On the determination of the steady film profile for a non-Newtonian thin droplet

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A shooting method is used to determine a solution to a third-order ODE modeling the steady profile of a non-Newtonian thin droplet. We compare a direct approach to an iterative approach using a secant method. We obtain a nonlinear relationship between the contact angle $\phi$ and the position of the contact line $r$. From this nonlinear relationship we use curve fitting to obtain an empirical law of the form $\tan \phi \propto f(k)r^f$ where $k$ is the power law coefficient and $f$ is a nonlinear function of $k$.

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1. Introduction

In this paper we consider the spreading of a thin droplet on a solid substrate. The time evolution of the free surface, $h(x, t)$, of the thin droplet is modeled by the generalized diffusion equation given by

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x} \left( h^k \frac{\partial^3 h}{\partial x^3} \right), \quad h \geq 0 \tag{1.1}$$

where $x$ is the spatial coordinate and $t$ is the time. For a Newtonian fluid, when the constant $k = 1$, (1.1) models the thickness of a thin film in a Hele-Shaw cell [1–5]. When $k = 3$, (1.1) models the surface tension driven spreading of a thin viscous film on a solid substrate [6–10]. A generalization of (1.1) given by

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x} \left( h^{(2q+1)/q} \frac{\partial^3 h}{\partial x^3} \right) \tag{1.2}$$

has been derived by King [11]. Eq. (1.2) models the spreading of a non-Newtonian fluid on a solid substrate. The mapping $q = 1/(k - 2)$ transforms (1.1) into (1.2). King [11] shows that for $0 < q < 1$, (1.2) models a shear-thinning fluid. For $q = 1$, (1.2) models a Newtonian fluid and for $q > 1$, a shear-thickening fluid. This implies that for $k > 3$, (1.1) models a shear-thinning fluid. For $2 < k < 3$, (1.1) models a shear-thickening fluid and for $k = 3$, a Newtonian fluid. Myers [12] has made an extensive review of the applications of the generalized diffusion equation and the importance of surface tension dominated flows in coating. Surface tension dominated flows are also used to model the motion of a thin layer of tears on a contact lens and the formation of foams and bubbles. Lie symmetry solutions admitted by (1.1) have been investigated by Gandarias and Medina [13].

In this paper we use a shooting method to determine a numerical solution to a third-order ordinary differential equation (ODE) obtained by investigating steady solutions of (1.1). As a consequence of using a shooting method we are able to
determine an explicit relationship between the static contact angle \( \phi \) and the position of the contact line at \( x = r \). More specifically, we obtain an empirical representation of Tanner’s law in terms of the constant \( k \), where in the light of the work by King [11], \( k \) can be thought of as a power law coefficient. The contact angle \( \phi \) is defined as the angle made by the droplet with the solid substrate at the air/liquid–solid interface. The contact line gives the position of the contact angle. The contact angle is important in determining the kind of wetting that takes place. For \( 0 < \phi < \pi/2 \), the film is defined as being highly wettable. For contact angles \( \phi \geq \pi/2 \), the film has low wettability. Knowing the wettability is important in industrial processes in which the coating of the solid substrate by the liquid is important. In coating flows it is important to ensure that the contact angle is small to ensure that complete wetting takes place. Hocking and Rivers [14] investigate the surface tension driven spreading of a drop and the relationship between the contact angle and wetting. Further investigations on the nonlinear relationship between wetting and the contact angle have been made by Dussan [15], de Gennes [16], de Gennes et al. [17], Neogi [18] and Shikhmurzaev [19].

Substituting the steady solution \( h(x, t) = y(x) \) into (1.1) we obtain

\[
\frac{d}{dx} \left(y'y''(x)\right) = 0 \quad (1.3)
\]

where \( \prime = d/dx \). Integrating (1.3) we obtain

\[
y'y'' = d_0 \quad (1.4)
\]

where \( d_0 \) is a constant. Substituting the transformations

\[
y = e^{a\xi}, \quad x = e^{b\xi}
\]

where \( a \) and \( b \) are constants into (1.4) we obtain

\[
e^{(ak+a-3b)}y'''' = c. \quad (1.6)
\]

Tanner [10] has shown that by choosing \( c = e^{ak+a-3b} \) we can reduce (1.4) to

\[
y'''' = y^{-k} \quad (1.7)
\]

where we have suppressed the overbars. Alternatively, substituting the traveling wave ansatz \( h(x, t) = y(\xi) \) where \( \xi = x - Vt \) into (1.1) we obtain

\[
Vy = y^{(k+1)}y'' + d_1 \quad (1.8)
\]

where \( d_1 \) is a constant. Choosing \( d_1 = 0 \) and \( V = 1 \) we obtain (1.7). The behavior of (1.8) has been extensively studied by Boatto et al. [20]. Boatto et al. [20] characterize the behavior of soliton like solutions and moving front solutions for different values of \( k \).

