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Mathematical and Numerical Modeling of Liquids Dynamics in a Horizontal Capillary

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1 Introduction

Starting from the beginning of the last century several publications were devoted to study the dynamics of liquid flow into a capillary, leading to the derivation of the celebrated Washburn equation, the Bosanquet model, and, more recently, to the SNC model by Szekely, Neumann and Chuang. Washburn [13] considered the liquid penetration as being determined by a balance among capillarity, gravitational and viscous forces and used Poiseuille profile for the velocity. The Washburn equation has been confirmed by a lot of experimental data and also by molecular dynamic simulations; it 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. Those inertial effects were considered in a model proposed by Bosanquet [2]. The SNC model introduced by Szekely et al. [12] takes into account also the outside flow effects, including within the inertial terms an apparent mass parameter. Meanwhile, the research on the dynamics of capillary phenomena and their applications was blooming and several reviews appeared within the specialized literature: see Dussan [9], de Gennes [6], Leger and Joanny [11], Clanet and Quéré [5], Zhmud et al. [14], the recent book by de Gennet et al. [7] and the references quoted therein.

This paper was written in order to introduce a simple one-dimensional model for two immiscible liquids penetration, see for instance Chan and Yang [4] or Blake and De Coninck [1], and to report on preliminary numerical results for the one liquid case.

2 Mathematical modeling

With reference to figure 1, we consider a column of liquid 1, usually water, of fixed length ℓ_0 entrapped within a horizontal cylindrical capillary of radius R and finite length L. At the left end of the capillary we have a reservoir filled with a penetrant liquid 2. We are interested to model the dynamics of both liquids under the action of the surface tension. For the validity of the one-dimensional analysis we assume that both menisci can be approximated by spherical caps and this implies that the Weber, Bond and capillary numbers are small, that is $We = 2\rho RU^2/\gamma \ll 1$,

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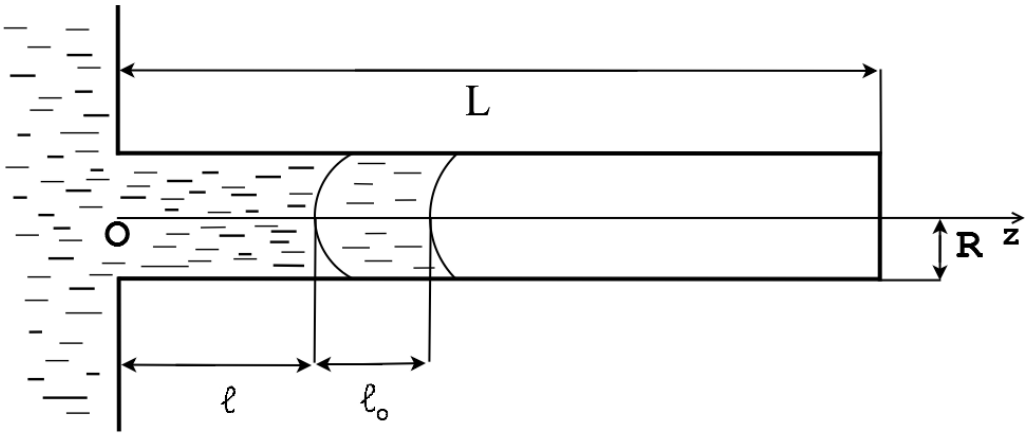

Figure 1: Draft of a cylindrical capillary section.

$Bo = 4\rho g R^2/\gamma \ll 1$, and $Ca = \mu U/\gamma \ll 1$, where ρ, γ, and μ are the liquid density, surface tension and viscosity, respectively, g is the acceleration due to gravity, and U is the average axial velocity within the capillary. Of course, we should have that $R/L \ll 1$, a quasi-steady Poiseuille velocity profile, and a dynamic contact angle simplification. The Newtonian equation of motion can be written as follows

$$\frac{d(mU)}{dt} = F_{drive} - F_{drag} \tag{1}$$

where $m(t)$ is the mass of the two liquids, t is the time and F_{drive}, and F_{drag} are the drive and the drag forces respectively. We can express the average axial velocity as $U = d\ell/dt$, where ℓ is the moving liquid-liquid interface coordinate, so that the momentum can be specified as

$$\begin{aligned} \frac{d(mU)}{dt} &= m\frac{dU}{dt} + \frac{dm}{dt}U \\ &= \pi R^2 \left(\rho_1 \ell_0 + \rho_2 \ell\right) \frac{d^2\ell}{dt^2} + \pi R^2 \rho_2 \left(\frac{d\ell}{dt}\right)^2 \end{aligned} \tag{2}$$

