Electronic Supplementary Material (ESI) for Lab on a Chip.

Supplementary Text

Phaseguides as Tunable Passive Microvalves for Liquid Routing in Complex Microfluidic Networks

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Analytical Model

The phaseguide pressure was calculated using the Young-Laplace relation given by

$$P_{phg} = \gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right) \quad \text{(S1)}$$

where γ is the surface tension, R_1 and R_2 are the principle radii of curvature of the meniscus at the instant of overflow. Fig. S1 illustrates the cut out section of the channel and the phaseguide at the instant of overflow, showing the global coordinate frame, the phaseguide, and the meniscus.

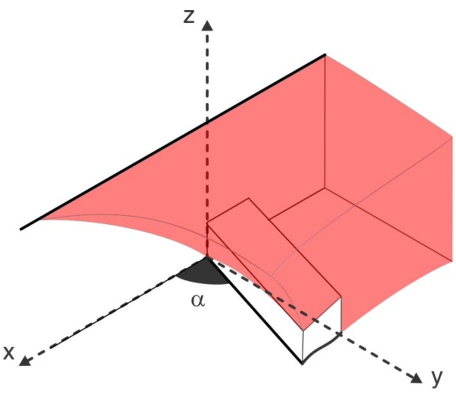

Fig. S1. Cut out section of the microchannel with phaseguide. The global coordinate system is located such that the z axis is directing upward and collinear with the edge created by the phaseguide and the channel wall, and x is pointing towards the liquid advancing direction.

At the instant of overflow, equilibrium requires that the pressure across liquid-air interface is uniform throughout the meniscus. It follows that the mean curvature at any point on the interface must be the same according to Equation S1. However, this does not necessarily mean that the principle curvatures $1/R_1$ and $1/R_2$ in Equation S1 are the same at any point on the interface. Therefore, to calculate the mean curvature, hence the phaseguide pressure, a specific point on the interface must be chosen such that the principle curves can be defined analytically.

Common interpretation of meniscus pinning considers only the principle curve on the vertical plane passing through the pinning barrier. However, this assumption disregards the effects of the other principle curve, which mainly describes the horizontal curvature of the interface. In derivation of the phaseguide pressure, we took the effect of both principle curves into account.

To determine the principle curvatures, a local frame was defined as shown in Figure S2.a. This frame was defined such that x'z' plane dissects the wedge created by the phaseguide and the channel wall to make a dihedral angle of $\alpha/2$ with the channel wall.

Here, since the plane x'z' dissects the wedge, it can be assumed that the angle between the curve C_1 and the top substrate measured on x'z' plane is approximately equal to the advancing contact angle θ_1 between the liquid and the top substrate (Figure S2.b). On the other hand, angle θ_2' between the edge created by intersection of the phaseguide and the channel wall, and curve C_1 can be found as[S1]:

$$\cos\theta_2'\cos\left(90^\circ-\frac{\alpha}{2}\right)=\cos\theta_2 \tag{S2}$$

where θ_2 is the advancing contact angle between the liquid and the wedge material. Here it should be noted that both the phaseguide and the channel wall, which constructs the wedge, are made of the same material with contact angle θ_2.

As a result, referring to Figure S2.b it can be written that:

$$\begin{aligned}\sin\theta_2' &= \frac{l_2}{R_1} \quad \cos\theta_2' = \frac{l_1+x'}{R_1}\\ \sin\theta_1 &= \frac{l_1}{R_1} \quad \cos\theta_1 = \frac{l_2+h}{R_1}\end{aligned} \tag{S3}$$

Since

$$l_2=R_1\sin\theta_2' \tag{S4}$$

it can be written that

$$R_1\cos\theta_1=R_1\sin\theta_2'+h \tag{S5}$$

As a result R_1 can be found as

$$R_1=\frac{h}{\cos\theta_1-\sin\theta_2'} \tag{S6}$$

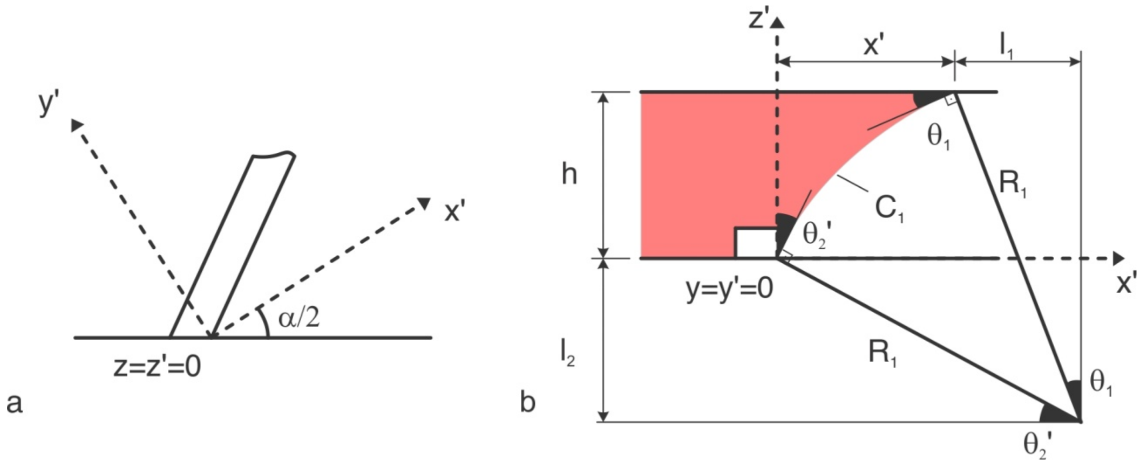

Fig. S2. (a) Orientation of the local coordinate frame for calculation of R_1. (b) Curve C_1 lying on x'z' plane.

