EDEW Version 2.0
A simulation and optimization tool for fluid handling by electrowetting effects

D 4.1: Report for the EU project “Micrometer scale patterning of Protein and DNA-Chips”

Jan Lienemann, Andreas Greiner, and Jan G. Korvink

IMTEK – Institute for Microsystem Technology, Albert Ludwig University
Georges Köhler Allee 103, D-79110 Freiburg, Germany
lieneman@imtek.de Contract No. EU G5RD-CT-2002-00744

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Abstract

We present an extended version of EDEW (**E**volve **d**roplets by **e**lectro**w**etting) [5], an application for the simulation of microscale fluid handling by electrowetting effects, which includes options for optimizing the shape of a fluidic array. It allows the user to input her own electrode shapes and study the effects on the energy landscape. Installation instructions and theoretical background are given in the previous report [5].

1 Introduction

Electrowetting devices are microfluidic components which allow for the motion of droplets on a substrate with a given grid of electrodes. Since on a 2D grid, the motion of a droplet is free in the plane as long as it sticks to the grid lines, these devices are particularly suitable for the design of reconfigurable fluidic circuits with programmable fluid paths [3, 6].

The usual setup for electrowetting actuation is shown in Fig. 1. The system consists of a dielectric layer with electrodes attached to the bottom of the layer. It is essential that the dielectric layer is a good insulator with no pinholes, and that ions can not easily be trapped inside the layer; this would inhibit the correct function of the device.

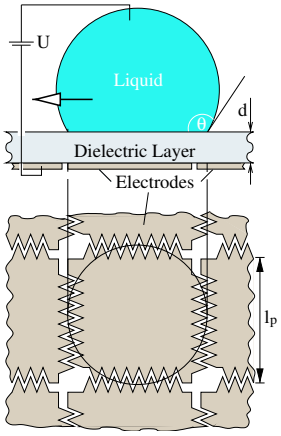

Figure 1: Setup for electrowetting. The top electrode is usually replaced by a glass lid with conducting ITO layer at the bottom.

The droplets are placed on top of the dielectric layer. The droplet is contacted either with a wire as shown in Fig. 1, or is confined between the dielectric layer and a conducting top layer, e.g., a metal or indium tin oxide (ITO, a transparent but conducting material) layer, forming a single large electrode.

By applying an electric voltage between the top and the bottom electrode a change of the contact angle results. By applying the voltage not to the electrode on which the droplet is sitting on, but to the adjacent electrode, the droplet tends to increase its area of support on that electrode and therefore a motion to the next electrode takes place. Subsequent application of the algorithm to the next pair allows to transport the droplet over the complete area.

The success and speed of this procedure is a function of the drag force on the contact line of the droplet. Understanding the dynamic effects at the beginning of the droplet motion is crucial for the optimization of electrode structures with respect to fast switching and tolerance against droplet volume variations. Consider a square electrode shape and a droplet sitting on this electrode, but with no overlap to the neighboring electrode (Fig. 2). The acceleration at the start of the motion is determined by the energy gradient. The energy change is proportional to the overlap area of the electrode and the droplet's contact area. With flat electrode edges, a small motion of the contact line of the droplet will not result in a change of energy due to the (necessary) gap between the electrodes. However, if interdigital edge structures are present, a small overlap is formed which can initiate the motion of the droplet.

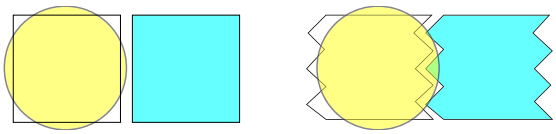

Figure 2: Droplet on a square electrode (left) and on an electrode with a ridged edge (right).

The shape of these interdigital structures determines the drag force on the contact line and thus the character of the inital motion. By optimizing its shape, it is possible to account for different droplet sizes and possible chemical contaminations on the substrate which can resist and even inhibit the motion of the droplet.

2 Modelling of electrode shapes

The modelling of these effects is based on the energy balance of the system and its desire to move to an energy minimum along the negative energy gradient. The analytic model for the contact angle of a droplet states that the free energy F for a thin dielectric layer reads [7] in differential form (see Fig. 3):

$$\mathrm{d}F = \gamma_{SL}\mathrm{d}A - \gamma_{SV}\mathrm{d}A + \gamma_{LV}\mathrm{d}A\cos\theta + \mathrm{d}U - \mathrm{d}W_B \quad (1)$$

where U is the energy stored in the electric field in the dielectric layer between droplet and electrode, γ_{SL}, γ_{SV} and γ_{LV} are the surface/interfacial tensions of the system at $V = 0$ (see Fig. 4), and W_B is the work the voltage must perform to built up the potential between droplet and electrode.

