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Some dry facts about dynamic wetting

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Abstract. Some aspects of research into the dynamic wetting phenomenon are discussed where multidisciplinarity of the dynamic wetting community becomes a hindrance rather than an advantage. An instance of this is when the accumulated knowledge is cast into mathematical models that mix conceptual frameworks inherent in different levels of description. An attempt is made to establish some common reference points for the modelling and outline a research programme that utilizes the already obtained results and the complementary expertise of several sectors of the research community.

1 Introduction

An important role played by the dynamic wetting phenomenon in numerous applications makes it the subject of research in many disciplines, from chemistry to mathematics. Such a multidisciplinary approach has both advantages and drawbacks. Whilst the advantages of viewing dynamic wetting from different perspectives are rather obvious, the drawbacks are much less visible, and as a result very often a substantial part of research effort, especially experimental, appears to be misdirected and the outcomes misinterpreted.

In this paper, we will attempt to establish some common ground for the mathematical modelling of dynamic wetting and consider typical misconceptions that have recurred in the field for many years. This part should facilitate communication between researchers with different backgrounds and especially help a newcomer to the field to make sense of the growing body of literature on the subject. Then, we will discuss the physics that holds the key to the dynamic wetting phenomenon and outline a research programme where experimental, computational and molecular-dynamics/statistical physics approaches are brought together in a way that promises a substantial progress in how dynamic wetting is described quantitatively. Some of the issues raised below are discussed in more detail in [1], where one can also find a review of theoretical and experimental works on dynamic wetting and related phenomena.

2 A few words about mathematical models and modelling practices

The ultimate goal of research, in our case on dynamic wetting, is to arrive at a *theory* which would accumulate our understanding of the phenomenon in question.

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However, in what follows we will discard the term "theory" as too imprecise and much abused. "A reasoned supposition put forward to explain facts", which is how "theory" is defined by a dictionary, can refer to almost any set of views and beliefs regarding material and/or spiritual entities, and there are no clear criteria that could be applied to decide how "reasoned" a supposition is and hence whether or not it constitutes a "theory". We will be interested in a quantitative description of dynamic wetting and, since it is mathematics that deals with quantities, consider what forms the skeleton of any quantitative theory – a *mathematical model* of the phenomenon.

The term "mathematical model" needs clarification. Does an equation relating two quantities, say, the contact angle and the wetting speed, constitute a mathematical model of dynamic wetting? Or do we need a set of equations? If so, how many? More generally: what distinguishes a mathematical model of a physical phenomenon from just a mathematical object or a set of such objects, say, equations of various kind?

A short answer to the last question is that a mathematical model must have a certain structural form which employs the intrinsic logic of mathematics and therefore makes it possible to extract more information about the phenomenon from the model than what has been put into it. For example, a well-posed problem for a partial differential equation allows one to obtain the function *everywhere* in the specified domain whilst the "input" is only the equation, which is supposed to describe a certain physical law, and the appropriate set of initial and/or boundary conditions, which provide information additional to that incorporated into the equation. By contrast, an isolated element of mathematics can, at best, be just an approximating formula for already obtained experimental data, with its predictive power limited to simple interpolation/extrapolation.

In other words, once we decide what type of quantitative concepts are to be used to describe a phenomenon, it is mathematics that imposes the framework in which these concepts must be used and dictates the criteria that the resulting model must satisfy. As one might have expected, the expertise needed to formulate mathematical models of physical (chemical, biological, etc) systems is acquired via special training, both in the modelling and in mathematics itself, and does not come as a by-product of experimental, engineering or any other activity.

This remark is called for by the current state of mathematical modelling in the area of dynamic wetting, where multidisciplinarity has led to the recurring appearance of "models" that are incompatible with the very basics of the modelling frameworks they use. Ironically, whilst no-one would venture, say, into chemistry with one's own freshly-invented periodic table, researchers of all creeds and persuasions happily manipulate bits and pieces of mathematics, assembling them into "mathematical models" (calling them, of course, "theories") that would not stand even a passing glance of a mathematician. This tendency is so wide-spread that it is very rare that an experimental paper is not accompanied by a "mathematical model" of one sort or another. One can even come across monographs, full of formulas "describing" various features of "wetting and spreading" but without a single closed mathematical model, not to mention a clear-cut mathematical problem formulation.

