Supplementary Material (ESI) for Lab on a Chip

Supplementary information

to

Computation of transient flow rates in passive pumping micro-fluidic systems

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Derivation of modified Young-Laplace Equation (Equation 4b in the paper)

For calculating the volume of a droplet sinking into the cylindrical entry port of a micro-fluidic device with a pseudo-concentric descend pattern (Fig. 2c and 2d in the paper) the continuously changing shape of the droplet is approximated as a stack of thin disks. At each t_i time instant the radii, volumes, and surface areas of the disks depend of their position in the stack that is represented by the angle $\theta_{i,j}$ (Fig. S1), which varies between zero, at the apex, and $\theta_{i,max}$, at the circumference of the contour line. When $h/a > 1$

$$\theta_{i,\max} = \frac{\pi}{2} + \cos^{-1}\left(\frac{a}{R_i}\right)$$

When $h/a \leq 1$, $\theta_{i,max}$ can be calculated with the inverse sine function:

$$\theta_{i,\max} = \sin^{-1}\left(\frac{a}{R_i}\right)$$

The radius of the disk j ($\rho_{i,j}$) in the stack is

$$\rho_{i,j} = R_i \sin\theta_{i,j}$$

and the pertinent area of disk j is denoted as:

$$A_{i,j} = 2\pi R_i^2 \sin\theta_{i,j} d\theta_{i,j}$$

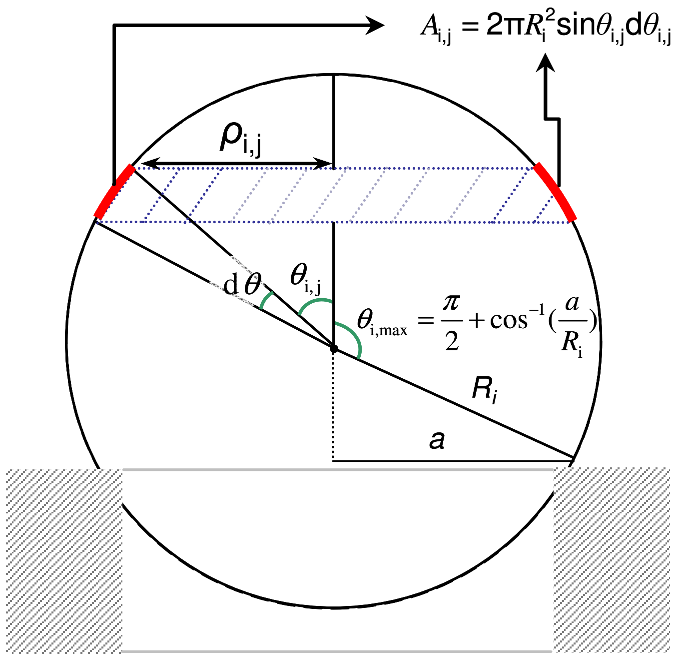

Fig. S1: Cross sectional snapshot of a droplet at a time instant t_i with notations utilized in our model calculations: $\rho_{i,j}$ is the radius disc j, $A_{i,j}$ is the pertinent area of disk j, R_i is the radius of the droplet, a is the half cord length, and $\Theta_{i,j}$, dΘ, and $\Theta_{i,max}$ are angles used to designate individual discs in the stack of hypothetical discs.

As shown in Fig. 2d in the paper, the changing droplet surface is depicted with its surface points descending $dh_{i,j}$ distances ranging between $dh_{i,max}$ (at the apex) and zero (at the circumference of the contour line). These $dh_{i,j}$ distances are space and time dependent and can be approximated by a cosine function:

$$dh_{i,j} = dh_{i,max} \cdot \cos(\frac{\pi}{2} * \frac{\theta_{i,j}}{\theta_{i,max}}) \quad \text{(S1)}$$

The quality of this approximation is demonstrated in Fig. S2 where the $dh_{i,j}$ distances were calculated from the drop geometry and by using Eq. S1 for the limiting cases: (i) hemispherical droplet, $h = a$ and (ii) a droplet completely sunken into the entry port of the microfluidic device, $h = 0.3a$ (where h is the height of the droplet and a is the cord of the contour line). As shown in the figure, the trigonometric function provides an excellent approximation for assessing $dh_{i,j}$

values during the entire sinking process; however, the cosine function gives best approximation when h/a=1.

