Numerical Study of Thin Viscoelastic Films on Substrates

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Abstract

We numerically study the interfacial dynamics and instability of a thin viscoelastic film on a substrate. We use the long wave approximation to describe the non-linear evolution of the interface. We consider different regimes of slippage, and in each regime, we investigate the role of the liquid viscoelasticity and of the contact angle on the thin film break-up. Numerical solutions of the full non-linear equations are compared with the results of the linear stability analysis.

Introduction

Numerical solutions are of fundamental importance in the understanding of the dynamics, and in particular of the instability, of thin films of viscoelastic fluids, such as polymeric fluids. In this study, we are interested in the instabilities that cause the dewetting of the liquid on a solid substrate. We simplify the generalized Maxwell model of Jeffreys type for the moving interface of viscoelastic liquids in the $2D$ lubrication approximation. This model describes the non-Newtonian nature of the stress tensor, linearly interpolating a purely elastic and a purely viscous behavior, characterized by two time constants λ_1 and λ_2 respectively, namely *relaxation time* and *retardation time*. We carry out our analysis on a thin film of fluid of constant initial thickness h_0 that is perturbed, in regimes that transit from no-slip to weak-slip and see how the slippage together with the viscoelasticity affect the instability.

Governing Equations

The equation governing the hydrodynamics for the fluid interface of viscoelastic media is derived as a long-wave approximation of the conservation laws. The liquid is considered incompressible, with mass density ρ. The equation of conservation of mass and continuity of momentum are:

$$\nabla \cdot \mathbf{u} = 0\,, \tag{1}$$

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p_R + \nabla\cdot\tau\,,$$

where $\mathbf{u} = (u,v,w)$ is the velocity vector field, and p_R the reduced pressure such that $p_R = p - \Pi$, where p is the hydrostatic pressure, while Π is the pressure induced by body forces of van der Waals type (attractive or repulsive). The stress tensor τ follows the Jeffreys model for viscoelastic fluids, which describes the non-Newtonian relation $\tau(\dot\gamma)$ between the stress tensor τ and the *strain rate* $\dot\gamma$:

$$\tau + \lambda_1\partial_t\tau = \eta(\dot\gamma + \lambda_2\partial_t\dot\gamma) \tag{2}$$

in which η is the shear viscosity coefficient and $\lambda_1,\ \lambda_2$ are the two relaxation times of the liquid when it shrinks back to its original shape after deformation, with $\lambda_1 > \lambda_2$.
In figure 1 we can see a scheme of the fluid's interface. At the solid substrate we have Navier boundary conditions where $b \geq 0$ is the *slip length* ($b = 0$ means no slip, and $b \gg 1$ means strong-slip).

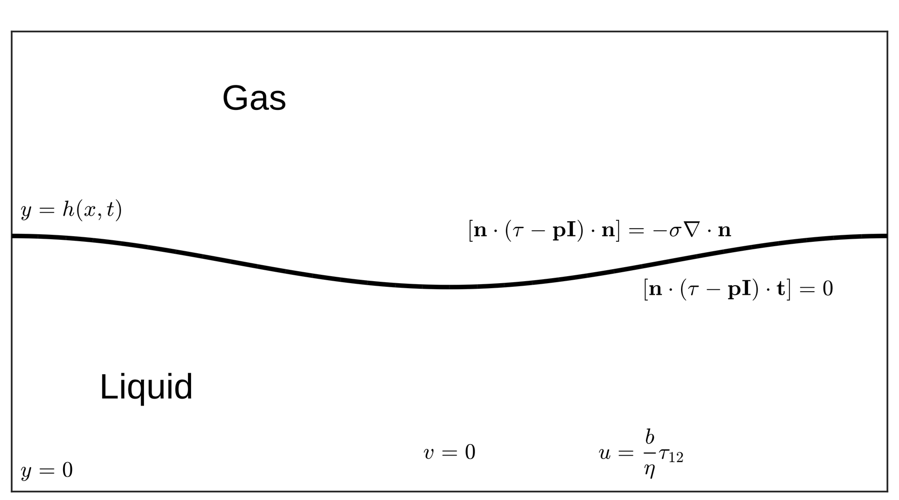

Figure 1: *Scheme of the fluid interface and boundary conditions.*

We nondimensionalize these equations, using: $(x,y) = L(x^*,y^*)$, $z = Hz^*$, $(u,v) = U(u^*,v^*)$, $w = \varepsilon U w^*$, $t = Tt^*$, with $T = L/U$, and $H/L = \varepsilon$, where ε is the small parameter. In the weak-slip regime the slip length $b = O(1)$ and the pressure is scaled as $PH/\eta U \sim \varepsilon^{-1}$ [3].

