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Finite-time thin film rupture driven by modified evaporative loss

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HIGHLIGHTS

- A fourth-order thin film equation with modified non-conservative flux is analyzed.
- Non-conservative loss can overcome disjoining pressure and cause finite-time singularities.
- The generalized PDE yields various forms of rupture dynamics.
- A bifurcation diagram for rupture regimes is obtained from the model.
- Analytical predictions are supported by high-precision PDE simulations.

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ABSTRACT

Rupture is a nonlinear instability resulting in a finite-time singularity as a film layer approaches zero thickness at a point. We study the dynamics of rupture in a generalized mathematical model of thin films of viscous fluids with modified evaporative effects. The governing lubrication model is a fourth-order nonlinear parabolic partial differential equation with a non-conservative loss term. Several different types of finite-time singularities are observed due to balances between conservative and non-conservative terms. Non-self-similar behavior and two classes of self-similar rupture solutions are analyzed and validated against high resolution PDE simulations.

1. Introduction

This paper is devoted to studying the development of rupture singularities in a one-dimensional partial differential equation on a finite domain, $0 \le x \le L$,

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^3 \frac{\partial p}{\partial x}\right) - J, \tag{1a}$$

where the non-conservative flux is

$$J = -\frac{\gamma p(h)}{h + K_0}, \tag{1b}$$

where γ is a scaling constant, $K_0 > 0$ and the dynamic pressure is defined as

$$p(h) \equiv \Pi(h) - h_{xx}, \tag{1c}$$

including a disjoining pressure function, $\Pi(h)$, and the linearized curvature, h_{xx}. The form of $\Pi(h)$ is motivated by a physical model and will be given later. Starting from a given initial condition $h_0(x)$ at $t = 0$, the dynamics will be subject to no-flux and normal-contact boundary conditions at the edges of the domain,

$$p_x(0, t) = p_x(L, t) = 0, \qquad h_x(0, t) = h_x(L, t) = 0, \tag{1d}$$

which are equivalent to specifying homogeneous Neumann conditions $h_x = h_{xxx} = 0$. This class of PDE is motivated by lubrication models of free surface flow of thin viscous films, for the evolution of the thickness (or height h of the free-surface) of the fluid layer.

The scaling coefficient for the non-conservative term, γ, will be seen to play an important role in determining the qualitative behavior of the model. While the case $\gamma \le 0$ corresponds to physical models of thin fluid films where some analytic results were obtained, for $\gamma > 0$ rich and interesting PDE dynamics of singularity formation [1] occur and this will be the main focus of our paper.

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1.1. Related physical models with $\gamma \le 0$

When $\gamma = 0$ (1a) is the Reynolds equation for one-dimensional coating flows which takes the form of a fourth-order nonlinear differential equation,

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^3 \frac{\partial}{\partial x}\left[\Pi(h) - \frac{\partial^2 h}{\partial x^2}\right]\right). \tag{2}$$

This model characterizes the behavior of the fluid which is strongly affected by surface tension [2] and the wetting properties of the substrate, namely whether the solid attracts and encourages the spreading (called a hydrophilic or wetting material), or repels the fluid (called a hydrophobic or non-wetting material). This is achieved by including a contribution in the dynamic pressure representing molecular interactions between the fluid and the solid, the disjoining pressure $\Pi(h)$, in addition to the influence of surface tension which is manifested through the linearized curvature of the free-surface, h_{xx}. This equation is derived using the lubrication approximation from the classic Navier Stokes equations in the limit of low Reynolds number. The disjoining pressure characterizes key material properties in the model and qualitatively changes solution behaviors. For hydrophobic substrates, the disjoining pressure will act to oppose the diffusive spreading driven by surface tension and can generate instabilities in uniform coatings. For ideal hydrophobic materials, the simplest model for the disjoining pressure is $\Pi(h) = A/h^3$ [3], where A is called a Hamaker constant. The case $A > 0$ represents disjoining intermolecular forces, while $A < 0$ corresponds to conjoining pressure for hydrophilic surfaces. For $A > 0$, early studies demonstrated this model has instabilities in the film thickness [4]. These instabilities lead to rupture at a finite critical time, $t = t_c$, with $h \to 0$ at an isolated point, $x = x_c$ and the nonlinear dynamics were shown to be given by a self-similar solution [5,6],

$$h(x,t) \sim \tau^{1/5} H(\eta), \quad \tau = t_c - t,\ \eta = \frac{x - x_c}{\tau^{2/5}}, \text{ as } t \to t_c. \tag{3}$$

This model is problematic since the solution cannot be continued past the time of the first rupture, however, this can be avoided by considering more detailed models for $\Pi(h)$. In [7], conditions on the form of $\Pi(h)$ were determined so that the solutions of (2) remain positive for all times, $\Pi(h) = Ah^{-3}(1 - \epsilon/h)$ with $A > 0$ is a simple example that includes both attractive van der Waals forces and short range repulsive forces (Born repulsion). Physically, there is a film thickness $h = O(\epsilon) > 0$ set by the intermolecular forces that acts as a lower bound [8]. The solutions follow (3) until the minimum thickness approaches $h_{\min} = O(\epsilon)$, thereafter, that minimum will spread to form a growing "dry spot" while the bulk of the fluid moves to form droplets [9], see Fig. 1(left). The film breakup, the development of dry spot and further morphological changes are usually called "dewetting".

