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Ill and Well-Posed One-Dimensional Models of Liquid Dynamics in a Horizontal Capillary

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Abstract

In this paper, we report a mathematical and numerical study of liquid dynamics models in a horizontal capillary. In particular, we prove that the classical model is ill-posed at initial time, and we present two different approaches in order to overcome this ill-posedness. By numerical viewpoint, we apply an adaptive strategy based on an one-step one-method approach, and we compare the obtained numerical approximations with suitable asymptotic solutions.

Keywords: Ill and well-posed models, horizontal capillary, asymptotic solutions, adaptive numerical method.

1. Introduction

The present study was motivated by the non-destructive control named "liquid penetrant testing" used in the production of airplane parts and in many industrial applications where the detection of open defects is of interest. Liquid penetrants, involving capillary action, are used to locate surface-accessible defects in solid parts.

In this paper, we present some mathematical models that describe the dynamics of a liquid inside an open ended capillary. In particular, we prove that the classical model is ill-posed at initial time, and we present two different approaches in order to overcome this ill-posedness. A first model was obtained by Bosanquet, modifying the usual initial conditions [1], another one was derived by Szekely et al. [12], taking into account the flow effects outside the capillary. Finally, with reference to the academic test case presented in Cavaccini et al. [4], we compare the numerical approximations, obtained by an adaptive procedure based on an one-step one-method approach, with the solutions derived by an asymptotic study.

With reference to figure 1, we consider a liquid freely flowing within a horizontal cylindrical capillary of radius R. At the left end of the capillary

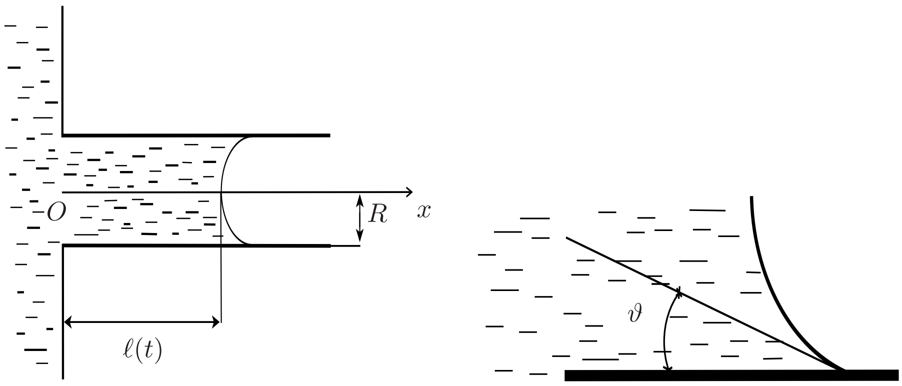

Fig. 1. Left frame: geometrical setup of a horizontal capillary section. Right frame: definition of the contact angle ϑ.

we have a reservoir filled with the penetrant liquid. The model governing the dynamics of a liquid inside an open ended capillary is given by

$$\rho \frac{d}{dt}\left[\ell \frac{d\ell}{dt}\right] = 2\frac{\gamma \cos\vartheta}{R} - 8\frac{\mu\ell}{R^2}\frac{d\ell}{dt} \tag{1}$$

where ℓ is the moving liquid-gas interface coordinate, $d\ell/dt$ can be interpreted as the average axial velocity. Moreover, ρ, γ, and μ are the liquid density, surface tension and viscosity, respectively. The contact angle between the liquid and the capillary wall is denoted by ϑ, with $0^\circ \le \vartheta << 90^\circ$. The left-hand side term describes the inertial resistance. The effect of inertia are usually significant only in the early stages of penetration or when the radius R is large and/or μ is small. The first term of the right-hand side is the capillary driving force, the second one gives the viscous resistance of the liquid in the capillary. For the mathematical derivation of the governing equation we refer to Cavaccini et al. [4] and the references quoted therein.

