocapillary effects. In the same 1997 issue of *Reviews of Modern Physics*, Eggers [28] gave a comprehensive review of research on the break-up of free-surface fluid flows in free-space (i.e. rupture of liquid sheets and jets). This included a review of the classical stability theory given by Rayleigh as well as recent experimental and computational studies showing finite-time break-up of fluid filaments into droplets. Later studies showed many relations between break-up of fluids in free-space with the finite-time rupture of thin films coating solid substrates. The broad array of applications of lubrication models with surface tension effects was presented in [58]. Many of the fundamental issues of rigorous mathematical analysis of contact line dynamics and the associated weak solutions of the nonlinear thin film PDE were given in [11], where computational issues for contact lines and related regularized forms of the PDE were also examined.

The year 2009 brought more notable review articles of the field. Craster and Matar [23] surveyed the state of the art in mathematical models of thin film flows including thermal effects, surfactants, and models including evaporation or inertial effects. Special attention was given to intermolecular effects and other physical properties of the solid substrate (topography, elasticity, porosity). Connecting back to de Gennes' article, [12] gave an overview of modern developments on models and experimental studies of contact line dynamics. [30] surveyed the progress in the study of stability and break-up of fluid jets and sprays, and a closely related survey highlighted the role of self-similar solutions in representing the dynamics leading to finite-time singularities of nonlinear PDEs in fluid dynamics and other applications [29].

The above survey articles and the body of research overviewed by them form the background and general scope of research that the workshop contributed to. The 2012 workshop also builds on other BIRS workshops that have been run on thin film dynamics [1, 22], free-surface flows [39] and dynamics of complex fluids [33, 9].

3 Presentation Highlights

The format of the workshop was designed to provide for extensive time for questions following-up on research talks. These questions often led to very lively discussions on a wide range of mathematical, modeling, and experimental aspects. Further research connecting to various workshop themes was also presented in evening poster sessions. Below we briefly review some of the results covered in the workshop, grouped together by different aspects of the research along with useful related references.

3.1 Contact line dynamics

As described above, studies of moving contact line behavior in various system configurations are active areas of interest. David Sibley [64] presented a comprehensive comparison of different mathematical models for motion of contact lines, including slip effects, precursor films, diffusive interface equations and others. In the context of coating flows, Satish Kumar [70] illustrated the considerations needed to accurately model contact line dynamics that can allow for wetting failure and the entrainment of air between the film and the solid substrate. Gunter Auernhammer's work made use of an experimental system with a rotating cylindrical drum to examine the dynamics of the contact line and the influence of the drum's surface roughness and the presence of surfactant in the fluid [32, 31]. Daniel Herde described his work on numerical simulations of contact line dynamics and measurements of the contact angle in shear-driven flows over substrates with varying chemical (wetting) properties. Joshua Dijksman described his work on tracking the radially-collapsing contact line in a circular spinning bucket in a poster presentation [57, 56].

3.2 Influence of substrate properties

Work relating to the influence of substrate properties on the spreading of fluid layers spanned a wide range of directions from experimental physics to PDE analysis. Lou Kondic presented molecular dynamics computations that showed dramatic behaviors of nanoscale drops of liquid metals on dewetting substrates. Break-up of the drop was illustrated in different geometries – finite line segments and rings [59, 45, 37]. Karin Jacobs reviewed research on nanoscale polymer films on substrates with different surface properties. Good agreement on dewetting characteristics of the films in experiments has been obtained from analytic models that include slip effects [5, 8, 7, 4, 6, 34, 35]. Ralf Seemann carried out experimental studies of fluids filling grooves on solid substrates. The geometry of the fluid free-surface depends on the fluid volume and the groove shape (triangular or rectangular) and the fluid-solid contact angle [62, 42, 38, 43, 41, 10]. Electowetting was used to control the contact angle. This facilitated an exploration of whether the spreading is reversible. In some cases, break up into droplets was observed. When the substrate was an elastic solid, fluid capillary forces could deform groove walls and yield coupling to behavior in adjacent grooves. Joao Cabral described how elastic instabilities of film coatings could be used to control desired patterns down to very small lengthscales for improved microfabrication of structured substrates [18, 71]. Elastic deformation of the substrate played an even stronger role in the research of Joshua Bostwick, who considered the spreading of liquid droplets on soft gels. Capillary forces at the liquid-gel contact line can drive fracture of the gel. Elasticity theory applied to the gel can predict the rate of spreading of the drop and the instabilities that had been seen in earlier experiments [25].

Longer-scale substrate topography effects, namely flows on curved surfaces, were also considered. Yvonne Stokes talked about her work modeling and computing flows in helical channels [50]. The geometry of the channel was used to separate out particles in slurries. Stephen Wilson presented joint work with Brian Duffy on fluid rings on the outside of rotating horizontal cylinders. Colin Paterson presented further related work in a poster presentation [51, 27, 67]. Marina Chugunova described analytical techniques she has used for studying the thin films on rotating and fixed horizontal cylinders and how these approaches can also be applied to the fourth order Mullins equation for thermal grooving under surface diffusion [19, 16].