Momoniat [21] investigates a finite difference solution to the third-order ODE (1.7) solved subject to (1.9) and (1.11). Momoniat [21] shows how the instability of solutions obtained from a symmetric difference scheme are overcome by using a non-symmetric difference scheme. In this approach the position \( r \) of the contact line must be specified before the domain discretization can take place. Other investigations of the third-order ODE (1.7) based on asymptotic methods [22], numerical methods [23,24], series solutions [25] and analytical solutions [26–28] have focused on boundary conditions related to the problem of drainage of a thin film down a dry wall or boundary conditions with a non-zero initial derivative. Momoniat and Mahomed [29] have performed a Lie symmetry analysis on (1.7) for the initial value problem \( y(0) = \alpha, y'(0) = \beta \) and \( y''(0) = \gamma \) for \( \alpha, \beta \) and \( \gamma \) constants.

Boundary conditions appropriate to our investigation come from a problem originally considered by Tanner [10]. Tanner investigated the surface tension dominated spreading of a thin oil droplet. Tanner’s boundary conditions are given by

\[
y(0) = 1, \quad y'(0) = 0 \quad (1.9)
\]

and

\[
y(r) = 0 \quad (1.10)
\]

where \( r \) is a constant satisfying \( r > 0 \). The boundary condition (1.10) gives the position of the contact line \( y = 0 \) at \( x = r \). The contact line singularity of the third-order ODE (1.7) is overcome by replacing \( y(r) = 0 \) by

\[
y(r) = \epsilon \quad (1.11)
\]

for \( \epsilon \ll 1 \) [30,31]. The constant \( \epsilon \) is the height of a precursor film (see Fig. 1).

The paper is divided up as follows. In Section 2 we consider an asymptotic solution of (1.7) for \( k < 2 \) at the contact line \( y = 0 \). From this asymptotic solution we derive a nonlinear relationship between the contact angle and the position of the contact line. In Section 3 we compare two formulations of a shooting method to determine a numerical solution to the boundary value problem. Concluding remarks are made in Section 4.
2. An asymptotic solution at the contact line

In this section we investigate an asymptotic solution admitted by (1.7) in order to determine a relationship between \( r \) and \( \phi \). It is well known that the investigation of invariant solutions effects a reduction in the order of the differential equation under consideration. The order of the autonomous third-order ODE (1.7) can be reduced by 1 by making the substitution

\[
y' = v(y)
\]  
(2.1)

that makes the dependent variable \( y \) an independent variable. Substituting (2.1) into (1.7), we obtain the second-order ODE

\[
v^2 \frac{d^2 v}{dy^2} + v \left( \frac{dv}{dy} \right)^2 = y^{-k}.
\]  
(2.2)

By including a contact angle boundary condition

\[
y'(r) = -\tan \phi
\]  
(2.3)

at the contact line \( y = 0 \), the boundary conditions (1.9) and (1.11) are transformed by (2.1) into

\[
v(\epsilon) = -\tan \phi, \quad v(1) = 0.
\]  
(2.4)

The second-order ODE (2.2) is singular when touchdown occurs, i.e. \( y = 0 \). To investigate the asymptotic behavior of (2.2) at the contact line we make the coordinate transformation:

\[
y = e^\xi.
\]  
(2.5)

Eq. (2.2) reduces to

\[
v^2 \left( \frac{d^2 v}{d\xi^2} - \frac{dv}{d\xi} \right) + v \left( \frac{dv}{d\xi} \right)^2 = e^{(2-k)\xi}.
\]  
(2.6)

The boundary conditions (1.9), (1.11) and (2.3) reduce to

\[
v(\epsilon) = -\tan \phi, \quad v(1) = 0.
\]  
(2.7)

Choosing \( k = 2 \) simplifies (2.6) to

\[
v^2 \left( \frac{d^2 v}{d\xi^2} - \frac{dv}{d\xi} \right) + v \left( \frac{dv}{d\xi} \right)^2 = 1.
\]  
(2.8)

