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THE ASYMPTOTIC DESCRIPTION OF THE MOVING CONTACT LINE AS A TEXTBOOK SINGULAR PERTURBATION PROBLEM: CRACKING AN OLD NUT

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Abstract: *We revisit the classical matched asymptotic analysis of the moving contact line, a problem that has received considerable attention for several decades. The prevalent solution to the problem, considered classical now, involves a three-region asymptotic structure with an intermediate region deemed necessary as the inner and outer regions do not directly match. In this work, we describe why this classical solution is not the end of the story. In fact, we show that the textbook singular perturbation method of matching overlapping outer and boundary layer regions directly applies even to the moving contact line problem, thus correcting a several decades misconception.*

1 INTRODUCTION

In perturbation theory, a singular perturbation problem occurs when model equations are reduced by setting a small parameter to zero, and the resulting solution no longer holds for the physical problem being modelled [1, 2].

Often a singular perturbation problem arises when the terms including the highest derivative in the governing differential equation are neglected. However amongst other cases, they may also occur where boundary conditions are no longer satisfied due to the approximation.

The moving contact line problem is an example of this second case. A moving contact line occurs where the interface between two fluid phases is in contact with a solid substrate, and the interface between the fluids moves relative to the solid due to some physical process. For example, this motion can be due to chemical driving forces in droplet spreading, forced wetting when dipping a substrate into a fluid, or it can be driven by gravitational forces. We refer to several recent reviews on the moving contact line problem [3, 4, 5]. The first studies of the moving contact line problem were presented by Moffatt [6] and Huh and Scriven [7].

The moving contact line problem is a singular perturbation one due to the following: When the usual continuum mechanics equations (e.g. Navier-Stokes) are considered with a sharp interface between two immiscible fluids, and with the classical no-slip boundary condition applied at the wall, the contact line *cannot* move. This is as the solution to the equations will claim that the motion requires infinite energy to proceed, giving infinite values of stresses and pressure, and a multi-valued velocity at the contact line.

There are many approaches that change either the boundary conditions or the governing equations to alleviate this singularity, many of which are discussed in a recent paper by the present authors [8].

The crucial point for this work, however, is that while all of the possible alterations act to overcome the singularity of the pressure in the vicinity of the contact line, the classical equations still dominate in most of the domain away from the contact line. All of these alterations, whether ad-hoc or with physical basis, give significant effects near the contact line in essentially a *boundary layer*. The remaining domain is the core (outer) flow, which is still well modelled (at leading order in this singular perturbation problem) by the classical equations.

In this work, we frame the moving contact line as singular perturbation problem with perturbation parameter λ, where λ is a microscopic length scale. On scales of $O(1)$, the classical continuum mechanical equations hold. On scales of $O(\lambda)$ we are in the inner ("boundary-layer") region where something else occurs, and an overlap and matching happens somewhere in between.

1.1 Why hasn't this been performed already?

A natural question is why this approach is not already well discussed in the literature. To understand this, we introduce the capillary number Ca, which can be interpreted in the current setting as the dimensionless contact line velocity. In most works [9, 10], the singular perturbation in λ is subsequently followed by a regular perturbation in Ca. This is as many works assume slow contact line motion ($\mathrm{Ca} \ll 1$). In this procedure, only the leading orders in both Ca and λ expansions are retained, and an overlap between outer and inner regions does not occur. For this reason, in the literature a third intermediate region is introduced which bridges the "boundary layer" (contact line) and outer regions. Concluding, the moving contact line has been treated as a *special case*, rather than a usual textbook singular perturbation problem.

1.2 What is the textbook solution, instead of this special case treatment?

Having understood that it is the interplay between Ca and λ that causes the breakdown of the overlap, the textbook solution becomes clear. The equations should not be truncated in the Capillary number Ca, but instead an infinite series of significant terms be found, so that the matching between inner and outer regions (defined only through the singular perturbation problem in λ) can be performed. In what follows, the existence of a direct overlap region will not only be shown analytically, but will also be illustrated with numerical computations, in which the overlap becomes increasingly visible as more terms in the Ca series are retained.

Our method is described here. Further details, and specific examples, can also be found in another publication by the present authors [11].

