Principle behind droplet formation in microfluidic devices based on force balance

Prinzip der Tröpfchenbildung in mikrofluidischen Geräten basierend auf Kräftegleichgewicht

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Abstract — The work presents a numerical study of the mechanisms responsible for the droplet formation in a flow-focusing microfluidic device. The three stages of droplet formation in the dripping regime and the responsible forces for their formation were analysed. Surface tension $\Delta p\sigma$, the pressure difference between inside and outside of the droplet Δp_{int} and the shear stresses $\tau x_i x_j$ are taken into account as the main parameters responsible for droplet generation. The results show that the whole process is driven by a force disbalance. In the first stage of droplet formation, in which the droplet is growing in diameter, the surface tension is the domination force. The second stage however, in which the actuall neck squeezing and droplet detachment accur, can be described by the increase of the outside channel pressure on the surface. This analyse was confirmed by the development of the neck diameter of the forming bubble.

Zusammenfassung — Die Arbeit präsentiert eine numerische Studie der Mechanismen, die für die Tröpfchenbildung in einem mikrofluidischen Gerät verantwortlich sind. Analysiert wurden die drei Stadien der Tropfenbildung im sogenannten Dripping regime und die verantwortlichen Kräfte für ihre Bildung. Als hauptsächlich verantwortliche Parameter werden die Oberflächenspannung $\Delta p\sigma$, die Druckdifferenz zwischen dem Inneren und Äußeren des Tropfens Δp_{int} und die Schubspannungen $\tau x_i x_j$ berücksichtigt. Die Ergebnisse zeigen, dass der gesamte Prozess durch ein Kräfteungleichgewicht angetrieben wird. In der ersten Stufe der Tröpfchenbildung, in der der Tröpfchendurchmesser zunimmt, ist die Oberflächenspannung die dominierende Kraft. Die zweite Stufe jedoch, in der die eigentliche Halsquetschung und Tropfenablösung erfolgt, lässt sich durch die Erhöhung des Außenkanaldrucks auf der Oberfläche beschreiben. Diese Analyse wurde durch die Entwicklung des Halsdurchmessers der sich bildenden Blase bestätigt.

I. INTRO DUCTION

In recent years, microfluidics developed as a novel ap- proach for solving numerous questions arising from the re- alization of different biological, chemical and medical pro- cesses [citeee]. Having fluidic channels with dimensions smaller than a millimetre, i.e. micro-scale, microfluidic de- vices can significantly reduce reaction times and energy consumption for a certain process [citeee]. The extremely low Reynolds number result in strictly laminar flow condi- tions in the channels and thus providing an absolute con- trol over fluidic flows supply in different chip regions. With well-defined microenvironments which mimic the habitants of living cells, microfluidic devices enable the successful in- tegration and replacement of expensive and demanding lab- oratory equipment in these small chips [citeee]. An emerg- ing microfluidic technology based on hydrodynamics princi- ples, utilized as a precise and reliable tool for the automati- zation of assays is the so-called droplet-based microfluidics. Encapsulating different chemical or biological compounds into individual picolitre-droplets, allows the isolation of the occurring reactions from their surroundings, avoiding un- wanted mixing and disruption of fragile compounds. These small microreactors allow a cheap and easily implementable method for a broad range of processes including cell ly- sis [citeee], antibiotics susceptibility screening [cite], digital polymerase chain reaction (PCR) [citeee] etc. The massive number of possible independent reactions in the droplets adds also a high parallelization factor into the conducted experiments. Three main geometry types for droplet gen- eration are widely utilized in the microfluidic world: co- flow of dispersed and continuous phases, cross-flow in T- junction and flow-focusing (Figure 1).

All of these potential advantages come at the price of a high hydrodynamic complexity of the microfluidic sys- tem due to the dynamic interaction between forces acting on the interface of the two phases. One of the phenom- ena characterizing these multiphase microfluidic flows and their complexity is the occurring of different flow regimes depending on the systems boundary conditions.

For the design of microfluidic devices operating in droplet flow regime, prior knowledge of droplet size, shape, forma- tion frequency or pressure drop are essential.