The substitution

\[
\frac{dv}{d\xi} = h(v), \quad \frac{d^2 v}{d\xi^2} = h \frac{dh}{dv}
\]  
(2.9)

reduces the autonomous second-order ODE (2.8) to

\[
v^2 \left( \frac{dh}{dv} - h \right) + vh^2 = 1.
\]  
(2.10)

Once again we are unable to make analytical progress with (2.10).
We consider an asymptotic solution of (2.6) for \( \xi \to -\infty \) (\( y \to 0 \)). Eq. (2.6) reduces to

\[
v^2 \left( \frac{d^2 v}{d\xi^2} - \frac{dv}{d\xi} \right) + v \left( \frac{dv}{d\xi} \right)^2 = 0.
\]  

(2.11)

The reduction to (2.11) is valid for \( k < 2 \). The substitution (2.9) reduces the second-order autonomous ODE (2.11) to the first-order ordinary differential equation

\[
v^2 \left( \frac{dh}{dv} - h \right) + vh^2 = 0.
\]  

(2.12)

Solving (2.12) we find that

\[ h = \frac{v}{2} + \frac{c_1}{v}, \]  

(2.13)

where \( c_1 \) is a constant. From (2.9), Eq. (2.13) can be written as the first-order ordinary differential equation

\[
\frac{dv}{d\xi} = \frac{1}{2} v + \frac{c_1}{v},
\]  

(2.14)

and integrating (2.14) we find that

\[ v^2 + 2c_1 = c_2 e^{\xi}. \]  

(2.15)

Substituting (1.9) and (2.5) into (2.15) we obtain

\[ y^2 + 2c_1 = c_2 y. \]  

(2.16)

Imposing the boundary conditions (1.9) on (2.16) we find that

\[ c_2 = 2c_1 \]  

(2.17)

giving

\[ y^2 = 2c_1 (y - 1). \]  

(2.18)

Imposing (1.10) and (1.11) on (2.18) we obtain

\[ c_1 = \frac{\tan^2 \phi}{2 (\epsilon - 1)} \]  

(2.19)

and therefore

\[ y' = \pm \tan \phi \sqrt{\frac{y - 1}{\epsilon - 1}}. \]  

(2.20)

In the asymptotic limit \( \epsilon \to 0 \), (2.20) simplifies to (for the negative case)

\[ y' = - \tan \phi \sqrt{1 - y}. \]  

(2.21)

Integrating (2.21) and imposing the initial condition \( y(0) = 1 \) we obtain

\[ y = 1 - \frac{1}{4} x^2 \tan^2 \phi. \]  

(2.22)

Therefore, at the contact line \( y(r) = 0 \), we find that

\[ r = \pm \frac{2}{\tan \phi}. \]  

(2.23)

The asymptotic solution considered in this section has shown the dependence of the contact angle \( \phi \) on the position of the contact line \( x = r \).
3. The shooting method

In this section we use a shooting method to investigate numerical solutions of (1.7). We write (1.7) as the system of first-order ODEs

\[ \begin{align*}
  y' &= v, \quad v' = w, \quad w' = y^{-k}. 
\end{align*} \tag{3.1} \]

We discretize the system (3.1) by defining \( y_j = y(x_j) \), \( v_j = v(x_j) \) and \( w_j = w(x_j) \). The domain \( x \in [0, r] \) is divided up into \( n + 1 \) equidistant intervals where \( x_j = jh, h = r/n, x_0 = 0 \) and \( x_n = r \).

In order to implement a shooting method we solve the third-order ODE (1.7) subject to

\[ y(0) = 1, \quad y'(0) = 0, \quad y''(0) = \alpha. \tag{3.2} \]

The constant \( \alpha \) must be determined such that (1.11) is satisfied. In terms of the discretization given above, the initial conditions (3.2) are written as

\[ y_0 = 1, \quad v_0 = 0, \quad w_0 = \alpha. \tag{3.3} \]

The physical boundary conditions of the problem (1.9) and (1.11) give

\[ y_0 = 1, \quad v_0 = 0, \quad y_n = \epsilon. \tag{3.4} \]

A high-order Taylor approximation to \( y_{j+1} \) is given by

\[ y_{j+1} = y_j + hy'_j + \frac{h^2}{2}y''_j + \frac{h^3}{3!}y'''_j + O(h^4). \tag{3.5} \]

