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Theoretical evaluation of the dispensing well plate method (DWP part II)

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Abstract

The "dispensing well plate" (DWP^{TM}) method is a technique to deliver fluidic jets or droplets with volumes of several nanoliters contact free to targets like micro well plates or slides. A cheap and simple pneumatic actuation mechanism allows for the simultaneous delivery of a large number of different liquids. In this paper the dispensing dynamics of a DWP-type nanodispenser is studied theoretically. The device is modelled using computational fluid dynamics (CFD) simulations which are benchmarked to experimental data. Furthermore an analytical discussion is presented providing some insight into the dispensing dynamics. Based on these modelling approaches the dispensing process is studied in detail. Influence of system parameters like driving pressure, nozzle size, channel layout etc. on the jet formation and dispensed volume are quantified and design rules are given to improve the performance.

Keywords: Droplet dispensing; Jets; CFD-simulation; Microfluidics

1. Introduction

The massive parallel dispensing of nanoliter volumes of liquid reagents is an essential enabling technology in many modern biotechnical applications and within pharmaceutical research [1–4]. The dispensing well plate (DWP) method studied in this paper from a theoretical point of view is a method for the simultaneous delivery of chemical reagents into micro well plates or onto flat substrates. A single dispensing unit of a DWP-type dispenser consists of three basic elements: a reservoir, a connection channel and a nozzle chamber as depicted in Fig. 1a. Many individual dispensing units can be arranged very closely to form an array like demonstrated in [5]. The working principle of the dispenser is then as follows: Each reservoir is filled with a specific liquid which is drawn by capillary forces via the connection channel into the nozzle chamber (Fig. 1b and c). By applying a pressure pulse to the whole upper surface of the DWP, the liquid contained in the nozzle chamber is driven out completely (Fig. 1d and e). Because reservoir and nozzle channel are exposed to the same pressure no pressure driven flow occurs within the connection channel. Thus essentially the volume confined in the nozzle chamber is dispensed. After switching off the driving pressure, the nozzles refill again from the reservoirs by capillary forces (Fig. 1f)). The DWP method is described in detail in [5] along with fabrication requirements and experimental results obtained with various prototype devices. In the remainder of this paper the working principle of the DWP method is analysed from a theoretical point of view.

2. CFD modelling

The computational fluid dynamic (CFD) simulations of the dispensing process presented in this section have been carried out using the software package ACE+ from CFDRC [6]. The software uses the finite volume method (FVM) [7] for solving the Navier–Stokes equations and applies the volume of fluid (VOF) technique [8] to simulate the free surface. The aim of the simulations was to study the fluid flow within the system as well as the jet ejection. These quantities are very difficult to access by experimental techniques, but contain essential information about the dynamical behaviour.

2.1. Model setup

For the CFD-simulations a full 3D model of one DWP dispensing unit has been set up making use of the symmetry

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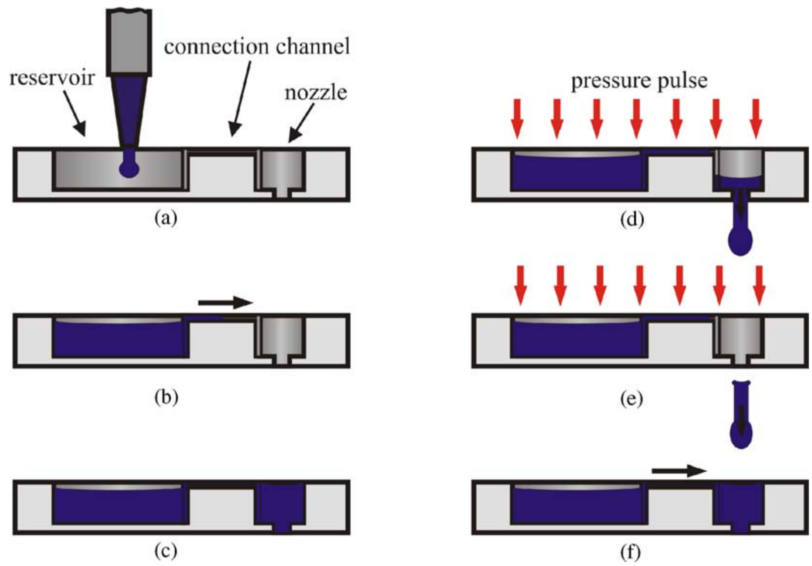

