Axisymmetric self-similar rupture of thin films with general disjoining pressure

This item was submitted to Loughborough University’s Institutional Repository by the/an author.


Additional Information:

- This is a conference paper.

Metadata Record: https://dspace.lboro.ac.uk/2134/22476

Version: Accepted for publication

Publisher: International Union of Theoretical and Applied Mechanics

Rights: This work is made available according to the conditions of the Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International (CC BY-NC-ND 4.0) licence. Full details of this licence are available at: https://creativecommons.org/licenses/by-nc-nd/4.0/

Please cite the published version.
A thin film coating a dewetting substrate may be unstable to perturbations in the thickness, which leads to finite time rupture. The parameters in question may be model parameters, or artificial parameters introduced for numerical expediency, as we use here.

Michael Dallaston∗1, Dmitri Tseluiko2, Serafim Kalliadasis3, Zhong Zheng3, Marco Fontelos4, and Howard Stone3

1Department of Chemical Engineering, Imperial College London, London, UK
2Department of Mathematical Sciences, Loughborough University, Loughborough, UK
3Mechanical and Aerospace Engineering, Princeton University, Princeton NJ, USA
4Departamento de Ciencia e Ingeniería, Universidad Rey Juan Carlos, Madrid, Spain

Summary A thin film coating a dewetting substrate may be unstable to perturbations in the thickness, which leads to finite time rupture. The self-similar nature of the rupture has been studied by numerous authors for a particular form of the disjoining pressure, with exponent \( n = 3 \). In the present study we use a numerical continuation method to compute discrete solutions to self-similar rupture for a general disjoining pressure exponent \( n \). Pairs of solution branches merge when \( n \) is close to unity, indicating that a more detailed examination of the dynamics of a thin film in this regime is warranted. We also numerically evaluate the power law behaviour of characteristic quantities of solutions in the limit of large branch number.

FORMULATION

A thin film on a dewetting substrate is dominated by the effects of surface tension and van der Waals forces. Invoking the lubrication or thin film approximation [3], the thickness of the film \( h(x, t) \) may be modelled by the (dimensionless) equation

\[
\frac{\partial h}{\partial t} = -\nabla \cdot \left[ h^3 \nabla \left( \nabla^2 h + \Pi(h) \right) \right], \quad \Pi(h) = -\frac{1}{nh^n}. \tag{1}
\]

As long as \( n > 1 \), the disjoining pressure \( \Pi(h) \), which captures the effect of van der Waals forces, destabilises the film. This leads to finite time rupture, where \( h \) vanishes at a point or line at time \( t_0 \). Assuming axisymmetry and self-similarity near a rupture point \( (r = 0) \), the film thickness may be expressed as \( h(r, t) = (t_0 - t)^\alpha f(\xi), \xi = r/(t_0 - t)^\beta \), where \( f \) satisfies the following ordinary differential equation

\[
-\alpha f + \beta \xi f' = -\frac{1}{\xi} \left[ \xi f^3 \left( f'' + \frac{1}{2} f' \right) + \xi f^{2-n} f' \right], \quad f'(0) = f''(0) = 0, \quad f \sim c \xi^{\alpha/\beta}, \xi \rightarrow \infty. \tag{2}
\]

The similarity exponents \( \alpha \) and \( \beta \) are simple functions of the exponent \( n \), while the far field condition is derived from the assumption of quasi-steadiness away from the rupture point. The conditions at \( \xi = 0 \) are required for symmetry and boundedness of the solution at the origin.

For \( n = 3 \), it has been shown that (2) has a discrete family of solutions, which may be characterised by the scaled film thickness at the origin \( f_0 = f(0) \). Previously, these solutions have been computed numerically, using a shooting method [7], and Newton iteration on a discretised boundary value problem [5]. In each case, the numerical computation is highly sensitive to an initial guess (the right-hand initial condition for shooting, or the initial guess of the Newton scheme, respectively). The selection mechanism in the plane symmetry (line-rupture) version of (2) was explored in [1], where the exponential asymptotics of the large branch-number (equivalent to small \( f_0 \) was performed). The plane-symmetric version has also recently been resolved numerically [4] using the continuation algorithms implemented in the open source package AUTO07p [2].