Equilibrium and thus an energy minimum is reached when $\mathrm{d}F/\mathrm{d}A = 0$. For $V = 0$ (and thus $\mathrm{d}U = \mathrm{d}W_B = 0$), this leads to the Young equation

$$\cos\theta = \frac{\gamma_{SV} - \gamma_{SL}}{\gamma_{LV}}. \quad (2)$$

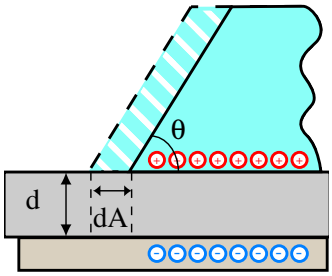

Figure 3: Schematic picture of the virtual displacement of the contact line.

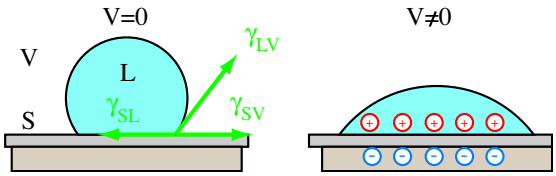

Figure 4: A droplet changing its contact angle by electrowetting. The arrows denote the surface/interfacial tensions.

The energy stored in a capacitor with large area A, small plate distance d and relative dielectric constant ε_r of the material inbetween for a voltage V is approximately given as

$$U = \frac{1}{2}CV^2 = \frac{1}{2}\frac{\varepsilon_r\varepsilon_0 A}{d}V^2, \tag{3}$$

where ε_0 is the dielectric constant of vacuum.

Now we assume that the droplet changes its area by dA because of moving the contact line. Then the energy of the electric field changes by

$$\frac{\mathrm{d}U}{\mathrm{d}A} = \frac{1}{2}\frac{\varepsilon_r\varepsilon_0}{d}V^2. \tag{4}$$

The additional energy is fed into the system by the voltage source, so that [7]

$$\frac{\mathrm{d}W_B}{\mathrm{d}A} = \frac{\varepsilon_r\varepsilon_0}{d}V^2. \tag{5}$$

$\mathrm{d}U/\mathrm{d}A$ and $\mathrm{d}W_B/\mathrm{d}A$ can be combined to an electrowetting term $\gamma_{EW} = \mathrm{d}W_B/\mathrm{d}A - \mathrm{d}U/\mathrm{d}A$, whereupon (1) reads

$$\frac{\mathrm{d}F}{\mathrm{d}A} = \gamma_{SL}\mathrm{d}A - \gamma_{SV}\mathrm{d}A + \gamma_{LV}\mathrm{d}A\cos\theta - \gamma_{EW} \tag{6}$$

with

$$\gamma_{EW} = \frac{1}{2}\frac{\varepsilon_r\varepsilon_0}{d}V^2. \tag{7}$$

The Young equation (2) then becomes

$$\cos\theta = \frac{\gamma_{SV} - \gamma_{SL} + \frac{1}{2}\frac{\varepsilon_r\varepsilon_0}{d}V^2}{\gamma_{LV}}. \tag{8}$$

We implement this model by modifying the interfacial tension of the droplet to the substrate, i.e., $\gamma_{SL} = \gamma_{SL,V=0} - \varepsilon_r\varepsilon_0 V^2/2d$ on the parts of the contact area where it overlaps with the respective electrode.

The surface evolver model has no explicit representation of the (redundant) interface S between droplet and substrate (this is only the bottom, if the droplet is not confined; if it is confined, this also applies to the top of the droplet). Its energy must be added to the total energy by other means. Since the boundary ∂S of this interface is known, we can convert the surface integral to a line integral by the Green-Gauss theorem [2] which states

$$\int_S \vec{f}\,\mathrm{d}\vec{A} = \int_{\partial S}\vec{g}\,\mathrm{d}\vec{l} \tag{9}$$

with

$$\vec{f} = \nabla\times\vec{g}. \tag{10}$$

Since on the bottom $\mathrm{d}\vec{A} = \vec{k}\mathrm{d}A$, where $\vec{k}$ is the unit vector in the z direction, we require a $\vec{g}$ such that the third component of its rotation, $f_z = \partial g_y/\partial x - \partial g_x/\partial y$, is equal to the interfacial tension γ_{SL}. Choosing $g_x = 0$, we get

$$\vec{g} = \begin{pmatrix} 0 \\ \int_x \gamma_{SL}\mathrm{d}x \\ 0 \end{pmatrix}. \tag{11}$$

On the top (confined droplet), the sign is reverted.