Fig. 1. Schematic illustration of the DWP working principle.

along the connection channel as displayed in Fig. 2a. To reduce the number of grid elements—hence computing time—the reservoir was not included in the model. This is justified because the flow within the reservoir or out of the reservoir is negligible compared to the flow through the nozzle. Thus the fluidic CFD model consists of the elements connection channel, nozzle chamber and orifice. Additionally a control volume for visualization of the ejected jet has been added. Initially the whole fluidic part was set to be filled completely with dimethylsulfoxide (DMSO)—a solvent commonly used in pharmaceutical research. The control volume was filled with air.

The boundary conditions applied to the geometry are visualized in Fig. 2: The upper surface and the distant end of the connection channel are defined as inlets and a pressure boundary condition is applied there to drive the ejection (arrows in Fig. 2a). The incoming fluid at the top inlet surface is set to supply air, while the inlet at the end of the connection channels is set to provide DMSO. The surfaces of the control volume are defined as outlets and a constant pressure boundary condition ($P = 0$) is applied there. All other surfaces are wall boundary conditions with a contact angle of $\theta = 35^{\circ}$ inside the connection channel and nozzle chamber and $\theta = 110^{\circ}$ on the nozzle plate (i.e. the surface

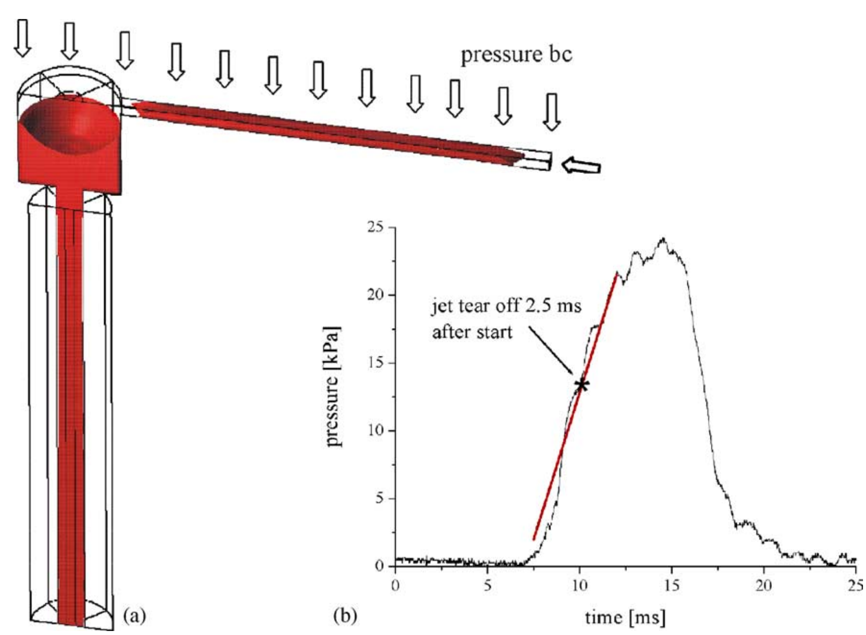

Fig. 2. (a) Grid model and boundary conditions used for CFD-simulation ($d_{nc} = 385\,\mu m$, $d_o = 100\,\mu m$, $l_c = 1800\,\mu m$); (b) measured pressure history of a DWP prototype device and applied pressure run for CFD-simulation (straight line).

surrounding the orifice). The contact angle on the nozzle plate was determined by measurements using DWP prototypes described in [5]. These prototypes were preconditioned by a silane treatment to enhance the contact angle.