2 THE MAIN RESULT

Our main result is that matching between outer and inner regions indeed occurs in a standard textbook fashion for moving contact line problems. An overlap exists, but formulating the solutions as a regular perturbation in Ca and only retaining a finite number of terms (as commonly done) leads to the breakdown of this overlap. If we instead regroup the series of solutions by isolating and retaining the terms that cause this breakdown when omitted, thus incorporating this infinite series of non-negligible terms into our solution, the overlap region persists.

In slow motion of contact lines that we consider, the behaviour of the free-surface slope in outer and inner regions can be written in a general form as

$$H'_{\text{out}}(x) \sim \Theta_{\text{out}} + \mathrm{Ca}\left[f(\Theta_{\text{out}})\ln x + c_{\text{out}}\right] + O(\lambda, x, \mathrm{Ca}^2, \mathrm{Ca}\, x\ln x), \qquad \text{as } x \to 0, \tag{1a}$$

$$H'_{\text{in}}(x) \sim \Theta_{\text{in}} + \mathrm{Ca}\left[f(\Theta_{\text{in}})\ln\frac{x}{\lambda} + c_{\text{in}}\right] + O\left(\lambda, \mathrm{Ca}^2, \frac{\lambda\,\mathrm{Ca}}{x}\ln\frac{x}{\lambda}\right), \qquad \text{as } \frac{x}{\lambda} \to \infty. \tag{1b}$$

Here $x \geq 0$ is the spatial variable ($x = 0$ giving the location of the contact line), H' denotes the slope of the free surface. The parameters $\{\Theta_{\text{out}}, \Theta_{\text{in}}, c_{\text{out}}, c_{\text{in}}\}$ and the function f are different for each specific situation being considered, but could depend on quantities such as the droplet radius (if a droplet is considered) or viscosity ratio of the fluids in contact. The variables H' and Θ have been used, rather than more common choices in the literature, to show how this analysis is general, and not only for e.g. thin-film problems.

The difficulties arise when some of the neglected terms are no longer small, which occurs when as $x \to 0$ from the outer region, terms of $O(|\mathrm{Ca}\ln x|)$ become $O(1)$ before the region of validity of the inner region expansion is approached. This means that neglecting all terms of $O(\mathrm{Ca}^2)$ in the expansions (1) is not uniformly possible. Similar reasoning suggests that terms $(\mathrm{Ca}\ln x)^n$ for any positive integer n, may not be neglected. We define the region where overlap occurs by $|\,\mathrm{Ca}\ln x| = O(1)$. Using this, we consider the outer expansion (1a), and regroup the terms to retain any that will become significant in an expansion of the form

$$H'_{\text{out}}(x) \sim \sum_{n=0}^{\infty} a_n (\mathrm{Ca}\ln x)^n + \mathrm{Ca}\sum_{n=0}^{\infty} b_n (\mathrm{Ca}\ln x)^n + O(\mathrm{Ca}^2, x, \mathrm{Ca}\, x\ln x, \lambda), \quad \text{as } x \to 0. \tag{2}$$

Here two terms have been retained in an expansion in Ca, which will mean achieving a correction of $O(\mathrm{Ca}^2)$ in our final result.

Now considering (2) in the form of (1a) we obtain

$$H'_{\text{out}}(x) \sim \Theta_{\text{out}} + \mathrm{Ca}\left[f(\Theta_{\text{out}})\ln x + c_{\text{out}}\right] + \sum_{n=2}^{\infty} a_n(\mathrm{Ca}\ln x)^n + \sum_{n=1}^{\infty}\mathrm{Ca}\, b_n(\mathrm{Ca}\ln x)^n + O(\mathrm{Ca}^2, x, \mathrm{Ca}\, x\ln x, \lambda), \quad \text{as } x \to 0, \tag{3}$$

where now all terms significant in the outer and the overlap region, are retained, and the neglected terms will always be negligible in comparison to those retained. To more clearly write the analysis to follow, we introduce the variable

$$z = \mathrm{Ca}\ln x, \tag{4}$$

which is an $O(1)$ quantity in the overlap region, and we collect terms in (3) to obtain

$$H'_{\text{out}}(z) \sim S_0(z) + \mathrm{Ca}\, S_1(z) + O(\mathrm{Ca}^2, \mathrm{e}^{z/\mathrm{Ca}}, z\mathrm{e}^{z/\mathrm{Ca}}, \lambda), \quad \text{as } x \to 0, \tag{5a}$$

$$\text{where} \quad S_0(z) = \Theta_{\text{out}} + f(\Theta_{\text{out}})z + \sum_{n=2}^{\infty} a_n z^n, \qquad S_1(z) = c_{\text{out}} + \sum_{n=1}^{\infty} b_n z^n. \tag{5b}$$

We now need to determine forms of $S_0(z)$ and $S_1(z)$. Theoretically, all of the non-negligible terms in (3) could be determined through an iterative procedure to find solutions at higher orders of Ca, but alternatively we can use physical reasoning to describe the dominant balance that holds throughout the overlap between outer and inner regions.