Keeping only $O(1)$ terms in the boundary conditions we obtain $p_R = -\nabla^2 h - \Pi$, and using this together with the kinematic boundary condition into the governing equations (dropping the *) leads to system of equations for the fluid's interface:

$$(1+\lambda_2\partial_t)h_t + (\lambda_2-\lambda_1)\nabla\cdot\left[\left(\frac{h^2}{2}\mathbf{Q} - h\mathbf{R}\right)h_t\right] =$$
$$\nabla\cdot\left\{\left[(+\lambda_1\partial_t)\frac{h^3}{3}\nabla p_R + (1+\lambda_2\partial_t)bh^2\nabla p_R\right]\right\} \tag{3}$$

where $\mathbf{Q}$ and $\mathbf{R}$ satisfy

$$\mathbf{Q} + \lambda_2\mathbf{Q}_t = \nabla p_R,\ \ \mathbf{R} + \lambda_2\mathbf{R}_t = h\nabla p_R \tag{4}$$

and the van der Waals potential is defined by:

$$\Pi(h) = \frac{\sigma(1-cos\theta)}{Mh_\star}\left[\left(\frac{h_\star}{h}\right)^n - \left(\frac{h_\star}{h}\right)^m\right],$$

with θ the contact angle, $M = (n-m)/[(m-1)(n-1)]$ (generally $n > m$) [2], $h_\star$ the precursor film thickness, and σ the surface tension.

Linear Stability Analysis

To study the film's response to a perturbation we consider $h = h_0 + \delta h_0 e^{ikx+\omega t}$, $Q = \delta Q_1$, $R = \delta R_1$, where h_0 is the flat initial thickness, k the wave number $k = 2\pi/\lambda$, and ω the growth rate. Using these into equation (3) and keeping only terms up to $O(\delta)$, we obtain the following disperion/dissipation relation:

$$\lambda_2\omega^2 + \left[1 + (k^4 - k^2\Pi'(h_0))\left(\lambda_1\frac{h_0^3}{3} + \lambda_2 bh_0^2\right)\right]\omega + (k^4 - k^2\Pi'(h_0))\left(\frac{h_0^3}{3} + bh_0^2\right) = 0\,. \tag{5}$$

Solving for the two roots of this quadratic equation we obtain one root strictly negative, let us say ω_2, and one root with varying sign, call it ω_1. The latter one is positive (unstable) for $-\sqrt{\Pi'(h_0)} < \omega_1 < \sqrt{\Pi'(h_0)}$. The most unstable mode is given by $k_m = \pm\sqrt{\Pi'(h_0)/2}$. Therefore from the definition above we can see that both $k_c = \pm\sqrt{\Pi'(h_0)}$ and k_m do not depend on the viscoelasticity times λ_1 and λ_2 and neither on the slip length b.

