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The Effect of Surface Tension on the Gravity-driven Thin Film Flow of Newtonian and Power-law Fluids

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Abstract

Gravity-driven thin film flow is of importance in many fields, as well as for the design of polymeric drug delivery vehicles, such as anti-HIV topical microbicides. There have been many prior works on gravity-driven thin films. However, the incorporation of surface tension effect has not been well studied for non-Newtonian fluids. After surface tension effect was incorporated into our 2D (i.e. 1D spreading) power-law model, we found that surface tension effect not only impacted the spreading speed of the microbicide gel, but also had an influence on the shape of the 2D spreading profile. We observed a capillary ridge at the front of the fluid bolus. Previous literature shows that the emergence of a capillary ridge is strongly related to the contact line fingering instability. Fingering instabilities during epithelial coating may change the microbicide gel distribution and therefore impact how well it can protect the epithelium. In this study, we focused on the capillary ridge in 2D flow and performed a series of simulations and showed how the capillary ridge height varies with other parameters, such as surface tension coefficient, inclination angle, initial thickness, and power-law parameters. As shown in our results, we found that capillary ridge height increased with higher surface tension, steeper inclination angle, bigger initial thickness, and more Newtonian fluids. This study provides the initial insights of how to optimize the flow and prevent the appearance of a capillary ridge and fingering instability.

Keywords

Thin film flows; Surface tension; Shear-thinning effect; Capillary ridge

1. Introduction

There are many industrial applications in which gravity-driven thin film flow is of interest. Among these are paints [1], contact lens manufacture [2] and microchip fabrication [3]. Gravity-driven thin film flow also occurs throughout nature, including a variety of gravity currents, such as lava flow and glacier flow [4–5]. All these flows can be modeled with very similar methods. However, since the study of these flows focuses on tracing the change of the free surface, a question must be raised here: is surface tension important? This paper is intended to develop a mathematical tool for understanding how important a role the surface tension plays in such flows.

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This paper is also one of the components of our research on how to design polymer solutions for optimal performance. One of the applications is in the topical drug delivery of anti-HIV products called microbicides [6–8]. Microbicides are delivered to vaginal or rectal epithelium to protect it from HIV and other sexually transmitted pathogens [9]. Microbicides may provide a physical barrier [10] amplifying the normal vaginal defense, as well as destroy the pathogens chemically or inhibit viral infection [11]. The microbicide may consist of an anti-HIV active agent in some delivery vehicle, such as a gel, cream, or foam. Microbicides are a promising solution to provide a low-cost, female-controlled method for protection against HIV and other sexually transmitted pathogens.

Our long-term goal is to design delivery vehicles (e.g. polymer solutions or “gels”) for one or more active microbicidal ingredients. As a step towards this goal, we develop mathematical tools to optimize the physicochemical properties of the delivery vehicle. The mathematical tools will be used to make a microbicide delivery vehicle that broadly and durably coats target epithelial surfaces.

To connect vehicle rheological properties to performance, we use non-Newtonian fluid mechanics to describe the flow of gels in response to forces experienced when delivered to the vagina. These forces can include gravity, squeezing, and surface tension. Here we focus on the gravity-driven coating process and consider surface tension. A gel may flow along the epithelial surface due to gravity because of the orientation of the vaginal axis and/or changes in posture. In our previous work on gravity-driven spreading, we developed experimental and numerical models (2D, i.e. 1D spreading) of a finite bolus of non-Newtonian fluids (power-law or Herschel-Bulkley) flowing down an incline [7, 12]. This new study considers the effect of surface tension of the liquid in the 2D power-law model.

To simulate surface tension, many studies have used the Volume of Fluids (VOF) Method coupled with the continuum surface force (CSF) method [13–17], which was originally developed by Brackbill et al. [18]. Basically, they treat surface tension as the volumetric force acting on the fluid near an interface and incorporate the surface tension effect as a source term in the Navier-Stokes equations. Therefore, VOF+CSF can be used to solve full Navier-Stokes equations for general fluid dynamics problems. However, for the thin film flow problems we are studying, we can reduce the Navier-Stokes equations down to a single thin film equation using the well-known lubrication approximation. Through this approach, we used the Young–Laplace equation, which states that surface tension results in a net normal force directed toward the center of curvature of the interface. Thus, we can incorporate the surface tension effect as a boundary condition for the pressure, as done in many studies (e.g., [19–22]). Although the computational scheme and post-analysis can both benefit from the simplified model, the limitation for this method is that it is hard to simulate the influence of contact angle. However, contact angles vanish when assuming complete wetting, as done in this study.