All this amateurish model-building activity would have been relatively innocuous if it were not for the fact that it is misdirecting a substantial part of experimental research effort. As Einstein famously remarked, "it is the theory that decides what we can observe", and, when experiments are viewed through the prism of, or even designed to verify, a "theory" whose quantitative basis – the mathematical model – is fundamentally inconsistent, they can only obscure the picture and slow down developments in the field. For example, many experiments are carried out in a hope to decide, say, whether it is molecular dynamic simulations or fluid mechanics that is better suited to describe dynamic wetting, clearly not understanding that the very dichotomy is wrong – it is like proposing a mutually exclusive choice between individuals and the people these individuals form. Furthermore, there are numerous papers (e.g. [2]) contrasting "hydrodynamics" with "molecular kinetics", whilst the latter is just an *element* of the former, as it serves to provide inputs (reaction rates, etc) into an embracing continuum model.

Below, we outline the basics of the main modelling frameworks and discuss specifically some of the typical misconceptions in the modelling that recur in publications on dynamic wetting. All references in this brief overview are, of course, only representative, and their list can easily be expanded; a detailed review and analysis of works in the field can be found in [1].

3 Basics and reality of modelling

3.1 Modelling frameworks, their mathematical structure and constraints

One can distinguish the following three levels of description of fluid flow where the corresponding conceptual and mathematical frameworks have been developed, enabling one to produce closed mathematical models applicable to entire classes of fluid motion, as opposed to being *ad hoc* tools designed specifically for dynamic wetting.

Continuum mechanics considers a fluid's parameters as *field variables* and describes them in terms of smooth functions of spatial coordinates and time. This conceptual framework brings in the necessity to use partial differential equations into which physical laws have to be cast. In its turn, this dictates that the space must be split into the domains, referred to as "bulk phases", where these equations operate, and boundaries/interfaces, where one has to formulate boundary conditions that must reflect the physics *additional* to that incorporated into the bulk equations. The initial/boundary conditions must also be mathematically compatible with the bulk equations, i.e. they must provide the information to select a solution in the form that these equations require. The boundary conditions can themselves contain derivatives along the interfaces and in this case will themselves require boundary conditions at the (contact) lines that confine the interfaces.

Incorporating the physical reality into this framework is a nontrivial task but the pay-off is that the variables featuring in continuum mechanics do not need any sophisticated interpretation as they are supposed to be the ones that can be observed experimentally.

After the discrete (molecular) structure of matter was discovered and the appropriate methods of statistical physics developed, it has been shown that smooth field variables and the corresponding equations of continuum mechanics are the result of the so-called "thermodynamic" (or "continuum") limit, i.e. they appear as the 0th-order approximation as the ratios of molecular-to-macroscopic length and time scales go to zero. Therefore, mathematical models formulated in the framework of continuum mechanics should *not* contain any molecular length or time scales – these scales are negligible compared to the length/time scales on which equations of continuum mechanics operate. In these equations, all intermolecular effects must be incorporated into encompassing macroscopic (field) quantities. Conversely, all length and time scales that feature in such models are, *by definition*, macroscopic, not molecular. As we will see below, the understanding of these basic constraints alone helps to detect inconsistencies in many models.

Statistical physics makes explicit some of molecular effects by introducing, again, *field variables* describing statistical distributions of molecular properties. Such models are regularly applied to describe fluid flows, notably in the form of the lattice-Boltzmann method [3].

In the statistical physics framework, the picture becomes more detailed than what can be described by continuum mechanics at the expense of both the loss of relative transparency of how (macroscopic or microscopic) physics is incorporated and the loss of direct observability of the results, which now need an averaging procedure to be compared with experiments. The latter reflects the fact that, unlike continuum mechanics, models formulated in the framework of statistical physics operate on length and time scales *comparable* with those of intermolecular interactions and hence deal with a different space of independent variables.

Molecular dynamics simulations (MDS) consider the medium as a set of interacting molecules and, mathematically, come down to solving initial-value problems for very large systems of ordinary differential equations. This approach, essentially aimed at "mimicking nature" *on the molecular scale*, is simple conceptually but the price for this simplicity is not only formidable technical difficulties and the necessity to average (often very noisy) data to compare the simulation results with physical experiments; more importantly, it is the fact that the variables and equations used in MDS provide no conceptual macroscopic framework, not to mention relationships between macroscopic quantities, into which the obtained computational data could be cast. For example, the equations used and the data produced by MDS on their own give no indication that, say, a layer, where molecules of two neighbouring bulk phases interact, will – when viewed on the macroscopic level – possess the surface tension.

This last aspect becomes crucial for essentially new systems and/or phenomena where the already known macroscopic concepts and especially relationships may be insufficient or even misleading (as, for example, in [4]). Therefore, molecular dynamics simulations need macroscopic theoretical guidance that would help to make sense of the masses of computational data.

