An analytical model for the prediction of microdrop extraction and splitting in digital microfluidics systems

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ABSTRACT

Digital microfluidics, especially electrowetting on dielectric (EWOD) has gained momentum in the recent years and it is now foreseen to be a promising way to perform many biological processes like DNA or protein manipulation and detection, and cell analysis.
It has been shown that surface energy minimization is an adequate approach to predict the behavior of drops on the electrodes. In the light of the minimization theory, we propose a model to determine the conditions under which drop extraction is possible.
***Keywords*:** electrowetting, EWOD, topology, surface tension, Laplace law, curvature radius.

INTRODUCTION

ElectroWetting On Dielectric (EWOD) is a major component of digital microfluidics [1,2,3]. Using such a technique, many applications in biotechnology are under way for DNA, proteins, cell manipulations and chemical reactions. It has also been demonstrated recently that EWOD microsystems may be used as calibration unit for drop dispensing systems [4].

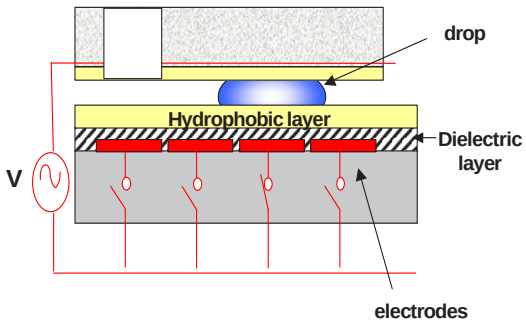

Fig. 1. Schematic view of a covered EWOD design.

Basically, the principle of electrowetting is to take advantage of the reduction of contact angle with an increase of electric charges, according to the Lippmann-Young law. Thus a gradient of wettability on a conducting drop can be created by an adequate arrangement of electrodes and drop displacement is then possible [5]. The dielectric prevents liquid droplet to be hydrolyzed and the hydrophobic layer permits the highest possible change in contact angle (fig.1). Precise modeling EWOD Microsystems is a complicated task [6]. However the problem may be simplified by a dimensional analysis showing that inertia and viscosity may be neglected in front of surface tension because the Weber and the Ohnesorge numbers are small. Thus the surface tension is the dominating force and the problem is principally topological [7]. Under this assumption, the drop location and shape are determined by minimization of its surface energy.
In an EWOD microsystem, drop motion or drop merging are rather straightforward operations but drop extraction from reservoir and drop division are much more complex. In the light of the surface minimization theory, we derive an analytical model aimed at the prediction of drop extraction. This model requires first a constitutive law ("modified" Lippmann law) for the correspondence between applied tension and contact angle, and second, the calculation of the relations between the different curvature radius in the different parts of the drop.
The model produces an "extraction" equation which relates the electric potential necessary for drop extraction as a function of the parameters of the system, i.e. vertical gap, surface tension, size of the electrodes, contact angles on the different surfaces, and reservoir volume. A direct by-product of this equation is the derivation of a limiting vertical gap beyond which the extraction becomes impossible.

THE PRINCIPLE OF EXTRACTION

It has been shown experimentally [1,2] and numerically [7] (with the help of the Surface Evolver numerical software [8]) that drop extraction is obtained by three successive operations (fig.2):

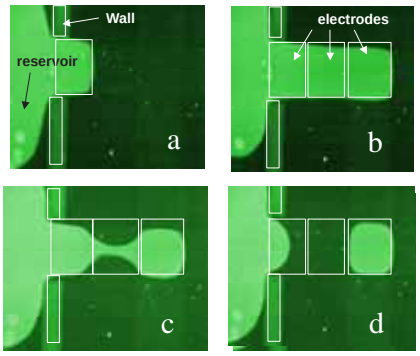

Fig.2. (a) and (b) liquid extrusion from reservoir, (c) pinching of the drop and back pumping, (d) separation

First, liquid extrusion from the reservoir onto the electrode row; second, drop pinching by de-actuating the "cutting" electrode; third back-pumping into the reservoir in order to reduce the internal pressure of the drop so that the pinching effect becomes effective. The delicate point here is the splitting of the drop and the present model is aimed at producing a characteristic equation for this splitting of the drop.