The pressure history applied to the inlets was measured on the actuation device used in [5] to perform experiments. Since it was not possible to run the CFD-software with the measured pressure profile, the pressure history has been approximated within the simulations by a straight line like depicted in Fig. 2b. Before this pressure history could be applied the equilibrium positions of the menisci in the nozzle chamber and the orifice had to be determined in a separate simulation. This is necessary, because the liquid volume contained in the nozzle chamber is smaller than its geometrical volume. The actual liquid volume contained in the nozzle chamber depends on the curvature of the menisci at both ends as can be seen in Fig. 4 at $t = 0$. To determine this equilibrium situation a separate simulation run was performed beforehand where all pressure boundary conditions were set to zero and the simulation was run for 0.19 μs until the menisci had relaxed to a stable position. The result of this simulation ($t = 0$ in Fig. 4) was then taken as initial condition for the transient simulation and the linear pressure history was applied as described before.

The presented CFD model consists of a structured hexahedral grid of 65 923 cells. The minimal grid distance of 3 μm occurs in radial direction along the middle axis of the 100 μm wide orifice. At this location the grid is fine enough to resolve all features of the jet. Typically only 8–12 computational cells are claimed to be sufficient to resolve the flow profile within a channel respectively jet. Due to the size of the CFD model and the long computing times caused by the VOF method a thorough grid dependence study could not be performed. Instead the model was validated by comparison with experiment as described in the next section.

2.2. Validation

In order to validate the CFD model the jet ejection has been recorded using stroboscopic imaging: A real 96-channel DWP-chip with identical dimensions has been filled with DMSO and was actuated with the prototype system described in [5]. Snapshots of the thereby ejected jet are displayed in Fig. 3 for various time intervals after opening of the pneumatic valves. Since it is not possible to determine an exact value of the beginning of the pressure run (cf. Fig. 2b) the time stamp of the photographs displayed in Fig. 3 are furnished with an estimated error of ±0.1 ms. The small droplets visible in the experiment close to the orifice are remains of the spray generated after jet tear off, which will be discussed in detail in the last section.

For comparison with the stroboscopic photographs also snapshots of the CFD-simulation are displayed in Fig. 3 showing the ejected jet. Since the graphics are drawn to scale with respect to the photographs a direct comparison of the pictures is possible. Obviously the correspondence between simulation and measurement is reasonable. The ejection speed as well as the qualitative jet shape are correctly reproduced. Also the jet duration is the same within the estimated error limit. Minor deviations like the larger head of the jet predicted by the simulations might be explained by the slightly different pressure pulse or by deviating material data: Due to the fact that DMSO is hygroscopic it might has changed density and viscosity slightly during the measurements. Also surface properties might have changed over time, since the applied silane coatings are not very stable and the contact angle has an essential influence on the jet shape.

2.3. Dynamics of the ejection process and proof of the DWP principle

In the previous section the externally visible part of the dispensing process, the jet ejection, has been discussed. However, of greater interest is the dynamics inside the dispenser which is difficult to access by experiments. The simulation displayed in Fig. 4 shows the dynamics of the liquid contained in the nozzle chamber: The applied pressure drives out this liquid creating a jet with an outlet speed of up to 4 m/s and a moving meniscus inside the channel. The meniscus moves towards the orifice due to depletion of the nozzle

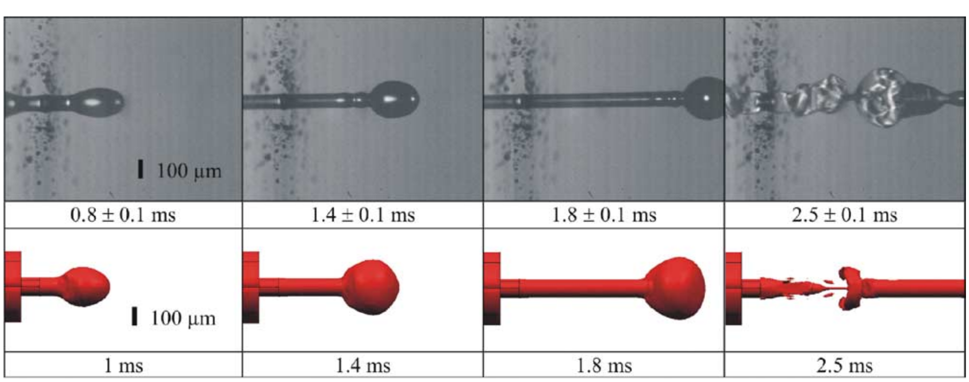

Fig. 3. Sequence of the jet ejection obtained from stroboscopic measurements (top) and CFD-simulations respectively (bottom). Both picture series are drawn to scale (see scale in the first picture).

