M3P.104

CAPACITIVE DETECTION OF NANOLITER DROPLETS ON THE FLY - INVESTIGATION OF ELECTRIC FIELD DURING DROPLET FORMATION USING CFD-SIMULATION

K. Mutschler[1], A. Ernst[3], N. Paust[2], R. Zengerle[1,2] and P. Koltay[1,3]
[1]Laboratory for MEMS Applications, IMTEK, University of Freiburg, Germany
[2] HSG-IMIT - Institut für Mikro- und Informationstechnik, Villingen-Schwenningen, Germany
[3]BioFluidix GmbH, Georges-Köhler-Allee 106, 79110 Freiburg, Germany

ABSTRACT

Recently we presented a capacitive droplet sensor that enables the characterization of volume and velocity of dispensed nanoliter liquid droplets on the fly in a contact free manner [1]. In this work we perform a multi-physics simulation study to understand the physical effects behind the sensor signal. We combine a two-phase fluid dynamics model for droplet generation and droplet flight with an electrostatic model for analyzing the electric field distribution inside an open plate capacitor while the droplet is passing through. Beside droplet volume and velocity, also droplet tear-off point as well as droplet oscillations are reflected in the electric field distribution. The characteristic negative dip of the transient sensor signal which was observed in experiments can be explained by capacitive coupling of the liquid column with the sensor and is correctly reflected by the model. The detected changes in charge on the sensor capacitor, are in the range of 2 – 28 fC and correspond to droplet volumes in the range of $5\ \text{nl} < V_{drop} < 100\ \text{nl}$. This is in good agreement with experimental findings and analytical approximations.

KEYWORDS

Non-contact nanolitre dispensing, detection of nanolitre droplets, capacitive coupling, multi-physics simulation, CFD-Simulation

1. INTRODUCTION

The online process control of low volume dispensing systems is an important topic in the field of automated liquid handling. The increasingly smaller liquid quantities as well as the high throughput and regulatory requirements have created a need for specific non-contact sensors for droplet monitoring. The presented multi - disciplinary simulation was realized to study the performance of a capacitive measurement method presented in [1]. The basic principle of this method is based on the change in charge on a capacitor plate while a dispensed droplet passes through the capacitor's electric field. This change in charge is amplified to a readable voltage signal by the sensor electronics and provides information about the volume and velocity of the dispensed droplet. In this work a model for the physical system description was deduced and implemented by means of computational fluid dynamics (CFD). The established computational model includes a droplet generation process as well as the electrodes of the sensor capacitor that generate the electrical field. The main purpose of the simulations study performed with this model is to study the influence of different droplet parameters like volume, velocity and droplet shape on the resulting charge on the capacitor i.e. the capacity of the sensor.

2. SIMULATION MODEL

The implementation of the numerical simulation of the droplet generation process as well as the impact of these droplets on the electric field of a measurement capacitor was realised by the use of the commercial CFD software package CFD-ACE+ [2]. This software features the numerical simulation of the Navier-Stokes equations, the modeling of free liquid surfaces by the Volume of Fluid (VOF) method and solution of the Maxwell equations on the same computational grid.

The simulation domain i.e. the computational grid is shown in Figure 1. It consists of a short fluidic inlet representing the dispenser nozzle, the two capacitor plates and the bulk material representing the material that encloses the plate electrodes (see Figure 2).

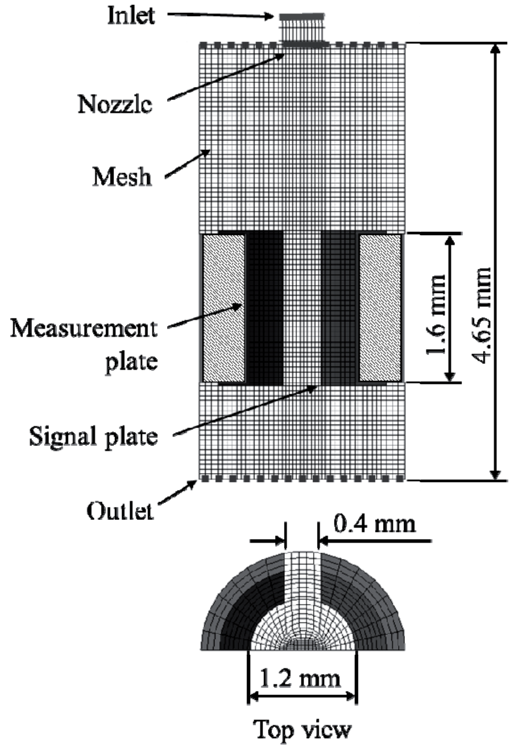

Figure 1: Computational domain showing the computation grid and boundary conditions (BC).

