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

Electronic Supplementary Information for

Moving droplets between closed and open microfluidic systems

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Electromechanical model for actuation force calculation

There are two approaches, both based on energy arguments and thus equivalent, for calculating the electromechanical forces acting on droplets: the Maxwell stress tensor method [S1-S3] and the method of lumped parameter electromechanics [S4,S5]. Because it is generally more convenient for microfluidic systems, we use the lumped parameter method here.

Electromechanical force for the parallel-plate scheme

To calculate the electromechanical forces exerted on a droplet, the first step is to obtain an expression identifying the system capacitance. Figure S1 shows a parallel-plate microfluidic device and its equivalent circuit. The droplet is modeled as a resistor and capacitor in parallel. The hydrophobic layer (Teflon-AF) on the top plate, and the hydrophobic (Teflon-AF) / dielectric (SOG) layers on the bottom plate are assumed to be perfect dielectrics represented by pure capacitors. For simplicity, the Teflon-AF layer on the top plate and the Teflon-AF / SOG layers on the bottom plate are grouped together as capacitor C_{cl} in the following calculation.

For the simplified circuit shown in Figure S1 (b), the capacitances and conductance of each element are:

$$C_L = \frac{\varepsilon_0 k_L x w}{D} \tag{S1-a}$$

$$G_L = \frac{\sigma_L x w}{D} \tag{S1-b}$$

$$C_M = \frac{\varepsilon_0 k_{air} x w}{D} \tag{S1-c}$$

$$C_{cl} = \frac{1}{\dfrac{1}{C_t} + \dfrac{1}{C_t} + \dfrac{1}{C_d}} \tag{S1-d}$$

$$C_{cl}^{'} = \frac{1}{\frac{1}{C_t^{'}} + \frac{1}{C_t^{'}} + \frac{1}{C_d^{'}}} \quad \text{(S1-e)}$$

where $C_t = \frac{\varepsilon_0 k_t x w}{d^{'}}$, $C_d = \frac{\varepsilon_0 k_d x w}{d}$, $C_t^{'} = \frac{\varepsilon_0 k_t (L-x) w}{d^{'}}$, $C_d^{'} = \frac{\varepsilon_0 k_d (L-x) w}{d}$.

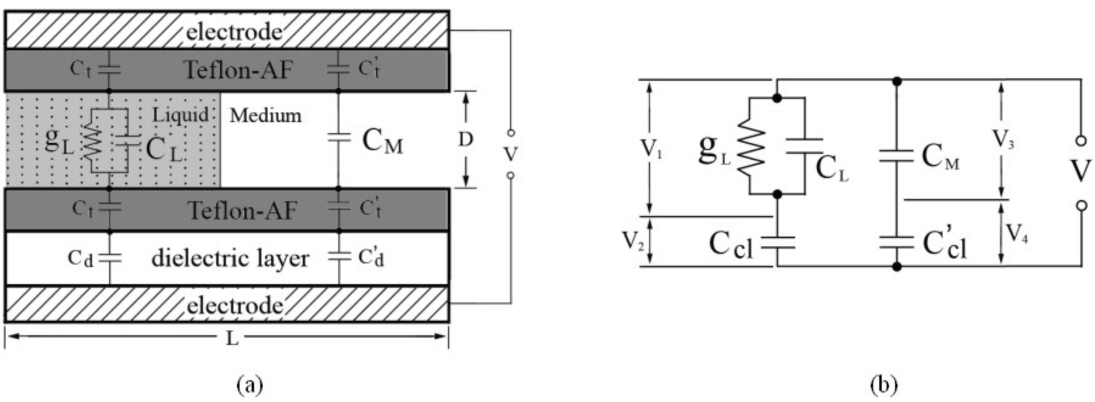

Fig. S1 (a) Equivalent circuit model for parallel-plate microfluidic device. (b) Simplified circuit for the model. Teflon-AF layer on top plate and Teflon-AF/SOG layers on bottom plate are grouped together and represented by one capacitor.

The device parameters and liquid properties used in the calculation are detailed in Table S1. We evaluate the voltages across each circuit element using standard AC circuit methods. Let $\underline{Z}_1$, $\underline{Z}_2$ be the impedances of the liquid and the combined dielectric/hydrophobic layers for the liquid filled side, and $\underline{Z}_3$, $\underline{Z}_4$ be the impedance of air and the combined layers for the medium side.

$$\underline{Z}_1 = \frac{1}{G_L + j\omega C_L},\ \underline{Z}_2 = \frac{1}{j\omega C_{cl}},\ \underline{Z}_3 = \frac{1}{j\omega C_M},\ \underline{Z}_4 = \frac{1}{j\omega C_{cl}^{'}} \quad \text{(S2)}$$

where $j = \sqrt{-1}$. From the voltage divider relation, the voltages defined in Fig. S1 are:

$$V_1 = \frac{\underline{Z}_1}{\underline{Z}_1 + \underline{Z}_2} V,\ V_2 = \frac{\underline{Z}_2}{\underline{Z}_1 + \underline{Z}_2} V,\ V_3 = \frac{\underline{Z}_3}{\underline{Z}_3 + \underline{Z}_4} V,\ V_4 = \frac{\underline{Z}_4}{\underline{Z}_3 + \underline{Z}_4} V \quad \text{(S3)}$$

Table S1 List of symbols and constants used in the electromechanical force calculation.