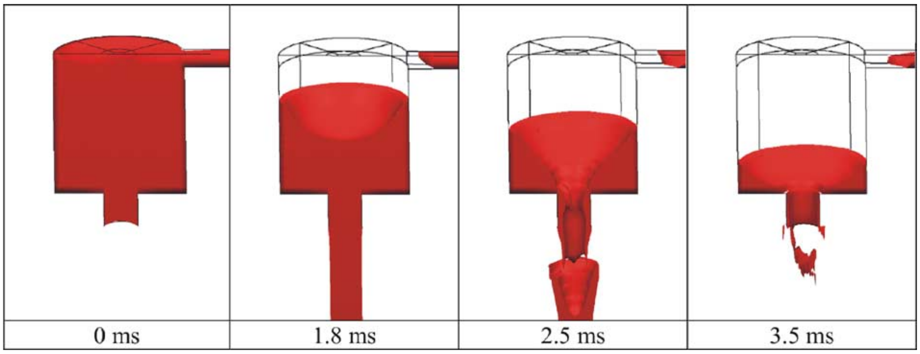

Fig. 4. Depletion of the nozzle chamber during dispensing simulated by CFD.

chamber. After jet tear off (2.5 ms after start of the dispensing) a certain rest volume remains in the nozzle chamber. When the meniscus breaks through the orifice a high speed air flow of about 70 m/s sets in which rapidly increases up to 180 m/s. This is due to the fact that the density of air is approximately 1000 times smaller than the one of DMSO. By this air flow the rest volume is continuously driven out by the Venturi-effect creating a spray. This spraying has also been observed in experiments and will be discussed later on in detail. Except for the spraying, the dispensing indeed proceeds like anticipated in Fig. 1.

In order to prove that at maximum only the volume contained in the nozzle chamber is dispensed and no substantial flow through the connection channel occurs during dispensing, the flow through the connection channel as well as through the orifice have to be quantified. The total integral flow through the nozzle (i.e. the total ejected volume up to a certain point in time) as well as the total integral flow through the connection channel are displayed in Fig. 5 as a function of time. It can be seen that the total integral flow through the nozzle increases quite linearly after the jet has formed and reaches a plateau after jet tear off. The integral flow through the connection channel during that time is one or two orders of magnitude smaller if the layout of the DWP is properly chosen (see Section 4 for a detailed discussion) and thus negligible. In the considered case less than 0.2 nL are provided through the channel, while the dispensed volume reaches roughly 43 nL.

Due to the fact, that the integral flow through the nozzle reaches a plateau after jet tear off the duration of the pressure pulse is not critical with respect to the dosage volume. Even if the pulse stays on after jet tear off the dosage volume hardly increases, because the flow provided by the spray decreases rapidly. The plateau signifying the dispensed volume stays stable even if the pressure head is changed. As can be seen in Fig. 5b) the pressure head influences only the slope of the curve and thus the jet duration, but hardly the saturation value and therefore the dispensed volume.

However, in any case the geometrical volume of the nozzle chamber (displayed as dashed line in Fig. 5) is greater than the dispensed volume. This has two reasons: First, the initially contained liquid volume is smaller than the geometrical volume of the nozzle chamber as discussed before. Secondly a certain fraction of the liquid might remain in the nozzle channel as visible in Fig. 4. This rest volume is very difficult to predict and gives rise to the spray effect. Therefore the main optimisation effort has to concern the reduction of the rest volume. One simple measure to reduce it slightly is to make the pressure head as small as possible. As can be deduced from Fig. 5b), the smaller the slope of the dosed volume the more liquid is already ejected when the jet tears off. Less liquid remains in the nozzle channel and can be transported by the spray.