By definition, the principal curves should be perpendicular to each other. Therefore, since the first principle curve (C_1) is lying on the plane x'z', the second principle curve (C_2) must be on a plane, which is orthogonal to x'z'. To determine this orthogonal plane, a secondary coordinate frame x"y"z" was defined such that the axis z" is tangent to the curve C_1 and the axis x" is collinear with the line connecting the center of the curve C_1 and the edge of the phaseguide (Fig. S3.a). Thus, we obtained the plane x"y", which is orthogonal to x'z'. Therefore, the curve lying on this plane and passing through the origin of the coordinate frame x"y"z" should be the second principle curve C_2 (Fig. S3.b). This implies that the location of the point on the interface, at which the principle curvatures are calculated, is the origin of the new coordinate frame x"y"z".

Assumption of a shallow phaseguide implies that the angle ϕ on Fig. S3.a is approximately equal to the angle θ_2' given by Equation S2 ($\phi\approx\theta_2'$). Therefore, the distance δ between the origin of the coordinate frame x"y"z" and the edge of the phaseguide along x" can be approximated as:

$$\delta=h_{phg}\sin\theta_2' \tag{S7}$$

Referring to Figure S3.b, it can be written that

$$\frac{R_2}{\sin\alpha'} = \frac{R_2 + \delta}{\sin\left(90^\circ + \theta_2\right)} \tag{S8}$$

As a result the radius of curvature of the second principle curve C_2 can be found as:

$$R_2 = \frac{\delta \sin\alpha'}{\sin\left(90^\circ + \theta_2\right) - \sin\alpha'} \tag{S9}$$

Here α' is the half phaseguide angle tilted approximately by θ_2', which can be stated as:

$$\tan\alpha' = \tan\frac{\alpha}{2}\cos\theta_2' \tag{S10}$$

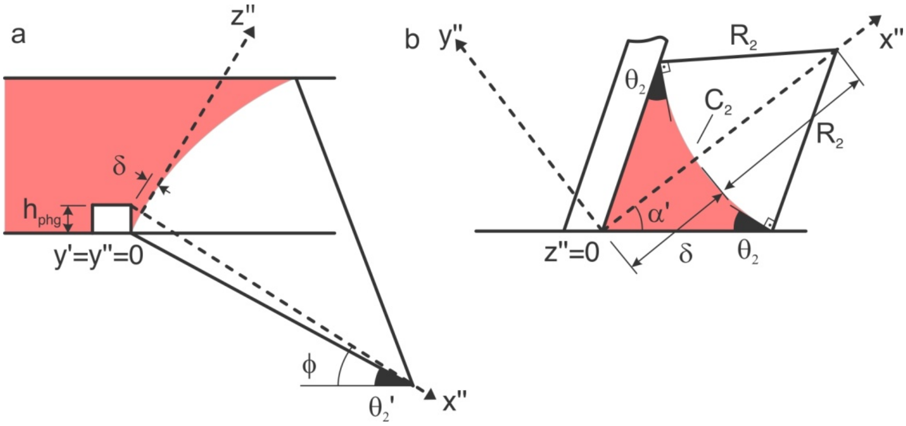

Fig. S3. (a) Orientation of the local coordinate frame for calculation of R_2. (b) Curve C_2 lying on x'z' plane.

As a result, inserting the expressions derived for the radii of curvature into Young-Laplace equation (Equation S1), the phaseguide pressure can be found.

By rearranging the terms, Young-Laplace equation for the phaseguide pressure can be rewritten as:

$$P_{phg} = \frac{\gamma}{R_1} + \frac{\gamma}{R_2} \tag{S11}$$

Here γ/R_1 and γ/R_2 can be interpreted as the pressure contribution of the first principle curve C_1 and the second principle curve C_2 respectively. Plotting γ/R_1, γ/R_2, and P_{phg} (Figure S4) reveals that P_{phg} is dominated by γ/R_2, which is mainly controlled by the phaseguide angle. This result shows that, on the contrary to the common interpretation, which relates the pinning behavior to the vertical meniscus profile, the pinning is mainly characterized by the horizontal geometry.