Replacing the third derivative from (1.7) and using (3.1), the Taylor approximation (3.5) becomes

\[ y_{j+1} = y_j + hu_j + \frac{h^2}{2}w_j + \frac{h^3}{3!}y_j^{-k} + O(h^4). \tag{3.6} \]

Similarly, we find that

\[ \begin{align*}
  v_{j+1} &= v_j + hw_j + \frac{h^2}{2}y_j^{-k} + O(h^2), \\
  w_{j+1} &= w_j + hy_j^{-k} + O(h^2). \tag{3.7, 3.8} \end{align*} \]

The truncation error of the high-order Taylor approximation to \( y_j \) is \( O(h^4) \). Fourth-order Runge–Kutta methods have truncation errors of the same order. Cortell [32] has recently discussed the advantages of using a shooting method to solve nonlinear ordinary differential equations that arise in the study of nonlinear fin equations. The combination of a shooting method with a fourth-order Runge–Kutta method has been applied by Cortell to a variety of physical problems [33–35]. The same approach as was discussed by Cortell [32] has been used by Tuck and Schwartz [24] to solve a third-order ODE modelling the draining of a thin film down a dry wall. The model equation is given by

\[ y'' = y^{-2} + 1 \tag{3.9} \]

solved subject to the boundary conditions \( y \to 1 \) as \( x \to -\infty \) and \( y \to \delta \) as \( x \to +\infty \).

3.1. The direct approach

There are two approaches to this problem. In the first instance we fix \( k \) and vary \( \alpha \) to determine \( r \) such that the boundary condition \( y_n = \epsilon \) is satisfied. In this case we have a stopping criterion based on the height of the precursor film stated as follows: if \( 0 < y_j \leq \epsilon \) then stop marching; if \( y_j \) becomes negative, take one step back and halve the step length and then continue until \( 0 < y_j \leq \epsilon \). The value of \( r \) is determined by iterating the difference equation \( x_{i+1} = x_i + h \) and halving the step length \( h \) as indicated for the height of the precursor film. To implement this approach we choose \( \alpha \in [-20, -3] \) taking an initial value of \( h = 0.01 \). We show the results for \( k = 1 \). There is little variation in the results for \( k \in [0, 2] \), the range of \( k \) values for touchdown. We plot the results obtained from this approach in Figs. 2 and 3.

In Fig. 2 we plot the values of \( y_n \) for \( \alpha \) values in the range \( \alpha \in [-20, -3] \). We note that the stopping criterion \( 0 < y_j \leq \epsilon \) has worked very well. We obtained a wide range of values for \( y_n \) in the interval \( 0 < y_n \leq \epsilon \).

In Fig. 3 we plot the contact angle obtained by using the backward difference approximation \( y_n' \approx (y_n - y_{n-1})/(x_n - x_{n-1}) \) against the derivative at \( y_n \). The contact angle \( \phi \) in degrees is obtained by taking \( \phi = \arctan \left(-y_n'\right) \). We plot the asymptotic relationship (2.23) on the same system of axes. We note that the asymptotic solution is valid for small values of \( r \), comparing to the nonlinear relationship between \( r \) and \( \phi \) obtained using the direct approach and the iterative approach. The limited range of validity of the asymptotic solution is due to the fact that it is only valid in the domain \( \epsilon \to 0 \).
3.2. The iterative approach

We initially evaluate (3.6)–(3.8) for two different values of $\alpha$ which we label $\alpha_0$ and $\alpha_1$. We choose $\alpha_0 = -10$ and $\alpha_1 = -20$. We get two estimates of $y_n$ which we label $y_n(\alpha_0)$ and $y_n(\alpha_1)$. Subsequent estimates of $\alpha$ are determined from the secant method:

$$\alpha_{z+1} = \alpha_z - \frac{\alpha_z - \alpha_{z-1}}{y_n(\alpha_z) - y_n(\alpha_{z-1})} (y_n(\alpha_z) - \epsilon)$$  \hspace{1cm} \text{(3.10)}$$

for $z = 2, 3, \ldots$. We stop iterating when $|\alpha_{z+1} - \alpha_z| \leq 10^{-12}$. In this case, $y_n = \epsilon$ is a fixed boundary value. We do not get the spread of values for $y_n$ as indicated in Fig. 2. We plot the corresponding results for $\phi$ against $r$ in Fig. 3 and the number of iterations for each value of $r$ in Fig. 4.