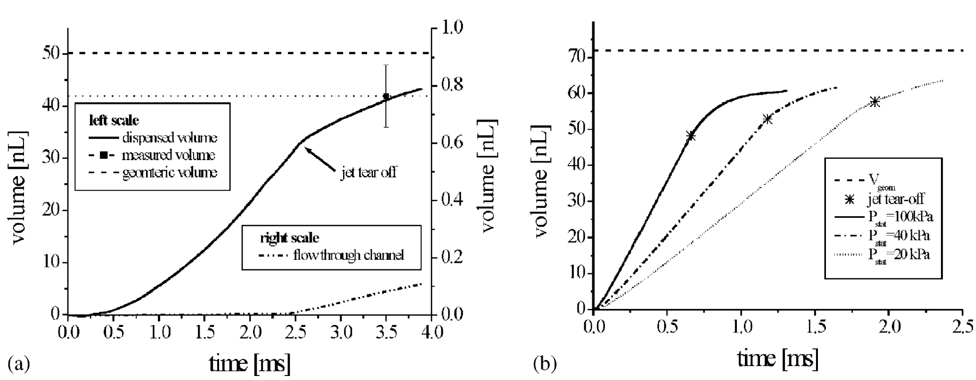

Fig. 5. Dispensed volume as a function of time. (a) As simulated with the geometry displayed in Fig. 2. (b) Simulation of a dispenser according to Table 1 driven by a constant pressure P_{stat}.

Table 1
Typical system parameters used for computing the data displayed in Figs. 7 and 8

b_c (μm)	h_c (μm)	l_c (μm)	d_{nc} (μm)	h_{nc} (μm)	d_o (μm)	h_o (μm)	η (mPa s)	θ (°)	σ (N/m)	ρ (kg/m^3)	P_{stat} (kPa)
140	115	4000	300	1000	100	100	1.022	15	0.0725	1	20

3. Parameter studies

In order to study the dispensing dynamics as a function of the various system parameters a series of CFD-simulations was performed using the presented model. A typical device has been chosen like sketched in Fig. 6 with the system parameters listed in Table 1. A connection channel of rectangular cross section $h_c \times b_c$ and length l_c is assumed. In contrast to the CFD model discussed before the upper side of the channel is considered now as wall with a no slip boundary condition (i.e. the connection channel is considered to be sealed from the top). The nozzle chamber has a circular cross section with the radii given in Fig. 6 and Table 1. To simplify the calculation the driving pressure (denoted by P_{stat}) is considered to be constant.

Since the CFD-simulations are extremely time consuming—a typical dispensing process like shown in Fig. 4 requires several days computation time on a state of the art PC—a faster and simpler modelling approach would be beneficial for engineering purposes. Such a model can also provide more insight into the dependence of the dosage volume on the various model parameters. Therefore we have derived analytical approximations to describe the flow which are compared subsequently to full CFD-simulations.

3.1. Analytical approximation

As we have seen, the dispensing dynamics of the DWP device is quite complex. Nevertheless, the flow through the orifice respectively nozzle chamber can be considered as quite constant during the major part of the dispensing time before the jet tears off. Especially if a constant pressure pulse is applied (cf. Fig. 5b). Thus the flow through the orifice can be very well approximated by a stationary flow. The simplest way to do so is to neglect all viscous and capillary forces and to model the flow through the nozzle chamber ϕ_{nc} simply by Toricelli's formula [9].

