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Abstract. In this work we numerically study the stability of the steady state displacement of a liquid plug in a capillary tube when gravity, inertia and surface forces are important. The methodology employed is based on the analysis of steady state solutions and has been presented in previous publications. Gravity is assumed to act only along the axis of the tube.

1. Introduction

The propagation of liquid plugs in small conduits has been studied for many applications including the extraction of oil from a porous rock and medical treatments requiring a liquid plug to be instilled in the pulmonary airway such as in mechanical ventilation and surfactant replacement therapy. Also, due to their small size distal airways are prone to closure in various respiratory disorders creating liquid plugs which obstruct the airflow.

A simplified model of those problems is the motion of a liquid slug inside a capillary whose wall is coated with a thin film of the same fluid. Therefore, the liquid plug propagates on that preexisting film, the precursor film, whose thickness is H_∞^F and leaves behind a trailing film with thickness H_∞^T which, for a given liquid and tube radius, depends on the speed of plug propagation. If the displacement of the plug is steady, mass conservation requires $H_\infty^T = H_\infty^F = H_\infty$ since otherwise liquid would accumulate in ($H_\infty^F > H_\infty^T$) or evacuate from ($H_\infty^F < H_\infty^T$) the plug. This quantity (H_∞) as well as the length of the slug, L_P, will depend on the relative strength of capillary, inertia, viscous and gravity forces. When the length of the plug exceeds a certain value (L_P^{max}) which depends on the magnitude of the forces acting on the system, the phenomena is similar to the propagation of the rear and front menisci of two consecutive semi-infinite bubbles separated by a distance L_P^{max}. The propagation of semi-infinite bubbles has received considerable attention since the pioneering work by Bretherton [9]; in fact it has been studied analytically ([1], [2]), experimentally ([3]-[5]), and numerically ([6]-[8]) by a number of authors.

When the plug is short, the flow is affected by the interaction between the menisci and the velocity and pressure fields must be simultaneously solved in the whole domain. This case has received considerable less attention in the literature, and most works have been published by the team led by Professor Grotberg; they are motivated by the displacement of liquid plugs in the pulmonary airways. In particular, Fujioka and Grotberg [10] presented a numerical study on the steady propagation of a

liquid plug in the gap formed by two horizontal parallel plates separated by a small distance. The governing equations and their boundary conditions were solved using the finite volume technique; the authors could not obtain solutions for capillary numbers larger than 0.4 and plugs shorter than half the gap of the channel. Based on this issue, they conjecture that the lack of convergence of the numerical algorithm employed might be related to the non existence of stable steady states, meaning that if the steady state solution is perturbed, the distance between the menisci will either continuously increase or decrease until the collapse of the plug occurs.

To determine if the above speculation was correct, we numerically investigated the stability of the displacement of a liquid plug in a capillary tube under the effects of surface, inertia, and viscous forces. The following two cases were considered in previous papers: i) an instant perturbation to the plug length occurs [11], and b) the pressure drop between the rear and front gas phases suffers a perturbation [12]. The main outcome of those works is that the stability of a liquid plug may be derived from the shape of the curves illustrating the steady state film thickness as a function of the plug length. In none of those papers the effect of gravity was considered. From a practical point of view, the more attractive case is that in which the disturbance affects the driving pressure drop; therefore, in this work we apply the methodology presented in [12] to study the effect of gravity on the stability of a liquid plug moving inside a capillary tube when the constant pressure difference applied between the front and rear gas phases is slightly perturbed. We consider the case in which the tube radius is small enough so that the flow can be regarded as symmetric around the centre of the tube. The Bond number that measures the ratio between gravity and surface tension forces may be positive or negative depending on whether the plug propagates against or with the direction of gravity, respectively.

The paper is organized as follows. In the next section we present the governing equations with their boundary conditions and briefly discuss the numerical methodology used to solve them. In Section 3, we present selected numerical results that show how gravity affects the stability of the plug. Finally, Section 4 concludes the paper.

