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Phase diagrams for two-phase flow in circular capillary tubes under the influence of a dynamic contact angle

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ABSTRACT

We analyze theoretically gas–liquid flow in a circular capillary tube, the inlet of which is connected to a constant-pressure liquid reservoir. Based on previously derived analytical solutions, we present for the first time comprehensive, two-dimensional phase diagrams, which predict the flow scenario from only two nondimensional numbers: a nondimensional pressure and a nondimensional gravity parameter. Diagrams are developed for both a constant and a dynamic contact angle where in the latter case the non-equilibrium Young force depends monotonically on the capillary number. The diagrams subdivide the entire parameter space into regions that are associated with either liquid withdrawal, liquid infiltration, or metastable and stable equilibrium states.

1. Introduction

Two-phase flow in capillary tubes occurs in engineering applications such as microfluidics. However, flow in capillary tubes is also indicative of flow in geometrically and topologically much more complex porous media such as soil, water filters, and fuel cells. Often flow is induced by a constant-pressure liquid reservoir that is connected to the tube inlet while the other end of the tube is connected to a constant-pressure gas reservoir, e.g., the atmosphere. Infiltration into soil due to ponding of a thin film of water is, for example, also frequently modeled by imposing a constant-pressure boundary condition for the water on the soil surface.

Traditionally two-phase flows in circular capillary tubes have been described by the Lucas–Washburn theory (Green and Ampt, 1911; Lucas, 1918; Washburn, 1921). This theory is based on the following assumptions:

1. Inertial forces can be neglected (small Weber number).
2. The viscosity of the gas can be neglected.
3. The pressure drop in the liquid can be described by Poiseuille's equation for axi-symmetric flow in a circular tube, thereby neglecting deviations from the parabolic velocity profile at the tube inlet and the gas–liquid interface.
4. The tube radius R is small enough such that gravity does not affect the shape of the gas–liquid interface, i.e., the interface has the shape of a spherical cap.
5. Contact angle θ is constant.

With these assumptions, flow is mathematically described by the following ordinary differential equation:

$$\frac{p_{l,0} - p_g}{l} + \frac{2\gamma}{Rl}\cos\theta = \frac{8\eta}{R^2}\dot{l} + \rho g \sin\Psi \tag{1}$$

where $l \geqslant 0$ is the distance between the tube inlet and the gas–liquid interface, $p_{l,0}$ is the pressure of the liquid reservoir, p_g is the constant gas pressure, γ is interfacial tension, θ is the contact angle that is measured in the liquid, η is dynamic viscosity of the liquid, ρ is the density of the liquid, g is the gravitational acceleration, and Ψ is the angle between the horizontal axis and the capillary tube. When the tube points downwards or upwards as seen from the tube inlet, $0^\circ > \Psi > -90^\circ$ or $0^\circ < \Psi \leqslant 90^\circ$, respectively.

The flow scenarios of downward liquid infiltration, capillary rise, and horizontal infiltration appear to be the flow scenarios that received the most attention when it came to the application of the Lucas–Washburn theory. Nonetheless it has been understood that the Lucas–Washburn theory can also be used to describe other types of flow such as liquid withdrawal (Blake and De Coninck, 2004). Our recent work revealed that all together 10 different flow scenarios may occur if one accounts for a dynamic contact angle. These flows differ in the orientation of the flow (horizontal, upward, or downward), the acceleration (positive, negative, or zero), and the direction of the flow (infiltration or withdrawal). The

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model for dynamic contact angle assumed the nonequilibrium Young force to be a function of the capillary number:

$$\cos\theta_{eq} - \cos\theta = \begin{cases} f(\eta\dot{l}/\gamma) & \text{for liquid infiltration} \\ -f(-\eta\dot{l}/\gamma) & \text{for liquid withdrawal} \end{cases} \quad (2)$$

where $f \geqslant 0$ is a nondimensional function that represented either a power law model or a polynomial. Note that the arguments of f are nonnegative, because $\dot{l} > 0$ for liquid infiltration and $\dot{l} < 0$ for liquid withdrawal.

Until only recently, no phase diagrams were available that allowed one to predict which type of flow occurs depending on the applied pressure, the fluid properties, the inclination angle of the tube, and the tube radius. In light of this lack of knowledge, Hilpert (2010b,c) developed such phase diagrams based on analytical solutions (Asthana, 2002; Martic et al., 2002; Hilpert, 2009a,b, 2010c,a,b). These phase diagrams assumed a linear contact angle model, $f = \alpha\eta\dot{l}/\gamma$. For the initial condition $l(t=0) = l_0 = 0$, these phase diagrams were 2D, while for $l_0 > 0$, they were 3D. In this paper, we show that 2D phase diagrams can be developed for any strictly increasing $f \geqslant 0$ with $f(0) = 0$. Since most physically-based contact angle models are not linear (Blake and Haynes, 1969; Jiang et al., 1979; Cox, 1986), this paper allows for more realistic predictions of capillary flows.

2. Phase diagrams

The right hand side of Eq. (2) can be written as $g(\eta\dot{l}/\gamma)$ where

$$g(x) = \text{sgn}(x)f(|x|) = \text{sgn}(x)f(x\,\text{sgn}(x)) \quad (3)$$

and sgn is the sign function. The function g inherits from the function f that it is strictly increasing and that $g(0) = 0$. Eq. (1) can be expressed in the following nondimensional fashion (Hilpert, 2010a,c):

$$4\lambda(\lambda' + \Gamma) = \overline{P} - g(\lambda') \quad (4)$$

where $\lambda(\tau) = l(t)/R$ is the nondimensional interface position, $\tau = t\gamma/(\eta R)$ is the nondimensional time, $\Gamma = \rho g R^2 \sin\Psi/(8\gamma)$ is a gravity number, $\lambda' = d\lambda/d\tau$ is the nondimensional interface velocity, and $\overline{P} = \frac{R(p_{l,0}-p_g)}{2\gamma} + \cos\theta_{eq}$ is a nondimensional pressure which accounts for the reservoir pressure and the equilibrium capillary suction.