Previous literature using linear stability analysis (LSA) has shown that the “capillary ridge” occurring in the lengthwise direction was strongly related to the contact line “fingering instability” in the transverse direction [21–26]. The term capillary ridge describes the bump showing at the front of the spreading fluid, while fingering instability describes how the moving contact line at the front corrugates during flow. Schwartz [27] studied the contact line instability numerically and for the first time showed that surface tension effects controlled the instability. Troian et al. [25] initially developed LSA on thin film flow and illustrated that the “bump” was responsible for the linear instability. Bertozzi and Brenner [22] showed that the transient growth of contact line instability explained why the critical inclination angle observed in LSA did not match experiments. They also verified that when a capillary ridge in the profile disappears, the front contact line is linearly stable. Kondic and

his research group [21–23, 26, 28–29] also numerically studied the 3D flow to simulate the fingering instability in the transverse direction. These studies provided insights for our future 3D flow study. Recently, Lin and Kondic [30] studied the instability of the thin film flowing down an inverted incline. Because hanging flow also occurs in microbicide epithelial coating processes, it is also one of our future research interests.

All above mentioned studies have been done using a constant flux assumption, which means the thickness of fluid behind and in front of the contact line is constant [21, 23–24, 26, 28, 30–31]. The constant flux assumption is not appropriate in our case, because the epithelial spreading flow case is “constant volume,” rather than constant flux, and the fluid layer thins over time. There are some limitations and complications to apply LSA on constant volume flow. Gonzalez et al. [32] developed a predictive model for the constant volume by applying the LSA results of the constant flux case. Gomba et al. [33] developed an integral method to study the linear stability of the constant volume flow.

The above mentioned studies provided us the idea of using capillary ridge as an indicator for the fingering instability and motivated this study, because when we add surface tension effect to our 2D numerical simulation of a power-law fluid, in some cases we observe a capillary ridge in the 2D profile at the front of the fluid bolus. We also found that most of the studies mentioned above have assumed Newtonian fluids [21–30, 32–33], except Balmforth et al. [31] studied the instability of Bingham fluids using LSA and showed the effect of yield stress stabilized the contact line. To the authors’ knowledge, connection between surface tension effect and the shear-thinning rheological properties for non-Newtonian fluids has not appeared in the literature. But capillary ridge and fingering instability can also be observed in our experimental studies for shear-thinning fluids.

The goal of this study is to incorporate surface tension in the numerical 2D power-law model and use it for a parametric analysis. The main research questions are: (1) Under what flow parametric conditions does surface tension have an influence on shape or spreading? (2) When and under what kind of circumstances does the capillary ridge occur and increase?

2. Methods

2.1 Evolution equation

In this section, we develop an evolution equation to apply numerical methods for flow calculations. The equation uses the height of the fluid as a function of space and time ($h(x, t)$) to describe the movement of the fluid’s free surface. FIG. 1 illustrates the coordinate system diagram for flow down an incline with inclination angle α . Only x and z directions are considered in this 2D model.

We follow the theoretical approach from our previous work [7], and combine conservation of momentum and mass, no-slip boundary condition, and thin film lubrication approximations [34], and the power-law constitutive equation, $\tau_{zx} = m |u|^{n-1} u / z$, where τ is shear stress tensor, u is velocity in the axial direction, m is consistency, n is the shear-thinning index.

To incorporate the surface tension effect, we use the Young–Laplace equation [18] $\Delta p = \gamma k$ to get pressure equilibrium at the free surface, where Δp is the pressure difference at the fluid-air interface, γ is surface tension coefficient, k is curvature of the interface. The free surface in this study is a 1D curve. The curvature for a 1D curve is $k = |h''(x)| / (1 + h'(x)^2)^{3/2}$, which is positive and indicates $\Delta p > 0$ in the Young–Laplace equation. Because surface tension results in a net normal force directed toward the center of curvature of the interface [18], we can get a pressure formulation at the gel-air interface,

$$p_{gel} = p_{air} - \gamma \frac{h''(x)}{(1+h'(x)^2)^{\frac{3}{2}}}. \quad (1)$$

This holds for both the convex curve ($h''(x) < 0$) and the concave curve ($h''(x) > 0$). A small slope is assumed according to the thin film approximation, and Eq. (1) reduces to

$$p_{gel} = p_{air} - \gamma h''(x). \quad (2)$$

We used this pressure formulation (Eq. (2)) for the pressure term in the conservation of momentum equation and we derived our governing evolution equation. Refer to [35–36] for more details about the derivation.