To resolve a ridged electrode shape in all its complexity, a very fine resolution of the contact line would be necessary. Since, on the other hand, the effect of the spike pitch is rather low, but it decreases also the stability and precission of the integration, we have decided to use a mean interfacial tension: γ_{SL} is averaged along the edge direction. The structures are still drawn in the graphical output, but are for display purposes only.

3 EDEW model

The EDEW model for the electrode shape optimization is based on the 1DPath model. This model simulates a row of electrodes with a single droplet on them. The configurable parameters that can be specified are listed in Table 1 (values with "*" only if "Confined" is checked) with dimensions as in Figure 5. Dimensions not shown in the figure are the distance of the bottom dielectric layer to the top layer for the confined droplet, the thickness of the dielectric layer and the droplet volume.

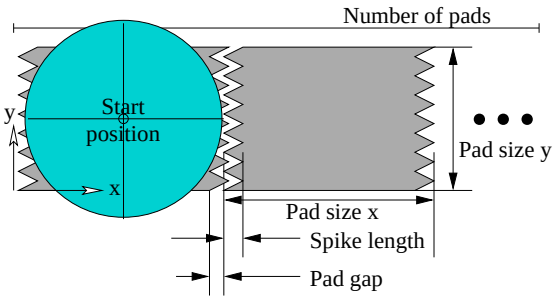

Figure 5: Dimensions for the EDEW model.

There are also three shape specific parameters par1, par2 and par3. They can be used to further influence the ridges at the electrode edges, e.g., a pulsewidth can be given for a rectangular shape.

Parameter	Default	Confined?
Confined droplet	no	
Surface tension	72 J/m^2	
Contact angle top	110 °	*
Distance to top	1 mm	*
Contact angle bottom	110 °	
Droplet volume	1 nl	
Actuation voltage	40 V	
Layer thickness	1 µm	
Rel. dielectric constant	3	
Number (#) of pads	2	
Pad size x	1 mm	
Pad size y	1.5 mm	
Pad gap	0.1 mm	
Spike length	0.1 mm	
Start position x	0.5 mm	
Parameter par1:		
Parameter par2:		
Parameter par3:		

Table 1: Parameters for EDEW model. Parameters with * only if “Confined” is checked.

It is possible to select from predefined shapes or from user defined ones (see fig. 6):

- Sinusoidal
- Rectangular
- Rectangular with a user definable pulse width. The pulse width is defined as ratio of the area occupied by electrode metal devided by the total area of the fine structure region and is specified as par1. A pulse width of 0.5 gives the standard rectangular shape.
- Triangular

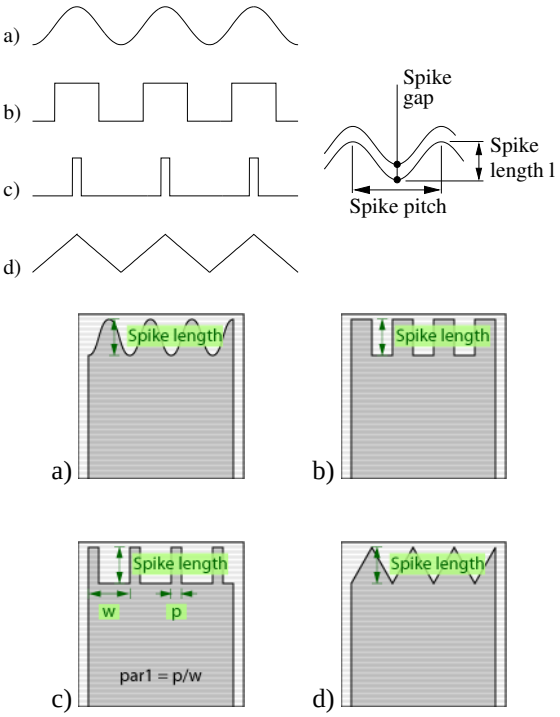

Figure 6: Predefined edge shapes and the corresponding icon in EDEW

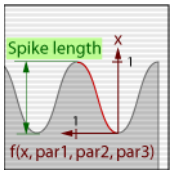

Figure 7: Icon for user defined shape in EDEW

For employing a user defined shape, two steps are necessary:

1. Find the function for $\gamma_{EW}(x)$ and normalize its support to the interval $[0,1]$ such that the normalized new function $f(x)$ fulfills $f(0) = 0$ and $f(1) = 1$. It should be noted that the shape is defined in x-direction (see example).