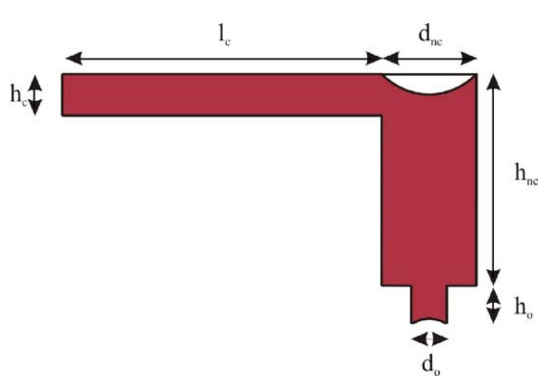

Fig. 6. Sketch of the considered DWP dispensing unit and corresponding parameters.

$$\phi_{nc} \approx A_o \sqrt{\frac{2P_{stat}}{\rho}} \tag{1}$$

where P_{stat} is the stationary driving pressure, ρ the density and A_o denotes the cross sectional area of the orifice. To improve this approximation the specific shape of the nozzle can be accounted for like commonly done in fluidic engineering and described in detail in [9]. A dimensionless number μ is introduced characterizing the nozzle geometry. For all presented calculations μ has been fixed to 0.82, which corresponds to a cylindrical orifice with aspect ratio $h_o/d_o = 1$. Thus the approximation for ϕ_{nc} reads:

$$\phi_{nc} \approx \mu A_o \sqrt{\frac{2P_{stat}}{\rho}} \tag{2}$$

Due to the fact that viscous dissipation and capillary forces tend to reduce the flow in reality, Eqs. (1) and (2) yield upper estimates of the mean flow encountered in the real device.

In order to assess the significance of liquid supply from the reservoir, the flow occurring in the nozzle chamber needs to be compared to the flow through the connection channel ϕ_c. The dispensed volume can be considered to be limited by the geometrical volume of the nozzle chamber only if $\phi_{nc} \gg \phi_c$. In this case no significant flow from the reservoir takes place during the dispensing and not more liquid than initially contained in the nozzle chamber is dispensed. To obtain an estimate if this condition is indeed fulfilled, the flow through the connection channel can be calculated as follows: Since the connection channel is much smaller and longer than the nozzle chamber viscous dissipation cannot be neglected. It can be modelled by a constant fluidic resistance R_c of the connection channel. For example for the case of an open channel (like studied in the previous section) a formula given in [10] can be applied. For the case of a closed rectangular channel the well known formula applies [11]:

$$R_c = 8\eta \frac{l_c (h_c b_c)^2}{h_c^3 b_c^3} \tag{3}$$

The flow through the connection channel is determined by this resistance and the pressure difference between both of its ends.

$$\phi_c = \frac{\Delta P}{R_c} \tag{4}$$

The pressure difference ΔP can be considered as independent of the driving pressure P_{stat} which is applied equally to both ends of the channel. The difference is essentially caused by the capillary pressure P_{cap} created by the meniscus residing in the nozzle chamber. Neglecting surface forces in the reservoir and dynamical effects at the junction for the moment, the capillary pressure in the equilibrium situation reads

$$P_{cap} = \frac{4\sigma}{d_{nc}} \cos\theta \tag{5}$$

where σ is the surface tension and θ the contact angle.

Setting $\Delta P = P_{cap}$ we approximate the flow through the connection channel during dispensing by the same flow which takes place during self priming of the nozzle chamber.

$$\phi_c \approx \frac{P_{cap}}{R_c} \tag{6}$$

Putting together the approximations for the flow through the nozzle chamber respectively the connection channel given in Eqs. (2) and (6) the ratio ϕ_c/ϕ_{nc} can be calculated. As explained before this relative flow should be as small as possible to obtain a good correspondence between the geometrical volume of the nozzle channel V_{geom} and the dispensed volume V_d. In the framework of this approximation the dispensed volume is given by

$$V_d = (\phi_{nc} + \phi_c) t_d \tag{7}$$

where the dispensing time t_d can be estimated by

$$t_d \leq \frac{V_{geom}}{\phi_{nc} - \phi_c} \tag{8}$$

Here the smaller sign needs to be applied because the volume V_{geom} defined by the geometry of the nozzle chamber is an upper estimate of the liquid volume initially contained in the nozzle chamber like explained in Section 2. The dispensing time might also further be reduced by a rest volume which potentially remains in the nozzle chamber. Thus Eqs. (2), (6), (7) and (8) provide an upper estimate for the dosage volume to be expected.