2. Mathematical formulation and numerical solution

2.1 Governing equations and boundary conditions
We investigate the stability of the displacement of an incompressible and Newtonian liquid plug following the methodology presented in [12]. To that end, we consider the steady-state propagation of a plug of length L_P inside a capillary tube of radius R coated with a film of the same liquid whose thickness is uniform and equal to H_∞^{F}. Viscosity (μ), density (ρ), and surface tension (σ) are constant, and the gas phase is regarded as inviscid. The pressure drop, $\Delta P = P_{BT} - P_{BF}$, between the rear and front air phases drives the motion of the liquid plug with a constant velocity U. The pressure of the leading bubble, P_{BF} is taken as reference and it is arbitrarily set equal to zero. As the plug displaces inside the tube, it leaves behind a liquid film, the trailing film, with thickness H_∞^{T}. Since the displacement is steady, $H_\infty^{\mathrm{T}} = H_\infty^{\mathrm{F}} = H_\infty$; i.e., the trailing and precursor films have the same thickness. In this formulation, the frame of reference moves with the displacement velocity of the liquid plug, U. Then, the flow is described by the Navier-Stokes and continuity equations, that in dimensionless form read as follows,

$$\lambda Ca\, \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{Ca}\nabla p + \nabla^2 \mathbf{v} + \frac{Bo}{Ca}\mathbf{e}_z, \qquad (1)$$

$$\nabla \cdot \mathbf{v} = 0, \qquad (2)$$

where $\mathbf{v}(v_r, v_z)$ is the velocity vector scaled with U, the pressure is scaled with σ/R, and the coordinates (r, z) are scaled with R; $\lambda = Re/Ca = \rho\sigma R/\mu^2$ is the Laplace number, $Ca = \mu U/\sigma$ is the capillary number, and $Bo = \rho g R^2/\sigma$ is the Bond number and measures the ratio between gravitational and

surface tension forces. It is worth to note that a positive value of the Bond number represents a plug moving in the opposite direction of the gravity force; on the contrary, a negative value of that parameter corresponds to a plug which moves in the direction of gravity (see Fig. 1).
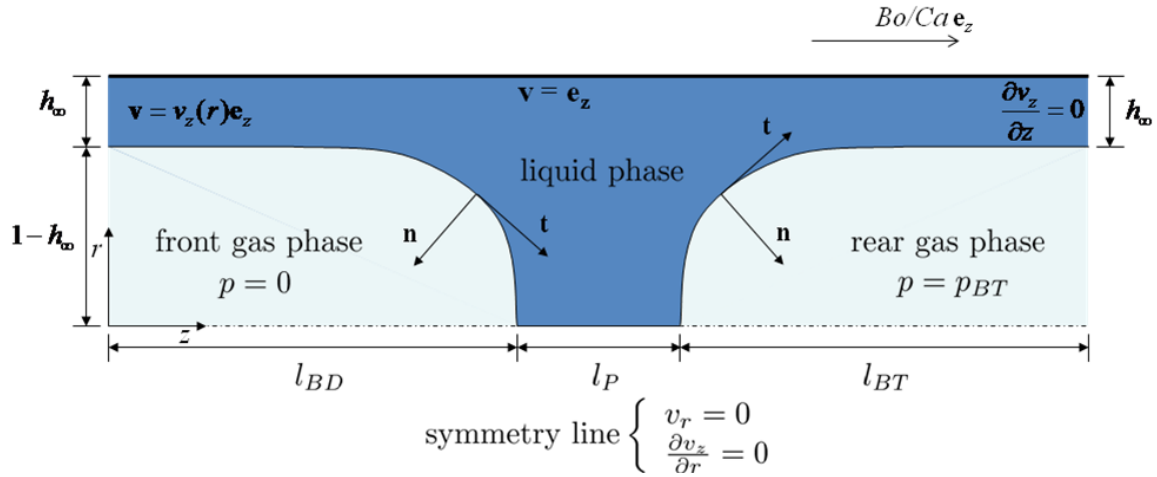

Figure 1. Sketch of the flow domain and coordinate system adopted.