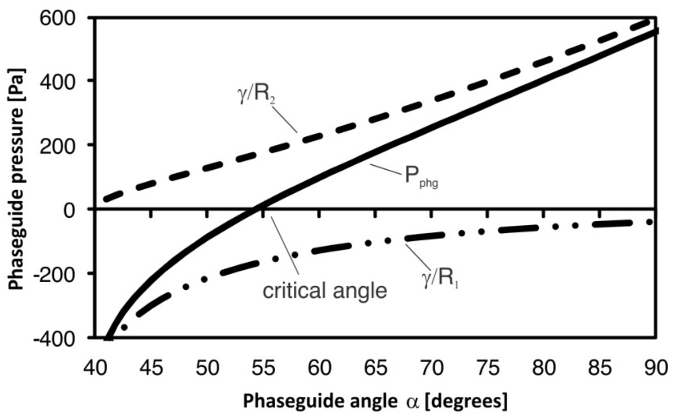

Fig. S4. Contribution of the first principle curve represented by the radius R_1 and the second principle curve represented by the radius R_2 on phaseguide pressure. θ_1 and θ_2 are 20 and 70 degrees respectively. Channel height and phaseguide height are 30 µm and 120 µm respectively. Intersection of the curve γ/R_2 with the horizontal gives the critical angle prescribed by the Concus-Finn criterion ($180^o – 2\theta_2$). However, the analytical model results in a larger critical angle, which is caused by the effect of γ/R_1.

Simulation Model

To determine the phaseguide pressure using Surface Evolver, the phaseguide was modeled as a ridge patterned on the bottom of a rectangular channel while the initial geometry of the meniscus was defined as a plane leaning slightly towards the advancing direction as illustrated on Fig. S5.a. Boundary conditions were set as listed in Table S1.

As the first step, meniscus geometry at zero pressure was determined (Fig. S5.b) by evolving the initial meniscus shown in Fig. S5.a. The new meniscus was re-evolved by incrementally changing the pressure (Fig. S5.c). These iterations were carried out until the meniscus reaches the bottom of the channel (Fig. S5.d). The pressure on the meniscus at this instant was recorded as the phaseguide pressure.

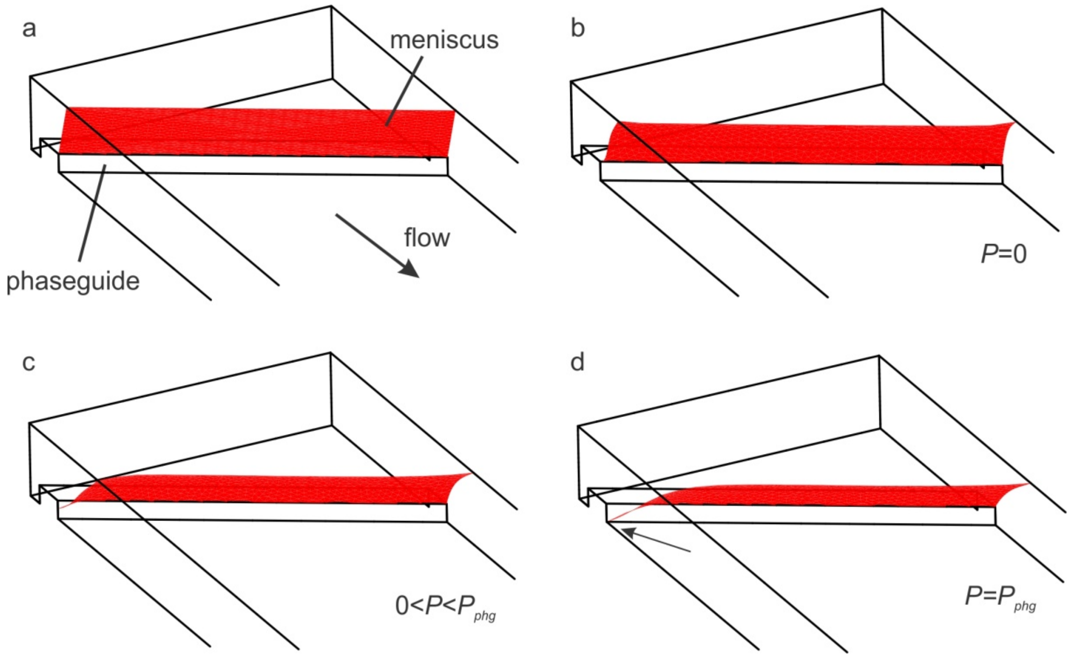

Fig. S5. Surface Evolver model of the meniscus pinned on a phaseguide. (a) The meniscus is initially modeled as a plane slightly leaning towards the advancing direction. Initial meniscus is evolved to determine the (b) meniscus geometry at zero pressure. (c) Pressure is incrementally changed to simulate the meniscus advancement. (d) Simulation is stopped when the meniscus touches the bottom of the channel.

Table S1. Parameters and boundary conditions used in the simulation model. Channel and phaseguide dimensions were selected as defined in the manuscript.

Parameter or Boundary Condition	Value
Contact angle on the channel top (implemented using glass)	20^o
Contact angle on the phaseguide front face (implemented using dry film photoresist)	70^o
Contact angle on the channel side walls (implemented using dry film photoresist)	70^o
Surface tension on the meniscus (water-air)	72.9x10^{-3} N/m

Reference

S1 Shuttleworth, R., Bailey, G. L. J., *Discuss. Faraday Soc.*, 1948, **3**, 16.