$$\frac{\partial h}{\partial t} + m^{-\frac{1}{n}} \frac{n}{2n+1} \frac{\partial}{\partial x} \left\{ h^{\frac{1}{n}+2} \left[\rho g (\sin \alpha - \cos \alpha \frac{\partial h}{\partial x}) + \gamma \frac{\partial^3 h}{\partial x^3} \right]^{\frac{1}{n}-1} \left[\rho g (\sin \alpha - \cos \alpha \frac{\partial h}{\partial x}) + \gamma \frac{\partial^3 h}{\partial x^3} \right] \right\} = 0. \quad (3)$$

All the parameters in Eq. (3) were kept in dimensional form for the rest of this study because we want this study to provide insight on our future experimental work. Thus, showing isolated parameters and the critical values of these parameters in dimensional form is very important to this analysis. A non-dimensional study of Eq. (3) was also carried out and compared to existing Newtonian results in the literature in Appendix D (which also utilizes Appendix A–C).

2.2 Numerical method

The numerical method used to solve this nonlinear PDE was an implicit finite difference scheme. We applied backward difference for the time derivative and central difference for the space derivatives. We then used Newton's method to solve the full set of nonlinear algebraic equations resulting from finite difference discretization. Each iteration of Newton's method then involved a large set of linear equations, which was solved by LU decomposition method. The above processes were coded using C++.

The computational domain for the simulations in this study was 10cm long [0,10cm] in the x direction. We used a parabolic initial condition profile to start the flow. The free surface for this parabolic initial condition can be described with a function,

$$h(x) = \begin{cases} H(1 - (x-2)^2), & 1 \leq x \leq 3 \\ b, & \text{other domain} \end{cases},$$

where H is the initial center height of the parabola, and b is the thickness of the thin film preceding the front, called the precursor. We added a precursor because there is a surface tension singularity caused by the 4th order derivatives in Eq. (3). Refer to [37] for details. We used $b=0.01\text{cm}$ for all simulations in this study. Appendix A shows the sensitivity study on the precursor thickness b . The error tolerances for the LU decomposition method and Newton's method were both set to $1e-4$. The time step Δt was set to 0.001sec and the spatial mesh interval was 0.002cm .

2.3 Model validation

We validated our new model in the following four ways:

1. We performed the convergence test; the free surface height $h(x, t)$ converges for both space and time mesh refinement.
2. We monitored the total volume of the gel as a function of time and the results showed it holds for conservation of mass.
3. The results of the new surface tension model for $\gamma=0$ agreed with the similarity solution for power-law fluids, as well as the results of the previous model for a power-law fluid without consideration of surface tension [7]. Comparison between the numerical model results and the similarity solution is discussed in more details in Appendix B.
4. By assuming a simplified constant flux flow, we compared the result from our numerical model to the traveling wave solution. We found they greatly agreed with each other. Please refer to the Appendix C for details.

3. Results and discussion

In Sec. 3.1, we highlight the surface tension effect and appearance of the capillary ridge. In Sec. 3.2, first, we isolate the effect of surface tension on capillary ridge height and the spreading speed for both Newtonian and shear-thinning fluids. We also selected a surface tension coefficient value for the other parametric studies. Then, we explored how the other terms in the evolution equation (Eq. (3)) interact with each other and impact the capillary ridge height. The relevant parameters in the evolution equation (Eq. (3)) are:

- m : consistency of the gel,
- n : shear-thinning index of the gel,
- α : inclination angle,
- H : initial thickness, and
- γ : surface tension coefficient.

3.1 Capillary ridge

In Sec. 1, we mentioned that surface tension dominates at the front of the flow and therefore causes the capillary ridge. We also witnessed this phenomenon in our simulations when we added the surface tension effect.

The following simulations use a Newtonian fluid with initial thickness $H=0.3\text{cm}$, consistency $m=100\text{Psec}^{n-1}$, shear-thinning index $n=1$, inclination angle $\alpha=60^\circ$ and surface tension coefficient $\gamma=70\text{dyn/cm}$, as an example. A variety of parametric studies for non-Newtonian fluids are covered in the parametric study section.

FIG. 2 shows the free surface plot for the new surface tension model during a 110sec period with 10sec time sampling. A very similar side profile is also obtained in Gomba et al.'s constant volume study for Newtonian fluids [33]. We can compare our new surface tension model with our previous model [7] as shown in FIG. 3.