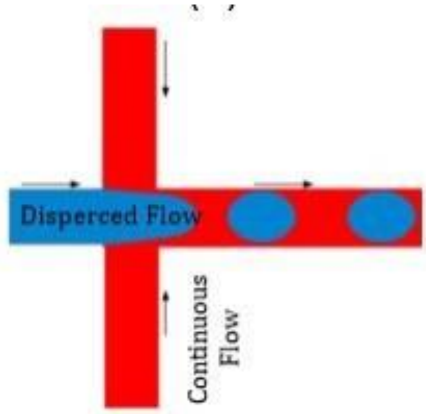

Fig. 1. Flow-focusing microfluidical setup for the droplet generation.

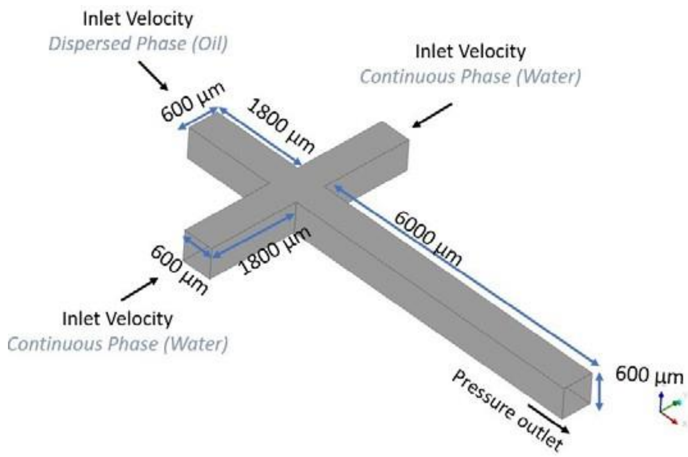

Fig. 2. Model geometry, dimensions and boundary conditions.

Even though the principles of droplet formation are well understood, there is, in our opinion still a lack of detailed explanation of the influence of the responsible parameters during the process. Although there are plenty of existing theoretical/experimental works for the flow-focusing geom-etry, there is a need to fill the gap between the limitations of the experimental measurements and theoretical assump- tions, simplifying the problem. A good way to collect in advance this information for a new setup is by utilizing a predictive CFD (Computational Fluid Dynamics) model and interpreting the influences of some fluid properties on the droplet breakup. Few numerical studies on droplet-based microfluidics were carried out in the past years uti-lizing different numerical techniques (for example level set (LS) [11] or Lattice Boltzmann method (LBM) [12-13]). In this article we investigate numerically the droplet cause of bubble formation in a flow-focusing microfluidic chan-nel by utilizing the volume of fluid (VOF) method. The three main pressures responsible for droplet formation are analysed. The mechanism behind droplet formation is de-scribed through a pressure (dis) balance.

II. Mathematical model, geometrical setup and boundary conditions

In the present study three-dimensional simulations of droplet formation in a flow-focusing geometry are carried out utillizing a finite volume method based CFD solver from ANSYS Fluent 21. The two immiscible fluids, water and oil as well as their interface, are modelled by the Vol-ume of fluid (VOF) method. A phase fraction parameter, α, is used to indicate the presence of each phase at every location of the domain. Fluid properties such as viscosity and density are smoothed and the surface tension force is distributed near the interface as a body force in the Navier-Stokes equations. With this, the system of coupled partial differential equation consists of the continuity equation (1) the momentum balance equation (2), and the phase frac-tion equation for α (3) becomes [14]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho U = 0 \tag{1}$$

$$\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U U) = -\nabla p + \nabla \cdot (\mu [\nabla U + \nabla U^T]) + F_s \tag{2}$$

$$\frac{\partial \rho\alpha}{\partial t} + \nabla \cdot \rho\alpha U = 0 \tag{3}$$

In the equations above, U is the velocity vector field, p is the pressure field and μ the viscosity of the fluid. F s rep-resents the surface tension force, which can be calculated as follows:

$$F_s = \sigma \cdot \kappa(\nabla\alpha) = \sigma \cdot \nabla \cdot \left(\frac{\nabla \alpha}{|\nabla\alpha|} \right) \cdot (\nabla\alpha) \tag{4}$$

κ describes the curvature of the interface between the fluids. Only one such transport equation (3) needs to be solved since the volume fraction of the other phase can be inferred from the constraint:

$$\alpha_c + \alpha_d = 1 \tag{5}$$

where the index ‘c’ stands for continuous and ‘d’ for dis-persed phase. The continuous phase (water) is introduced through the two side channels and the dispersed phase (oil: octane +2,5 % SPAN 80) is entered from the main (cen-tral) channel. The information about the fluid properties is obtained from the experimental results of Yao et al. [15]. All the measurements were conducted under atmospheric pressure conditions and room temperature.