2. Ill and Well-Posed One-Dimensional Models

Rewriting equation (1), and assuming that, at initial time, the liquid starts to flow inside the capillary, we have

$$\begin{cases} \ell \dfrac{d^2\ell}{dt^2} = 2\dfrac{\gamma\cos\vartheta}{\rho R} - 8\dfrac{\mu\ell}{\rho R^2}\dfrac{d\ell}{dt} - \left(\dfrac{d\ell}{dt}\right)^2 , \\ \ell(0) = \dfrac{d\ell}{dt}(0) = 0 \ . \end{cases} \tag{2}$$

The right-hand side of the governing differential equation is a function of ℓ and its first derivative, that can be abbreviated by F:

$$F\left(\ell, \frac{d\ell}{dt}\right) = 2\frac{\gamma\cos\vartheta}{\rho R} - 8\frac{\mu\ell}{\rho R^2}\frac{d\ell}{dt} - \left(\frac{d\ell}{dt}\right)^2 , \tag{3}$$

so that we can rewrite the governing equation in (2) as

$$\ell\frac{d^2\ell}{dt^2} = F\left(\ell, \frac{d\ell}{dt}\right) \tag{4}$$

to be taken with zero initial conditions. Therefore, by evaluating F at the initial time we get

$$F(0,0) = 2\frac{\gamma\cos\vartheta}{\rho R} , \tag{5}$$

which is positive and ensures that the fluid flows inside the capillary. This implies that, at the same initial time, the left-hand side of the governing equation in (2) should be positive as well. However, because of the initial conditions the left-hand side of the governing equation in (2) must be zero which hints at a contradiction. However, this alone does not invalidate the derived modeling. In fact, the considered equation may possibly hold for all $t > 0$, and there may be a solution which assumes the required initial values. Here we show that this is not the case for the considered model.

In order to understand the ill-posedness of our model, we examine the simple model defined by

$$\begin{cases} \ell\dfrac{d^2\ell}{dt^2} = C \\ \ell(0) = \dfrac{d\ell}{dt}(0) = 0 , \end{cases} \tag{6}$$

where C is a positive constant. Now, if we assume that a solution $\ell(t)$ of (6) exists with $\ell(t) > 0$ for $t > 0$, then solving for the second derivative and multiplying both sides by the first derivative yields

$$\frac{d\ell}{dt}\frac{d^2\ell}{dt^2} = C\frac{\frac{d\ell}{dt}}{\ell} . \tag{7}$$

By considering solutions on the interval $[\delta, t]$ with $\delta > 0$, we integrate both sides of (7), with respect to t, to get

$$\frac{1}{2}\left[\frac{d\ell}{dt}(t)\right]^2 - \frac{1}{2}\left[\frac{d\ell}{dt}(\delta)\right]^2 = C\left[\ln\ell(t) - \ln\ell(\delta)\right] . \tag{8}$$

Fixing t and taking the limit as $\delta \to 0^+$, the left-hand side of equation (8) takes a positive finite value, but the right-hand side goes to infinity which is a contradiction. Therefore, there is no solution to the problem (6). This ill-posedness also applies to our problem with zero initial data.

Now, we define two different ways to revise the considered model in order to get a well-posed one.

As first revision, we can modify the given initial conditions. Assuming that, at the initial time, the liquid is inside the capillary, we obtain the model, so called Bosanquet one [1],

$$\left\{ \begin{array}{l} \rho \dfrac{d}{dt}\left[\ell \dfrac{d\ell}{dt}\right] = 2\dfrac{\gamma\cos\vartheta}{R} - 8\dfrac{\mu\ell}{R^2}\dfrac{d\ell}{dt} \\ \ell(0) = R \ , \qquad \dfrac{d\ell}{dt}(0) = \left(2\dfrac{\gamma\cos\vartheta}{\rho R}\right)^{1/2} \end{array} \right. , \tag{9}$$

derived by rewriting the momentum balance for the moving column neglecting viscosity and external hydrodynamics. As shown below by numerical results, the Bosanquet velocity gives an accurate upper estimate of the initial velocity of liquid penetration into a horizontal capillary.

