Numerical Study of Thin Layers of Viscoelastic Fluids

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Abstract

This study is developed in the field of Computational Fluid Dynamics, focusing on thin films of viscoelastic liquids, such as polymeric fluids. Polymeric liquids combine characteristics of viscous fluids with features typical of elastic matter. They are present in a broad variety of real life aspects and therefore studied and used by a wide spectrum of industries and Sciences. The aim in this study is to give a full mathematical analysis and to provide numerical simulations for the moving interface of viscoelastic liquids. The goal is to deepen the comprehension of key features of the dynamics, and in particular of the interfacial instability, of viscoelastic fluids through the tools of mathematical modeling and numerical simulations. We are interested in the instabilities that cause the dewetting of the liquid on a solid substrate. The model we take into consideration is characterized by a non-linear PDE that describes the motion of the fluid interface in time and space, and includes a generalized Maxwell model of Jeffreys type to incorporate the viscoelastic behavior. Through our study we find that the viscoelastic physical parameters, together with other physical quantities involved such as slippage and molecular interactions with the substrate, affect the dynamics of the instability and the final configuration of the fluid in blobs and droplets. Our findings are in agreement with the theoretical framework and have been verified through the tool of Linear Stability Analysis.

Introduction

Thin liquid films are ubiquitous in nature and widely studied in industry for their innumerable types of application. In particular, thin layers of viscoelastic fluids, such as polymeric liquids are commonly used in the food industry, the chemical, pharmaceutical and biomedical industries, and material science related disciplines. Our investigations are motivated by applications of thin polymer films in wetting/dewetting processes on solid substrates (see figure 1). We are interested in understanding how the interface of a thin layer of fluid surrounded by an ambient gas destabilizes, and separates so that the fluid exposes the solid substrate (dewetting) and reorganizes in blobs and droplets. To solve this free-interface problem, we first use mathematical tools like modeling and linear stability analysis to describe the theoretical framework. We then drive numerical simulations to solve the highly non-linear partial differential equation (PDE) that governs the motion of the liquid interface. Numerical investigations allow us to approximate the solution otherwise impossible to obtain analytically.

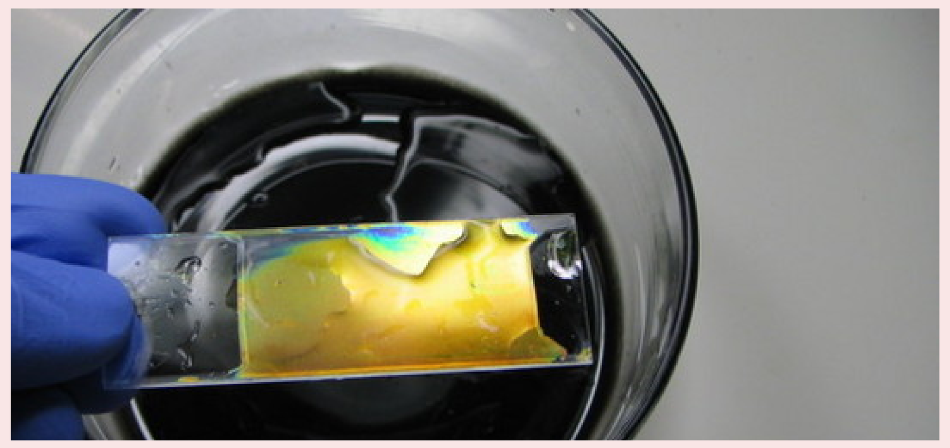

Figure 1: An application of a thin polymeric liquid film. Picture from www.foodproductiondaily.com - MIT research.

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:

$$\nabla \cdot \mathbf{u} = 0\,, \quad \rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p_R + \nabla\cdot\tau\,, \tag{1}$$

where $\mathbf{u} = (u(x,y), v(x,y))$ is the velocity vector field, $\nabla = (\partial_x, \partial_y)$, 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 λ_1, λ_2 are, respectively, the *relaxation time* and the *retardation time*. In figure 2 we can see a schematic of the fluid interface described parametrically by the function $y = h(x,t)$, where $y = 0$ is the solid substrate. At $y = 0$ we have Navier boundary conditions where $b \geq 0$ is the *slip length* ($b = 0$ means no slip, and $b \gg O(1)$ means strong-slip). We nondimensionalize these equations, using: $x = Lx^*$, $y = Hy^*$, $u = Uu^*$, $v = \varepsilon Uv^*$, $t = Tt^*$, with $T = L/U$, and $H/L = \varepsilon$, where ε is the small parameter, and the pressure is scaled as $PH/\eta U \sim \varepsilon^{-1}$. Keeping only $O(1)$ terms in the governing equations and boundary conditions, and dropping the "*" for simplicity sake, leads to the closed form equation for the interface of a thin layer of viscoelastic fluid (3). The full derivation can be found in [1].