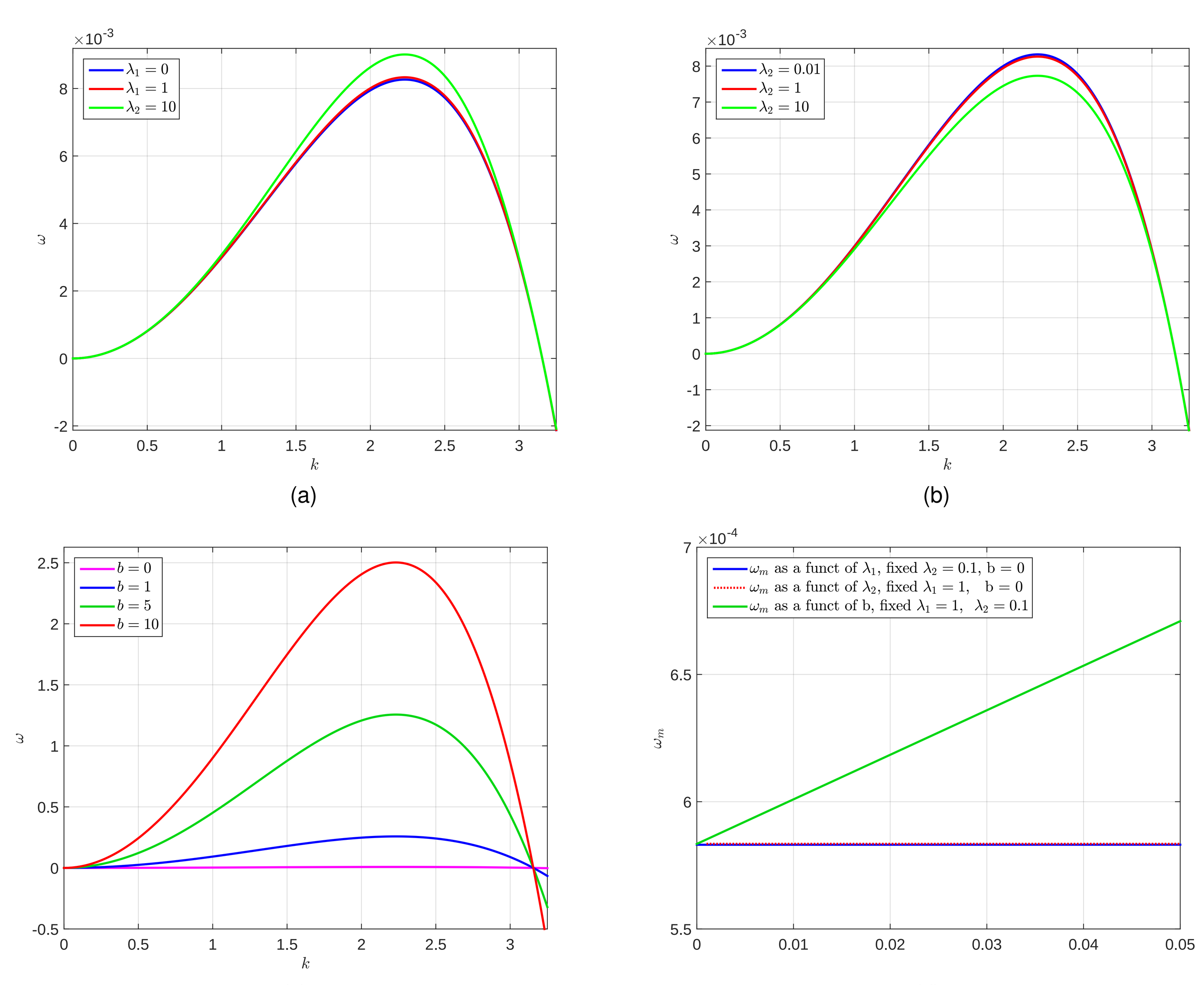

Figure 2: *(a), (b) Influence of the dispersion curve $\omega_1(k)$ on λ_1, λ_2 respectively. (c) Influence of the dispersion curve $\omega_1(k)$ on the slippage b. (d) The direct dependence of the fastest growth rate $\omega_m(k)$ on λ_1, λ_2 and b respectively.*

Numerical Results

We drove simulations using Newton linearization of the nonlinear terms, Crank-Nicolson scheme for the spacial derivatives and central finite differences for the time second order derivative. The two ODEs for the terms (4) can be solved with any Euler's method.