978-1-4577-0156-6/11/$26.00 ©2011 IEEE

An inlet at the top of the domain serves for implementation of a droplet ejection process from the nozzle by suitable fluidic boundary conditions (BC) at the inlet. The inlet was set to an electrical BC of U = 0V (GND) to implement the effect of capacitive coupling like described in more detail below. The change in charge induced by the droplet is monitored on the measurement plate of the capacitor using the integral output function on the whole surface. The signal plate is set to a constant potential of U = +10 V for all simulations. The simulations were realised considering the mirror symmetry of the problem that allows for reducing the simulation domain to half of the problem.

The droplet ejection process is implemented by the supply of a liquid flow via the inlet for a short period of time. Figure 2 presents the simulation results as an example showing the droplet passing through the capacitor plates as well as the electric field lines. The BC at the inlet was u = 2.5 m/s for t = 65 µs in this case. The presented simulation study includes variations of this BC to generate droplets of variable volume and velocity.

In order to understand the requirement for an electrical BC at the inlet and the effect of capacitive coupling, the experimental setup of the capacitive droplet sensor has to be considered in detail: The sensor signal determined by experiments previously [1] can be divided into two phases A and B corresponding to different electrical equivalent circuits as far as the system consisting of dispenser/droplet/capacitor is concerned.

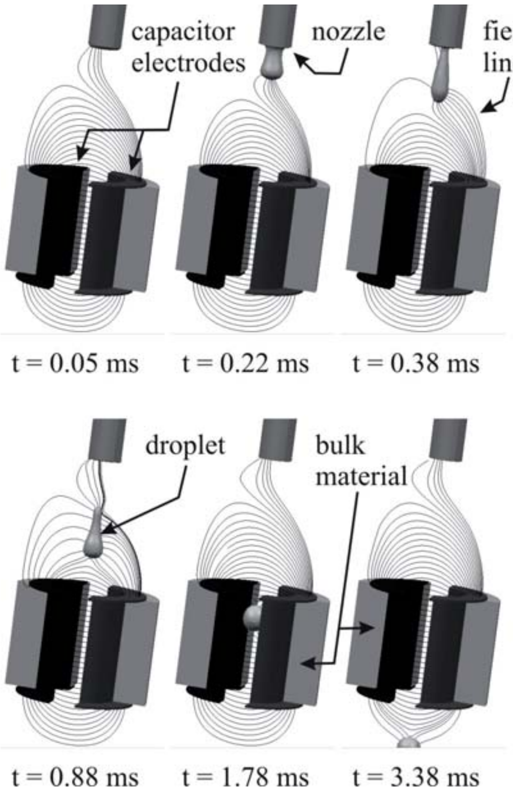

Figure 2: 3D Simulation of tear-off process of the droplet, including the electrical field lines while a droplet is passing the measurement capacitor

The two situations are depicted in Figure 2 by sketches of charge distribution and electrical field lines as well as by equivalent electrical circuits. While a droplet is protruding from the dispenser nozzle (phase A) it is still connected to the electrical GND potential of the dispenser until it has teared off. During this time the distance between liquid surface and capacitor plates is continuously reduced. Thus, an increasing capacitive coupling takes place because the GND potential serves as reference potential for the amplification circuitry, over the capacitors C_{wall} and C_{solid} (c.f. Figure 3), which represent the capacities of the nozzle wall and the adjacent solid material of the dispenser.

After droplet tear-off (phase B), entailing the cut-off of the electrical connection to the GND potential, the capacitive coupling suddenly stops. The droplet can now be considered as dielectric body which passes the electric field of the capacitor.

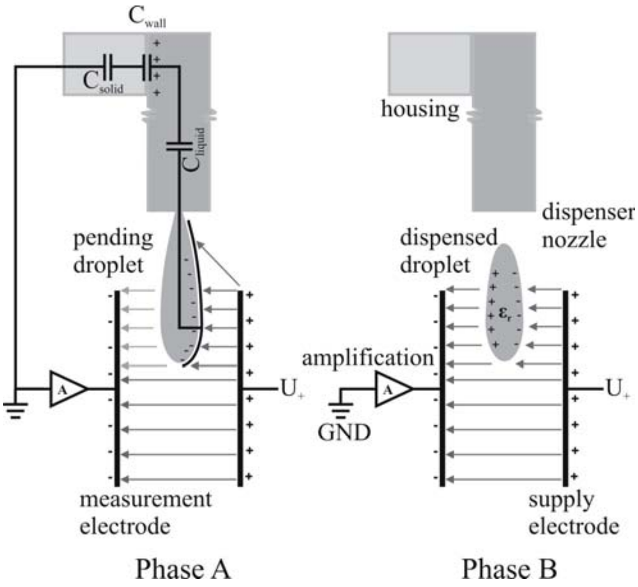

Figure 3: Electrical equivalent circuits representing the situation during droplet ejection (Phase A) a pending droplet is still connected to the electrical ground potential through the dispenser (Phase B) a droplet after tear-off acts as dielectric body.