The purpose of the present study is two-fold: firstly, we compute discrete solutions to (2) using numerical continuation, which has been shown to be highly effective on the plane-symmetric version of this problem [4]. Secondly, numerical continuation allows us to compute the discrete solution branches as the disjoining pressure exponent \( n \) is varied.

NUMERICAL CONTINUATION

The idea behind numerical continuation is to compute a solution to a boundary value problem that features a number of parameters, then gradually vary one or more of those parameters, using the previous solution as an initial guess (say, in a Newton iteration) to compute the new solution. The smooth dependence of the solution on parameters may thus be harnessed. The parameters in question may be model parameters, or artificial parameters introduced for numerical expediency, as we use here.

∗Corresponding author. Email: m.dallaston@imperial.ac.uk
As a starting point, we note that when \( n = 3 \), (2) has the exact solution \( f_c(ξ) = c\sqrt{ξ} \) satisfying the far field conditions, but not the conditions at \( r = 0 \). We thus introduce the artificial parameters \( δ_1 \) and \( δ_2 \) into the boundary conditions, as well as an approximate left hand boundary location \( ξ_0 \ll 1 \), and enforce the conditions

\[
f(ξ_0) = f_0, \quad f'(ξ_0) = δ_1, \quad f''(ξ_0) = δ_2.
\]

The far field boundary conditions are also enforced at a large but finite value \( ξ = L \). Given appropriate values of \( δ_1 \) and \( δ_2 \), \( f_c(ξ) \) also satisfies these boundary conditions, so may be used as an initial guess in our computation. Using numerical continuation, we now take \( δ_2 \) and \( δ_1 \) to zero, allowing \( f_0 \) to be free in each case. Now as \( ξ_0 \) is taken to zero, we approach a solution to the original problem (2).

The introduction of the artificial parameters also provides a systematic way of computing the other members of the discrete family of solutions. For \( δ_1 = 0 \) and \( ξ_0 > 0 \) we allow \( f_0 \) to vary, letting \( δ_2 \) be free. The curve of \( δ_2 \) against \( f_0 \) oscillates around \( δ_2 = 0 \), each intersection corresponding to a solution of (2). This approach is similar to that used for the plane symmetric problem [4], although in our case the variation of the artificial parameters in the boundary conditions cannot take place on \( ξ = 0 \) due to the coordinate singularity.

Finally, after finding the discrete solutions for \( n = 3 \), we continue in \( n \) to trace out discrete solution branches.

RESULTS

In figure 1a we plot the curve of the artificial parameter \( δ \) against \( f_0 \) for \( n = 3 \), showing the selection of discrete solutions where \( δ_2 = 0 \). In figure 1b we plot the discrete branches of solutions, characterised by \( f_0 \), over a range of values of \( n \). The most interesting phenomenon we observe is the merging of pairs of branches at a value \( n > 1 \) as \( n \) decreases. Thus, for small values of \( n \), the branch with largest \( f_0 \) (the only which is stable [5]) disappears. The dynamical behaviour of the time-dependent problem (1) in this regime is therefore of further interest, something which we intend to explore further by numerical computation of (1).

In addition we compute the relationship between \( f_0 \) on the discrete solution branches and the index \( N \) of the branch (starting with the largest value as \( N = 1 \), particularly in the limit that \( N \) is large. As shown in figure 1c, the discrete values of \( f_0 \) appear to behave as \( ∝ N^{-1/n} \) as \( N \to \infty \) for \( n = 3, 4 \) and 5. When \( n = 3 \), the far field coefficient \( c \) behaves as \( N^{-0.43} \), as previously computed [6, 4]. The relationship between these numerically observed power laws, as well as the connection with the asymptotic result of [1], is ongoing work.

References