For $\gamma < 0$, Eq. (1) describes the dynamics of thin films subject to fluid evaporation and vapor condensation with applications to precorneal tear film [10,11] and thermal management [12]. Several models [13–15] have been constructed to characterize the evaporating/condensing liquid films. Burelbach et al. [15] first proposed a one-sided model to describe the dynamics of the liquid decoupled from the dynamics of the surrounding vapor. Based on this model, Oron and Bankoff [16,17] studied the dynamics of evaporating/condensing thin liquid films but neglected effects like thermocapillarity and vapor thrust. The evaporation loss or condensation source term in these models takes the form of

$$J(h) = \frac{E_0}{h + K_0},$$

where K_0 measures the thermal resistances to mass transfer due to the temperature jump at the liquid–vapor interface as described in [15], and E_0 is called the dimensionless evaporation number, which can be interpreted as a temperature difference and gives the ratio of the viscous timescale to the evaporative timescale. The case $E_0 > 0$ corresponds to evaporation [16], while $E_0 < 0$ is for condensing films [17]. A more detailed evaporation model was derived by Ajaev and Homsy [18,14,13] with an evaporative loss term of the form

$$J(h) = \frac{E_0 - \delta(h_{xx} - Ah^{-3})}{h + K_0}, \tag{4}$$

which incorporates surface tension, h_{xx}, and conjoining pressure, Ah^{-3} with $A < 0$ for wetting substrates, by taking into consideration the pressure jump at the liquid–vapor interface. The effect of the pressure jump during the phase-change is characterized by the positive nondimensional parameter $\delta > 0$. For a thorough discussion on the modeling and numerical studies of evaporating thin films, see [19].

1.2. Mathematical model (1) with $\gamma > 0$

Seeking to write a class of PDEs that can include (4) we generalize $\Pi(h)$ in (1) to include a constant P_0 pressure offset,

$$\Pi(h) = \frac{A}{h^3}\left(1 - \frac{\epsilon}{h}\right) + P_0, \tag{5}$$

where $A > 0$ describes a dewetting substrate and $\epsilon > 0$ characterizes the scale of the ultrathin film where the intermolecular forces are dominant (see Fig. 1 (left)). Combining (5) with (1c), Eq. (1b) can match the form of the flux (4) with the parameters related by $\gamma = -\delta$ and $P_0 = E_0/\delta$. We restrict the pressure offset to be a constant to be consistent with the conservative flux due to the gradient of p in (1a). In this paper, we set $A = 1$ and $\epsilon = 1$, letting h be normalized with respect to the van der Waals film thickness scale on a dewetting substrate.

While the model for evaporation/condensation given by (4) determines the physical range for γ to be $\gamma < 0$, we relax this condition and consider $\gamma > 0$ to explore the possible behaviors that can occur from competing conservative and nonconservative fluxes built from a common pressure function (1c).

It is important to note that $\delta > 0$ in (4) (equivalent to $\gamma < 0$ in (1b)) yields a stabilizing influence of evaporation or condensation in reducing spatial gradients while increasing or decreasing film thickness. We will show that allowing this term to have opposite sign will lead to interesting behavior with non-conservative destabilizing effects. For instance, with $\gamma < 0$ and P_0 being negative as in Fig. 1 (middle), condensation can occur with spatial variations decaying over time. However, with $\gamma > 0$ model (1) exhibits dramatically different and mathematically interesting singularity formation dynamics in Fig. 1 (right). While it is straightforward to see that the sign of γ is the cause of the difference between losing and gaining mass, it is not clear that this kind of change can create singularities. Specifically, although previous studies [7] have analytically established that with $\gamma = 0$ the disjoining pressure involved in (2) precludes the film from rupturing, the positivity of solutions cannot be guaranteed with instabilities enhanced by the non-conservative flux term in (1) with $\gamma > 0$. In particular, Fig. 1(right) shows that for some choices of parameters the non-conservative flux can overcome the regularizing influence of the disjoining pressure to yield finite-time rupture singularities.

Rupture and long-time dynamics of dewetting in (2) have attracted extensive applied interest, and some rigorous analyses have also been developed [20,21]. For an extensive study of singularity formation including rupture and blow-up we refer to [1]. While (2) conserves fluid mass for all times and describes non-volatile liquids, what has not been studied to the same degree

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