Microfluidic Dynamic Wetting Flows: Modelling and Simulation

J.E. Sprittles[1] & Y.D. Shikhmurzaev[2]

[1] University of Oxford, Mathematical Institute, 24-29 St Giles', OX1 3LB, U.K.
[2] University of Birmingham, School of Mathematics, Edgbaston, B15 2TT, U.K.

June 20, 2012

1 Introduction

Reliable simulation of flows in which a liquid wets a solid at a moving contact line is the key to the understanding of a whole host of technologically important processes, such as in the coating of optical fibres or in the use of inkjet printed microdrops as an alternative fabrication method. Such flows can be considered as microfluidic phenomena and are characterized by large surface area to volume ratios in which interfacial effects become dominant. The trend towards miniaturization has continued with much recent speculation about the nature of dynamic wetting in nanofluidics, and in particular the imbibition of liquids into carbon nanotubes. Here, it is known that experiments cannot be described using current models for the interfacial dynamics [1] and a new approach is sought after.

To extract reliable unambiguous experimental data from micro and nanofluidic flows is difficult and/or costly and, consequently, there is a desire to have a flexible and robust computational tool, which can quickly map parameter space of interest to allow a specific process to be optimized. Such computational software could be validated against experiments at scales and geometries easily accessible to accurate measurement and then used to make predictions in processes inaccessible to experimental analysis.

A physical phenomenon which distinguishes between the predictions of the many different models proposed in the literature for this class of flows is the 'hydrodynamic assist to dynamic wetting', which was first observed in high accuracy experiments on the curtain coating process [2]. It was shown that if a given liquid wets a given solid at a fixed contact line speed, the dynamic contact angle can still be manipulated by altering the flow field in other ways, for example by changing the flow rate or curtain height, to allow the process to be optimized. Similar dependencies have been noted in the spreading of a liquid between parallel plates [3], the imbibition of liquid into capillaries [4], in the spreading of impacted drops over solid substrates [5] and in the coating of fibres [6]. Our aim is to determine if these are flows in which 'assist' also occurs or whether the results can be attributed to low spatial resolution in the experiments.

Currently, the only model able to even qualitatively describe the aforementioned phenomena is the interface formation model [7]. This model captures the key physics of wetting, that is the process in which fresh liquid-solid interface is formed, and shows how the global flow influences the dynamic contact angle by altering the relaxation of dynamic surface variables along the interfaces. To compare the predictions of this model to experiments requires the development of CFD code, which has been the aim of many investigators coming from a range of backgrounds, but thus far has not been achieved due to the mathematical complexity of the model.

Progress in the development of the aforementioned CFD code was achieved in [8], where the mathematically less complex conventional models were incorporated into an accurate computational framework. The developed finite element code uses an arbitrary Lagrangian Eulerian description, in order to accurate capture the free surface motion, which is based on the spine method developed by Scriven and co-workers [9] for coating flow simulation, whilst time derivatives are handled using the second-order accurate BDF2 method described in [10]. It was shown that many of the previous numerical results obtained for dynamic wetting processes are unreliable as they contain uncontrolled errors caused by not resolving all the scales in the conventional model, most notably the dynamics of slip and the curvature of the free surface near the contact line.

Recently, the interface formation model has been incorporated into the finite element framework, with a detailed description of the implementation, as well as benchmark calculations, of the first full implementation of this model provided in [11]. Following on from this, the code has been used to describe the dynamics of liquid drops on both homogeneous and chemically patterned surfaces in [12]. Here, we present benchmark calculations from the code, highlighting key newly discovered physical effects and then proceed to discuss the potential capabilities of the developed computational tool.

2 Benchmark Simulations of Dynamic Wetting Processes

Results from a programme of comparative study of how dynamic wetting flows are described by different theories are presented. Two completely different flows, namely the imbibition of a liquid into a capillary and the impact and spreading of microdrops, are used to validate our simulations against experimental results which already exist in the literature. Then, benchmark simulations are provided which highlight experimentally verifiable differences between the interface formation model's predictions and those from previous models of wetting proposed in the literature. In particular, the effect of the system size on the relationship between the dynamic contact angle and the contact line speed, which is not included in conventional models of dynamic wetting, is a new path of investigation which will be shown to be critical to industrially-relevant micro and nanofluidic flows.