The second revision was already done by Szekely et al. [12] by taking into account the flow effects outside the capillary. These authors introduced a coefficient of apparent mass $c = O(1)$ and obtained the following model

$$\left\{ \begin{array}{l} \rho \dfrac{d}{dt}\left[(\ell + cR)\dfrac{d\ell}{dt}\right] = 2\dfrac{\gamma\cos\vartheta}{R} - 8\dfrac{\mu\ell}{R^2}\dfrac{d\ell}{dt} \\ \ell(0) = \dfrac{d\ell}{dt}(0) = 0 \ . \end{array} \right. \tag{10}$$

Note that, starting with zeroth velocity, the liquid accelerates and attains a maximum velocity within a short interval. The most challenging model, by a numerical viewpoint, is the one proposed by Szekely et al. Therefore, we discuss numerical results comparing them with asymptotic ones obtained by solving an academic test case presented in [4]. Several numerical computations, related to real liquids, can be found, by the interested reader, in the paper by Cavaccini et al. [4]. Further numerical results were presented at the ICIAM congress held in Zurich, 16-20 July 2007, see Fazio et al. [6].

3. Academic test case

As an academic test case, we report on the numerical results for the model

$$\left\{ \begin{array}{l} \dfrac{d}{dt}\left[(\ell + R)\dfrac{d\ell}{dt}\right] = 1 - \ell\dfrac{d\ell}{dt} \ , \\ \ell(0) = \dfrac{d\ell}{dt}(0) = 0 \ , \end{array} \right. \tag{11}$$

derived by equation (10) setting the following parameters

$$c = \rho = 2\frac{\gamma \cos\vartheta}{R} = 8\frac{\mu}{R^2} = 1 \ . \tag{12}$$

Now, we present asymptotic solutions of the model (11) that will be used, in the following, in order to validate the numerical approximations, of the models (9) and (10) with parameters defined in (12), obtained by an adaptive numerical approach.

3.1. *Washburn equation*

For very small radii, viscous forces are dominant, the inertial terms at the left-hand side of the (11) can be neglected, and one obtains the differential equation, named Washburn one [13]. As far as our academic test case is concerned, by using the relations (12), the Washburn equation specializes to

$$\ell \frac{d\ell}{dt} = 1 \ . \tag{13}$$

By integrating, taking into account the initial condition $\ell = 0$, at $t = 0$, we get the solution

$$\ell_W(t) = (2t)^{1/2} \ , \tag{14}$$

valid only for $t >> 8$. Note that, at initial time

$$\frac{d\ell_W}{dt}(0) = +\infty \ ,$$

and this is an evident paradox [8]. However, Washburn approximation is still considered as a valid approximation, although it fails to describe the initial transient, since it neglects the inertial effects which are relevant at the beginning of the process. In fact, this approximation has been confirmed by a lot of experimental data and also by molecular dynamic simulations, see for instance Martic et al. [11,10,9], and lattice-Boltzmann computations, see Chibbaro [5].

3.2. *Budd and Huang asymptotic analysis*

An asymptotic analysis has been developed by Budd and Huang [2], who used the method of matched asymptotic expansions to tackle the problem (11). Now, observe that the equation (11) has a first integral given by

$$(\ell + R)\frac{d\ell}{dt} = t - \frac{\ell^2}{2} \ . \tag{15}$$

In the inner region, where t is of order R, Budd and Huang rescaled the solution and then developed a series expansion of ℓ in powers of R, obtaining the asymptotic solution

$$(16) \qquad \ell_{in}(t) = \sqrt{R^2 + t^2} - R \qquad \text{valid for } 0 < t << 1 \; .$$