The radius of the tube is small enough so that surface tension tends to dominate over other forces and the flow can be regarded as symmetric around the tube centerline; at the tube wall the no-slip condition is imposed,

$$v_r = \frac{\partial v_z}{\partial r} = 0, \text{ at } r=0, \qquad (3)$$

$$v_r = 0, v_z = 1, \text{ at } r=1. \qquad (4)$$

At both ends of the domain, the interfaces are parallel to the z-axe and the flow is fully developed; therefore, the following conditions must be satisfied at the ends of the domain (see Fig. 1):

$$v_r = 0, v_z = -\frac{Bo}{4Ca}\left[r^2 - 1 - 2(1-h_\infty)^2 \ln r\right]+1, \text{ at } z=0, (1\text{-}h_\infty) \leq r \leq 1; \qquad (5)$$

$$\frac{\partial v_z}{\partial z} = 0, \text{ at } z=l_{BD}+l_P+ l_{BT}, (1\text{-}h_\infty) \leq r \leq 1. \qquad (6)$$

In (6) l_P is the dimensionless length of the plug. The gas/liquid interfaces are material surfaces; therefore, the kinematic condition applies at both free surfaces

$$\mathbf{v} \cdot \mathbf{n} = 0 . \qquad (7)$$

The tangential component of the stress balance vanishes at the interfaces and the normal component adopts the following expression,

$$- p + Ca\, S_{nn} = \begin{cases} 2\mathsf{H} - 0 \\ 2\mathsf{H} - p_{BT} \end{cases}, \qquad (8)$$

where $S_{nn} = \mathbf{n} \cdot \mathbf{S} \cdot \mathbf{n}$, $\mathbf{S}$ being the rate of strain tensor and $\mathsf{H} = -1/2\nabla_s \cdot \mathbf{n}$ the interface curvature. The governing equations (1) and (2) with boundary conditions (3) – (8) are numerically solved as described in the next paragraphs; their solution provide pressure and velocity fields as well as the location of the free surface. Since under steady state propagation the length of the plug is fixed, the position of the tips of the front and rear gas bubbles is fixed. The symmetry of the interface at those points supplies the two additional equations needed to obtain the film thickness, h_∞, and the dimensionless pressure of the back gas phase, p_{BT}, to complete the solution.

2.1. Numerical method.

The numerical technique employed uses the Galerkin/finite element method with the parameterization of the free surface by means of spines. The physical domain is tessellated into quadrilateral elements; mixed interpolation is used to approximate the velocity and pressure fields, and the coefficients that locate the free surface are interpolated by the one-dimensional specialization of the bi-quadratic basis functions that interpolate the velocity.

Weighted residuals are built in the usual form and the resulting set of algebraic equations is simultaneously solved through a Newton loop. The iterative process is stopped when the norm of the difference between two consecutive iterations is smaller than or equal to 10^{-6}. Further details are provided in refs. [11] and [12].

Similar tests to those described in ref. [12] were carried out to select an appropriate finite element mesh; in particular we seek for the invariance of the film thickness and the pressure drop with the mesh and elements size. As a result of those trials, the meshes used to compute the solutions presented in this work have between 10016 and 12608 elements depending on l_P.
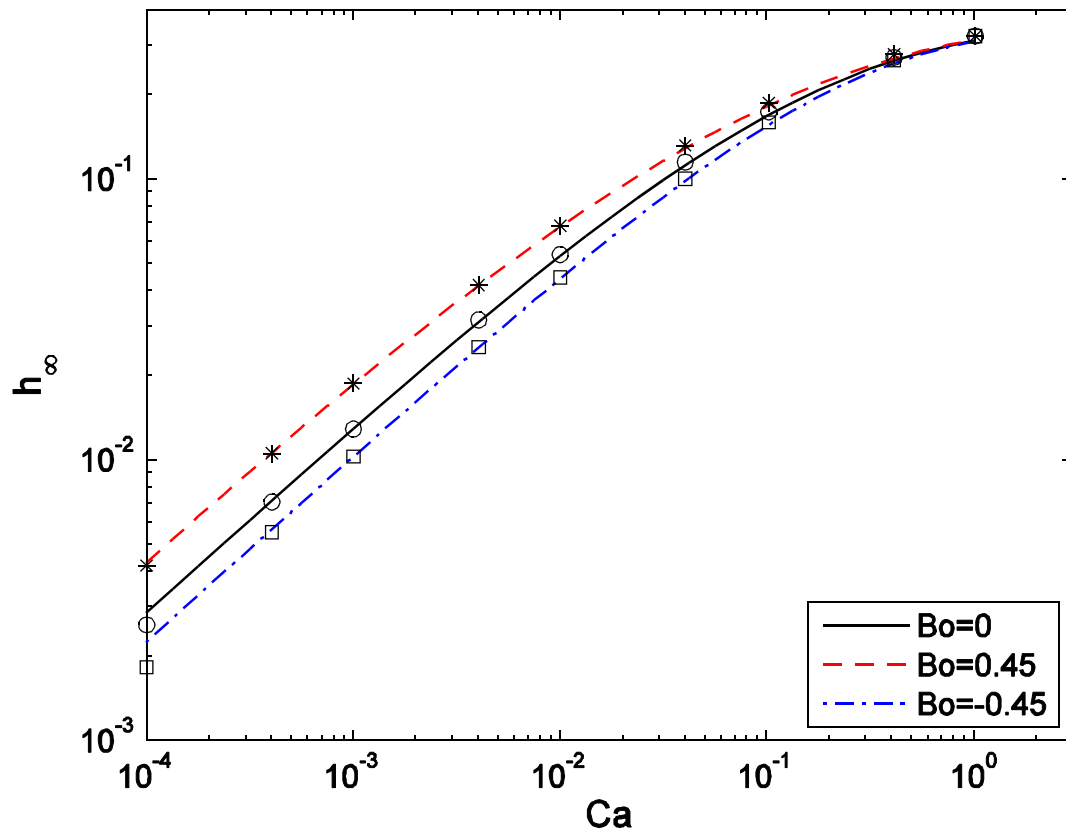