The height z_a of a meniscus propagating into vertical completely wetting capillaries of radius 0.036cm and 0.074cm is plotted in Figure 1. Comparison is made between experimental results in [13], the Lucas-Washburn curve which is often used to describe this class of flows and our simulation. Considering that no parameters have been fitted, our computations are seen to approximate the data exceptionally well and are vastly superior to the Lucas-Washburn curve which hugely overpredicts the speed of the meniscus through the capillary. Our code will be used to compare all the models proposed for imbibition into a capillary, establish the individual effects contributing to the meniscus' behaviour and ascertain bounds of applicability on models previously proposed.

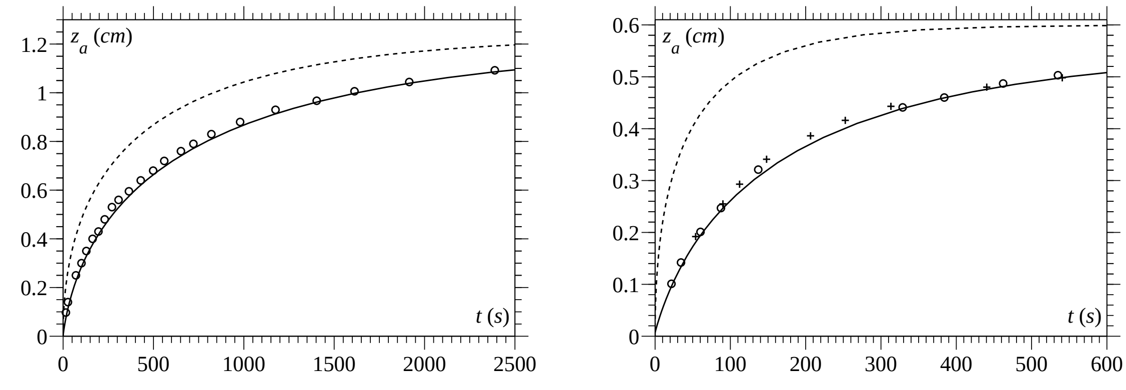

Figure 1: Apex height z_a of a meniscus in a capillary of radius 0.036cm (left) and 0.074cm (right) as a function of time t. Experimental results are circles and crosses, our simulations are the solid lines whilst the dashed line is the Lucas-Washburn result.

Secondly, we consider the impact and spreading of microdrops on solid surfaces in the parameter range applicable to inkjet printing technologies. In Figure 2, a typical simulation is compared to experiments in [14] and, again without any fitted parameters, excellent agreement is seen. After this validation, an extensive analysis of parameter space using our computational tool will be shown to indicate clear, experimentally verifiable, deviations between the predictions of different models used for the microdrop spreading process and, finally, additional physical effects will be added, such as the use of chemically patterned surfaces to gain flow control on the process.

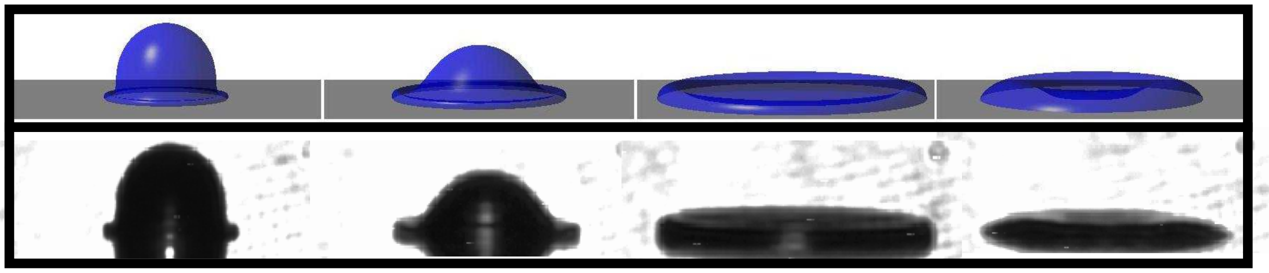

Figure 2: Simulation of a 25μm radius drop of water impacting a partially wettable solid at 12.2m s^{-1} compared to experiment of [14].