In the outer region, they ignored the contributions involving R to leading order and integrated again. This led to the following asymptotic formula

$$(17) \qquad \ell_{out}(t) = \sqrt{2}\sqrt{t - 1 - \exp(-t)} \qquad \text{valid for } R << t \; .$$

The two expansions match when $R << t$, where they both have the form

$$\ell(t) \approx t \; .$$

4. Validation of numerical results

In this section, we show the numerical approximations of the mathematical models, presented in section 2. These results, obtained by an adaptive approach developed by Jannelli and Fazio [7] and briefly described in the next section, are validated by comparing with the above asymptotic solutions. All computations were performed with MATLAB.

First, we consider the numerical results of the Bosanquet model (9), with the conditions (12) and $R = 0.01$. In this case, at the beginning of the

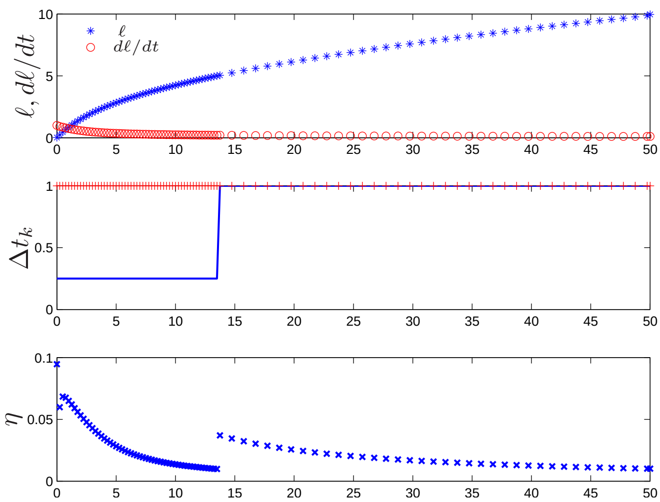

Fig. 2. From top to bottom: $\ell(t)$ and its first derivative; adaptive step-size selection Δt_k; monitor function η.

process, there is not fast transitory of first derivative, the liquid is inside the capillary and it has a maximum velocity that, after decreases. Therefore, even a simple integration with constant step size would be suitable in this case. In the top frame of figure 2, we show the numerical solution ℓ and its first derivative. The step-size selection Δt_k and the monitor function $\eta(t_k)$ are reported in the middle and in the bottom frames, respectively. Note that, in this case our adaptive strategy used only 92 steps, with no rejections, to complete the integration in $[0, 50]$. The minimum value of Δt used was 0.25 and only in this case we magnified the time step by a factor of 4.

Now, we report the numerical results of the academic test case (11) with $R = 0.01$. In the top frame of figure 3, we show the numerical solution ℓ

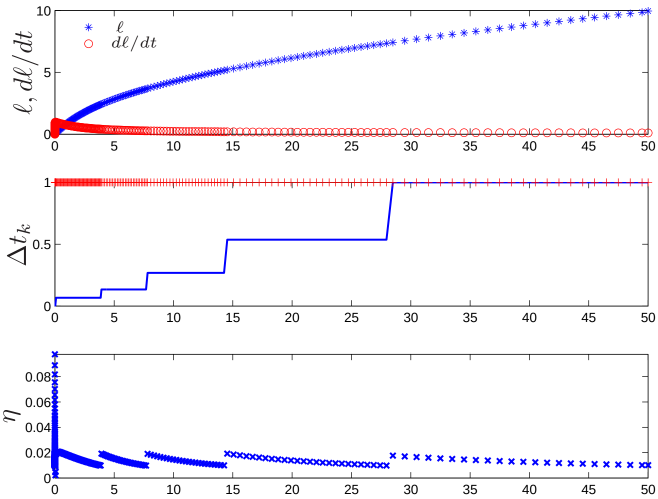

Fig. 3. Adaptive step-size results. From top to bottom: $\ell(t)$ and its first derivative; adaptive step-size selection Δt_k; monitor function η.