TABLE I. Summary of the fluid properties

Fluid	Density ρ - [kg m^{-3}]	Viscosity μ - [mPa s]
Water	1004,4	3,32
Oil	689,9	0,53

For the boundary conditions, constant velocity block profile was utilized for both continuous and dispersed phase inlets. We set α = 1 at the inlet of the dispersed phase and α = 0 at the inlet of the continuous phase. No slip boundary conditions are applied at the walls. Pressure boundary was specified at the outlet of the main channel. The inlet veloc- ities of both fluids were kept equal at ud = 0,009 25 m s^{-1} for the simulated case. The surface tension coeficient be- tween the two fluids is σ = 5,04 mN m^{-1}. The lengths and dimensions of the square cross-section, the inlet and outlet channels are presented in Figure 2.

III. CONSIDERED FORCES

In this section we discribe the considered pressures (forces) on the interface between the two fluids, respon- sible for the droplet generation. The main pressure, which acts in the negative x-direction (trying to pull back the forming bubble) is the surface tension:

$$\Delta p_\sigma = \sigma/\kappa \qquad (6)$$

In our analysis the value of κ are directly taken from Equation 4 precisely from the Fluent Solver, which is di- rectly accessible in the post processing stage. When the fluids are at rest and for perfect geometries of the interface (sphere, cylinder etc.) this pressure force is balanced by the pressure difference through the interface:

$$\Delta p_{int} = p_i - p_o \qquad (7)$$

In our case pi is always defined as the static pressure in- side the droplet, whereas po is the static pressure of the sur- rounding continuous phase, entering the domain through the two side channels.

When the two fluids move in the microchannel, the above-mentioned forces will deviate from these theoretical values. At this point it is important to take into account the influence of the forces acting in tangential direction of a fluid element. For an isotropic Newtonian fluid, the viscous stress tensor can be defined as follows:

$$\tau_{x_i x_j} = \mu_c \cdot \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \qquad (8)$$

In the present work we decided to do the analysis using local values available from the computations. Definition of forces would require to define also the exact areas these forces work on which would present rather global (as op- posed to local) quantities. Most often the local parameters available from the numerical method are in terms of nor- mal and tangential stresses with dimension Pa. That is the reason to define also Δpσ.

IV. RESULTS

In this work only the so-called dripping regime is dis-cussed. The latter is characterised by bigger emulsions and relative low detachment frequencie, as shown in a work [1]. The process of droplet detachment is marked by three main stages, as visible on the normalized neck (DD) of the advancing oil front, as shown in Figure 3. First, the so-called filling stage is observed, where the dispersed phase is injected into the cross section for a time of tfill. The diameter of the forming bubble becomes larger than the width of the channel. At some point the dispersed flow almost blocks the flow from the side channels, causing the upstream pressure to increase, see Figure 1b. In a second stage starting from t =0,109 s the diameter of the droplet starts to reduce, becoming smaller than the width of the channel, as shown for t = 119 s. This stage is known as necking stage. At the beginning of this second phase the pressure in the side channel continuous increasing until t = 0,123 s. One can see that the total increase in the side chan-nels pressure is above 17 Pa, which obviously will result in a pressure increase at the interface. In the last pinch-off stage, droplet detaching occurs, marked in Figure 3 by the black arrow.

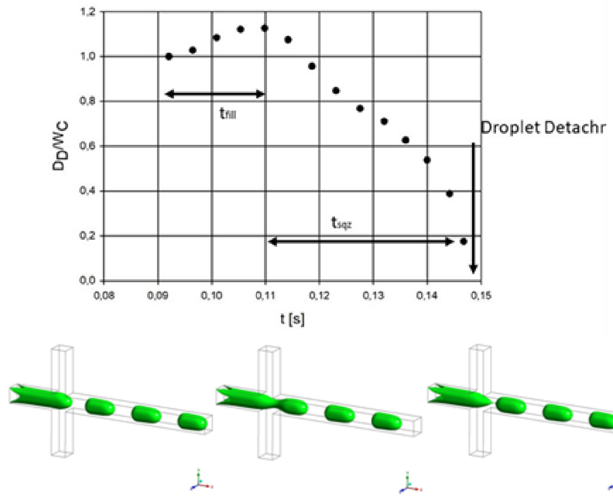

Fig. 3. The nondimensional diameter of the forming droplet as a function time and the iso-surfaces of the three stages (filling on the left, neck squeezing in the middle and droplet detachment on the right).