Figure 2. Comparison of the predictions of the film thickness of a large plug (lines) with those for a semi-infinite bubble reported by Hazel and Heil (symbols).

When the plug is sufficiently large, the front and rear menisci do not interact and the problem can be split into two smaller ones. Moreover, under these circumstances the film thickness is determined by the propagation of a semi-infinite bubble for the same value of λ, Ca, and Bo. Hazel and Heil [13] investigated the propagation of an air finger into a tube when gravity acts parallel to the tube axis. Even when that paper considers flexible tubes of elliptical or rectangular sections, the authors report numerical solutions for a circular tube within a wide range of capillary number, when inertia forces are

negligible and the Bond number is equal to 0.45 and -0.45. In order to validate our numerical code, we carried out computations for a large plug and the same values of *Ca* and *Bo* used by Hazel and Heil; in Figure 2 we compare our prediction for the film thickness with those reported in ref. [13].

3. Results

As we have mentioned in the Introduction to establish whether or not the steady displacement of a liquid plug is stable, it suffices to analyze the steady state results conveniently organized. To that end the curves of h_∞ for a fixed value of both the capillary number and the driving pressure drop are drawn as a function of l_P for selected values of the Bond and Laplace numbers. The analysis presented in ref. [12] for *Bo*=0, shows that the slope of those curves can be related to the stability of a given plug driven by a constant pressure drop (Δp) as follows:

✓ A liquid plug corresponding to a point where $\left(\partial h_\infty / \partial l_p\right)_{\Delta p} > 0$, is stable to small disturbances of Δp.

✓ Any steady plug located at a point where $\left(\partial h_\infty / \partial l_p\right)_{\Delta p} < 0$ is unstable.

Briefly, this result can be understood from the following analysis: when the driving pressure is perturbed, the speed of plug propagation is also affected, leading to a corresponding variation in the thickness of the trailing film (the precursor film is not affected by the perturbation). The resulting inflow/outflow imbalance modifies the volume —i.e. length— of the liquid plug. Once the perturbation disappears, whatever the change underwent by l_P, h_∞ will suffer a variation of the same sign if $\left(\partial h_\infty / \partial l_p\right)_{\Delta p} > 0$, leading to a new inflow/outflow imbalance that tends to recover the original plug volume. At this point the inflow/outflow ratio becomes one. The opposite happens when $\left(\partial h_\infty / \partial l_p\right)_{\Delta p} < 0$.