We can see the capillary ridge occurs in the new model after incorporating the surface tension effect – in FIG. 3, the red dashed plot shows a capillary ridge at the front of the flow. Moreover, the surface tension effect influences the spreading speed by holding the fluid and making it flow slower.

3.2 Parametric study

In this section, a series of simulations were carried out to investigate how the parameters influence the capillary ridge size. Here, we first focused on our main subject – surface tension. Then, we examined how the other terms in the evolution equation interact with each other and influence the capillary ridge.

We defined the capillary ridge height function as $h_{cr} = h_{max} - h_{max}|_{\gamma=0}$, where h_{max} is the maximum height of the free surface for a certain case, and $h_{max}|_{\gamma=0}$ is the maximum height of the free surface under the assumption that all other parameters in the simulation are the same, and only surface tension effect is not incorporated. Note that this calculation of h_{cr} is only an approximation of the capillary ridge height due to the flow behavior difference between the non-zero surface tension case and zero surface tension case. An alternate definition can be defined for a true capillary ridge height, but we did not select that method because it requires an arbitrary selection of the beginning of the ridge.

Due to different values of parameters, the spreading shape and speed of the simulations were very different. So for better comparison, we didn't choose a certain instance in time to compare the difference among these cases. Instead, we calculated the capillary ridge height for each case when the flowing front reached the same position: $x=4\text{cm}$.

Because surface tension is the actual cause of the capillary ridge, first, we varied the surface tension coefficient γ to examine the sensitivity. A large range of values [0, 0.01, 0.1, 1, 10, 100 dyn/cm] for the surface tension coefficient γ were investigated. Surface tension coefficient is generally much bigger than 0.01dyn/cm and 0.1dyn/cm for the polymer solutions we were studying, and is typically 40 to 80 dyn/cm. However, as a theoretical study, we want to see how surface tension affects the capillary ridge height over a large range.

FIG. 4 shows the results of changing capillary ridge height (black solid and dotted lines, left axis) and spreading time (red dashed and dash-dot lines, right axis) with different surface tension coefficients γ for both Newtonian ($n=1$) and shear-thinning fluids ($n=0.5$).

For both Newtonian and shear-thinning fluids, the capillary ridge height increased with increasing surface tension coefficient. The impact of surface tension on the capillary ridge height had a sharper increase in the range of [0.1, 10] dyn/cm than in other regions. The figure also showed the capillary ridge height of a shear-thinning fluid is less sensitive to changes in surface tension than for Newtonian fluids. Moreover, it took longer time for a larger surface tension fluid to reach to $x=4\text{cm}$, which means the surface tension can hold the spreading. In addition, surface tension slowed the shear-thinning fluids more than the Newtonian fluids. In the range of [0, 0.1] dyn/cm, the surface tension was not very important to both the spreading shape and speed.

We can conclude that an increase in surface tension coefficient will always increase the capillary ridge height. So for the rest of this study, we also want to know how the capillary ridge height depends on the other parameters: consistency m , shear-thinning index n , initial thickness H , and incline angle α , with a constant surface tension coefficient γ . We used $\gamma = 70\text{dyn/cm}$ for the rest of the simulations, referring to the surface tension coefficient measured for a hydroxyethylcellulose (Sigma-Aldrich, viscosity average molecular weight, $M_v=250,000$) polymer solution.

Over many cases of parametric study, we found that the consistency m affected the capillary ridge very slightly. Therefore, we considered consistency as constant for the following

simulations as well. We chose $m=400\text{Psec}^{n-1}$, approximately middle range of consistency for typical gels used in our lab's experiments (range of [91.95, 506.58] Psec^{n-1}).

In order to better monitor how the capillary ridge height changed with respect to the other three parameters n , H , and α , we set up coupling parametric studies. The approach is to take one of these parameters as a constant and vary the other two parameters as one series of studies. In total, there are three series varying the following parameter sets:

1. n and H
2. α and H
3. n and α

The range for the shear-thinning index n was set to [0.5, 1] with 0.1 increment, which brackets the range of n values for typical gels used in our experiments. The range for initial thickness H was [0.2, 0.45] cm with 0.05 increment, because 0.5 cm is the biggest thickness to make sure it is still within the lubrication approximation scope. We also varied the inclination angle α from 10° to 90° with 10° increment (5° increment from 10° to 30°).

In total, there were 360 cases involved in this parametric study. For efficiency, we submitted our simulations to run on the Bioinformatics cluster at the KU Information and Telecommunication Technology Center (ITTC).