and its first derivative. The step-size selection Δt_k and the monitor function $\eta(t_k)$ are reported in the middle and in the bottom frames. It is easy to note, how, the adaptive procedure modifies the time step in relation to the value of the monitor function. Initially, at the beginning of the process, the adaptive procedure reduces Δt_k corresponding to first derivative fast transitory. Then, when the solution becomes smooth, the procedure amplifies the step-size. Our adaptive strategy used 1603 successful steps, plus 10 rejections, to complete the integration in $[0, 50]$. For this test case, the minimum value of Δt used was about 10^{-12}.

In the figure 4, we report the numerical solutions obtained on the time interval $[0, 1]$. The solution of Bosanquet model (9) is shown in the left frame, and the solution of model (10) developed by Szekely et al. is in the right frame. The physical parameters are given by (12) and $R = 0.01$. Note that, at the initial steps of the process, the model (10) describes the fast

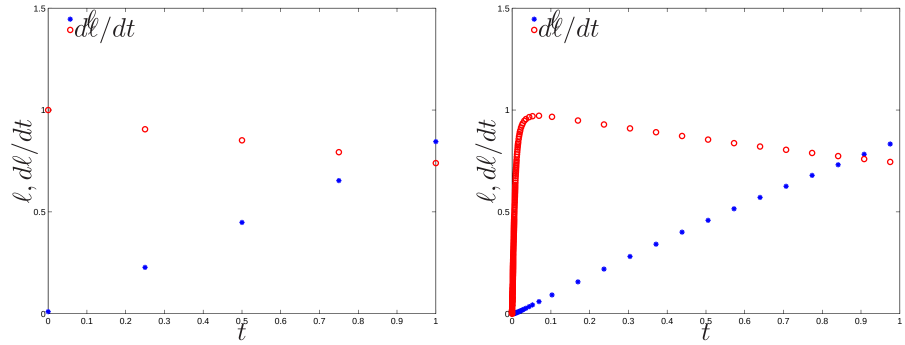

Fig. 4. Left frame: model (9); $\ell(t)$ and its first derivative. Right frame: model (10); adaptive step-size results, $\ell(t)$ and initial transient of its first derivative.

transient of first derivative of ℓ, developed by the increase of the velocity of the liquid entering the capillary. This large acceleration does not exist in the solution of the model (9), because, at initial time, the liquid is already inside the capillary. Note that, from the right frame of figure 4 the liquid entering the capillary is accelerated by capillary force ($\ell \approx t^2$ initially); but, soon thereafter the capillary force is compensated by the viscous drag so that a steady-state can be achieved ($\ell \approx t^{1/2}$ for t large enough). Moreover, we can notice how the Bosanquet velocity is an upper bound for the velocity of the Szekely et al. model.

In the left frame of figure 5, we report the asymptotic solution ℓ_{in} of (16), and its derivative, obtained for very short times. The numerical approximation, obtained by our adaptive procedure, is shown in the right frame of figure 5.

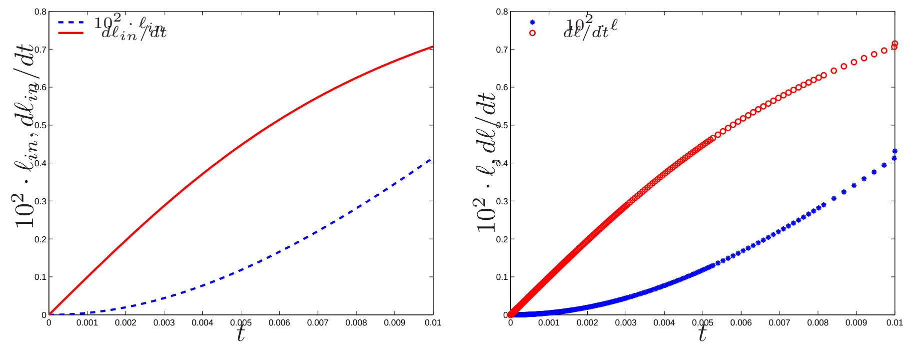

Fig. 5. Left frame: asymptotic solution: $10^2 \cdot \ell_{in}(t)$ and its derivative. Right frame: adaptive step-size results, $10^2 \cdot \ell(t)$ and its first derivative.