The frameworks outlined above are not limited to any particular medium or type of flow and, in principle, could be applied to describe a wide range of phenomena, from microfluidic flows to tsunami waves.

3.2 Typical misconceptions in the modelling of dynamic wetting

Thus, as discussed above, each of the three approaches has its own conceptual framework, mathematical structure and the characteristic length and time scales on which the corresponding concepts and equations apply. A model assembled by combining concepts plucked from different modelling frameworks is in danger of being inconsistent, and this will eventually show up in its properties. The brief overview below is intended to outline, in as simple terms as possible, some of the conceptual inconsistencies that have recurred in various couplings of continuum mechanics with other modelling approaches; it is by no means aimed at particular papers whose authors in many cases investigated the already formulated models and often themselves came across the points summarized below. However, the confusion persists with more inconsistent models appearing every year, so that it is worth at least to try to clarify at least some of the issues.

We begin by considering the mismatch of incompatible approaches in the so-called "hybrid atomistic-continuum formulation" [5,6]. This framework splits the "bulk" of the fluid into subregions, with molecular dynamics simulations used to describe the dynamics in the vicinity of the contact line and equations of macroscopic fluid mechanics employed further afield. In this case, one has both the fundamental conflict of scales and the conflict of concepts. Indeed, the size of the molecular-scale region where MDS operate is zero from the viewpoint of continuum mechanics. As we remember, the equations of continuum mechanics appear in the continuum *limit*, i.e.

as the number of molecules goes to infinity and their size to *zero* such that the product remains finite. Therefore, it is either the region where MDS operate should be viewed as a point from the continuum mechanics perspective or, for this region to be visible by fluid mechanics, its size and hence the size of the molecules there must be macroscopic. In other words, the approach either collapses or leads to absurdity.

The conceptual mismatch of the two models that form the "hybrid" manifests itself, in particular, at the interface separating the two subregions: the MDS data can be averaged to produce input (i.e. boundary conditions) for continuum equations at the separating interface but there is no way of "uncooking the egg" and justifiably extract such data from the continuum-mechanics solution to produce an input into the MDS. In other words, after the continuum limit is taken, the detailed information about the molecular motion is lost and there is no way to recover it. This fundamental problem cannot be resolved by replacing the separating interface with a "transition region" where matching is supposed to take place (see [7] for a recent review): the two models that form the hybrid operate on non-overlapping scales and *with different concepts*, and this cannot be helped by mimicking the method of matched asymptotic expansions[1].

A very popular way of producing "hybrids" is to "supplement" a model formulated in the framework of continuum mechanics with intermolecular forces [8–14], which then enter the model in the form of a body force. A remark that such "hybridization" introduces a molecular-dynamics concept and a molecular length scale into a macroscopic continuum model meets a routine "counter-argument" that "intermolecular forces exist", so that clearly more explanation is needed.

It is helpful to begin with a simple question: does the classical fluid-mechanical model, say, the Navier-Stokes equation for a viscous incompressible fluid, account for the existence of molecules and intermolecular forces? If not, then one can only marvel at how such model can describe anything at all. The fact is that a fluid-mechanical model does account for *all* intermolecular interactions as it incorporates them into its macroscopic concepts (stress, transport coefficients, parameters of constitutive equations, etc). Therefore, if some (macroscopically represented) intermolecular forces are added on top of a fluid-mechanical model, this means that these forces are *counted twice*. In order to explicitly add intermolecular forces to a fluid-mechanical model and avoid double-counting of the same physical effects, one must "subtract" these forces from the macroscopic parameters and variables that already incorporate them. An exposition of how to begin doing this subtraction and the level of difficulties involved even in the simplest case of a liquid film at rest can be found in [15], where it was shown that as even some of the intermolecular forces that give rise to the surface tension are "brought into the open", i.e. explicitly accounted for, the "remainder" of the surface tension is no longer equal to the surface tension used in macroscopic fluid mechanics. The gist of this argument is reproduced in [1, p. 389].

A telling detail of the continuum models "supplemented" with intermolecular forces is the non-mathematical use of mathematics that they require. The intermolecular forces added on top of a fluid-mechanical model are singular in the near field, i.e. as one approaches the solid boundary. In order to remedy this obvious flaw, these forces are truncated at a molecular distance from the solid surface. This truncation, "scientifically" referred to as "cut-off", not only introduces another molecular length scale into a continuum model; it employs an operation that has nothing to do with

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[1] The method of matched asymptotic expansions is just a technique of finding approximate solutions of mathematically formulated problems, which, in principle, could be solved using other methods, analytical or computational. This method is by no means a modelling tool, especially if one tries to "match" incompatible concepts.

mathematics. In mathematics, functions are not truncated at will, i.e. on the basis of considerations that lie outside mathematics. Interestingly, the "cut-off" arguments can be found even in purely fluid-mechanical papers where the model is not properly specified and hence requires non-mathematical "arguments" to hide the loose ends (e.g. [16]). As always, when a mathematical issue is countered using non-mathematical means, one should look for a flaw in the modelling.