2. Find the integral $F(x) = \int_0^x f(\bar{x})\mathrm{d}\bar{x}$.

For example, suppose we want to model a sinusoidal shape. Since the electrode spikes extend to the x direction, we need the width of the sinus for each x position, which is given by the inverse of $sin(y)$. So we have $f(x) = \arcsin(2*x-1)/\pi + 0.5$, where the argument $2*x-1$ normalizes to $[0,1]$, while the $/\pi + 0.5$ normalizes the amplitude. Integrating this

function yields

$$F(x) = \frac{\pi x + 2\sqrt{(1-x)x} + (1-2x)\arcsin(1-2x)}{2\pi}$$

By entering the R.H.S. properly into the text field, the user defined shape can be used for the calculations. Since the arcsin is singular near ± 1 and the square root near 0, numerical problems can be avoided by scaling their arguments such that they lie in an interval $[\varepsilon_1, 1-\varepsilon_2]$, e.g. by using $1e-5+(1-2e-5)*(1-2x)$.

It is very easy to turn a user defined shape into a predefined one: The integrated function is simply copied from the text field of the EDEW program to a file called <*libraryDir*>/Simulations/SimSpikeShape/Shape<*name*>.fkt. It will appear as a new choice. If further a .png image with dimensions 128 pixel×128 pixel and filename <*libraryDir*>/Simulations/SimSpikeShape/Shape<*name*>.png is provided, an icon is shown to the right of the buttons.

The GUI for the *Surface Evolver* control window is shown in Fig. 8. The first row after the general part consists of checkboxes to apply voltages to the individual pads. The voltage applied depends on the current voltage settings, which can be specified at the next row in the "Voltage" field. When changing the voltage, it is important to press Enter on your keyboard once so that the change is propagated to the *Surface Evolver* process. When switching on a pad, the voltage is applied only to this pad; the others remain at their current voltage. To change all selected pads, press the button "-> to all sel.".

Before the simulation can be started, it must first be initialized by pressing the "Init" button. In this step the mesh is refined and the droplet is evolved to an equilibrium state. Then, pads can be activated. To simulate like in the 1DPath model, click into the "Perform # steps" field, enter a number of simulation steps to perform, and press Enter. One simulation step consists of several *Surface Evolver* iterations and mesh averaging and equiangulation steps which keep the dimensions of the mesh elements at about the same scale and prohibit large aspect ratios.

After every step, the step number, centroid x position of the droplet and the system energy are written to a datafile (temp. filename + "_t-centrxE.dat"). The (empty) timestamp file (temp. filename + "_starttime.dat") helps to determine the start of the simulation. The data files can be postprocessed to recover the energy gradient and therefore the force acting on the droplet. It is also possible to save an image after every step by checking the "Save PS" checkbox (temp. filename + "_time" + step number + ".ps").

The centroid position is calculated by evaluating the integral

$$x_c = \int_V x \mathrm{d}v \Big/ V \qquad (12)$$

over the complete volume V. This integral is implemented as surface integral by means of the divergence theorem.

The lower button row can be used to calculate the energy versus centroid position curve for different spike parameters like presented in [4]. To fix the centroid of the droplet to its current position, activate the "centroid fixed" checkbox. To set it to a specific position, enter a value to the adjacent "Fix to:" text field and press enter, the checkbox will then be activated automatically. To fix the centroid to a position a certain amount away from the current droplet position, find the equilibrium and record the current centroid and energy values to the datafile, use the "+" and "-" buttons; the amount for the droplet motion is entered in the text field in the middle of the buttons. The "++" and "- -" buttons will perform this operation as many times as specified at the "Perform # steps:" text field (This number – contrary to the "voltage" field – does not need to be confirmed with the "Enter" key; otherwise the steps would be performed without moving the centroid as in the 1DPath model).

Sample results are available in [4].

4 Summary and Conclusions

We presented the second version of EDEW, which implements a new model for the optimization of fine interdigital structures at the electrowetting electrode edges. The tool helps designing the actuation process by giving insight into the energy configuration at the start of the motion and thus the forces acting on the droplet. This helps to find structures compensating for different droplet sizes and enabling the motion in spite of local minima caused by contaminations.

The tool is available from [1].

References

[1] http://www.imtek.de/simulation/microprotein.

[2] Kenneth A. Brakke. *Surface Evolver Manual, Version 2.20*. Susquehanna University, Selinsgrove, PA 17870, August 2003.