The selection of the range of values of the dimensionless parameters that characterize the problem depends on the particular application. In this work we consider a liquid with properties ρ=1 g/cm^3, μ=6 cP, and σ=50 dyn/cm; therefore for liquid plugs propagating with velocity between 0.08 m/s and 0.8 m/s in a conduit of radius approximately equal to 0.7mm, the resulting set of dimensionless parameters is λ=1000, *Bo*=0.1 and 0.01≤*Ca*≤0.1. This set may represent a liquid slug moving in the lung airways [14]. It is important to remember that in the coordinate system adopted, a positive Bond number represents a plug propagating against the direction of gravity while a negative Bond number accounts for the opposite situation (see Fig. 1). Also, the radius of the conduit chosen in this work is consistent with the assumption that gravity force does not affect the axial symmetry of the flow.

We carried out computations for plug lengths between 0.05 and 4.3 and *Bo* equal to ±0.1 and ±0.2. The predictions of h_∞ and Δp for each set (*Ca*, l_P) were used to build the stability charts corresponding to a selected value of the Laplace and Bond numbers. Each of the charts shown in Figs. 3-6 demanded about 400 individual simulations; curves for a fixed value of *Ca* (thin dashed blue lines) were plotted directly, while those for a fixed value of Δp (black solid lines) were obtained by interpolation. In Figures 3-6, we illustrate the maps for *Bo* equal to 0.1, 0 and -0.1. In those figures, the stable region is approximately enclosed by the thick-red-dashed line.

When the effect of gravity is negligible, i.e. when the axis of the tube is normal to gravity, the stable region encompasses short plugs (l_P<0.6) moving with a velocity corresponding to capillary numbers between 0.0562 and 0.112, approximately (see fig.3).

The map illustrated in Figure 4 represents plugs moving against gravity. If these results are compared with those depicted in Figure 3 for *Bo*=0, we see that the stable region is now smaller. The

length of the largest stable plugs is now equal to or smaller than 0.5 and the range of displacing velocities in which the steady motion is not affected by a perturbation of Δp is slightly narrower.
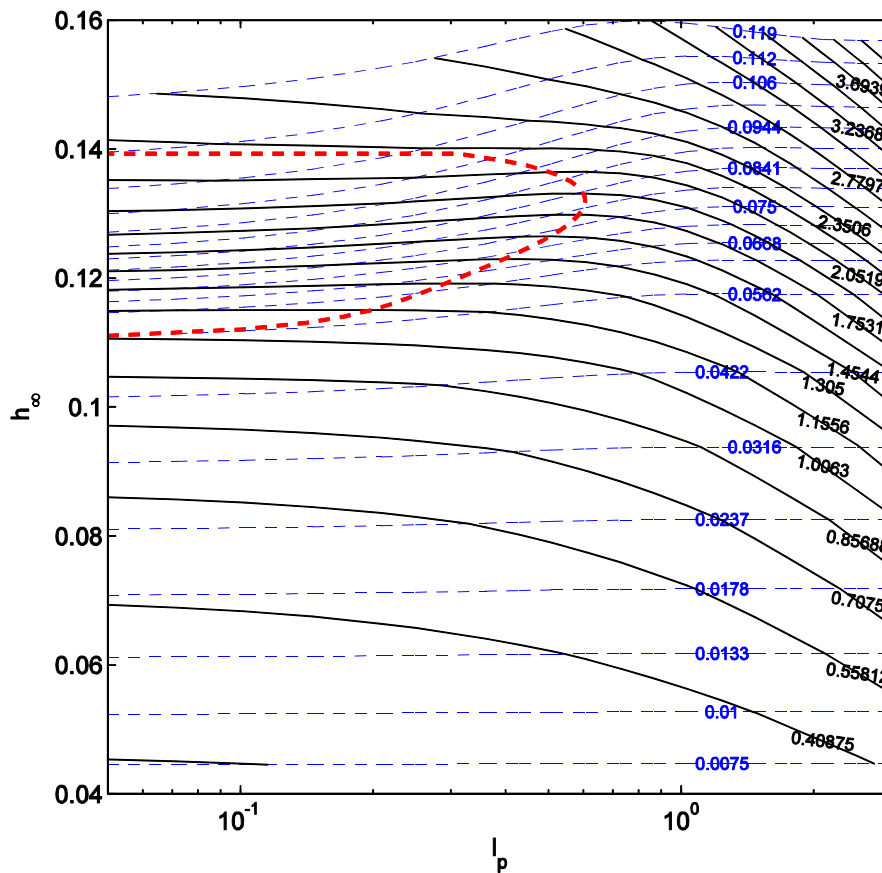

Figure 3. Steady state film thickness as a function of the plug length for λ=1000, *Bo*=0, and selected values of the capillary number (thin dashed blue lines). Black solid lines are curves of constant Δp. Steady state solutions within the region delimited by the thick dashed red line —where $\left(\partial h_\infty \big/ \partial l_p\right)_{\Delta p} > 0$ — are stable.