Another attempt at "hybridization" is the use of the so-called "diffuse-interface models" [17–24]. These models take Cahn-Hilliard's, i.e. essentially van der Waals', approach to the modelling of phase transitions and couple it with the continuum mechanics formulation. The result is an addition to the Navier-Stokes equations of a term intended to make them applicable across the fluid-liquid interface, which now becomes a transition layer of a finite thickness, as well as in each of the bulk phases. Thus, the interface's thickness, which is determined by intermolecular forces from the two bulk phases and is, as every chemist knows, on a molecular scale, is now made macroscopic and described in the continuum mechanics framework. This is despite the fact that this framework is based on the thermodynamic limit in which, by its definition, molecular dimensions are invisible and hence all interfaces must be sharp.

An obvious manifestation of the inconsistency of the diffuse-interface approach is in the flow field near the three-phase-interaction zone, i.e., macroscopically, the contact line. The defining feature of what is, physically, an interfacial layer is that the intermolecular forces experienced by molecules in there from the molecules of the two bulk phases are singularly strong compared with forces operating in the bulk hydrodynamics, and, as a result, the interfacial layer's thickness is on the molecular scale, i.e. singularly small compared with dimensions characterizing the bulk flow. It is the interplay of these two singularities that makes the interface a fluid-mechanical object in its own right, with its own physical properties such as the surface tension, and ensures the capacity of the interface to be impermeable, i.e. to be a *boundary* for the bulk flow. When the "diffuse-interface models" turn the sharp fluid-liquid interface into a diffuse transition region of a finite thickness, they reduce singularly strong intermolecular forces to the level of hydrodynamic forces, and, as a result, such an interface becomes *permeable*. It simply cannot resist the motion imposed by the drag from the solid, so that near the contact line the displaced fluid goes straight through such an interface into the displacing one [17,18,24]. A related effect is that, if one reduces the interfacial layer's thickness, the speed of propagation of the liquid-fluid interface also reduces [21,22], so that in the limit of a sharp interface the contact-line motion simply stops unless one keeps the diffusion-induced slip to prevent this from happening [24]. It is noteworthy that in this last case the Navier-Stokes equations in the bulk remain altered so that the "sharp-interface limit" considered in [24] is *not* the continuum limit of classical fluid mechanics.

Computers add their own flavour to the modelling as there appear models that (a) by-pass the stage of properly formulating the problem mathematically and go straight into creating a "numerical model" (e.g. [25]), (b) "circumvent" the moving contact-line problem outlined in §4 below by introducing "numerical slip", especially popular and often unnoticed in the volume-of-fluid method (e.g. [26]), (c) interpret a huge numerical error in computing the contact angle as a physical effect (e.g. [27]), etc. These trends, which are often present in the same paper (e.g. [25,27]), produce results that depend on numerical implementation and parameters of calculations [28]. For example, if the size of the mesh cell over which computer introduces "numerical slip" goes down, the contact-line motion slows down – and in the limit stops altogether; the computed contact angle differing by tens of degrees from the angle that the code tries to impose [27] will change should the computational mesh be refined; etc. In other words, instead of being an instrument for solving a mathematically-posed problem, the computer becomes an active contributor, adding numerical artifacts to the properties of the physical phenomenon under investigation. For obvious reasons, here we will not discuss this kind of modelling.

It is necessary to emphasize that there have always been close and fruitful interaction between the three modelling frameworks outlined in §3.1; however, this interaction has nothing to do with "importing" concepts into the frameworks where they do not belong.

4 Dynamic wetting as a modelling problem

As discussed in §3.1, the dynamic wetting phenomenon can be considered on different length and time scales. On what scale does its theoretical description become a *problem*? The answer is given by the very term "wetting" as it is essentially macroscopic. Indeed, a molecule does not "wet" a solid surface; it simply interacts with molecules of the solid, when it happens to be close to it, as well as with its fellow molecules of the liquid, being blissfully unaware that it takes part in what, on a macroscopic scale, is seen as "dynamic wetting". Similarly, there is also no "contact angle" on the molecular scale: this concept emerges as we "zoom out" (this "zooming out" is essentially what the thermodynamic limit is all about) and start seeing interfacial layers as sharp geometric surfaces and hence can define the angle they form. In other words, it is only when the flow is viewed macroscopically, we have "dynamic wetting" and a specific *problem* of how to describe it mathematically.