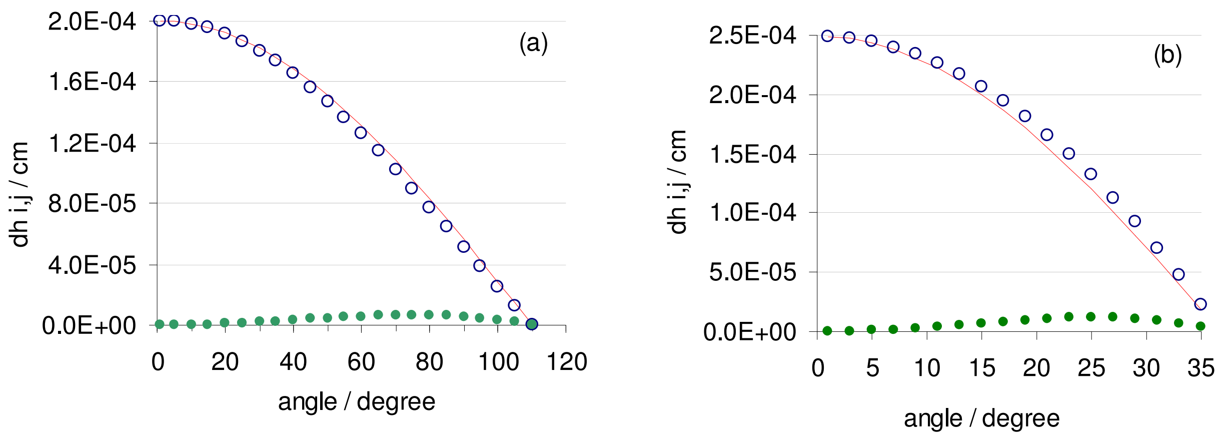

Fig. S2: $\mathrm{d}h_{i,j}$ distances as function of angle $\theta_{i,j}$ calculated from geometrical analysis (○) and by using Eq. S1 (solid lines). The filled circles (•) represent the difference between the two calculated values (absolute error). (a) Limiting condition for the sinking sample droplet ($h/a\approx$ 1.4), (b) Limiting condition for the emerging reservoir droplet ($h/a\approx$ 0.3).

The conversion of interfacial energy E_i between the two time instants t_i and t_{i+1}, which is apparent in the changing shape of the descending droplet, can be expressed by:

$$\mathrm{d}E_i = \int_{h_{i,\max}}^{h_{i,j}=0} \Delta P_i A_{i,j} \mathrm{d}h_{i,j} = \int_{t_i}^{t_{i+1}} \gamma \mathrm{d}A_i \qquad \text{(S2)}$$

where ΔP_i is the variation in the pressure in the sample droplet from time t_i to t_{i+1}, A_i is the whole surface area of the droplet on which the pressure does work, and γ denotes the surface tension. ΔP_i is a function of the droplet geometry, i.e., it is changing in time. However, its value is identical at every point on the cap.

The integration of the $A_{i,j}\mathrm{d}h_{i,j}$ function from $\theta_{i,j}$ = 0 to $\theta_{i,j}$ = $\theta_{i,\max}$ provides the surface energy at the water / air interface at each t_i time instant:

$$\int_{h_{i,\max}}^{h_{i,j}=0} \Delta P_i A_{i,j} \mathrm{d}h_{i,j} = \int_{\theta=0}^{\theta_{i,\max}} \Delta P_i 2\pi R_i^2 \cdot \mathrm{d}h_{i,\max} \cdot \cos\left(\frac{\pi\theta_{i,j}}{2\theta_{i,\max}}\right) \cdot \sin\theta_{i,j} \mathrm{d}\theta_{i,j} \qquad \text{(S3)}$$

The surface energy change between time intervals t_i and t_{i+1} can be expressed as

$$\int_{t_i}^{t_{i+1}} \gamma \mathrm{d}A_i = \gamma\pi(h_i^2 - h_{i+1}^2) \qquad \text{(S4)}$$

Calculation of the geometrical parameters of sample and reservoir droplets

Water droplets form different shapes when dispenses onto surfaces with different hydrophilicity. Images of droplets captured at time zero on untreated (hydrophobic) and air plasma treated (hydrophilic) sample wells of PDMS-based micro-channels are shown in Fig. S3a and S3b.

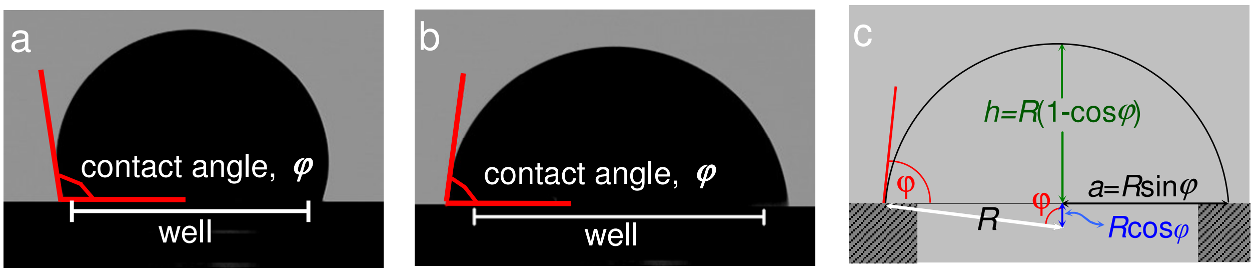

Fig. S3: Water droplets on top of hydrophobic (a) and hydrophilic (b) wells. The correlations between the contact angle (φ), the radius (R), the height (h), and the half-chord length (a) of a droplet cap are shown on the example of Fig. S3b.

The geometrical parameters of the sample and reservoir droplets were determined from the contact angle (φ) data as shown in Fig. S3c:

$$a = R\sin\varphi \qquad \text{(S5)}$$

$$h = R(1-\cos\varphi) \qquad \text{(S6)}$$

$$R = \left[\frac{3V}{\pi\left(2-3\cos\varphi+\cos^3\varphi\right)}\right]^{1/3} \qquad \text{(S7)}$$

When a sample droplet, with a diameter smaller than the diameter of the entry port of the micro-fluidic device, is dispensed over the filled entry port a spontaneously becomes equal to r and the radius (R_i) and volume (V_i) of the sinking droplet is calculated by using Eqs. 1 and 2.