3.2.1 Effect of shear-thinning index (n) and initial thickness (H)—Plots of the capillary ridge height for this n and H coupling parametric study are shown in FIG. 5. We can see that the height of the capillary ridge increased for both increasing shear-thinning index n and initial thickness H .

First, we compare between Newtonian fluids ($n=1$) and non-Newtonian shear-thinning fluids ($n<1$). If we look at the $H=0.3\text{cm}$ line in FIG. 5 and take the two ends $n=0.5$ and $n=1$ as examples, we can see the difference of the capillary ridge height between the two cases, as shown in the free surface profiles in FIG. 6. Obviously, a bigger capillary ridge occurred in the Newtonian fluid (red dashed) than the non-Newtonian fluid (black solid) with the same other parameters. The capillary ridge height is 0.0422 cm for the $n=0.5$ case, and 0.0530 cm for the $n=1$ case.

Likewise, we can compare between a thicker film and a thinner film – for example, $H=0.2\text{cm}$ and $H=0.45\text{cm}$ cases at the $n=0.7$ in FIG. 5. FIG. 7 shows the difference of the capillary ridge profile between the two cases. We found that the thicker film (red dashed) had a much bigger ridge than the thinner film (black solid). The capillary ridge height is 0.0311 cm for the $H=0.2\text{cm}$ case, and 0.0652 cm for the $H=0.45\text{cm}$ case.

In summary, increasing shear-thinning behavior reduces the capillary ridge height. Also, a thinner initial thickness will reduce the capillary ridge height as well. In addition, for thicker films, a change in shear-thinning behavior has more impact than in thinner films.

3.2.2 Effect of inclination angle (α) and initial thickness (H)—As shown in FIG. 8, the capillary ridge height is an increasing function for both increasing α and H . Inclination angle α plays a more important role than H , and the inclination angle's impact on the capillary ridge height increased at higher initial thickness. In addition, in the range of $[40^\circ, 90^\circ]$, H starts to have more influence than it does in the range of $[10^\circ, 30^\circ]$. Moreover, in the range of $[5^\circ, 15^\circ]$, the capillary ridge height is very small. An alternate definition of h_{cr} using the actual ridge height, as well as a side profile plot, indicated insignificant capillary ridge in the range of $[5^\circ, 15^\circ]$. Some previously published studies for Newtonian fluids [22]

showed there existed a critical angle where the capillary ridge just started to appear. This implies we can control the inclination angle in experiments to prevent the appearance of a capillary ridge. In summary, both α and H can be controlled to impact capillary ridge height.

3.2.3 Effect of shear-thinning index (n) and inclination angle (α)—Similarly, FIG. 9 shows that the capillary ridge height is an increasing function for both increasing n and α . In other words, as the fluid is more Newtonian or on a steeper incline, the capillary ridge gets bigger. Inclination angle α has more influence on the capillary ridge height than n . At greater inclination angles, shear-thinning behavior has a slightly greater impact than at smaller inclination angles. In summary, both changes in inclination angle and shear-thinning index can be used to control the capillary ridge height of a film, but the inclination angle has much greater influence.

4. Conclusions

In summary, according to our numerical model of spreading of power-law fluids on an incline, surface tension effect influences both the spreading shape and speed of the fluid. The dramatic difference between this surface tension model and the previous model is the capillary ridge in the front of the gel. We found in our parametric analysis that the capillary ridge height is an increasing function of surface tension coefficient γ , inclination angle α (when $\alpha >$ critical angle), initial thickness H , and shear-thinning index n . We also found consistency m affects the capillary ridge very slightly. Furthermore, a fluid flows slower if the surface tension coefficient γ increases.

In addition, our parameter analysis provided some useful conclusions about the relative impact of the parameters on the capillary ridge height. The capillary ridge height of a shear-thinning fluid is less sensitive to changes in surface tension than for Newtonian fluids. In thicker films, a change in shear-thinning behavior has more impact than it does for thinner films. Inclination angle plays a more important role than initial thickness, and the angle's impact is greater for thicker films. Initial thickness has a greater influence at steeper angles than flatter angles. There exists a critical angle where the capillary ridge just started to appear. Inclination angle also has a greater impact than shear-thinning behavior. But at steeper angles, shear-thinning behavior has a little more influence than at flatter angles.