The overlap occurs between regions of macroscopic hydrodynamical equations and microscopic inner equations. In the overlap, there will be a balance of viscous and surface tension effects, defining the mesoscopic hydrodynamic regime such as described by [4]. In practice, the balance comes as these contributions affect the free surface through the normal stress boundary condition, which leads to

$$\frac{dH'}{dz} = \frac{x}{\mathrm{Ca}}\frac{dH'}{dx} = f(H') + O\left(\mathrm{Ca}^2; \frac{x}{\mathrm{Ca}}, x\ln x; \frac{\lambda}{x}\ln\frac{x}{\lambda}\right), \tag{6}$$

which is also suggested by the behaviour of $d_z H'_{\text{out}}$ in (5). We further note that (6) is equivalent to the intermediate region equations found in the literature but we instead note that it holds for both outer and inner regions, and throughout their overlap—rather than being a separate entity. Hence from (6) we see that what is usually known as the intermediate region is in fact an overlap region, as it includes the limiting behaviour from both outer and inner regions, and that the breakdown of the overlap in the literature is an artifact due to the two-parameter expansion in λ and Ca.

For the outer region slope, (6) is

$$\frac{dH'_{\text{out}}}{dz} = f\left(H'_{\text{out}}\right) + O(\mathrm{Ca}^2, \mathrm{Ca}^{-1}\,\mathrm{e}^{z/\mathrm{Ca}}), \tag{7}$$

subject to a boundary condition suggested by (5) at $|z_0| = O(\mathrm{Ca}^2)$, $z_0 < 0$ of

$$H'_{\text{out}}(z_0) = \Theta_{\text{out}} + \mathrm{Ca}\, c_{\text{out}} + O(\mathrm{Ca}^2, \mathrm{e}^{-\mathrm{Ca}}). \tag{8}$$

Here, the second neglected term corresponds with the $O(x)$-term in the outer region expansion (1a), hence reflecting the accuracy of this expansion. It is worth noting that (8) does not reflect the accuracy of the matching procedure. This is because Θ_{out} is used here as a generic parameter to uniquely identify the the solution of (7), which is then determined *through* the matching procedure. We conclude that (8) only reflects the accuracy of using Θ_{out} as a boundary condition for the leading order contribution in Ca to the outer solution of the system.

Using (5) in (7) gives

$$d_z S_0(z) = f(S_0(z)), \qquad d_z S_1(z) = f'(S_0(z)) S_1(z), \tag{9}$$

and crucially these expressions now contain all terms $(\mathrm{Ca}\ln x)^n$ and $\mathrm{Ca}(\mathrm{Ca}\ln x)^n$ as they are assembled in S_0, and S_1, and thus no 'non-negligible' terms are discarded. By solving (9), we can now determine the infinite sum of the prefactors of all terms $(\mathrm{Ca}\ln x)^n$, and $\mathrm{Ca}(\mathrm{Ca}\ln x)^n$. S_0 is found through solving the leading order of (9):

$$S_0(z) = G^{-1}(z + A_c), \qquad \text{where} \qquad G(S_0) = \int_0^{S_0} \frac{1}{f(a)}\,\mathrm{d}a, \tag{10}$$

where A_c is a constant of integration. Similarly S_1 is found from the next order of (9):

$$S_1(z) = B_c f(S_0(z)) = B_c f(G^{-1}(z + A_c)), \tag{11}$$

to give

$$\begin{aligned} H'_{\text{out}} &\sim G^{-1}(z + A_c) + \mathrm{Ca}\, B_c f(G^{-1}(z + A_c)) + O(\mathrm{Ca}^2, \lambda, e^{z/\,\mathrm{Ca}}) \\ &\sim G^{-1}(z + A_c + \mathrm{Ca}\, B_c) + O(\mathrm{Ca}^2, \lambda, e^{z/\,\mathrm{Ca}}). \end{aligned} \tag{12}$$