One can construct a 2D phase diagram in terms of the initial interface velocity $\zeta_0 := \lambda'(0)$ and Γ based on previously derived analytical solutions (Hilpert, 2009a,b, 2010a). Table 1 shows the mathematical conditions for the occurrence of a flow scenario, and Fig. 1a shows the resulting phase diagram. The drawback of the $\zeta_0 - \Gamma$ phase diagram is that it predicts the scenarios from the initial interface velocity ζ_0 which is hard to control experimentally. For this reason we derive new 2D phase diagrams that depend on the initial interface position λ_0 which is easier to control experimentally than ζ_0. The initial interface position can be inferred from ζ_0 as follows:

$$\lambda_0 = \frac{\overline{P} - g(\zeta_0)}{4(\zeta_0 + \Gamma)} \quad (5)$$

The challenge now is to express the conditions for the possible flow scenarios listed in Table 1 in terms of λ_0 instead of ζ_0.

For $\lambda_0 > 0$, we define the following two nondimensional parameters:

$$\widehat{P} = \frac{\overline{P} + g(\Gamma)}{4\lambda_0}$$

$$\widehat{\Gamma} = \Gamma + \frac{g(\Gamma)}{4\lambda_0}$$

Using rigorous mathematical reasoning, the conditions from Table 1 can be reformulated in terms of $\widehat{P}$ and $\widehat{\Gamma}$ which in turn depend on λ_0. The second column in Table 2 shows these new conditions, and Fig. 1b shows the corresponding phase diagram. Appendix A.1 shows the corresponding mathematical derivation. Although this derivation does not work for the case of constant contact angle ($f \equiv 0$), it follows from Hilpert (2010b, Fig. 4a) that this case is still covered by the second column in Table 2 and Fig. 1b. Note that the conditions in terms of ζ_0 (see Table 1) are formally quite similar to those in terms of λ_0 in that the conditions are delineated by horizontal, vertical, one-to-one, and negative one-to-one lines. This is why the $\widehat{P} - \widehat{\Gamma}$ phase diagram is similar to the $\zeta_0 - \Gamma$ phase diagram.

For initial interface positions $\lambda_0 = 0$ and the case of a dynamic contact angle ($f > 0$), one can define the following new nondimensional gravity parameter that allows one to predict the flow scenarios from the conditions listed in the third column of Table 2 or from Fig. 1c:

$$\mathring{\Gamma} = g(\Gamma)$$

Appendix A.2 shows the corresponding mathematical derivation from the conditions listed in Table 1.

For the sake of completeness, we also address 2D phase diagrams in case of a constant contact angle, $f \equiv 0$, even though such diagrams have already been presented in the literature. For $\lambda_0 = 0$, we redisplay in the fourth column of Table 2 the conditions derived by Hilpert (2010c), and in Fig. 1d the corresponding phase diagram. It turns out that the case $\lambda_0 > 0$, which was already addressed by Hilpert (2010b) (using different independent variables to construct a phase diagram), is also accounted for by our analysis of the case $\lambda_0 > 0$ (see second column of Table 2 and Fig. 1b).

3. Discussion

Simple 2D phase diagrams (see Fig. 1) have been developed that allow one to predict which type of two-phase flow occurs in capillary tubes where flow is induced by a constant pressure reservoir. Flow can always be predicted from a nondimensional pressure variable and a nondimensional gravity number. The corresponding conditions are listed in Table 2. The 3D phase diagrams for capillary flow presented in Hilpert (2010b,c) have become obsolete, because they now have been replaced by 2D phase diagrams that account for dynamic contact angle models which allow for any monotonic dependence of the nonequilibrium Young force on the capillary number.

To the best of our knowledge, some of the flow scenarios (e.g. ADI, AHW, and AUW) have not been validated experimentally in

Table 1
Conditions for flow scenarios in terms of ζ_0 and Γ.

Scenario	Abbreviation	Condition
Decelerating horizontal liquid infiltration	DHI	$0 = -\Gamma < \zeta_0$
Accelerating horizontal liquid withdrawal	AHW	$\zeta_0 < -\Gamma = 0$
Equilibrium E0	E0	$\zeta_0 = -\Gamma = 0$
Equilibrium E+	E+	$-\Gamma < \zeta_0 = 0$
Equilibrium E−	E−	$\zeta_0 = 0 < -\Gamma$
Steady-state downward liquid infiltration	SDI	$0 < \zeta_0 = -\Gamma$
Steady-state downward liquid withdrawal	SDW	$\zeta_0 = -\Gamma < 0$
Decelerating downward liquid infiltration	DDI	$0 < -\Gamma < \zeta_0$
Decelerating downward withdrawal	DDW	$-\Gamma < \zeta_0 < 0$
Accelerating downward liquid infiltration	ADI	$0 < \zeta_0 < -\Gamma$
Accelerating downward liquid withdrawal	ADW	$\zeta_0 < -\Gamma < 0$
Decelerating upward liquid infiltration	DUI	$-\Gamma < 0 < \zeta_0$
Accelerating upward liquid withdrawal	AUW	$\zeta_0 < 0 < -\Gamma$