All of these above conclusions directly inform the experimental design for our planned experimental analysis of these flows. These conclusions are also very important because we can use them to optimize a polymer solution's properties for optimal flow and surface coverage. The literature suggests that the emergence of a capillary ridge may indicate fingering instabilities at the spreading front [22]. In our specific application in microbicide coating of epithelial surfaces, fingering instabilities during epithelial coating may change the microbicide gel distribution and impact how well it can protect the epithelium. Therefore, our study indicates we can control the inclination angle or optimize the shear-thinning index n to prevent the appearance of the fingering instabilities. For example, inclination angle results could be translated to package instructions for posture during microbicide gel application by the user. Additionally, gel structure or components could be altered to yield rheological parameters for optimal spreading with no fingering. The utility of this study's conclusions is not limited to drug delivery applications. The results we found here are applicable to other fields where gravity-driven thin film flows of shear-thinning fluids are present.

There are some limitations to this study, which guide our planned future studies. Future work should include implementing contact line stability analysis for the power-law model, setting up experiments to verify the model, using better constitutive equations to make the

model applicable for more types of fluids, involving a dilution/mixing influence and slip boundary condition, and extending to a 3D model. The findings in this study will directly guide us in experimental plans and 3D mathematical model development.

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Appendix A

Sensitivity study of precursor thickness

Many previous works have studied the influence of the precursor thickness. Both numerical [22, 33] and experimental [38] studies have indicated that increasing the thickness of the precursor can decrease the size of the capillary ridge and suppress the contact line instability. FIG. A.1 shows the comparison between different precursors: $b=0.001\text{cm}$ (black solid), $b=0.01\text{cm}$ (blue dotted) and $b=0.05\text{cm}$ (red dashed).

We can see the capillary ridge height goes down when we increase the precursor thickness b . This agrees with the previous literature.

Appendix B

Similarity solution for power-law fluids

Far behind the front region where surface tension dominates, the height profile of the gel can be described by a similarity solution. For Newtonian fluids, a similarity solution was obtained by Huppert [39],

$$h(x, t) = \sqrt{\frac{\mu x}{\rho g \sin \alpha t}}.$$

This expression indicates that the thickness of the free surface decreases on the scale of $H_N \sim t^{-1/3}$ at a relatively long time after initial condition, and it is independent of the initial condition.

Following the method outlined in [39], we can obtain the similarity solution for the power-law fluid as

$$h(x, t) = \left(\frac{m}{\rho g \sin \alpha} \right)^{\frac{1}{n+1}} \left(\frac{x}{t} \right)^{\frac{n}{n+1}}. \quad (\text{B.1})$$

By setting $n=1$, this expression reduced to Huppert's Newtonian similarity solution.

Assuming a zero surface tension in our model ($\gamma=0$), we compared the result from our numerical model to this power-law similarity solution. We compared for both Newtonian fluids (FIG. B.1) and shear-thinning fluids (FIG. B.2) using two different initial conditions

$H=0.2\text{cm}$ and $H=0.45\text{cm}$. As shown in the figures, all four cases agree with the similarity solution. We can see the gels start from different initial conditions, and after a relatively long spreading time (110 sec), the free surfaces approach the similarity solution profile. Although the Newtonian gels flow faster than the shear-thinning gels for these settings, the similarity solution very accurately describes the difference. Thus, through this study, we verified our numerical model using the similarity solution.

Appendix C

Traveling wave solution

By assuming a simplified constant flux flow, we compared the result from our numerical model to the traveling wave solution. We used the constant flux boundary conditions $x \rightarrow -\infty, h \rightarrow 1$ and $x \rightarrow \infty, h \rightarrow b$ for Eq. (3) (where b is thickness of the precursor). This boundary condition leads to a traveling wave solution $h(x, t)$ for Eq. (3). If we define $h(x, t) = h_0(x^*)$, where $x^* = x - Ut$, and U is the velocity of the traveling wave, then the function $h_0(x^*)$ must satisfy

$$-Uh_0 + m^{-\frac{1}{n}} \frac{n}{2n+1} \left\{ h_0^{\frac{1}{n}+2} \left| \rho g (\sin \alpha - \cos \alpha h_{0x^*}) + \gamma h_{0x^*} x^* \right|^{\frac{1}{n}-1} [\rho g (\sin \alpha - \cos \alpha h_{0x^*}) + \gamma h_{0x^*} x^*] \right\} = f.$$

Refer to [26] for more details about traveling wave solution of the thin film equation.