Symbol	description	Value
ε_0	Permittivity of free space	8.85×10^{-12} F/m
k_L	Dielectric constant of liquid	78 for water
k_t	Dielectric constant of Teflon-AF	1.93
k_d	Dielectric constant of SOG	4.5
σ_L	Conductivity of liquid	10^{-4} S/m for water
k_{oil}	Dielectric constant of oil	2.2 for mineral oil
f	Frequency of applied voltage	
ω	Angular frequency	$2\pi f$
x	Length of the liquid filled region	
w	Electrode width	1 mm
L	Electrode length	1 mm
D	Gap between top and bottom plates	100 μm
d	Thickness of the SOG layer	0.5 μm
d'	Thickness of the Teflon layer	1 μm
g	Lateral spacing between two coplanar electrodes	40 μm
w'	Electrode width for single plate scheme	280 μm
L'	Electrode length for single plate scheme	280 μm

The force is calculated using the coenergy method based on the *principle of virtual work*. [S5]. There are four capacitive energy terms recognized for the circuit shown in Figure S1(b). The total energy U of the system is $U = \sum_{i=1}^{4} \frac{1}{2} C_i V_i^2$. Thus, the total electromechanical force F acting on the liquid is $F = \frac{\partial U}{\partial x}$. Combining with equation (S1) (S2) and (S3), we obtain:

$$|V_1| = \left| \frac{j\omega\varepsilon_0 k_{eff} D}{j\omega\varepsilon_0 (k_L(2d' + d) + k_{eff} D) + \sigma_L (2d' + d)} \right| V \qquad \text{(S4-a)}$$

$$|V_2| = \left| \frac{j\omega\varepsilon_0 k_L + \sigma_L}{j\omega\varepsilon_0 (k_L + \frac{k_{eff} D}{2d^{'} + d}) + \sigma_L} \right| V \quad \text{(S4-b)}$$

$$F = \frac{1}{2}\varepsilon_0 w \{ \frac{k_L}{D} |V_1|^2 + \frac{k_{eff}}{(2d^{'} + d)} |V_2|^2 - \frac{k_{eff} k_{air}}{k_{eff} D + k_{air}(2d^{'} + d)} V^2 \} \quad \text{(S4-c)}$$

where k_{eff} is a convenient effective dielectric constant for the combined dielectric/ hydrophobic layers, $k_{eff} = \frac{k_t k_d (2d^{'} + d)}{k_t d + 2k_d d^{'}}$, and k_{air} is the dielectric constant for air medium, $k_{\text{air}} = 1$.

Electromechanical force for the single plate scheme

In the single-plate scheme, the electric field between coplanar electrodes is more complex than for the parallel-plate scheme, where the electric field is mostly uniform. To estimate the electromechanical force acting on the droplet in the single plate scheme, we assume the electric-field lines between two coplanar electrodes are approximately semicircular.

We model the single plate device by the equivalent circuit shown in Fig. S2. Once again the liquid is represented by as a resistor and capacitor in parallel, the hydrophobic (Teflon-AF) / dielectric (SOG) layers on the bottom substrate are combined and represented by a single capacitor, and the air gap takes the form of another capacitor. The expressions for the capacitances and the conductance are:

$$C_{water} = \varepsilon_0 k_L x A \quad \text{(S5-a)}$$

$$G_{water} = \sigma_L x A \quad \text{(S5-b)}$$

$$C_{air} = \varepsilon_0 (L^{'} - x) A \quad \text{(S5-c)}$$

$$C_1 = \frac{1}{\dfrac{d'}{\varepsilon_0 k_t x w'} + \dfrac{d}{\varepsilon_0 k_d x w'}} \qquad \text{(S5-d)}$$

$$C_2 = \frac{1}{\dfrac{d'}{\varepsilon_0 k_t (L' - x) w'} + \dfrac{d}{\varepsilon_0 k_d (L' - x) w'}} \qquad \text{(S5-e)}$$

where x = the length of liquid filled portion of the activated electrode, the geometric factor $A = K(1-k^2)/2K(k^2)$, and K is the complete elliptic integral of the first kind with modulus $k = g/(2w'+g)$ [S6].