The difficulties of describing dynamic wetting mathematically are two-fold.

(i) As can be shown analytically [1,29], the corresponding problem formulated in the framework of classical fluid mechanics, with the no-slip boundary condition on the solid surface, *has no solution*. In other words, no distribution of velocity and pressure exists that would simultaneously satisfy the Navier-Stokes equations and all the classical boundary conditions on the free surface and the solid boundary with the contact line moving across the solid. This is a mathematical fact.

(ii) Even if the above difficulty, known as "the moving contact-line problem", is resolved, to specify the shape of the flow domain where the Navier-Stokes equations are to be solved, one has to specify the angle formed at the intersection of the two parts of its boundary, i.e. the free surface and the solid. This angle, referred to as the *dynamic* contact angle to emphasize that it corresponds to the moving contact line, is part of what is to be described in a mathematical model regardless of a quite separate issue of what angle is actually measured in experiments whose spatial resolution is, of course, limited.

Thus, since "dynamic wetting" is an essentially macroscopic phenomenon, it is necessary to formulate a mathematical model that would be consistently within the framework of continuum mechanics. It should address the two issues outlined above and provide a quantitative description of the macroscopic features of the phenomenon observed experimentally. The description of dynamic wetting in the framework of MDS or statistical physics does not encounter specific difficulties associated with this type of flow, and we will show how these approaches can answer questions that the macroscopic modelling poses and provide information that is beyond its reach.

5 "Slip models" and experimental "moment of truth"

As was identified early on [30,31], mathematically, it is the no-slip condition that gives rise to the moving contact-line problem (understood at the time as a problem of “nonintegrable shear-stress singularity”[2]), and a lot of effort has gone into developing the so-called “slip models”. Representative examples of such models can be found in [32–44]. The basic idea of slip models is to use various physical justifications, and sometimes even the argument of mathematical convenience, to replace the no-slip condition with some form of slip. In a slip model, the second aspect of the dynamic wetting problem is treated completely independently of the first one, and it is simply assumed that the dynamic contact angle is a function of the contact-line speed as well as material constants of the contacting media. This approach allows one to arbitrarily couple the slip condition plucked from one slip model with the velocity dependence of the dynamic contact angle plucked from another to produce a new model (see [45, §9] for a schematic review). It is noteworthy that continuum models “supplemented” with intermolecular forces considered in §3.2 address the two sides of the dynamic wetting problem in exactly the same way as “slip models” [10] and hence the only contribution they make is the conceptual inconsistency we discussed earlier.

From a theoretical viewpoint, one can pick a number of flaws in slip models, from the contact line always being a stagnation point, which results in the flow kinematics different from what is observed experimentally [46–48], to the independent way in which the two sides of the same physical phenomenon are treated; however, at the very least, unlike “models” outlined in §3.2, each of the slip models is formulated consistently within the framework of fluid mechanics and produces well-posed mathematical problems. It is noteworthy, however, that although the slip length that the slip models introduce in one form or another must be, by definition, macroscopic, their comparison with experiment could be in conflict with this requirement [49].

The velocity dependence of the dynamic contact angle that the slip models use as an input ultimately comes from experiments: whatever form of the function is assumed, its parameters are determined by fitting the curve to the appropriate experimental data. Given that it is always possible to approximate the velocity dependence of the dynamic contact angle obtained experimentally and then plug the obtained dependence into a slip model to “describe” this (or similar) experiment, one has to ask a question of principle: is it possible to perform an experiment (more generally: indicate a class of experiments) that would test the very basis of slip models, their approach as a whole?

One such experiment should address the core issue as to whether the contact angle is indeed a mere function of the contact-line speed and hence can be used as an input into a model or whether it is an *output* determined by the flow field/geometry. In other words, the question is whether for a *fixed* contact-line speed the contact angle can be varied by manipulating the flow field/geometry sufficiently close to the moving contact line. If this is the case, then *no* function relating the contact angle and the contact-line speed will ever enable slip models to describe the behaviour of the dynamic contact angle.