Governing Equations (cont'd)

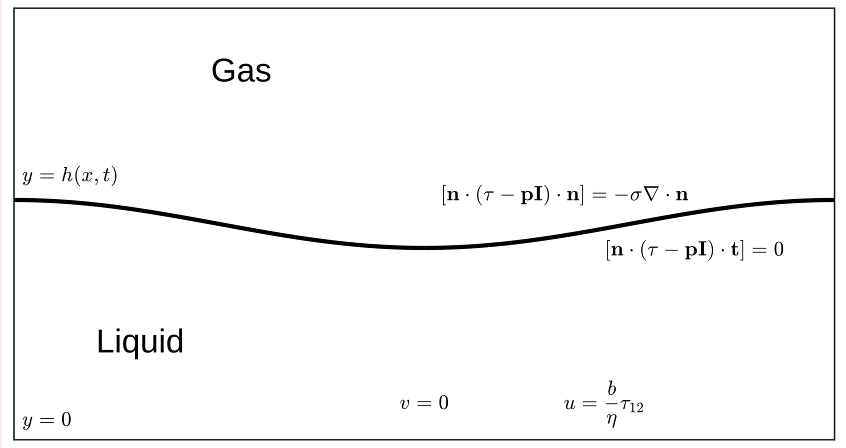

Figure 2: Scheme of the fluid interface and boundary conditions.

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

where Q and R satisfy respectively:

$$(1+\lambda_2\partial_t)Q = -\frac{\partial}{\partial x}(h_{xx} + \Pi(h))\,, \quad (1+\lambda_2\partial_t)R = -hh_{xxx} - h\Pi'(h)h_x \tag{4}$$

and the van der Waals potential is defined by:

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

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

Linear Stability Analysis

To study the film's response to a perturbation we consider $h = h_0 + \varepsilon h_0 e^{ikx+\omega t}$, 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 $O(\varepsilon)$, 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 $-\sqrt{\Pi'(h_0)} < \omega_1 < \sqrt{\Pi'(h_0)}$.