CONSTITUTIVE LAW

The technology of EWOD is based on the observation that an electrical field modifies the contact angle of a conducting liquid with the solid substrat, according to the Lippmann-Young relation [9]

$$\cos\theta = \cos\theta_0 + \frac{1}{2}\frac{C}{\gamma}V^2 \tag{1}$$

where θ, θ_0, C, γ and V are respectively the actuated and not-actuated contact angles, the capacitance of the substrat and the applied electric potential. However, a plot of the values of $\cos\theta - \cos\theta_0$ versus V^2 for different liquids and biologic buffers shows that the Lippmann-Young relation is only valid at low voltage (fig.3).

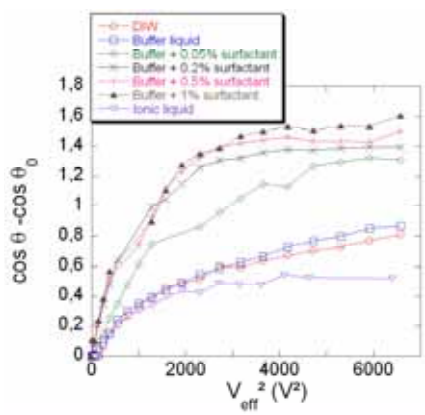

Fig. 3. Experimental Lippmann relations for different liquids (experimental conditions are described in [7])

Observing that the experimental curves are linear for low voltage (with a coefficient equal to $C/2\gamma$) and have a saturation threshold at high voltage, we find a clear similarity with the Langevin's equation for paramagnetic material, and verify that the Langevin's function fits well with the experimental results (fig.4)

$$\frac{\cos\theta - \cos\theta_0}{\cos\theta_S - \cos\theta_0} = \coth\left(\frac{3CV^2}{2\gamma\left(\cos\theta_S - \cos\theta_0\right)}\right) - \frac{1}{\dfrac{3CV^2}{2\gamma\left(\cos\theta_S - \cos\theta_0\right)}} \tag{2}$$

where θ_S is the saturation angle. Relation (2) may be called "modified" Lippmann law.

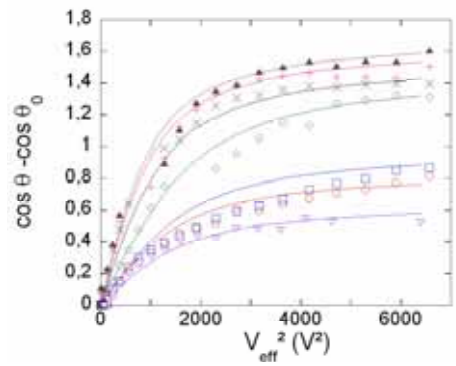

Fig. 4. Fit of the experimental results by Langevin's functions

ANALYTICAL MODEL

The analytical model requires four steps (1) calculation of the pressure in the reservoir; (2) calculation of the pressure at the pinching electrode; (3) determination of the curvature radius in the pinching zone by equating the calculated pressures of step 1 and 2; (4) derivation of an "extraction" equation by using the constitutive law derived in the preceding section.

Step 1: pressure in the reservoir

Pressure in the reservoir is given by Laplace law

$$P_R = \gamma\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \tag{3}$$

where R_1 and R_2 are the two curvature radius in a horizontal and vertical plane (fig. 5). It is easy to show that the vertical curvature radius R_1 is given by the relation

$$R_1 = \frac{h}{\left(-\cos\theta_0 - \cos\theta\right)} \tag{4}$$

where h is the vertical gap.

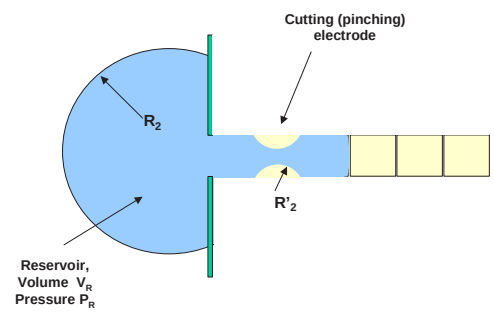

Fig.5. View from above of the drop morphology during extraction process

The horizontal curvature radius requires a little more algebra and is related to the volume in the reservoir by

$$R_2 \approx \sqrt{\frac{V_R}{\left(\theta_w - \dfrac{\sin 2\theta_w}{2}\right)h}} \tag{5}$$

where θ_w is the contact angle with the separation wall. Substitution of (4) and (5) in (3) yield the relation

$$P_R = \gamma \left(\frac{-\cos\theta_0 - \cos\theta}{h} + \frac{\sqrt{\left(\theta_w - \frac{\sin 2\theta_w}{2}\right)h}}{\sqrt{V_R}} \right) \quad (6)$$