where ρ_1 and ρ_2 are the densities of the two liquids. Moreover, from the Navier-Stokes model written in suitable cylindrical coordinates and applying no slip boundary conditions at the capillary wall, it is possible to derive the Poiseuille parabolic velocity profile

$$u(r) = \frac{1}{4\mu}\frac{\Delta p}{\Delta z}\left(R^2 - r^2\right) \ , \tag{3}$$

where r is the radial cylindrical coordinate. The volumetric flow rate is given by

$$Q = \frac{\pi R^4}{8\mu}\frac{\Delta p}{\Delta z} \ .$$

For a constant area tube, Q may also be written as

$$Q = \pi R^2 \frac{d\ell}{dt} \ .$$

So that equation (3) can be rewritten in the form

$$u(r) = 2U\left(1 - \frac{r^2}{R^2}\right) \ . \tag{4}$$

Then, the expression of the viscous drag force is given by

$$\begin{aligned} F_{drag} &= -2\pi R\left(\mu_1\ell_0+\mu_2\ell\right)\left.\frac{du}{dr}\right|_{r=R} \\ &= 8\pi\left(\mu_1\ell_0+\mu_2\ell\right)\frac{d\ell}{dt} \end{aligned} \tag{5}$$

where μ_1 and μ_2 are the dynamic viscosities of the two liquids. The driving force, due here to the surface tension only, can be defined as, see for instance Cartz [3],

$$F_{drive} = 2\pi R\left(\gamma_1\cos\vartheta_1+\gamma_{12}\cos\vartheta_{12}\right) \tag{6}$$

where γ_1 and γ_{12} are the surface free energies for the liquid 1-air and the liquid 1-liquid 2 interfaces, and ϑ_1 and ϑ_{12} are corresponding menisci contact angles. At the end of this derivation we get the following second order differential equation

$$\left(\rho_1\ell_0+\rho_2(\ell+cR)\right)\frac{d^2\ell}{dt^2}+\rho_2\left(\frac{d\ell}{dt}\right)^2 = 2\frac{\gamma_1\cos\vartheta_1+\gamma_{12}\cos\vartheta_{12}}{R}-8\frac{\mu_1\ell_0+\mu_2\ell}{R^2}\frac{d\ell}{dt}-\frac{p_aL}{L-\ell_0-\ell} \tag{7}$$

where $c = O(1)$ is the coefficient of apparent mass [12], and the term $\frac{p_aL}{L-\ell_0-\ell}$, being p_a the atmospheric pressure, is the pressure due to the entrapped gas within the capillary according to Deutsch [8]. The equation (7), with suitable initial conditions, accounts for the displacement of the two liquids due to the combined surface tensions action of both liquids.

3 A single liquid case and numerical results

In the simpler case of a single liquid dynamics without gas entrapment, that is $\ell_0 = \rho_1 = \gamma_1 = \mu_1 = p_a = 0$, the equation (7), dropping also all subscripts related to the considered fluid parameters, becomes

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

Moreover, within a steady flow assumption, equation (8) reduces to

$$\ell\frac{d\ell}{dt} = \frac{\gamma\cos\vartheta}{4\mu}R \tag{9}$$

that can be integrated, using the initial condition $\ell(0) = 0$, providing the solution

$$\ell^2 = \frac{\gamma R\cos\vartheta}{2\mu}t\ . \tag{10}$$

This is a Washburn equation, valid only for $t >> t_\mu$ where $t_\mu = \rho R^2/\mu$ is a viscous time scale.

As an academic test case we report on the numerical results for the model (8) supplemented with the following initial conditions

$$\ell(0) = 0\ , \qquad \frac{d\ell}{dt}(0) = 0\ , \tag{11}$$

and parameters

$$R = 0.01\ , \qquad c = \rho = 2\frac{\gamma\cos\vartheta}{R} = 8\frac{\mu}{R^2} = 1\ . \tag{12}$$

Figure 2 displays the numerical results obtained by a second order Heun's method implemented with an adaptive procedure developed by Jannelli and Fazio [10].

For this test case we used the following monitor function

$$\eta(t) = \frac{|\frac{d\ell}{dt}(t + \Delta t_k) - \frac{d\ell}{dt}(t)|}{\Gamma(t)} \tag{13}$$

where Δt_k is the current time-step and

$$\Gamma(t) = \begin{cases} |\frac{d\ell}{dt}(t)| & \text{if} \quad \frac{d\ell}{dt}(t) \neq 0 \\ 1 & \text{otherwise} . \end{cases} \tag{14}$$

We decided to define the above monitor function because we have found numerically that, for small values of R, the first derivative of $\ell(t)$ has initially a fast transient. More details on the adaptive strategy and alternative monitor functions can be found in [10]. We remark here that an adaptive approach is mandatory to resolve the fast transient, as well as to provide accurate results on the time interval of interest. Further numerical tests, involving the parameters characterizing several real liquids, as well as the entrapped gas pressure term, are in progress.