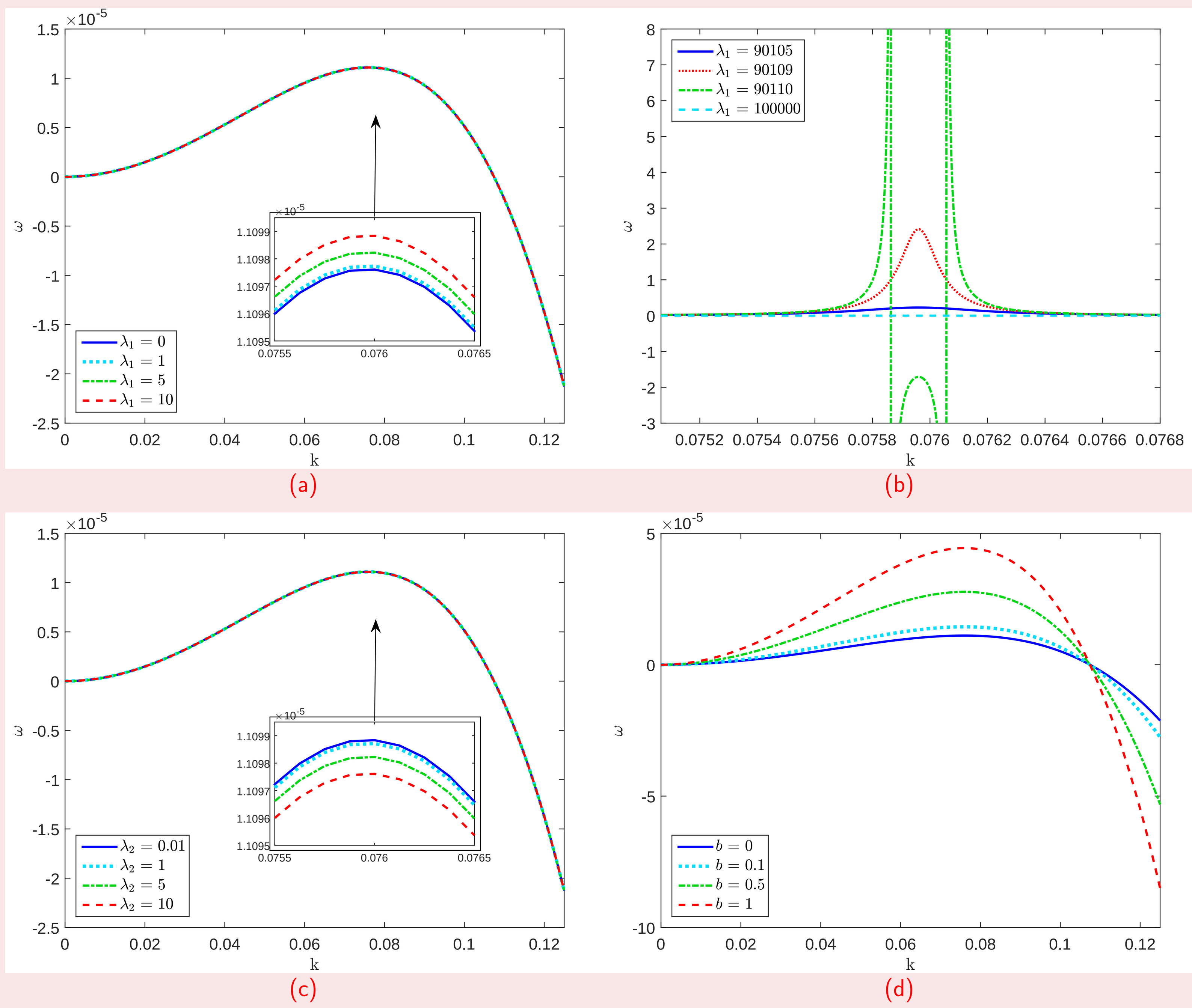

Figure 3: Linear Stability Analysis.

Results and Discussion

Through the LSA we investigate how the fastest growth rate ω_m varies with λ_1, λ_2, b. In figure 3(a) we see how ω_m increases with larger λ_1. In figure 3(b) we see how the growth rate blows up for this set of parameters, with $b = 0$, $\lambda_2 = 0$ at the value of $\lambda_1 = 9.011 \times 10^4$. In fact for $\lambda_2 = 0$ eq. (5) has a vertical asymptote for a certain value of λ_1. In figure 3(c) as λ_2 increases ω_m decreases, while in figure 3(d) as b increases ω_m increases remarkably.

We numerically solve eq. (3) using Newton linearization of the non-linear terms, Crank-Nicolson scheme for the spacial derivatives and central finite differences for the second order derivative in time. The two ODEs for eq. (4) can be solved with any Euler method.