Relation (6) can be satisfactorily compared to the results of the Evolver calculation (fig.6)

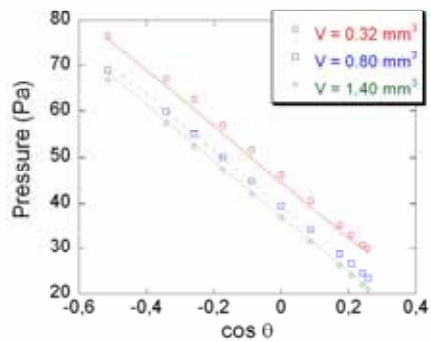

Fig. 6. Comparison of calculated pressure between Evolver results (dots) and present model (lines) for three different volumes of fluid in the reservoir

Step 2: pressure in the pinching region

In the pinching region (fig 7,8), Laplace law may be written under the form

$$P_E = \gamma \left(\frac{1}{R_1^{'}} - \frac{1}{R_2^{'}} \right) \quad (7)$$

and, the same reasoning as for eq.(4) leads to

$$R_1^{'} = \frac{h}{-2\cos\theta_0} \quad (8)$$

Note that $\theta_0 > \pi/2$ and $\cos\theta_0$ is negative. Thus, from (7) and (8), the pressure in the cutting electrode region is given by

$$P_E = \gamma \left(-\frac{2\cos\theta_0}{h} - \frac{1}{R_2^{'}} \right) \quad (9)$$

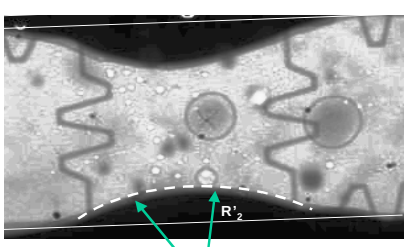

Fig. 7. Curvature radius R'_2 on the cutting electrode

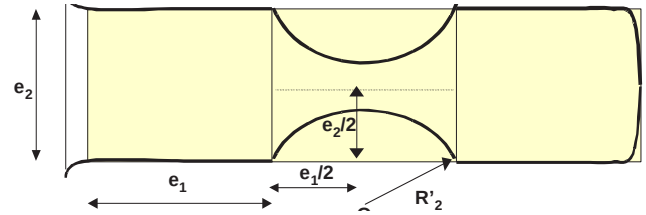

Fig. 8. Schematic view of the drop morphology on the cutting electrode

Step 3: calculation of R'_2 and first extraction equation

With the assumption of a quasi-steady state, the pressure is uniform at any time inside the drop. By equating the two calculated values of the pressure (6), (9), we find

$$\frac{1}{R_2^{'}} = -\frac{\cos\theta_0}{h} + \frac{\cos\theta}{h} - \frac{\sqrt{\left(\theta_w - \frac{\sin 2\theta_w}{2}\right)h}}{\sqrt{V_R}} \quad (10)$$

For square electrodes $e=e_1=e_2$, the curvature radius at the moment of the splitting is approximately

$$R_2^{'} \approx \frac{e}{2} \quad (11)$$

and we deduce a first equation for drop extraction, where $S_R=V_R/h$ is the surface of the drop inside the reservoir

$$\cos\theta - \cos\theta_0 = \frac{2h}{e} + \frac{h\sqrt{\left(\theta_w - \frac{\sin 2\theta_w}{2}\right)}}{\sqrt{S_R}} \quad (12)$$

The surface tension γ does not appear in (12). Using the Lippmann law (1) and relation (12), we find the value of the electric potential for extraction

$$V = \left(\frac{2h\gamma_{LG}}{C}\right)^{\frac{1}{2}} \left(\frac{2}{e} + \frac{\sqrt{\left(\theta_w - \frac{\sin 2\theta_w}{2}\right)}}{\sqrt{S_R}} \right)^{\frac{1}{2}} \quad (13)$$