Such an experiment has been reported in [50,51], where it was demonstrated that, for a given solid-liquid-fluid system, there is indeed no unique function that would relate the dynamic contact angle and the contact-line speed. As shown in [52], the situation cannot be saved by interpreting the experimental results in terms of the so-called “apparent” contact angle, a concept intended to account for the finite precision

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[2] The moving contact-line problem is usually referred to as “the problem of nonintegrable shear-stress singularity”, a notion that comes from an already simplified formulation of the problem [1, p. 102]. This mathematical, as opposed to physical, viewpoint on the problem is, perhaps, responsible for the ideology of “slip models” that dominated the field for many years.

of measurements and not inherent in the actual problem formulation, no matter how this “apparent” angle is defined.

The effect of the dependence of the dynamic contact angle on the flow field (to which the contact-line speed is a major but only one contributing factor) came to be known as “hydrodynamic assist of dynamic wetting” [53], owing its name to industrialists who are concerned with manipulating the flow field to promote wetting. Fluid dynamicists, perhaps, would have termed it “hydrodynamic resist”, as they have continued to ignore these and similar experimental findings (e.g. [49,54]) for many years.

Thus, as we have seen, neither “hybrids” of various kind nor mathematically-motivated slip models can be regarded as addressing the dynamic wetting problem even on the qualitative level. This outcome could be a consequence of the fact that the formidable difficulty of finding an adequate mathematical description of the dynamic wetting phenomenon has been treated as a unique “one-off” problem, with no serious attempt to embed this problem into a wider physical context and relate it to other physical processes that might share the same underlying physics. When a section of the scientific community starts acting like a sect, it is always a recipe for stagnation.

6 Physical essence of dynamic wetting

So, is there a physical mechanism that could be unquestionably put forward as the essence of dynamic wetting?

The answer is contained in the term itself. By its very definition, “dynamic wetting” means a process by which an initially dry solid surface becomes “wet”. In other words, it is the process of *formation* of a new liquid-solid interface, i.e. a “freshly wetted” solid surface. To deny this would mean to deny that a liquid ever gets in contact with a solid. There are, of course, other mechanisms by which a solid surface can become wet, e.g. evaporation-condensation, but these mechanisms are “additional”: even in their absence dynamic wetting still takes place when, say, a non-volatile liquid is poured down onto an initially dry solid surface. In other words, “dynamic wetting” and “the formation of a fresh liquid-solid interface as a result of the liquid spreading over the initially dry solid” are essentially synonymous expressions, and all other effects come on top of this basic physics of interface formation. Therefore, there is no chance that a mathematical model that does not have the physics of interface formation at its core will ever be able to adequately describe the dynamic wetting process[3].

It is now immediately clear that dynamic wetting is by no means a unique “one-off” phenomenon; one can point out many processes where interfaces form or disappear, so that dynamic wetting becomes just one in a wide class of fluid flows that share the same underlying physics. For example, coalescence and breakup of drops, rupture of films, expansion of a bubble are all flows where interfaces form or disappear. Interestingly, all problems considered in textbooks on fluid mechanics deal with interfaces that have already been formed, and whenever one comes across a phenomenon where interface formation (or disappearance) is important, there appears a difficulty in many ways similar to the “moving contact-line problem” [1].

The origin of the contact angle being “dynamic” and of the effect of “hydrodynamic assist” now become clear as well. The contact angle θ is introduced into

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[3] Clearly, a model aimed at describing additional physical effects (evaporation-condensation, influence of surfactants, etc) should be based on the correct model of dynamic wetting itself, i.e., when these effects are taken out, such a model should reduce to the model of dynamic wetting as an interface formation process.

macroscopic fluid mechanics via the Young equation which expresses the balance of forces acting on the contact line tangentially to the solid,

$$\sigma_1 \cos\theta = \sigma_3 - \sigma_2, \tag{1}$$

where σ_i $(i = 1, 2, 3)$ are the surface tensions in the three contacting interfaces. This equation dictates that the contact angle variation can *only* be caused by variation of at least one of the surface tensions[4]. When the contact line is moving, the liquid-solid interface in its immediate vicinity is forming, so that the surface tension there differs from the equilibrium surface tension this interface will have away from the contact line. As a result of the surface tension at the *moving* contact line being out of equilibrium, the *dynamic* contact angle is not equal to the static one, i.e. the one determined by equilibrium surface tensions in all contacting interfaces. Furthermore, since the "material" for the formation of the fresh liquid-solid interface is provided by the bulk flow, the surface tension distribution and hence the dynamic contact angle depend on the bulk flow in the vicinity of the contact line, and this is what "hydrodynamic assist of dynamic wetting" is all about.

Naturally, the main factor determining the flow field is the velocity at which the contact line moves with respect to the solid, so that, in the absence of other boundaries or sources of disturbance of the flow field located closely enough to the contact line, one ends up with a seemingly universal velocity dependence of the dynamic contact angle. However, this only disguises the full picture that emerges once the scale of the flow reduces, and it is this area of microfluidic flows, where capillarity and the effect of hydrodynamic assist of dynamic wetting become the dominant factors.