Applying the two boundary conditions, $x^* \rightarrow -\infty, h_0 \rightarrow 1$ and $x^* \rightarrow \infty, h_0 \rightarrow b$, we can get

$$U = m^{-\frac{1}{n}} \frac{n}{2n+1} (\rho g \sin \alpha)^{\frac{1}{n}} \left(\frac{1 - b^{\frac{1}{n}+2}}{1 - b} \right). \quad (\text{C.1})$$

$$f = m^{-\frac{1}{n}} \frac{n}{2n+1} (\rho g \sin \alpha)^{\frac{1}{n}} \left(\frac{-b + b^{\frac{1}{n}+2}}{1 - b} \right).$$

Using the 2D numerical model developed in this study, we can compare the result of our numerical solution to the traveling wave solution. We used a smooth step function as the initial condition,

$$h(x) = \frac{1}{1 + \exp(-4(-(x-10)))} \quad \begin{matrix} 0 \leq x \leq 10 \\ 10 < x \leq 40 \end{matrix},$$

in our 2D model. FIG. C.1 shows the numerical simulation results plotted over 10 seconds.

The velocity calculated in the simulation ($U=1.6200$) had a great agreement with the traveling wave solution ($U=1.6178$) (Eq. (C.1)).

Appendix D

Non-dimensional study with constant flux setup

Following the non-dimensionlization in [22], the dimensionless variables can be introduced using the characteristic film thickness H_N , film length L , time T and velocity U :

$$\tilde{h} = \frac{h}{H_N},$$

$$\tilde{x} = \frac{x}{L},$$

$$\tilde{t} = \frac{t}{T}.$$

Here, H_N is the thickness of the profile described in the power-law similarity solution, as introduced in Appendix B. $L = H_N/(C_a)^{1/3}$, where $C_a = \mu_0 U/\gamma$ is the power-law capillary number and $\mu_0 = m(U/H_N)^{n-1}$ is the characteristic viscosity.

Because the flow field away from the front determines the characteristic velocity, we can estimate the characteristic time scale, T , using the power-law similarity solution (Eq. (B.1)),

$$T = (H_N)^{-(\frac{1}{n}+1)} \left(\frac{m}{\rho g \sin \alpha} \right)^{\frac{1}{n}} L.$$

so that the characteristic velocity $U \sim L/T$, and the capillary number can be approximated as

$$C_a = \frac{\mu_0 U}{\gamma} \approx \frac{\rho g \sin \alpha H_N^2}{\gamma}.$$

Substituting these dimensionless variables as well as the capillary number C_a into Eq. (3), we get the non-dimensional evolution equation:

$$\frac{\partial \tilde{h}}{\partial \tilde{t}} + \frac{n}{2n+1} \frac{\partial}{\partial \tilde{x}} \left\{ \tilde{h}^{\frac{1}{n}+2} \left| 1 - \cot \alpha C_a^{\frac{1}{3}} \frac{\partial \tilde{h}}{\partial \tilde{x}} + \frac{\partial^3 \tilde{h}}{\partial \tilde{x}^3} \right|^{\frac{1}{n}-1} \left(1 - \cot \alpha C_a^{\frac{1}{3}} \frac{\partial \tilde{h}}{\partial \tilde{x}} + \frac{\partial^3 \tilde{h}}{\partial \tilde{x}^3} \right) \right\} = 0. \quad (\text{D.1})$$

If we define $D = \cot \alpha C_a^{1/3}$, which is an important quantity indicated in [22], then Eq. (D1) becomes only dependent on two dimensionless parameters: D and shear-thinning index n .

To directly compare to the literature, Eq. (D.1) was solved with the constant flux condition as introduced in Appendix C. The result is similar in shape to the result shown in FIG. C.1. The dependence of the dimensionless maximum height of the flow profiles on D and n is shown in FIG. D.1.

Because we used a constant flux setup, the capillary ridge height can be simply calculated by $h_{cr} = h_{max} - 1$. As we can see from FIG. D.1, for both Newtonian fluids ($n=1$) and non-Newtonian fluids ($n<1$), the capillary ridge height reduces as D increases. This result agrees with the parametric study of D for Newtonian fluids in [22]. Moreover, it indicates that the more shear-thinning the fluid is, the smaller capillary ridge occurs, as also found in our dimensional study.

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Highlights

- > We model gravity-driven flows of non-Newtonian fluids with surface tension effect.
- > Parametric study of surface tension, shearing-thinning, etc. is carried out.
- > Capillary ridge height increases with surface tension and shear-thinning index.
- > This study is to optimize polymeric liquids' properties for optimal flow performance.

FIG. 1.
Coordinate system diagram for our 2D model of 1D flow down an incline.

FIG. 2.