Solutions presented in Figure 5 for *Bo*= -0.1, i.e. for plugs moving in the same direction as gravity, show two regions of stable displacements. The upper one expands the stable zone delimited in Figure 3 for *Bo*=0: it comprises larger plugs which can propagate within a wider range of velocities. The lower one appears for *Ca* smaller than approximately 0.017 where it can be easily verified that the numerical predictions of the film thickness for a given value of the driving pressure drop monotonically increases with the length of the plug.

The above results point out that depending on the direction of the displacement of the slug with respect to gravity, the steady state propagation of a given plug may be stable or unstable. Also, for the three *Bo* considered the upper limit of the stable region seems to be a line where h_∞ is approximately constant for a certain Δp. This limit represents marginally stable plugs which move with decreasing velocity as the length of the plugs increases. Also, the propagation of a long liquid plug may be stable depending on the values of the capillary and the Bond number when λ is fixed. For instance, for λ=1000 and *Bo*= -0.1, the above statement is true for *Ca*< 0.013335, approximately.

Numerical solutions computed for other values of the Bond number (see Figure 6) show that the size of the stable region continuously increases (or decreases) as that parameter becomes bigger for

liquid plugs moving in the same (opposite) direction as gravity force. Moreover, the two stable regions present for Bo= -0.1 have merged into a larger one when that parameter is equal to -0.2.
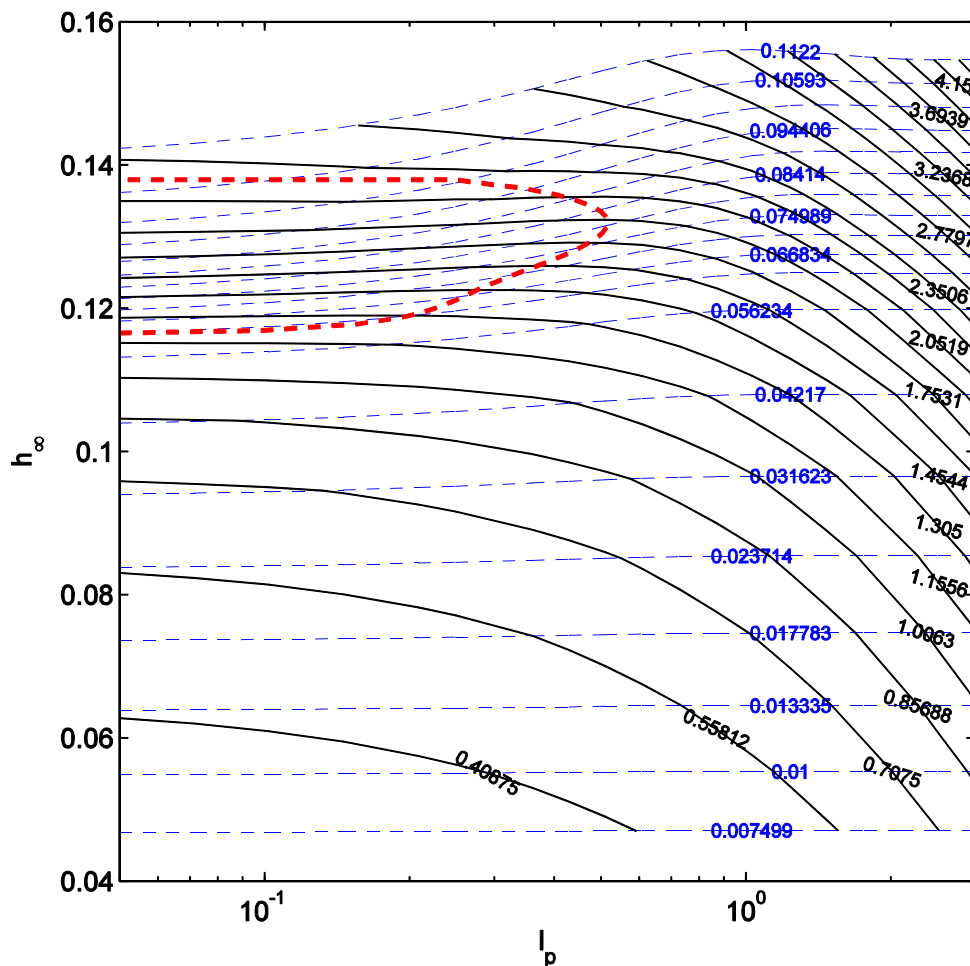