3.3 Complex fluids and surfactants

"Complex fluids" broadly refers to flows where more properties must be determined besides the local velocity field at each point. This can apply to non-Newtonian flows where a separate evolution equation is given for the stress field. But in the context of this workshop it describes: (i) nematic fluids, where a "director" molecular orientation vector field is present, and (ii) multi-component immiscible fluids. Linda Cummings presented a lubrication model for spreading nematic liquid crystal films with particular attention to the influence of the boundary conditions on the director field [52, 24]. Dimitri Papageorgiou described new results on the stability of the interfaces between three immiscible phases confined and flowing in a finite-width inclined channel. Dirk Peschka presented models (full Stokes flow and lubrication models with sharp contact lines vs. precursor films) and results from numerical simulations to capture the coupled spreading/draining of a drop of one fluid on a thin layer of another fluid [46]. Stephen Garoff described experimental studies on the spreading of surfactants over fluid mixtures having similar properties to biofluids in the lungs. While results imply that capillary effects are dominant, some aspects suggest that models must include effects like autophobing (finite spreading) [21, 44]. Further related results on autophobing of surfactants were presented in a poster by Ellen Swanson [63]. Rachel Levy presented a poster on intriguing experimental results in the complementary exterior problem on the spreading of a layer of surfactant spreading into a finite region of "clean" fluid film surface.

Uwe Thiele described an intriguing mathematical formulation for obtaining the evolution equations for complex fluids including two-layer flows [36, 61] and surfactant- or particle-ladened thin film flows as gradient dynamics based on an appropriate energy functional and mobility coefficient [68]

3.4 Fluid-structure interactions

While many of the studies described in the other sections involve the influence of contact with solids on the motion of a mass of fluid, we use the term "fluid-structure interaction" to describe systems where there is a significant coupling or feedback of the fluid dynamics to the structure or unsteady motion of the solid. Ofer Manor presented a poster on the instabilities that occur in fluid droplets subjected to acoustic forcing on vibrating solid substrates [54, 55, 20]. Stephen Wilson discussed the steady states for tilted rigid plates floating on thin film flows [17]. In a geophysical context, John Lister described the dynamics of *laccoliths* – intrusions of fluids (volcanic magma) between layers of deformable solids (sedimentary rock). Lister compared and contrasted the spreading behavior for the model, a lubrication flow coupled to an elastic membrane (yielding a sixth order PDE), against the contact line behaviors for the thin film equation and the second order porous medium equation for gravity currents. On a much smaller scale, Kara Maki described her work on modeling the elastic deformations of soft contact lenses and the influence of the tear film.

3.5 Jets, fluid sheets in free space, and draining flows

Several talks in the workshop considered the dynamics of interfacial flows in free-space. Burt Tilley presented results from continuing collaborative work with Mark Bowen on the rupture of a thin sheet of viscous fluid due to thermocapillary effects [13, 69]. Linda Smolka talked about her approach to the transient stability analysis of inertially driven thinning/expanding circular fluid sheets [65]. Both of these talks had interesting connections (through aspects of draining flows) to the very engaging talk by Stephen Davis on the complex dynamics of foams. Davis described the interaction of lamella sheets connected at Plateau border junctions forming dynamic networks that exhibit coarsening [66, 2, 3, 15]. Rouslan Krechetnikov talked about his continuing studies of the very unusual dynamics of droplet formation coming about as tip streaming from a larger pendant drop. Analysis of the Marangoni stresses and surface tension singularities accompanying droplet pinch-off incorporated fluid flow, chemical, and electrical effects [48, 47, 49].

3.6 Diffusion, evaporation, thermal, and other effects

Finally, other presentations had strong links to many of the previous areas (including complex fluids and contact lines) but also brought up different important fundamental effects to help model observed behaviors in different systems. Aaron Persad described very interesting results on thermal patterns and waves arising the the evaporation of sessile drops of volatile liquids [40]. Kara Maki presented other results on the influence of particle suspensions in evaporating droplets in a poster presentation [53]. While the influence of evaporation has received detailed attention in Richard Braun's extensive work on tear films coating the eye [14], at the workshop he considered the need to also include further analysis of heat transfer and osmolality from the eye to better describe the tear film [14]. Shilpa Khatri described her experimental studies of fluid droplets rising through layers of density-stratified fluids. While speeds of drops moving through homogeneous layers are well-understood, the influence of stratification interfaces can produce unexpected behaviors for rising drops and settling particles. Effects including fluid entrainment, convective mixing and time-scales for density diffusion can play important roles.

4 Outcome of the Meeting

The workshop was widely regarded as being successful in fostering a stimulating interaction across the broad range of research approaches being used in this area of fluid dynamics. The arrangement of talks given in the schedule could not predict or fully capture the interesting connections and interactions between the topics, participants, and problems that evolved during the meeting. While generally being strongly grounded in physical systems, all of the presentations were very suggestive of challenging problems for further mathematical modeling and analysis.

In addition to the notable talks and poster presentations mentioned in the previous sections, the workshop also included discussion periods drawing on the shared interests and expertise of the participants. Some of the topics considered in these discussions included: contact line hysteresis, contact lines for mixtures and with evaporation, modeling of wetting on rough surfaces, liquid lenses and instabilities of liquid bilayers, and formulating more general models for surfactant driven flows.

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