Obviously several effects are not considered in detail in the presented approximation like for example the influence of the rest volume of liquid in the nozzle chamber, the spraying after jet tear off or the time dependence of the flow. The presented formulas nevertheless do provide additional insight into the dispensing process by highlighting the mutual dependencies between certain system parameters.

3.2. Discussion of the CFD-simulations and comparison with the analytical approximations

Based on the initial parameter set given in Table 1 individual parameters have been varied separately and their influence on the flow through the nozzle has been studied. The results of the CFD-simulations and the analytical approximation according to Eq. (2) are summarized in Fig. 7. There the time averaged flow obtained from the CFD-simulations (before jet tear off) is compared to the analytically calculated stationary flow. As expected the analytical approximation provides a good upper estimate for the flow through the nozzle. The dependence of the flow on individual parameters is correctly reproduced: quadratic dependence on nozzle diameter, reciprocal square root dependence on density etc. The CFD-simulations prove, that parameters not accounted for in the analytical approximation like viscosity and surface tension do only weakly influence the flow in the considered parameter range.

One of the most relevant figures in designing a DWP is the residual flow through the connection channel compared to the flow through the nozzle f_c/f_{nc}. If this normalized, relative flow is sufficiently small and if the nozzle chamber is completely depleted after dispensing, then the dispensed volume corresponds essentially to the volume initially contained in the nozzle chamber. In this case the accuracy of the dispensing is mainly determined by the tolerances of the micro fabrication process. Since these tolerances are typically very small the accuracy can be excellent and homogenous over all dispensing units of a DWP (cf. [5]). However, it has to be pointed out that the accuracy is reduced, if an uncontrollable rest of liquid remains in the nozzle chamber. Therefore this rest volume has to be reduced as much as possible by an appropriate nozzle design. In the case of a vanishing residual flow through the connection channel the driving pressure head and liquid properties are of minor importance which provides additional robustness to the method.

In Fig. 8 the relative flow through the connection channel is displayed as a function of the main system parameters as calculated from Eqs. (2) and (6). The comparison with CFD data shows that the analytical approximation provides a good upper estimate for the relative flow. It turns out that the system parameters d_o, l_c and P_{stat} have the greatest influence on the residual flow and should be “sufficiently large” to reduce it. In other words the orifice should be not too small and the driving pressure and resistance of the connection channel should be sufficiently high.

As indicated before, the liquid’s viscosity and density are of minor importance in the studied parameter range which is reflected by the analytical approximation as well as by CFD-simulations. Only the surface tension has a considerable influence on the residual flow. However this effect is largely overestimated by the analytical approximation. This is due to the fact, that the exact curvature of the meniscus which defines the capillary pressure is quite crudely approximated. According to CFD-simulations the variation of surface tension causes a relative flow change of maximum 5% in the considered parameter range. Thus the DWP method can be still regarded as greatly media independent in the studied range of liquid properties. As far as the quality of the analytical approximations is concerned it can be concluded that the estimate for the flow through the nozzle channel (2) is exact in terms of providing an upper limit for the flow. The presented CFD-simulations prove that also the