3. SIMULATION RESULTS

To verify the presented model, first the situation in phase B was simulated and compared to analytical approximations for spherical droplets [3].

The spherical droplets with volumes of V = {5 to 100 nl} were realized in this case by spherical initial conditions for the VOF model and not by droplet ejection from the nozzle (i.e. BC u = 0 at inlet). Due to the absence of capacitive coupling in this case, the monitored change in charge on the measurement electrode resulted in a symmetric signal shape featuring a linear dependency of the signals amplitudes to the corresponding droplet volumes, see Figure 4.

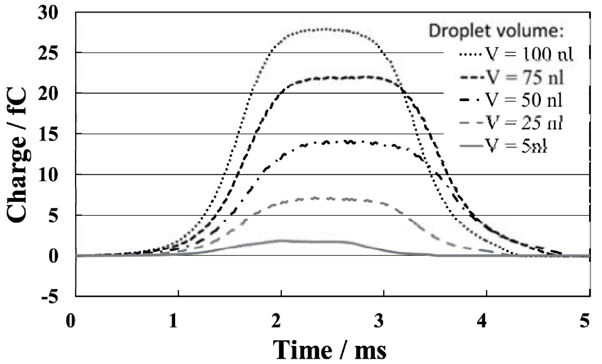

Figure 4: Spherically droplets with different volumes passing the capacitor with a velocity of u = 1 m/s causes a time dependent change of charge on the measurement plate.

To study the capacitive coupling effect that occurs in phase A pure water droplets of V = {17 to 33 nl} and velocities of u = {0.9 to 1.4 m/s} were generated by the adaption of the BC at the inlet. The change in charge first becomes negative until the droplet has detached from the nozzle and then increases to a volume dependent maximum value as shown in Figure 5.

The effect of capacitive coupling is also well illustrated by the electrical field lines determined from the simulations (cf. Figure 2). During growth of the pending droplet continuously more filed lines attach to the liquid surface (phase A). Due to that, fewer electrons have to be present on the measurement plate of the capacitor which yields a negative change of charge (cf. figure 5). After tear-off (phase B) the droplet acts as dielectric medium. This increases the capacity of the assembly and due to the constant voltage BC on the other plate more charges are stored on the measurement plate. This leads to an increase in the sensor signal while the droplet enters the capacitor. The established simulation model thus leads to the identical qualitative signal characteristics like presented in [1].

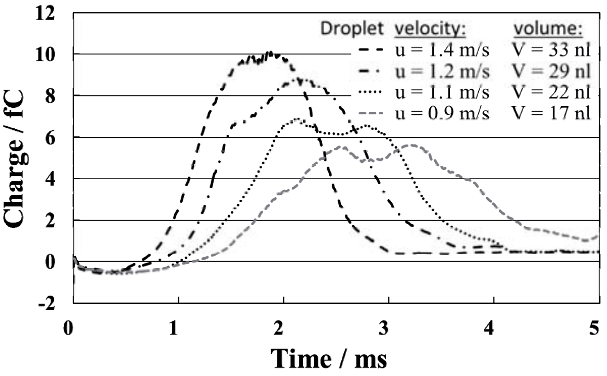

Figure 5: Change of charge caused by dispensed droplets of different volumes and velocities

A noticeable detail is the specific signal characteristics of some of the ejected droplets. In contrast to the signals generated by the spherical droplets (cf. Figure 4) multiple signal maxima can be observed for some of the droplets. Whereas the non-symmetric signal shape is induced by the effect of capacitive coupling, the multiple signal maxima are caused by droplet deformations during flight. The horizontal and vertical elongation of droplets as determined from the CFD simulation can clearly be related to maxima and minima of the sensor signal.

The correlation of the maximum signal peak to the corresponding droplet volume exhibits a clearly linear behaviour for both cases: for the dispensed droplets as well as of the spherical droplets. Also the linear fits shown in Figure 6 are in excellent agreement. This confirms that the maximum change in charge is a good quantitative measure for the droplet volume. It might only be disturbed by slight droplet oscillations discussed before.