This relation shows that the applied potential for extraction varies as the square root of the vertical gap. However, if we use the modified Lippmann law (2), we obtain the more accurate implicit extraction relation

$$h\left[\frac{2}{e} + \frac{\sqrt{\left(\theta_w - \frac{\sin 2\theta_w}{2}\right)}}{\sqrt{S_R}}\right] = (\cos\theta_S - \cos\theta_0) \left\{ \coth\left(\frac{3CV^2}{2\gamma_{LG}(\cos\theta_S - \cos\theta_0)}\right) - \frac{1}{\frac{3CV^2}{2\gamma_{LG}(\cos\theta_S - \cos\theta_0)}} \right\} \quad (14)$$

There are two elements in the relations (13) or (14): the term *2/e* refers to the "cutting" electrode and the other term to the reservoir. Relations (13) and (14) have been plotted in the figure 9.

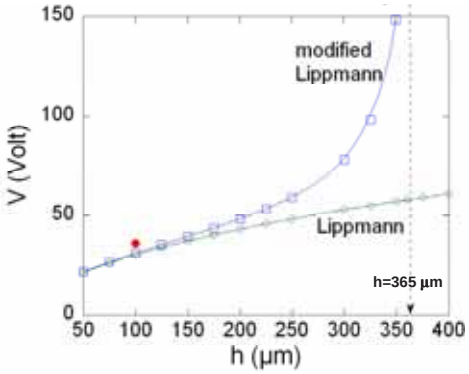

Fig. 9. Electric potential required to obtain extraction vs. vertical gap (buffer solution with 0.05% surfactant in silicon oil). Lippmann relation does not indicate a limiting distance whereas modified Lippmann law does. The red dot corresponds to the experimental potential for *h*=100µm and square electrodes of 800 µm, and *h*=365 µm corresponds to an experimental impossibility to extract droplets.

MAXIMUM VERTICAL GAP

It has been observed that there is a limit for the vertical gap beyond which extraction is not possible. We show here that the value of the maximum vertical gap can be derived from the present model.

The pressure in the drop must be positive (larger than the external pressure) and a first criteria for the maximum vertical gap may be deduced from (9)

$$h < h_{\max,1} = -e\cos\theta_0 \qquad (15)$$

This first criterion is a geometrical criterion. But, there is also an electrical criterion imposed by saturation. At saturation the right hand side of (14) is collapses to $\cos\theta - \cos\theta_0$, and we find a second condition for the vertical distance

$$h < h_{\max,2} = \frac{(\cos\theta_S - \cos\theta_0)}{\dfrac{2}{e} + \dfrac{\sqrt{\left(\theta_w - \dfrac{\sin 2\theta_w}{2}\right)}}{\sqrt{S_R}}} \qquad (16)$$

The first limit for the vertical gap (15) is based on geometrical conditions; the second (16) is based on electrical conditions. We have noticed that condition (16) is more restrictive than condition (15) for all the liquids we have tested. Remarking that $h_{max,2}$ is bounded by

$$h_{\max,2} < \frac{e(\cos\theta_S - \cos\theta_0)}{2}$$

then

$$h_{\max,1} - h_{\max,2} > -\frac{e}{2}(\cos\theta_0 + \cos\theta_s)$$

and $h_{\max,1} - h_{\max,2} > 0$ if $\theta_s > \pi - \theta_0$ which is the usual case.

We have checked experimentally on a buffer solution that the limiting vertical gap was around 365 µm for a square electrode of 800µm. It is in agreement with the value from (16) which indicate for the same liquid a distance of 384 µm. Besides, for a vertical gap of 100µm, the experimental limit potential was about 35 V, which is similar to the value given by the model (fig. 9).

CONCLUSION

In this work, a modified Lippmann equation based on a Langevin's function has been derived and an analytical model based on minimization theory (Laplace law) has been set up. The model produces an "extraction" relation that relates the required electric potential to obtain droplet extraction to the principal parameters of the EWOD system, such as the vertical gap, the electrode size, the liquid volume in the reservoir and the non-actuated contact angles. A consequence of this equation is the derivation of the limit vertical gap beyond which extraction becomes impossible.

The model predicts values of the vertical gap in agreement with the experimental values, and pressure in agreement with the Surface Evolver results. A more complete experimental verification is still needed, and extrusion from the reservoir - which is the first step of the extraction process - should also be investigated. However, this model contains interesting insights for the scaling down (or up) of an EWOD microsystem.

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