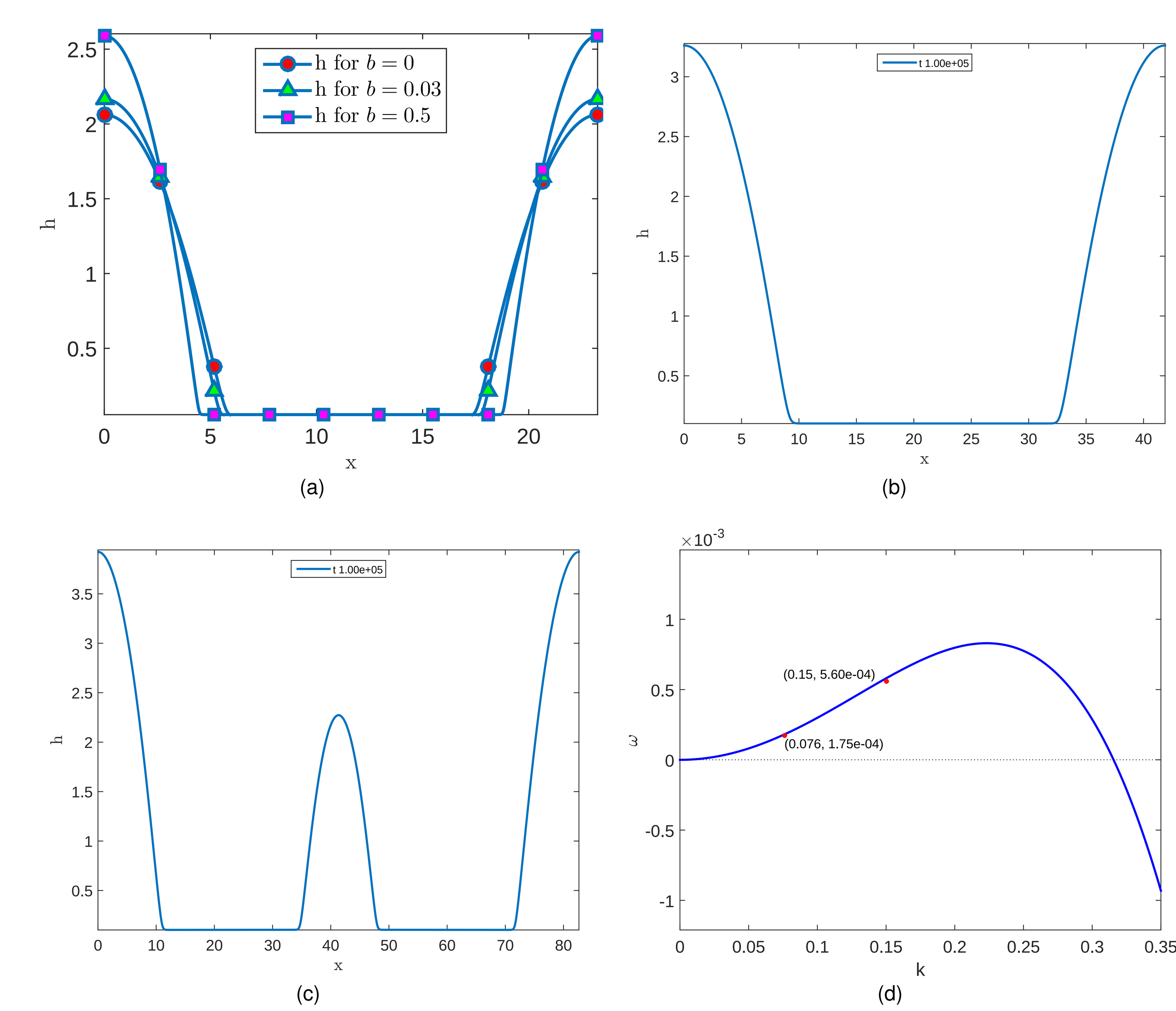

Figure 3: *(a) Fluid interface instability - transition from no slip to weak-slip regime. (b),(c) $\lambda_1 = 10$, $\lambda_2 = 5$, longer domain in (c) allows for a satellite droplet. (d) Growth rate of interfacial instability given by the numerical simulations compared with the theoretical LSA.*

In figure 4a we see the evolution in time of a film of initial thickness $h_0 = 0.1$: the liquid interface is perturbed and it does not returns to its flat profile, but it breaks up into two separate rims. The instability is due to van der Waals forces' interaction with a precursor film $h_\star = 0.01$ and contact angle $\theta = 45°$. In figure 4b and 4c we see the final film interface configuration for $\lambda_1 = 10$, and $\lambda_2 = 5$, for fixed initial height $h_0 = 1$, $h_\star = 0.1$ and $b = 0$, respectively for shorter and longer wave-lengths. The longer wave-length allows for the formation of a satellite droplet between the separate rims. In figure 4d instead we compare the growth rates of the instabilities for different wave lengths with the theoretical results given by the Linear Stability Analysis.

Conclusions and Future Work

The numerical results of our simulations are in agreement with the linear stability analysis. In our future work we will implement the full Navier-Stokes equation (1) for arbitrary geometries in the weak-slip regime and investigate how the transition from weak to moderate to strong-slip regimes affects the instability together with the viscoelastic effects.

References

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