Evolution of free surface, total time=110sec, sampling=10sec. (Parameters used in the simulation: $m=100\text{Psec}^{n-1}$, $n=1$, $\alpha=60^\circ$, $\gamma=70\text{dyn/cm}$, $H=0.3\text{cm}$, $b=0.01\text{cm}$)

FIG. 3.

(Color online) Comparison of free surfaces between the model without surface tension effect (black solid) and the surface tension model (red dashed) at $t=20\text{sec}$. (Parameters used in the simulation: $m=100\text{Psec}^{n-1}$, $n=1$, $\alpha=60^\circ$, $\gamma=70\text{dyn/cm}$, $H=0.3\text{cm}$, $b=0.01\text{cm}$)

FIG. 4.

(Color online) Plot of the capillary ridge height h_{cr} (black solid and dotted lines, left axis) and spreading time (red dashed and dash-dot lines, right axis) as a function of surface tension coefficient γ for both Newtonian ($n=1$, solid and dashed lines) and shear-thinning fluids ($n=0.5$, dotted and dash-dot lines). (Parameters used in the simulation: $m=100\text{Psec}^{n-1}$, $\alpha=60^\circ$, $H=0.3\text{cm}$, $b=0.01\text{cm}$)

FIG. 5. Plot of the capillary ridge height h_{cr} (cm) as a function of n for different values of initial thickness H , with constant $m = 400 \text{ Psec}^{n-1}$, $\alpha = 60^\circ$, $\gamma = 70 \text{ dyn/cm}$.

FIG. 6.
 (Color online) Comparison of free surfaces between shear-thinning index $n=0.5$ (black solid) and $n=1$ (red dashed) when gel reaches $x=4$ cm, with constant $m=400\text{Psec}^{n-1}$, $\alpha=60^\circ$, $\gamma=70\text{dyn/cm}$ and $H=0.3\text{cm}$.

FIG. 7.
 (Color online) Comparison of free surfaces between initial thickness $H=0.2\text{cm}$ (black solid) and $H=0.45\text{cm}$ (red dashed) when gel reaches $x=4\text{cm}$, with constant $m=400\text{Psec}^{n-1}$, $n=0.7$, $\alpha=60^\circ$ and $\gamma=70\text{dyn/cm}$.

FIG. 8.

Plot of the capillary ridge height h_{cr} (cm) as a function of α for different values of initial thickness H , with constant $m=400\text{Psec}^{n-1}$, $n=0.7$ and $\gamma=70\text{dyn/cm}$. Note: a finer mesh between 10° and 40° for α was applied to handle the rapid change.

FIG. 9.

Plot of the capillary ridge height h_{cr} (cm) as a function of α for different values of n , with constant $m=400\text{Psec}^{n-1}$, $H=0.3\text{cm}$ and $\gamma=70\text{dyn/cm}$. Note: a finer mesh between 10° and 40° for α was applied to handle the rapid change.

FIG. A.1.

(Color online) Comparison of the free surfaces between the results of different precursor thickness: $b=0.001$ cm (black solid), $b=0.01$ cm (blue dotted) and $b=0.05$ cm (red dashed).

(Parameters used in the simulation: $m=100\text{Psec}^{n-1}$, $n=0.8$, $\alpha=60^\circ$, $\gamma=70\text{dyn/cm}$, $H=0.3\text{cm}$)

FIG. B.1.

(Color online) Comparison of the free surface spreading of the similarity solution (black solid) and the numerical model at 110 sec for Newtonian fluids. Two different initial conditions: $H=0.2\text{cm}$ (red dashed) and $H=0.45\text{cm}$ (blue dotted). Parameters: $m=100\text{Psec}^{n-1}$, $n=1$, $\alpha=60^\circ$ and $\gamma=0\text{dyn/cm}$.

FIG. B.2.

(Color online) Comparison of the free surfaces spreading of the similarity solution (black solid) and the numerical model at 110 sec for shear-thinning fluids. Two different initial conditions: $H=0.2$ cm (red dashed) and $H=0.45$ cm (blue dotted). Parameters: $m=100\text{Psec}^{n-1}$, $n=0.5$, $\alpha=60^\circ$ and $\gamma=0\text{dyn/cm}$.

FIG. C.1.

Evolution of free surface using constant flux in the numerical simulation, total time=10sec, sampling=1sec. (Parameters used in the simulation: $m=200\text{Psec}^{n-1}$, $n=0.9$, $\alpha=60^\circ$, $\gamma=40\text{dyn/cm}$, $b=0.01\text{cm}$)

FIG. D.1.
Dimensionless maximum height of the flow profiles as a function of D for different values of shear-thinning index n .