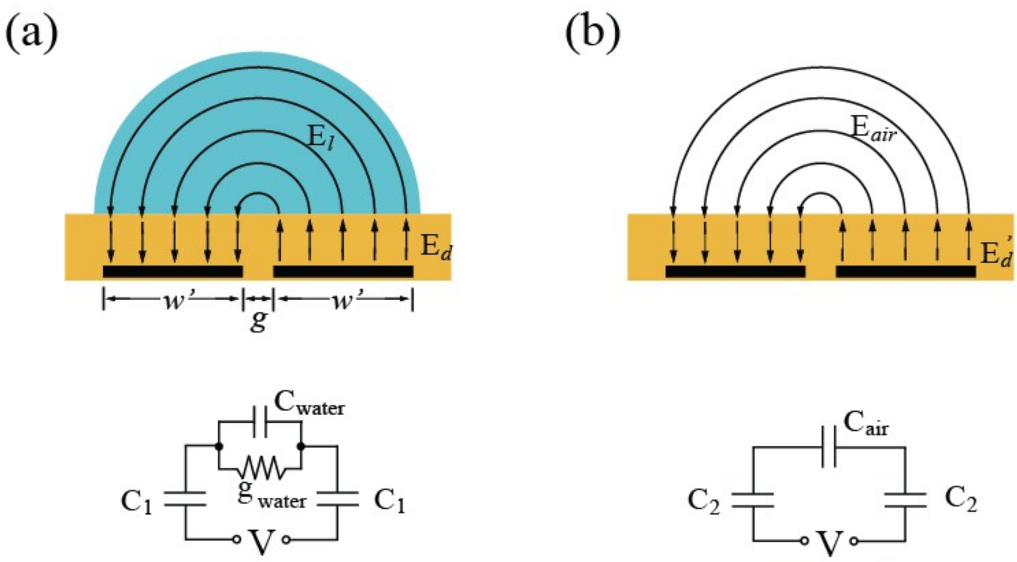

Fig. S2 Approximate E-field distribution on coplanar electrode structure and corresponding circuit model. (a) The liquid filled region. (b) The air filled region.

With these conductances and capacitances, it is easy to find the impedances for the liquid, air, and the combined dielectric layers.

$$\underline{Z}_{water} = \frac{1}{G_{water} + j\omega C_{water}}, \; \underline{Z}_1 = \frac{1}{j\omega C_1}, \; \underline{Z}_{air} = \frac{1}{j\omega C_{air}}, \; \underline{Z}_2 = \frac{1}{j\omega C_2} \qquad \text{(S6)}$$

The approximate voltage drops across the liquid, the air, and the dielectric layers are, respectively,

$$V_{water} = \frac{\underline{Z}_{water}}{\underline{Z}_{water} + 2\underline{Z}_1} V \text{ , } V_1 = \frac{\underline{Z}_1}{\underline{Z}_{water} + 2\underline{Z}_1} V \text{ , } V_{air} = \frac{\underline{Z}_{air}}{\underline{Z}_{air} + 2\underline{Z}_2} V \text{ , } V_2 = \frac{\underline{Z}_2}{\underline{Z}_{air} + 2\underline{Z}_2} V$$

(S7)

There are six energy storage elements for the system, so the total system coenergy of interest is $U = \sum_{i=1}^{6} \frac{1}{2} C_i V_i^2$. The total electromechanical force F acting on the liquid is $F = \frac{\partial U}{\partial x}$. Combing with equation (S5) (S6) and (S7), we obtain:

$$\left| V_{water} \right| = \left| \frac{j\omega\varepsilon_0 \frac{k_{eff}^{'} w^{'}}{(d + d^{'})}}{j\omega\varepsilon_0 (\frac{k_{eff}^{'} w^{'}}{d + d^{'}} + 2k_L A) + 2\sigma_L A} \right| V \quad \text{(S8-a)}$$

$$\left| V_1 \right| = \left| \frac{j\omega\varepsilon_0 k_L A + \sigma_L A}{j\omega\varepsilon_0 (\frac{k_{eff}^{'} w^{'}}{d + d^{'}} + 2k_L A) + 2\sigma_L A} \right| V \quad \text{(S8-b)}$$

$$F = \frac{1}{2} \varepsilon_0 \{ k_L A \left| V_{water} \right|^2 + \frac{2k_{eff}^{'} w^{'}}{(d^{'} + d)} \left| V_1 \right|^2 - \frac{A k_{eff}^{'} w^{'}}{k_{eff}^{'} w^{'} + 2A(d^{'} + d)} V^2 \} \quad \text{(S8-c)}$$

where k_{eff}’ is the effective dielectric constant for the combined dielectric/hydrophobic layers on the bottom substrate, $k_{eff}^{'} = \frac{k_t k_d (d^{'} + d)}{k_t d + k_d d^{'}}$.

Supporting references

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