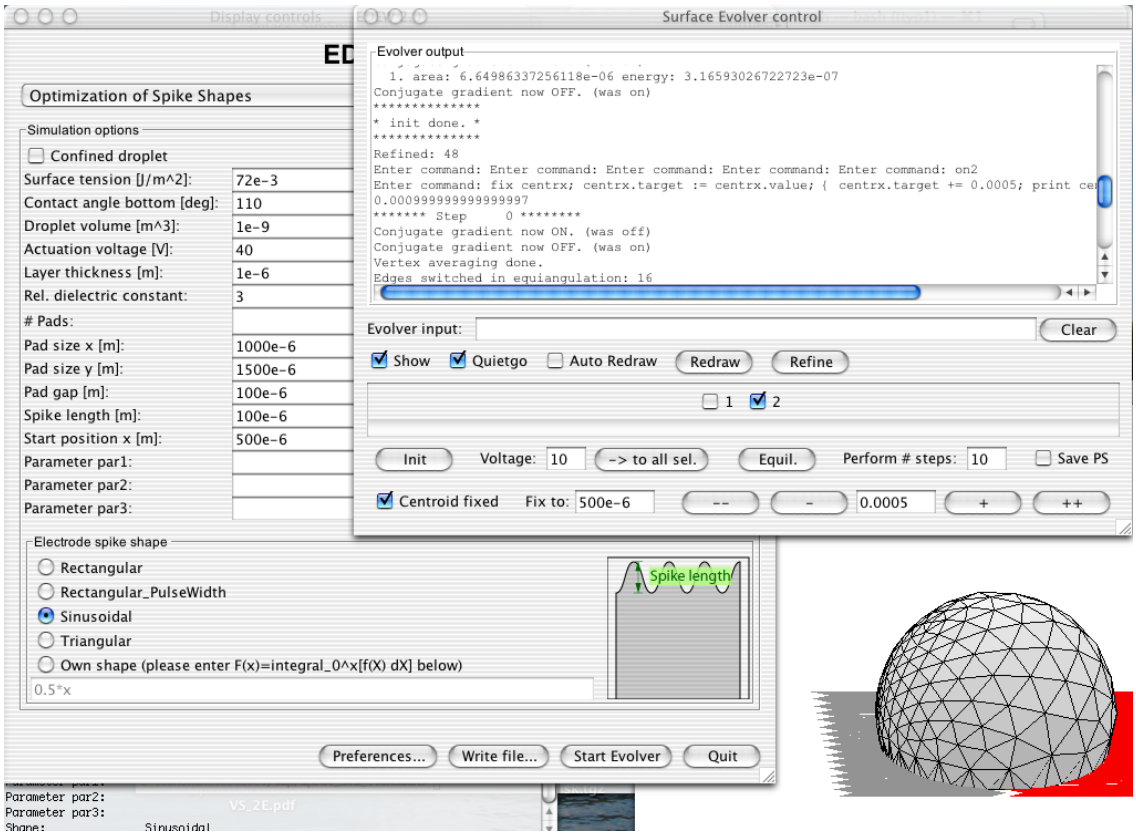

Figure 8: The GUI for the optimization tool.

[3] Jie Ding, Krishnendu Chakrabarty, and Richard B. Fair. Reconfigurable microfluidic system architecture based on two-dimensional electrowetting arrays. In *Proc. MSM 2001*, pages 181–185, Hilton Head Island, South Carolina, USA, March 19–21, 2001.

[4] Jan Lienemann, Andreas Greiner, and Jan G. Korvink. Electrode shapes for electrowetting arrays. In *Proc. Nanotech 2003*, volume 1, pages 94–97, Cambridge, USA, February 2003. NSTI.

[5] Jan Lienemann, Andreas Greiner, and Jan G. Korvink. EDEW version 1.0, a simulation tool for fluid handling by electrowetting effects. D 3.4: Report for EU project “Micrometer scale patterning of Protein and DNA-Chips”, IMTEK - Institute for Microsystem Technology, Albert Ludwig University Freiburg, Georges Köhler Allee 103, D-79110 Freiburg, Germany, January 2004.

[6] Michael G. Pollack, Richard B. Fair, and Alexander D. Shenderov. Electrowetting-based actuation of liquid droplets for microfluidic applications. *Applied Physics Letters*, 77(11):1725–1726, September 11, 2000.

[7] H. J. J. Verheijen and M. W. J. Prins. Reversible electrowetting and trapping of charge: model and experiments. *Langmuir*, 15(20):6616–6620, 1999.