7 Multidisciplinarity in the modelling of dynamic wetting

As explained in §4, the modelling of dynamic wetting as a macroscopic phenomenon must be carried out consistently in the framework of macroscopic fluid mechanics, and the key physics of this phenomenon is identified as the physics of interface formation. Starting from these two points, the simplest mathematical model that consistently incorporates the physics of interface formation into the conceptual framework of fluid mechanics has already been developed, analyzed in the limiting cases and verified using available experiments. This work, initiated in [55] and then published in a series of papers over the period of almost 20 years, has now been summarized in a monograph [1]. Thus, the problem, as outlined in §4, appears to be resolved.

As is invariably the case in science, the obtained result becomes just a starting point from which several interlinked research routes open up. Below, we briefly outline these routes, emphasizing how the specific expertise of different disciplines involved in research on dynamic wetting could have a synergic effect.

7.1 Computational Fluid Dynamics (CFD) route

The first route is the use of the already developed simplest model [1] for practical purposes, where new effects could be discovered, and as a guide for theoretical and experimental research. This makes it necessary to implement the model into full-scale

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[4] Here we do not discuss such ideas as attributing these variations to the bulk stresses acting on the contact line or the "friction" between the moving contact line and the solid; such views, as well as the notion of a "line tension", are fundamentally in conflict with the continuum limit and hence incompatible with the modelling framework into which such notions are inserted.

numerical codes capable of handling complex flows for a wide range of controlling parameters. Then, one would be able, firstly, to make predictions regarding practically important flows occurring in various engineering applications. As has already been shown, the interface formation model, where, contrary to the slip models, the dynamic contact angle is an *output*, is capable of describing experimental data for a series of fluids without ad hoc adjustments [1, p. 252] and incorporates the effect of "hydrodynamic assist" [1, p. 264], so that the already known properties of the model should make the code that fully incorporates it useful for engineering purposes.

Secondly, such a code would make it possible to interpret the results of more elaborate experiments than those that have already been analyzed. Thirdly, a sufficiently flexible numerical platform could become a vehicle for testing generalizations of the simplest model suggested by the analysis of results of experimental and MDS/statistical physics studies.

Given that even the simplest interface formation model [1] provides boundary conditions for the Navier-Stokes equations that are themselves differential equations along interfaces coupled with the bulk flow, its proper implementation into numerical codes is a very non-trivial task, especially for the situations where "hydrodynamic assist of dynamic wetting" is important. This task requires a high level of expertise in computational fluid dynamics as well as in applied mathematics.

7.2 MDS/statistical physics route

The second, and more fundamental, direction of research is the further development of the model itself, based on what can now be obtained using molecular dynamics simulations and the methods of statistical physics, notably the lattice-Boltzmann modelling. As mentioned in §3.1, MDS and statistical physics both employ averaging to produce a macroscopic quantity and hence both require a macroscopic conceptual framework into which their data could be cast. This framework is now provided by the developed interface formation model.

Basically, in MDS and statistical physics all macroscopic formulas, so often taken for granted, must be "earned", i.e. one has to compute all macroscopic quantities such formulas contain independently and verify that the formulas indeed hold. Then, the methods developed for computing all these macroscopic quantities can be used to investigate dynamic situations, where the quantities regarded as constants could become variables.

The research programme that the findings of the interface formation model suggest for MDS is almost entirely suitable also for the statistical physics research, so that below we refer to MDS simply for brevity. The gist of such a programme can look as follows:

1. The ability of MDS to describe the bulk flows, i.e. to reproduce the known exact solutions of the Navier-Stokes equations and/or, for a more robust validation, solutions obtained numerically, say, using available CFD codes, is the first to be verified. Such checks are routine in MDS but very often they are limited to the Couetta-Poiseuille flow, which is not a very informative case.
2. To be able to describe capillary flows, it is necessary to ensure that the surface tensions can be computed locally. For the surface tension on the free surface it is sufficient to verify Laplace's formula relating the surface tension σ on the free surface of a spherical drop with its radius R and the pressure p inside: $p = 2\sigma/R$.
3. Once the surface tension on the free surface is "earned", it is necessary to develop a method of calculating the surface tension in the liquid-solid interface and then verify it by checking whether the Young equation (1) holds, say, for a drop sitting on a solid surface.