We have here employed (10), and used that $(G^{-1})'(a) = 1/[G'(G^{-1}(a))]$, and $(G^{-1})'(T) = f(G^{-1}(T))$. By applying boundary condition (8) we find $A_c = G(\Theta_{\text{out}})$, and $B_c = c_{\text{out}}/f(\Theta_{\text{out}})$, and obtain the full asymptotic behaviour of the outer solution as $x \to 0$ as

$$H'_{\text{out}} \sim G^{-1}\left(\mathrm{Ca}\ln x + G(\Theta_{\text{out}}) + \mathrm{Ca}\,\frac{c_{\text{out}}}{f(\Theta_{\text{out}})}\right) + O(\mathrm{Ca}^2, \lambda, x). \tag{13}$$

Finally, an analogous procedure can be applied to the limiting behaviour of the inner region to give

$$H'_{\text{in}} \sim G^{-1}\left(\mathrm{Ca}\ln\left(\frac{x}{\lambda}\right) + G(\Theta_{\text{in}}) + \mathrm{Ca}\,\frac{c_{\text{in}}}{f(\Theta_{\text{in}})}\right) + O\left(\mathrm{Ca}^2, \lambda, \frac{\lambda}{x}\right). \tag{14}$$

Completing the analysis, by comparing (13) and (14), it is now clear that the outer and inner solutions have the same functional form and coincide in the full overlap region. Matching can then be performed in the textbook fashion, through

$$\lim_{x/\lambda\to\infty} H'_{\text{in}} = \lim_{x\to 0} H'_{\text{out}}, \tag{15}$$

and giving the result

$$G(\Theta_{\text{out}}) - G(\Theta_{\text{in}}) = \mathrm{Ca}\left[-\ln\lambda + \frac{c_{\text{in}}}{f(\Theta_{\text{in}})} - \frac{c_{\text{out}}}{f(\Theta_{\text{out}})}\right] + O(\mathrm{Ca}^2). \tag{16}$$

3 NUMERICAL COMPARISON

To provide a guide to the asymptotic regions and procedure, we show in figure 1 a comparison between full numerical and asymptotic solutions of the forced wetting problem in the thin-film regime [12, 11]. We show the extent of applicability of outer and inner regions (calculated analytically), and how the overlap breaks down when the Ca-series of solutions is truncated. As a greater number of terms in the Ca perturbation are retained, the extent of the breakdown of the overlap region reduces.

4 CONCLUSIONS

In this work, we have highlighted the fact that the moving contact line problem should not be treated uniquely, but in fact can be considered as a textbook problem in singular perturbation theory. Whilst further details are giving in [11], this summary allows us to give a pedagogical description of the result.

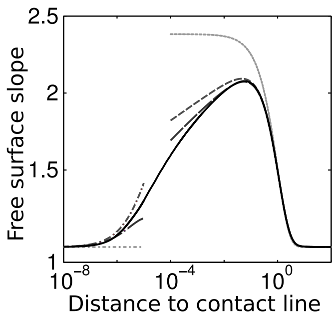

Figure 1: Comparison of outer and inner asymptotic solutions and full numerical solution (black line) of the free surface slope in the thin-film forced wetting problem. First three orders in Ca shown (respectively longer dashes for higher orders). $\lambda = 10^{-5}$, Ca= 0.3.

We note that (16) is the same result as the matched asymptotic derivations for Stokes and thin-film moving contact line problems, which employ a separate intermediate region, so that the result has not changed, and we do not call into question any comparison between analytical results and numerics/experiments. It is the procedure, however, that we hope to have significantly clarified. Additionally, Ca in (16) may be either positive or negative for advancing or receding flows, respectively. For receding flows the result holds only up to a critical value of $|\mathrm{Ca}|$ when it is negative due to the validity of (16) depending on (6), which holds only up to this critical value of $|\mathrm{Ca}|$ for receding flows.

The results in this work are far from merely a mathematical curiosity. The complex three-region asymptotic structure has been a barrier to analytical work where moving contact lines are present. Given that the fundamental structure is here shown to be in fact a standard two region (core and boundary layer) form, many of the unresolved issues such as for fully three-dimensional droplets and rapid dewetting flows may now be considered with renewed clarity.

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