To validate our results with respect to the iterative approach we consider an improvement on the secant method (3.10) that has been derived by Amat and Busquier [36], given by

$$\alpha_{z+1} = \alpha_z - \frac{\alpha_z - \gamma_z}{y_n(\alpha_z) - y_n(\gamma_z)} (y_n(\alpha_z) - \epsilon)$$  \hspace{1cm} \text{(3.11)}$$

for $z = 2, 3, \ldots$ where

$$\gamma_z = \alpha_z + \delta_z (\alpha_{z-1} - \alpha_z).$$  \hspace{1cm} \text{(3.12)}$$

The constant $\delta_z$ is chosen using the formula

$$\delta_{z+1} = \begin{cases} \delta_z^2 & \text{if } \delta_z^2 |\alpha_z - \alpha_{z+1}| \geq \text{tol}_c, \\ \text{tol}_c / |\alpha_z - \alpha_{z+1}|, & \text{elsewhere} \end{cases}$$  \hspace{1cm} \text{(3.13)}$$

where $\delta_0 = 0.1$ and $\text{tol}_c = 10^{-16}$ for single precision. As in the case above, we stop iterating when $|\alpha_{z+1} - \alpha_z| \leq 10^{-12}$. We plot the number of iterations for each value of $r$ in Fig. 5. We note when comparing the results in Fig. 4 to those from the modified secant method in Fig. 5 that the modified secant method needs fewer iterations than the standard secant method.
4. Results and concluding remarks

In this paper we have used a shooting method coupled with a secant method to determine a numerical solution to a boundary value problem modeling the steady profile of a thin droplet. In the first instance we use a direct approach in which we fix the value of the second derivative and determine the corresponding position of the contact line $x = r$ and the corresponding contact angle $\phi$. We then use an iterative approach in which the value of the second derivative is determined from a secant method such that the contact line condition $y(r) = \epsilon$ is satisfied. In this way we recover the position of the contact line $x = r$ and are able to determine the corresponding contact angle $\phi$. We validate the results obtained from the iterative approach by comparing these results with those obtained from using a modified secant method. The results obtained from the direct approach and iterative approach coincide, as indicated in Fig. 3.

The shooting method gives us more than just the results indicated in Figs. 2 and 3. As indicated in the introduction, we are able to determine an empirical law relating the contact angle to the position of the contact line. We use the curve fitting functionality of MATHEMATICA to determine values of the constants $\lambda$ and $\gamma$ such that the contact angle and position of the contact line are related by the power law

$$\tan \phi = \lambda r^\gamma.$$  \hspace{1cm} (4.1)

We implement the shooting method indicated above for different values of $k$ and then run the FindFit routine in MATHEMATICA to obtain the values of $\lambda$ and $\gamma$. We plot these values for $k \in [0, 3]$ in Fig. 6.

In Fig. 7 we plot $k/\lambda$ and $k/\gamma$ against $k$. We note that the curves are almost linear. We fit a straight line through the data and find that

$$\frac{k}{\lambda} = -0.0371074 + 0.548814k, \quad \frac{k}{\gamma} = -0.0299864 - 0.962504k.$$  \hspace{1cm} (4.2)

Therefore

$$\lambda = \frac{k}{-0.0371074 + 0.548814k}, \quad \gamma = \frac{k}{-0.0299864 - 0.962504k}. \hspace{1cm} (4.3)$$
Fig. 6. Plots showing the variation of $\lambda$ and $\gamma$ for $k \in [0, 3]$.

Fig. 7. Plot showing the relationships $k/\lambda$ and $k/\gamma$ against $k$ and the straight line fits given by (4.2) and (4.3) (---).

We therefore find that
\[ \tan \phi \propto r^{-\frac{k}{k-1}}. \quad (4.4) \]

We have therefore obtained a nonlinear relationship between the contact angle $\phi$ and the position of the contact line $r$ in terms of the power law coefficient $k$. This result would be useful in various experiments in which the contact angle and position of the contact line are determined for different fluids. The interested reader is referred to the papers of Hoffman [37], Bacri et al. [38] and Garnier et al. [39] for descriptions of these experiments.

An advantage of using a shooting method approach over a finite difference solution to the problem is that no initial guess to the solution profile is required. An incorrect initial guess can have a major impact on the solution. A finite difference approach requires the solution of linear systems of increasing size for improvements in accuracy. We note here that Ha [40] has introduced a new shooting method in which a sequence of solutions to an initial value problem that tend to the solution of the boundary value problem is constructed. It is not necessary to implement the shooting approach of Ha [40] here as we obtain good, accurate results from implementing the high-order Taylor approximation.

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References