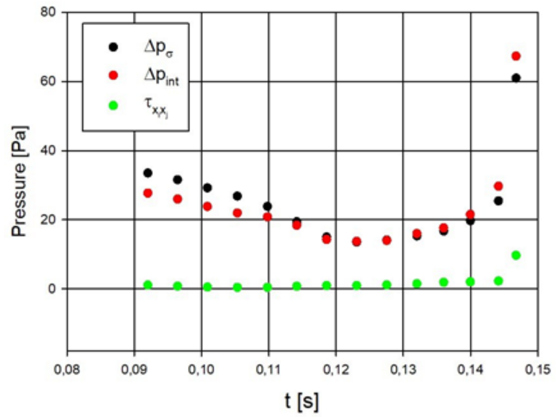

Fig. 4. Time development of the pressures, responsible for the droplet detachment.

This whole process characterizing the droplet formation in the dripping regime can be explained by the develop-ment of the pressure force caused by surface tension and the pressure difference through the interface, described in the previous section. Figure 4 shows the time development of the three pressures on the neck of the oil front. The effect of the shear stresses here is rather negligable. Com-paring Figures 3 and 4 clearly shows that the whole process of droplet dormation is characterized by a disbalance be-tween the interposing pressures. The domination of Δpσ on the growing bubble at the beginning determines the growth in diameter of the propagating front. With time the two pressures reach a point of balance (for t around 0,0095 s), characterizing the end of this filling stage. From this mo-ment on Δpint begins to dominate over Δpσ, giving start of the squeezing of the droplet neck.

As visible from Figure 5 the main cause for the starting decrease of the pressure difference between inside and outside of the bubble is attributed mostly to the increase in the pressure outside the bubble (at α = 0,02). The latter is atributed to the flow stagnation in the side chanels due to the propagation of the oil front. In the second part of the process one can see that the pressure in the side channel (outside the oil front) begins to decrease rapidly. This is atributed to the fact that the squeezing of the droplet neck is linked to a pressure release.

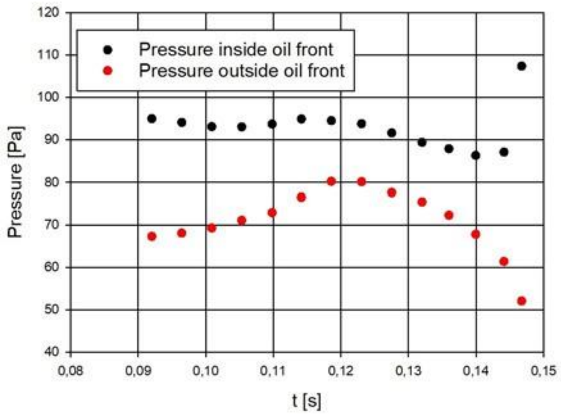

Fig. 5. Time development of the pressures inside and outside of the developing front of the disperced face.

V. CONCLUSION

In this work the droplet generation in a flow-focusing microfluidic device has been investigated. The continuous phase (water) was introduced through the two side chan- nels and the dispersed phase (oil: octane +2,5 % SPAN 80) was entered from the main channel. For all simulations the VOF method was utilized. For the first time in the liter- ature the responsible pressures for the droplet generation were described numerically. The surface tension, pressure difference between inside and outside of the forming bub- ble, and the shear stresses were considered for this analysis. It was shown that at the first stage of droplet generation, also known as filling stage, the surface tension dominates the two other forces, trying to minimize the area between the two fluids and thus increasing the diameter of the form- ing bubble. At some point the pressures in the two side channels increase, due to the stagnation of fluid flow there, thus increasing the influence of the outer pressures on the surface of the forming droplet. This increase of Δp in t over- comes the surface tension, giving begin to the second stage of droplet formation. This necking stage fininshes with the final droplet detachment. The effect of the shear stresses on the surface were rather neglegable, compared to the two other forces. As a whole, the present study shows that the VOF method is also a reliable technique for the simula tion and prediction of droplet generation in a flow-focusing channels. It will allow the future study of other diverse setups and various fluid combinations.

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