

AXISYMMETRIC SELF-SIMILAR RUPTURE OF THIN FILMS WITH GENERAL DISJOINING PRESSURE

Michael Dallaston^{* 1}, Dmitri Tseluiko², Serafim Kalliadasis¹, Zhong Zheng³, Marco Fontelos⁴, and Howard Stone³

¹*Department of Chemical Engineering, Imperial College London, London, UK*

²*Department of Mathematical Sciences, Loughborough University, Loughborough, UK*

³*Mechanical and Aerospace Engineering, Princeton University, Princeton NJ, USA*

⁴*Departamento de Ciencia e Ingenieria, 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 $h(\mathbf{x}, t)$ may be modelled by the (dimensionless) equation

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

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

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

The similarity exponents α and β 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

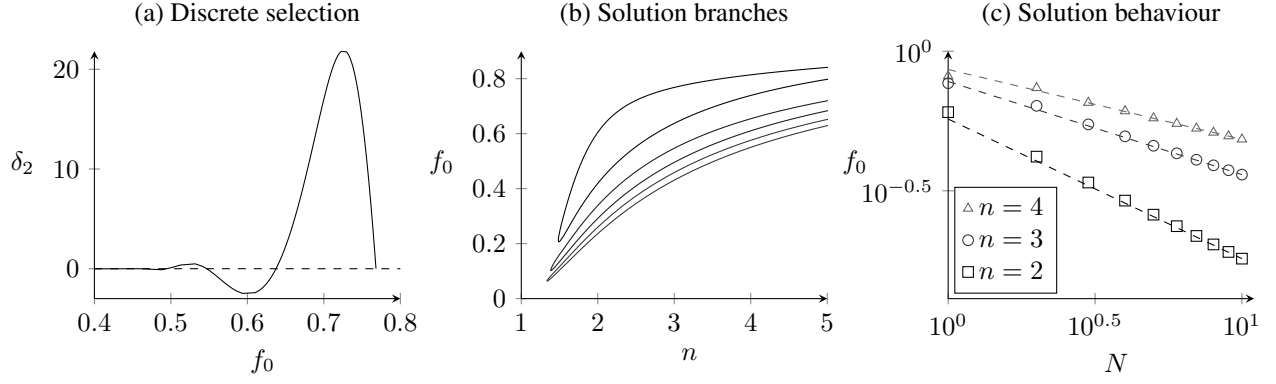


Figure 1: (a) The artificial parameter δ_2 as a function of the scaled film thickness at the origin f_0 ; The roots $\delta_2 = 0$ correspond to solutions of (2). (b) The first six solution branches vs the disjoining pressure exponent n . Pairs of solution branches merge near $n = 1$. (c) Discrete solutions f_0 vs solution index N ; solutions appear to asymptote to $\propto N^{-1/n}$ for large N .

As a starting point, we note that when $n = 3$, (2) has the exact solution $f_e(\xi) = c\sqrt{\xi}$ 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 $\xi_0 \ll 1$, and enforce the conditions

$$f(\xi_0) = f_0, \quad f'(\xi_0) = \delta_1, \quad f'''(\xi_0) = \delta_2.$$

(the far field boundary conditions are also enforced at a large but finite value $\xi = L$). Given appropriate values of δ_1 and δ_2 , $f_e(\xi)$ 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 $\delta_1 = 0$ and $\xi_0 > 0$ we allow f_0 to vary, letting δ_2 be free. The curve of δ_2 against f_0 oscillates around $\delta_2 = 0$, 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 $\xi = 0$ 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 $\delta_2 = 0$. 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 $\propto N^{-1/n}$ as $N \rightarrow \infty$ 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

- [1] S. J. Chapman, P. H. Trinh, and T. P. Witelski. Exponential asymptotics for thin film rupture. *SIAM J. Appl. Math.*, 73(1):232–253, 2013.
- [2] E. J. Doedel, A. R. Champneys, F. Dercole, T. F. Fairgrieve, Yu. A. Kuznetsov, B. Oldeman, R. C. Paffenroth, B. Sandstede, X. J. Wang, and C. H. Zhang. Auto-07p. *Continuation and bifurcation software for ordinary differential equations*, 2007.
- [3] A. Oron, S. H. Davis, and S. G. Bankoff. Long-scale evolution of thin liquid films. *Rev. Mod. Phys.*, 69(3):931–980, 1997.
- [4] D. Tseluiko, J. Baxter, and U. Thiele. A homotopy continuation approach for analysing finite-time singularities in thin liquid films. *IMA J. Appl. Math.*, 78(4):762–776, 2013.
- [5] T. P. Witelski and A. J. Bernoff. Stability of self-similar solutions for van der Waals driven thin film rupture. *Phys. Fluids*, 11(9):2443–2445, 1999.
- [6] T. P. Witelski and A. J. Bernoff. Dynamics of three-dimensional thin film rupture. *Physica D*, 147(1-2):155–176, 2000.
- [7] W. W. Zhang and J. R. Lister. Similarity solutions for van der Waals rupture of a thin film on a solid substrate. *Phys. Fluids*, 11(9):2454–2462, 1999.