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Finite element simulation of dynamic wetting flows as an interface formation process

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ABSTRACT

A mathematically challenging model of dynamic wetting as a process of interface formation has been, for the first time, fully incorporated into a numerical code based on the finite element method and applied, as a test case, to the problem of capillary rise. The motivation for this work comes from the fact that, as discovered experimentally more than a decade ago, the key variable in dynamic wetting flows — the dynamic contact angle — depends not just on the velocity of the three-phase contact line but on the entire flow field/geometry. Hence, to describe this effect, it becomes necessary to use the mathematical model that has this dependence as its integral part. A new physical effect, termed the 'hydrodynamic resist to dynamic wetting', is discovered where the influence of the capillary's radius on the dynamic contact angle, and hence on the global flow, is computed. The capabilities of the numerical framework are then demonstrated by comparing the results to experiments on the unsteady capillary rise, where excellent agreement is obtained. Practical recommendations on the spatial resolution required by the numerical scheme for a given set of non-dimensional similarity parameters are provided, and a comparison to asymptotic results available in limiting cases confirms that the code is converging to the correct solution. The appendix gives a user-friendly step-by-step guide specifying the entire implementation and allowing the reader to easily reproduce all presented results, including the benchmark calculations.

1. Introduction

Reliable simulation of flows in which a liquid advances over a solid, known as dynamic wetting flows, is the key to the understanding of a whole host of natural phenomena and technological processes. In the technological context, the study of these flows has often been motivated by the need to optimize *continuous* coating processes that are routinely used to create thin liquid films on a product [1], for example, in the coating of optical fibres [2,3]. However, more recently, *discrete* coating, in particular inkjet printing of microdrops [4], has matured into a viable, and often preferable, alternative to traditional fabrication processes, e.g. in the additive manufacturing of 3D structures or the creation of P-OLED displays [5,6], and it is becoming a new driving force behind research into dynamic wetting phenomena. In most cases, such flows can be regarded as microfluidic phenomena, where a large surface-to-volume ratio brings in interfacial effects on the flow that are not observed at larger scales.

Obtaining accurate information about micro and nanofluidic flows experimentally is often difficult and usually costly so that, consequently, a desired alternative is to have a reliable theory describing the physics that is dominant for this class of

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flows and incorporate it into a flexible and robust computational tool which can quickly map the 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.

The discovery that no solution exists for the moving contact-line problem in the framework of standard fluid mechanics [7,8] prompted a number of remedies to be proposed, which are summarized, for example, in [9, ch. 3]. Modelling approaches range from continuum theories through to mesoscopic approaches [10] right down to molecular dynamics simulations [11], see [12,13] for discussions of the various modelling approaches. Of these, most, based on continuum mechanics, are what we shall refer to as 'conventional' or 'slip' models, in which the no-slip condition on the solid surface is relaxed to allow a solution to exist, with the Navier-slip condition [14] being the most popular choice.

As a boundary condition on the free-surface shape at the contact line, one has to specify the contact angle formed between the free surface and solid. In conventional models, this angle is prescribed as a heuristic or empirical function of the contact-line speed and material parameters of the system, e.g. [15]. A variant of this approach is to claim that the actual contact angle is static, whilst the observed 'apparent' angle is produced as a result of viscous bending of the free surface near the contact line [16]. Such models provide predictions that adequately describe experiments at relatively large scales, often around the length scale of millimetres. It is well established that on such scales many of the proposed models work equally well and that finding significant deviations between their predictions, and hence ascertaining which best captures the key physical mechanisms of dynamic wetting, is practically impossible [17,18].

A physical phenomenon that gives an opportunity to distinguish between different models came to be known under a 'technological' name of the 'hydrodynamic assist of dynamic wetting' (henceforth 'hydrodynamic assist' or simply 'assist'). The essence of this effect, first observed in high accuracy experiments on the curtain coating process [19,20], is that for a given liquid spreading over a given solid at a fixed contact-line speed, the dynamic contact angle can still be manipulated by altering the flow field/geometry, for example, in the case of curtain coating, by changing the flow rate or the height from which the curtain falls. This effect has profound technological implications as it allows the process to be optimized by offsetting the increase of the contact angle with increasing contact-line speed by manipulating the flow conditions and hence postponing air entrainment [19].

The dependence of the dynamic contact angle on the flow field has also been reported in the imbibition of liquid into capillaries [21,22], in the spreading of impacted drops over solid substrates [23,24] and in the coating of fibres [3]. However, in many of these flows it is yet unclear whether hydrodynamic assist actually occurs, or whether the free surface bends significantly beneath the spatial resolution of the experiments, whereas for curtain coating the hope of attributing assist to the poor spatial resolution of experiments has been quashed by careful finite element simulations which show that the degree of free-surface bending under the reported resolution of the measurements is too small to account for the observed effect and that conventional models cannot in principle describe this important physical effect [25].

Currently, the only model known to be able to even qualitatively describe assist [26,27] is the model of dynamic wetting as an interface formation process, first introduced in [28] and discussed in detail in [9]. This model is based on the simple physical idea that dynamic wetting, as the very name suggests, is the process in which a fresh liquid–solid interface (a newly 'wetted' solid surface) forms. Qualitatively, the origin of the hydrodynamic assist is that the global flow influences the dynamics of the relaxation of the forming liquid–solid interface towards its equilibrium state and hence the value of this interface's surface tension at the contact line, which, together with the surface tension on the free surface, determines the value of the dynamic contact angle. When there is a separation of scales between the interface formation process and the global flow, the 'moving contact-line problem' can be considered locally and asymptotic analysis provides a speed-angle relationship which is seen to describe experiments just as well as formulae proposed in other models [9]. However, in the situation where the scale of the global flow and that of the interface formation are no longer separated, the influence of the flow field on the dynamic contact angle will occur and hence no unique speed-angle relationship will be able to describe experiments. Then, the interface formation model becomes the only modelling tool, and, given that the processes of practical interest are free-surface flows under the influence of, at least, viscosity, capillarity and inertia, it is inevitable that, to describe such flows, one needs computer simulation, i.e. the development of accurate CFD codes, which, for the effect of hydrodynamic assist to be captured, have to incorporate the interface formation model.

Since the interface formation model came into wider circulation, there has been considerable interest, e.g. [29,23,24], in using it in its entirety as a practical tool for describing dynamic wetting phenomena, especially on the microscale. Review articles have also referred to the description of assist using this model as one of the main challenges in the field [12,13]. Although robust computational codes based on the conventional models already exist, e.g. [30,31], the extension of these codes to a numerical tool that incorporates the interface formation model is far from trivial. In particular, one has to solve numerically the Navier–Stokes equations describing the bulk flow subject to boundary conditions which are themselves partial differential equations along the interfaces and in their turn have to satisfy certain boundary conditions at contact lines confining the interfaces. These conditions determine the dynamic contact angle and hence influence the free-surface shape, which exerts its influence back on the bulk flow. Thus, the bulk flow, the distribution of the surface parameters along the interfaces and the dynamic contact angle that these distributions 'negotiate' become interdependent, with the dynamic contact angle being an *outcome* of the solution as opposed to conventional models where it is an *input*. This interdependency is, on the one hand, the physical essence of the experimentally observed effect of hydrodynamic assist to be described but, on