The asymptotic solution ℓ_{out}, given by (17), and its first derivative, with the numerical approximations are compared, for large times, in figure 6. The solution of the Washburn equation $\ell_W(t)$ is plotted for comparison. This figure shows a good agreement for large times between the two asymptotic solutions.

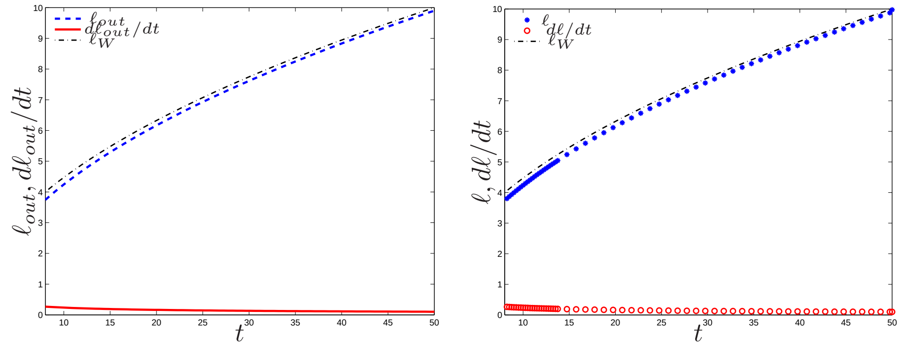

Fig. 6. Left frame: asymptotic solutions: $\ell_{out}(t)$ and its derivative obtained for $R << t$. Right frame: adaptive step-size results: $\ell(t)$ and its first derivative. The solution of the Washburn equation ℓ_W(t) is shown for comparison.

5. Numerical method and adaptive procedure

In this section we describe the considered adaptive procedure, developed by Jannelli and Fazio [7], used with the classical fourth order Runge-Kutta's method [3, p. 166]. For the reported test case we used the following monitor function

$$\eta(t_k) = \frac{\left| \frac{d\ell}{dt}(t_k + \Delta t_k) - \frac{d\ell}{dt}(t_k) \right|}{\Gamma_k} \tag{18}$$

where Δt_k is the current time-step and

$$\Gamma_k = \begin{cases} \left| \frac{d\ell}{dt}(t_k) \right| & \text{if} \quad \frac{d\ell}{dt}(t_k) \neq 0 \\ \epsilon & \text{otherwise} \end{cases}, \tag{19}$$

with $0 < \epsilon \ll 1$. The above monitor function has been chosen because, as far as the solution of the model (10) is concerned, we have found numerically that, for small values of R, initially the first derivative of $\ell(t)$ has a fast transient.

For the adaptive procedure we enforced the following conditions: $\Delta t_{\min} \leq \Delta t_k \leq \Delta t_{\max}$ with $\Delta t_{\min} = 10^{-15}$, $\Delta t_{\max} = 1$, and $\eta_{\min} \leq \eta(t_k) \leq \eta_{\max}$ with $\eta_{\min} = 10^{-2}$, $\eta_{\max} = 10\ \eta_{\min}$, and $\epsilon = 10^{-9}$. Moreover, the time step is modified in two cases: when $\eta(t_k) < \eta_{\min}$ we use $\Delta t_{k+1} = 2\,\Delta t_k$

as the next time step, whereas if $\eta(t_k) > \eta_{\max}$, then we repeat the same step using $\Delta t_k = \Delta t_k/2$. Full details on the adaptive strategy, as well as alternative monitor functions, can be found by the interested reader in [7].

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