3 Discussion

The developed framework has demonstrated its ability to accurately describe a range of technologically-relevant dynamic wetting phenomena and can now be adapted to consider other processes of industrial and/or fundamental interest. For example, the code can be adapted to simulate other situations where the influence of the flow field or geometry on the contact angle has been observed, for example in high-speed coating of fibres or in curtain coating technologies. Furthermore, the influence of system size on flow characteristics can easily be attained by, say, looking at drop impact phenomena from millimetre-size right down to nanometre size; at the bottom end of this scale a comparison with molecular dynamics simulations can be performed. Moreover, as additional physical effects, such as heat transfer or electromagnetic fields become relevant, these can be built into a code which has been thoroughly validated for the underlying wetting process.

The flexibility of the computational tool also allows other free surface flows of interest to be considered, in particular, the coalescence of liquid drops, whose dynamics are critical for a range of processes, such as the interaction between sessile and impacting drops ejected from 3D printers. In this phenomenon, recent experimental results, which capture exceptionally small spatio-temporal scales [15], demonstrate the failure of current models in describing this class of 'singular flows'. These results suggest that more complex physics, such as that brought in by the interface formation model, are required.

References

[1] L. Bocquet and E. Charlaix. Nanofluidics, from bulk to interfaces. *Chemical Society Reviews*, 39:1073–1095, 2010.

[2] T. D. Blake, A. Clarke, and K. J. Ruschak. Hydrodynamic assist of wetting. *AIChE Journal*, 40:229–242, 1994.

[3] C. G. Ngan and E. B. Dussan V. On the nature of the dynamic contact angle: An experimental study. *Journal of Fluid Mechanics*, 118:27–40, 1982.

[4] V. D. Sobolev, N. V. Churaev, M. G. Velarde, and Z. M. Zorin. Dynamic contact angles of water in ultrathin capillaries. *Colloid Journal*, 63:119–123, 2001.

[5] I. S. Bayer and C. M. Megaridis. Contact angle dynamics in droplets impacting on flat surfaces with different wetting characteristics. *Journal of Fluid Mechanics*, 558:415–449, 2006.

[6] P. G. Simpkins and V. J. Kuck. On air entrainment in coatings. *Journal of Colloid and Interface Science*, 263:562–571, 2003.

[7] Y. D. Shikhmurzaev. *Capillary Flows with Forming Interfaces*. Chapman & Hall/CRC, Boca Raton, 2007.

[8] J. E. Sprittles and Y. D. Shikhmurzaev. A finite element framework for describing dynamic wetting phenomena. *International Journal for Numerical Methods in Fluids*, 68:1257–1298, 2012.

[9] S. F. Kistler and L. E. Scriven. Coating flow theory by finite element and asymptotic analysis of the Navier-Stokes system. *International Journal for Numerical Methods in Fluids*, 4:207–229, 1984.

[10] P. M. Gresho and R. L. Sani. *Incompressible Flow and the Finite Element Method. Volume 2. Isothermal Laminar Flow*. John Wiley & Sons, LTD, 1999.

[11] J. E. Sprittles and Y. D. Shikhmurzaev. Finite element framework for simulating dynamic wetting flows as an interface formation process. *Submitted*, 2012. Preprint: http://arxiv.org/abs/1202.6463.

[12] J. E. Sprittles and Y. D. Shikhmurzaev. The dynamics of liquid drops and their interaction with solid of varying wettabilities. *Submitted*, 2012. Preprint: http://arxiv.org/abs/1202.3456.

[13] P. Joos, P. Van Remoortere, and M. Bracke. The kinetics of wetting in a capillary. *Journal of Colloid and Interface Science*, 136:189–197, 1990.

[14] H. Dong, W. W. Carr, D. G. Bucknall, and J. F. Morris. Temporally-resolved inkjet impaction on surfaces. *AIChE Journal*, 53:2606–2617, 2007.

[15] J. D. Paulsen, J. C. Burton, and S. R. Nagel. Viscous to inertial crossover in liquid drop coalescence. *Physical Review Letters*, 106:114501, 2011.