Figure 4. Steady state film thickness as a function of the plug length for λ=1000, Bo=0.1, and selected values of the capillary number (thin dashed blue lines). Black solid lines are curves of constant Δp. Steady state solutions within the region delimited by the thick dashed red line —where $\left(\partial h_\infty / \partial l_p\right)_{\Delta p} > 0$ — are stable.

4. Conclusion

In this paper we have applied the methodology presented in a previous work to analyze the effects of gravity on the stability of the steady state propagation of a liquid plug in a capillary tube lined with a uniform thin liquid film.

The stability maps show that the size of the stable region for a given Laplace number shrinks as the Bond number is augmented when the plug moves against gravity. On the other hand, if the plug propagates in the direction of gravity, one or two stable regions are detected depending on the value of Bo. Moreover, in this case the steady displacement of large plugs can be stable, a situation which is not observed when gravity effects are negligible.
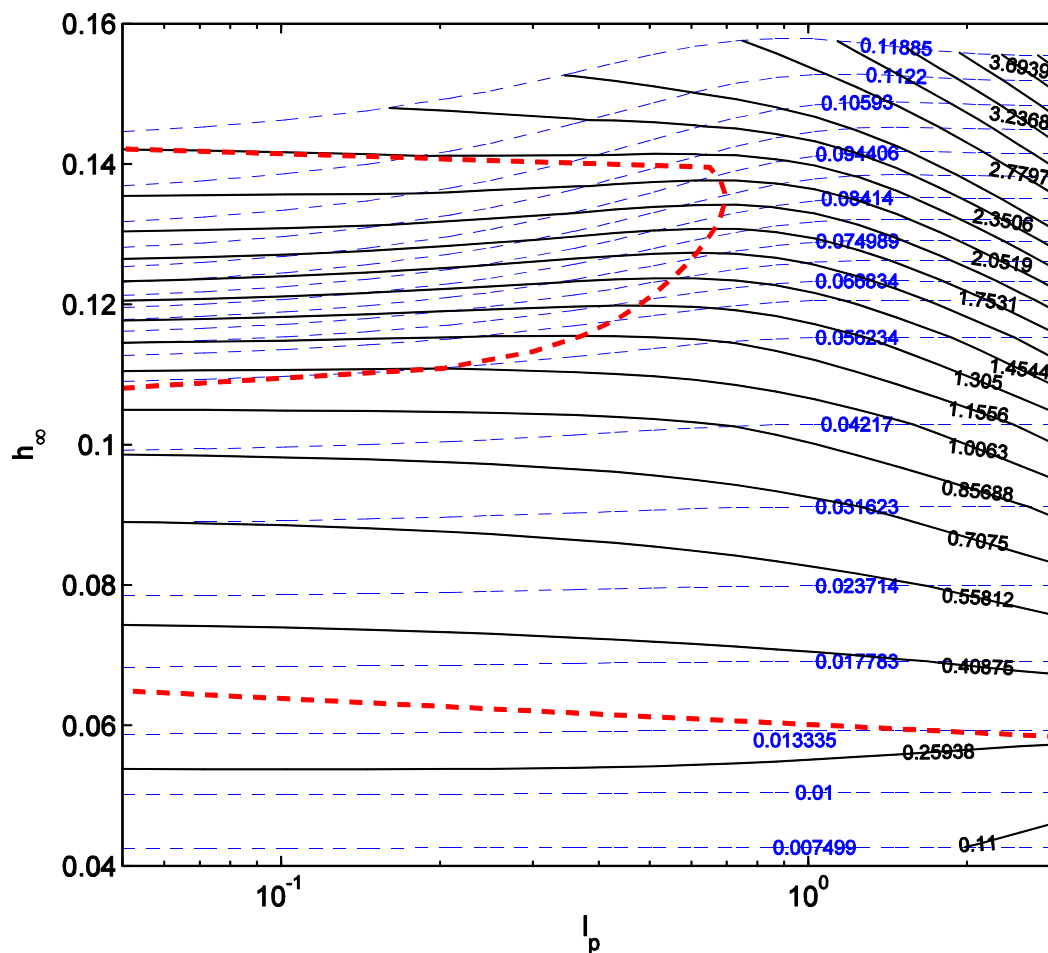
Figure 5. Steady state film thickness as a function of the plug length for λ=1000, *Bo*=-0.1, and selected values of the capillary number (thin dashed blue lines). Black solid lines are curves of constant Δ*p*. Steady state solutions within the region delimited by the thick dashed red line —where $\left(\partial h_{\infty}/\partial l_{p}\right)_{\Delta p} > 0$ — are stable.
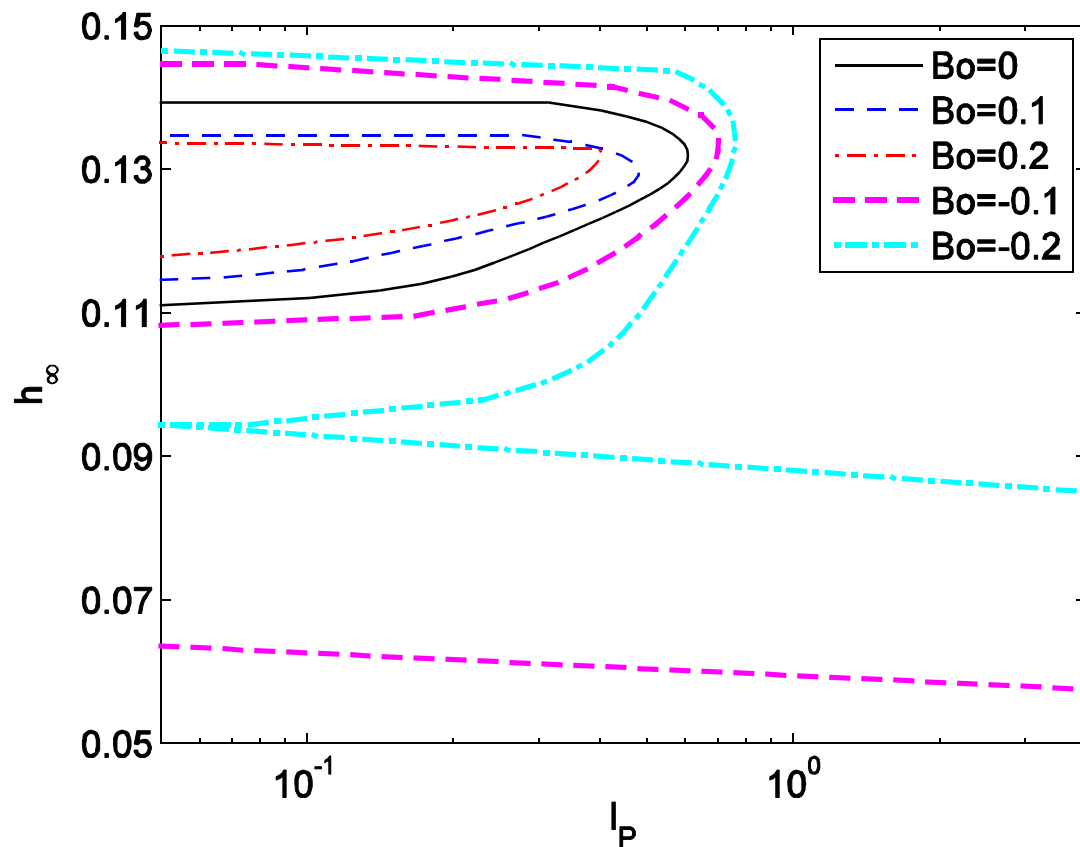
Figure 6. Marginally stable plugs for λ=1000 and selected Bond.

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