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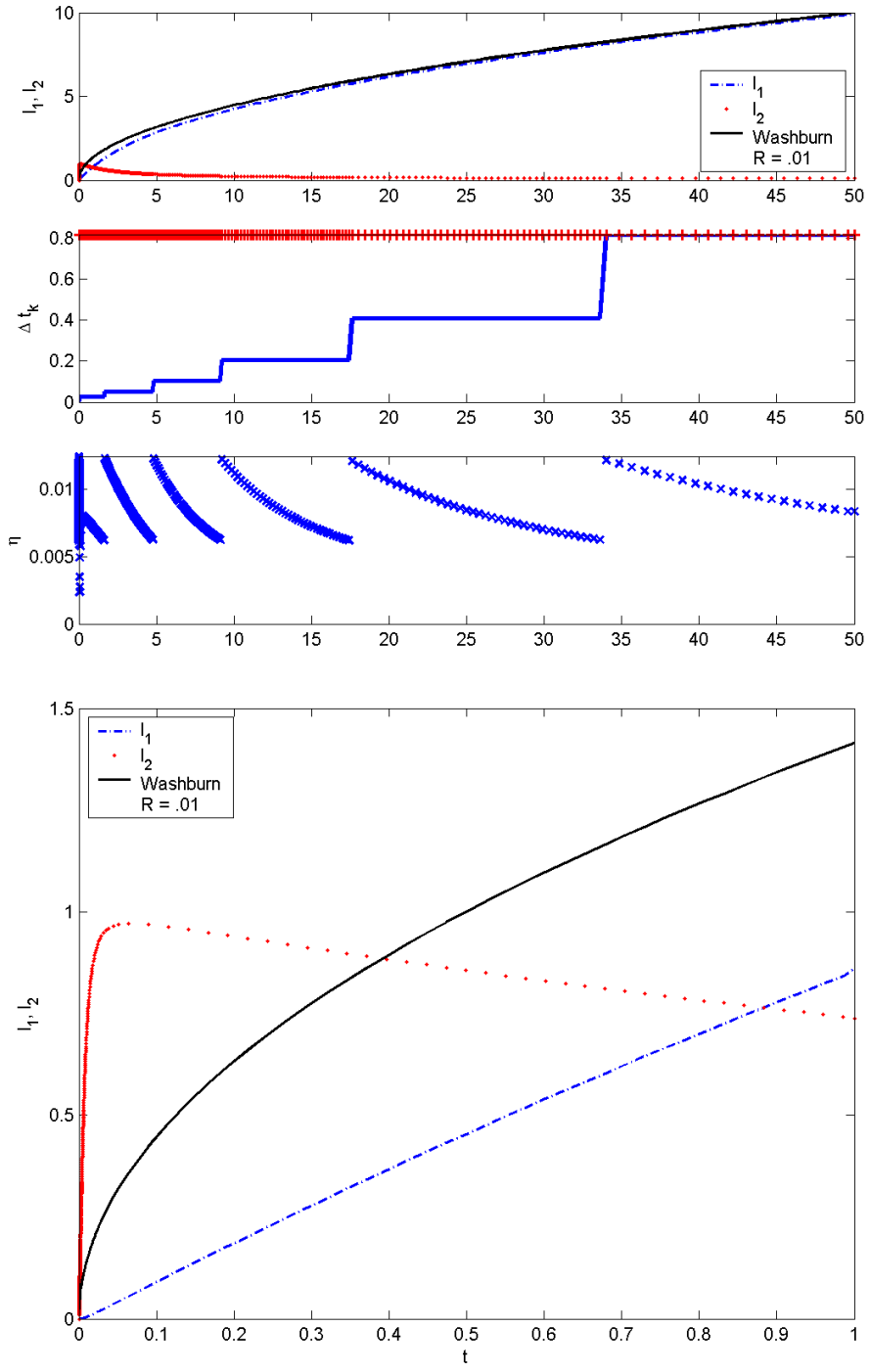

Figure 2: Adaptive results for the model (8)-(11)-(12). From top to bottom: $\ell(t)$, its first derivative (shown as l_1 and l_2 dotted-dashed and dotted lines respectively) and the Washburn solution (solid line); adaptive step-size selection Δt_k; monitor function η; and zoom of the initial transient.