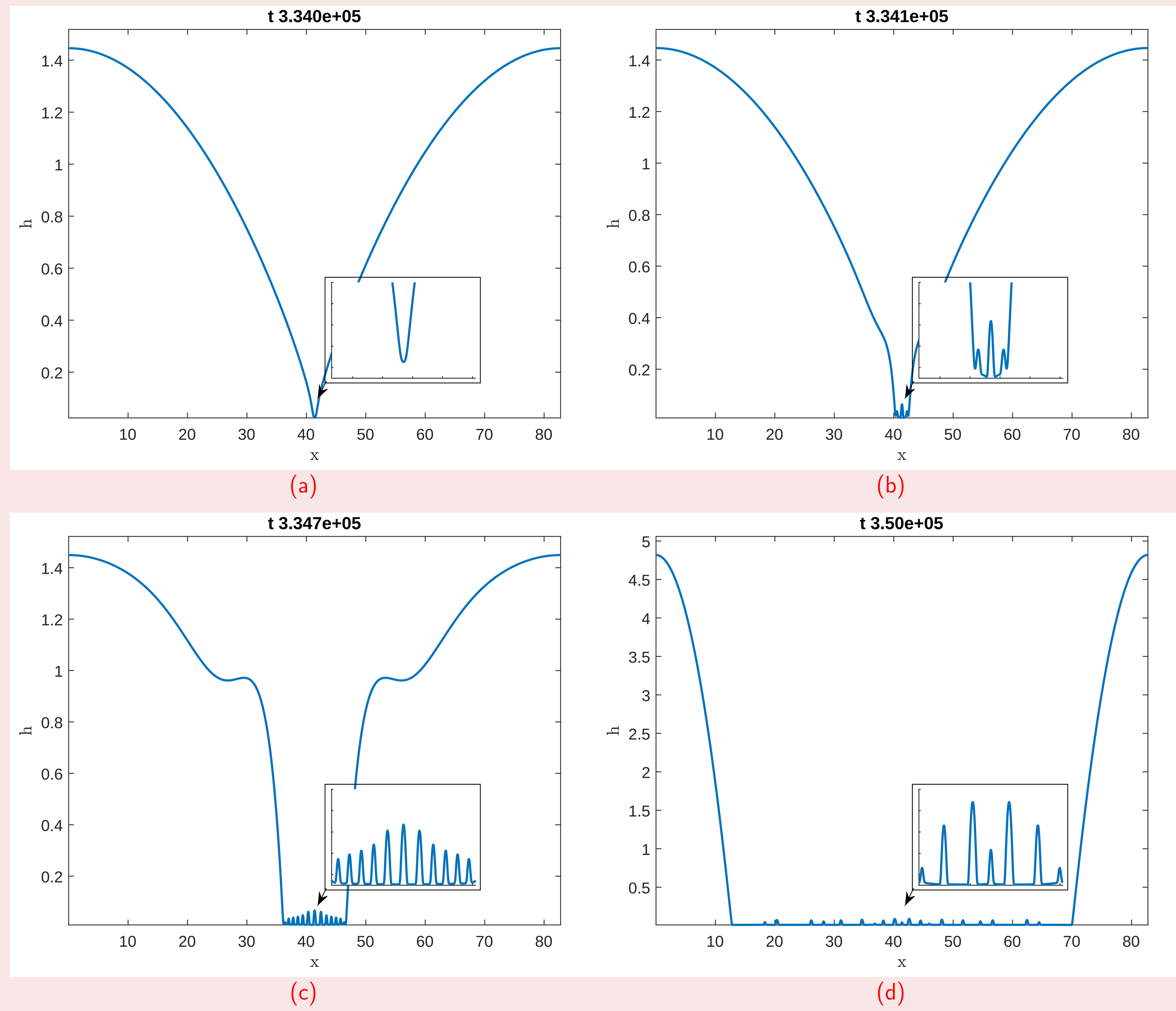

Figure 4: (a)-(d) Evolution for $h_0 = 1$ and $h_* = 0.01$, $b = 0$, $\lambda_1 = 10$, $\lambda_2 = 0.01$ at four selected times. In (a) the cusp formation. In (b) the separation of the two rims and the formation of wrinkles that lead to droplets in later times, e.g. in (c), and that stay until the final steady configuration (d).

In figures 4(a)-4(d) we see a numerical simulation of the evolution of the fluid interface. The unstable interface, initially flat, is perturbed, and it does not return to its initial profile, but it breaks up into two separate rims. The instability is due to the van der Waals force that drives the fluid interface towards the substrate (figure 4(a)) until the fluid thickness reaches a short-range value, the precursor film h_*. After this value the fluid separates in rims (figure 4(b)). The high elasticity of the fluid ($\lambda_1 = 10$) forms multiple wrinkles (figure 4(c)) that lead to the formation of satellite droplets between the two major blobs of fluid. These droplets remain even when the fluid reaches the steady state final configuration (figure 4(d)).

Conclusions and Future Work

Our numerical investigations allow to predict the dynamics of the moving interface of an unstable thin layer of polymeric liquid that dewets a solid substrate. Our findings are in agreement with the theoretical framework and have been verified through the tool of Linear Stability Analysis in the early times in which the fluid obeys the linear regime. We numerically solve the highly non-linear PDE governing the interface of the viscoelastic liquid, and our simulations show for the first time the dynamics of satellite droplets in thin films of viscoelastic fluids. This opens to future investigations in the characterization of droplets number, size and separation, depending on the physical parameters involved.

References

[1] Raucher M., Münch A., Wagner B., Blossey R., *A thin-film equation for viscoelastic liquids of Jeffreys type*, Eur. Phys. J. E **17**, 373 – 379, (2005)

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