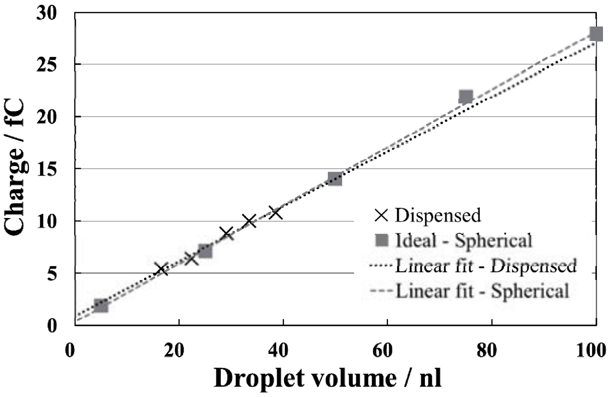

Figure 6: Droplet volume in correlation to the corresponding maximum change in charge for spherical and dispensed droplets

4. VALIDATION

The validation of the simulation results was realized by comparison to experimental results using the electronics and hardware presented in [1]. As first test a simulated signal for a droplet of 33 nl with a velocity of 1.4 m/s was qualitatively compared to an experimental signal generated by a droplet of equal properties. The result is shown in Figure 7 where the sensor signal is provided in units of [V] in comparison to the simulation results in [fC].

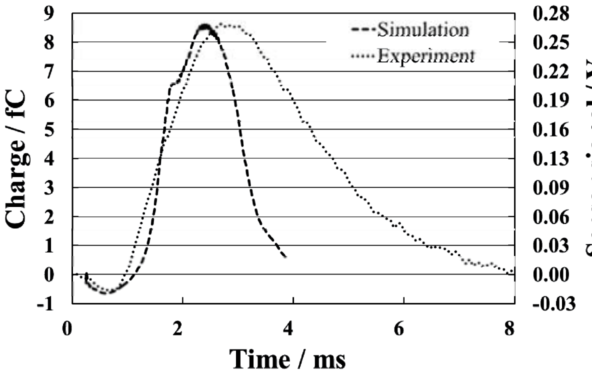

Figure 7: Quantitative correlation of experiment to CFD simulation in respect to a time dependent signal

In this respect, the quantitative agreement between simulation and experiment is excellent and also the slope of the rising edge looks similar. The decay of the falling edge examined by the experimentally gained signal is based on the applied measurement technique. By comparison of both peak signals a scaling factor of 32.7 fC/mV could be determined that can be used to relate simulations directly to experimental results. This scaling factor incorporates numerical errors from the simulation (e.g. resulting from the discretisation error of the grid) as well as the amplification factor of the electronic circuit used for experiments.

In order to improve the validity of the scaling factor, a linear fit was applied to the whole set of experimental data available to determine the most appropriate scaling over the whole range of volumes. The resulting mean scaling factor was determined to be 39.9 fC/mV with a determination coefficient of $R^2 = 0.9037$. The good agreement between experiment and data in Figure 8 reflects the fact the correlation between droplet volume and change of charge in the simulation model (cf. Figure 6), as well as the correlation between droplet volume and measured peak voltage in the experiments exhibits a very good linearity.

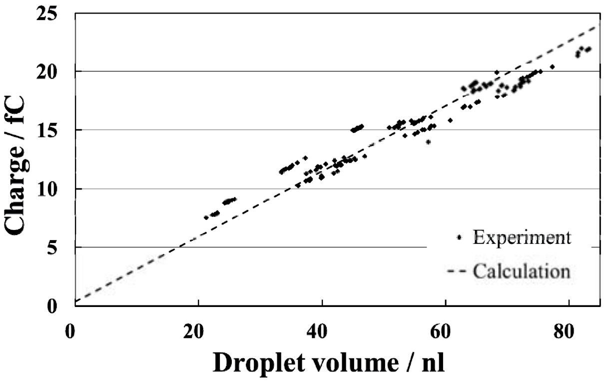

Figure 8: Comparison of experimentally measured signals which have been scaled with a scaling factor of 39.9 fC/mV to be correlated to the change in charge determined by simulation.

5. CONCLUSION

In summary, it can be concluded that the established model reflects the sensor performance with high accuracy and enables quantitative predictions regarding the change of charge caused by different droplet volumes. The simulation of the complete dispensing process leads to an improved understanding of the sensor's asymmetric signal characteristics, caused by the effect of capacitive coupling.

REFERENCES

[1] A. Ernst, W. Streule, N. Schmitt, R. Zengerle, P. Koltay, "A capacitive sensor for non-contact nanoliter droplet detection", Sensors and Actuators A 153 (2009) 57–63

[2] ESI-group, http://www.esi-group.com (2010)

[3] W. P. Winn, "An Electrostatic Theory for Instruments which Measure the Radii of Water Drops by Detecting a Change in Capacity Due to the Presence of a Drop", Journal of Applied Meteorology, vol. 7, no. 5, 1968

CONTACT

* K. Mutschler, tel: +49 761 203 7148;
klaus.mutschler@imtek.uni-freiburg.de

ACKNOLEDGEMENTS

The authors thank the Ministry of Science, Research and Art of the Federal State of Baden-Württemberg, Germany (Kap. 1499 Tit. Gr. 97) for financial support.