4. At this stage, the following lines of inquiry based on the conceptual framework of the interface formation model open up.
   (a) The first is to study the dynamics of wetting, for example, (i) detect and investigate the surface-tension-relaxation zone near the contact line where the formation of the liquid-solid interface takes place, (ii) verify the generalized Navier condition [1, pp. 198, 202], which in the model relates the velocity difference across the liquid-solid interface not only to the tangential stress acting on this interface from the bulk of the liquid, as the Navier-slip condition does, but also to the gradient of the surface tension along this interface, (iii) examine the state of the free surface as the flow drives it into the contact line, etc. It is noteworthy, that the surface-tension-relaxation zone has already been detected using the lattice-Boltzmann method [56], and a recent MDS study [57] gives further evidence for the effect of "hydrodynamic assist".
   (b) The second line of inquiry is to investigate the dynamics and thermodynamics of interfaces. This is a fundamental problem, and molecular dynamics simulations is a tool ideally suited for the task. With regard to dynamic wetting, an important issue is how the surface tension depends on other surface properties, in the first instance, the surface density. This is the starting point for obtaining realistic *surface equations of state* analogous to the equations of state used in thermodynamics of the bulk phases. The characteristic time (or times) associated with the interface formation is another topic, where MDS could provide vital information, especially for complex multicomponent systems.
   (c) The obtained information would allow one to develop the simplest interface formation model mentioned earlier into a more sophisticated macroscopic description of the process, especially with regard to the surface equation of state and possible non-Newtonian effects in the surface hydrodynamics. The developed macroscopic model in its turn would help to model and predict macroscopic effects that could be specifically looked for in experimental research.

7.3 Experimental route

On the experimental side, the identified physics of dynamic wetting as that of interface formation allows one to widen the class of flows whose investigation would highlight various aspects of this physics. This embedding of dynamic wetting into a wider context would also allow cross-checking of the parameter values obtained from experiments on different flows with formation or disappearance of interfaces.

Of particular interest in this respect is the convergent flow near a free surface that leads to the formation of two-dimensional singularities of curvature [58]. These singularities used to be thought of as "cusps", but a close inspection shows that they are actually corners [59]. This is a rare example of a *steady* flow with a disappearing interface, where, as shown by experiments [60], the free surface is swept into the bulk of the liquid and disappears as it loses its specific "surface" properties, such as the surface tension. Furthermore, this flow can be viewed as essentially representing the "hydrodynamic assist of dynamic wetting" in its purest form, i.e. with the dominant influence of the forced contact-line motion removed.

For almost all nontrivial interface formation/disappearance flows, including the one mentioned above, the main difficulty is not in measuring their observable features; it is in interpreting the results of measurements, since the flows involved are rather complex, and hence no "simple formula", like the velocity dependence of the contact angle so often "tested" in experiments on dynamic wetting, will be anywhere near what needs to be described. This situation makes it absolutely necessary to develop powerful CFD platforms capable of handling complex flow geometries and incorporating more and more sophisticated models for the interfacial physics. This makes the experimental route closely linked to the CFD route outlined earlier.

Thus, the developed fluid-mechanical model[5] of flows with forming interfaces [1] resolves and closes the dynamic wetting problem as described in §4, but at the same time it opens up several interlinked directions of research where interaction between different sections of the research community becomes vital for success.

8 Concluding remarks

The multi-faceted nature of the dynamic wetting phenomenon calls for a multidisciplinary approach to its study. However, when it comes to putting experimental findings into the form of a quantitative theory, the dynamic wetting community encounters the kind of difficulties that have already been experienced by the community that embarked on the construction of the Tower of Babel. As argued in the present paper, a way of avoiding a similar outcome is to use the expertise of participants as complementary, with interaction *at* the interfaces between disciplines, as opposed to making dilettante contributions *across* these interfaces. The history of science is already full of anecdotes about blunders that even great scientists have made when venturing outside their area of expertise, and this should perhaps caution against audacious cross-disciplinary interventions.

The research programme outlined in the present paper shows how multidisciplinarity of research on dynamic wetting could become its strength, produce independently verifiable results and save a considerable amount of resources and time. The interactive structure of this programme utilizes the specific expertise of different sectors of the dynamic wetting community, giving them a common language and a common objective. It also ensures that the results, ultimately incorporated into flexible CFD platforms, become transferable and could be channeled into practical engineering applications.

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[5] It should be pointed out that sometimes even the basic fact that the model in [1] is formulated strictly in the framework of classical fluid mechanics is not understood. For example, in [23] it is referred to as if it considers interfaces of a finite thickness despite the fact that it has been emphasized many times, starting from [55], that all interfaces are modelled as sharp and no “thickness of an interface” features anywhere in the model.

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