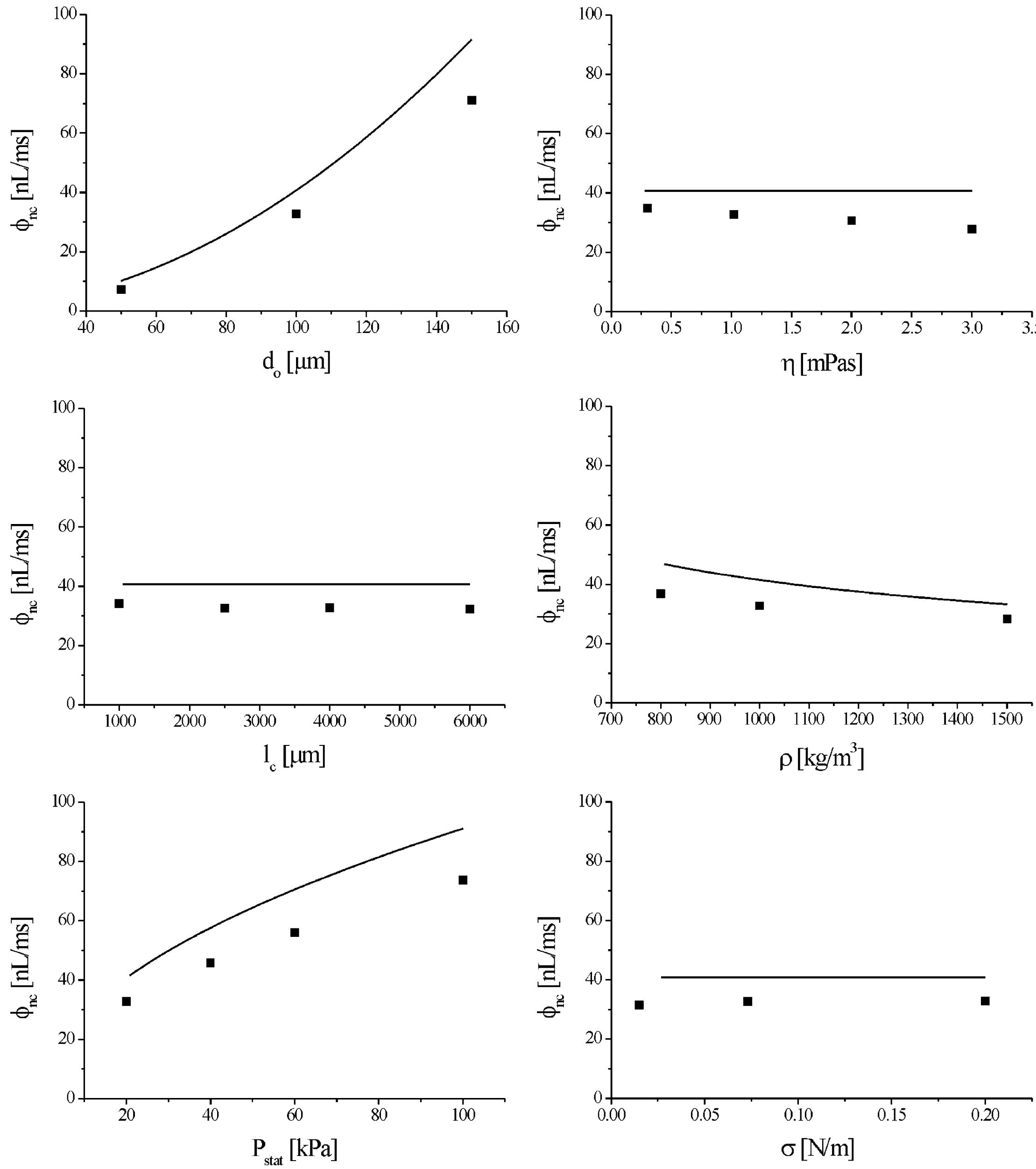

Fig. 7. Flow through the nozzle as function of various system parameters as calculated with the analytical model (line) and CFD-simulations driven by constant pressure (squares).

approximation of the flow trough the connection channel (6) is well applicable to estimate the residual flow from the reservoir for engineering purposes. In combination with the approximation for the dispensing time (8) an upper estimate for the dosage volume can be easily calculated for any given design.

4. System optimisation

After having studied the dispensing dynamics in detail the optimisation of the dispensing performance will be addressed in the following. The main factors influencing the dispensing performance of the DWP are

- The flow through the connection channel during dispensing;
- The rest volume remaining in the nozzle chamber at the end of the dispensing event;
- The spraying after jet tear off.

The flow through the connection channel and the rest volume in the nozzle chamber need to be as small as possible. Otherwise both can introduce systematic errors to the dosage volume. In case of a non-negligible flow trough the

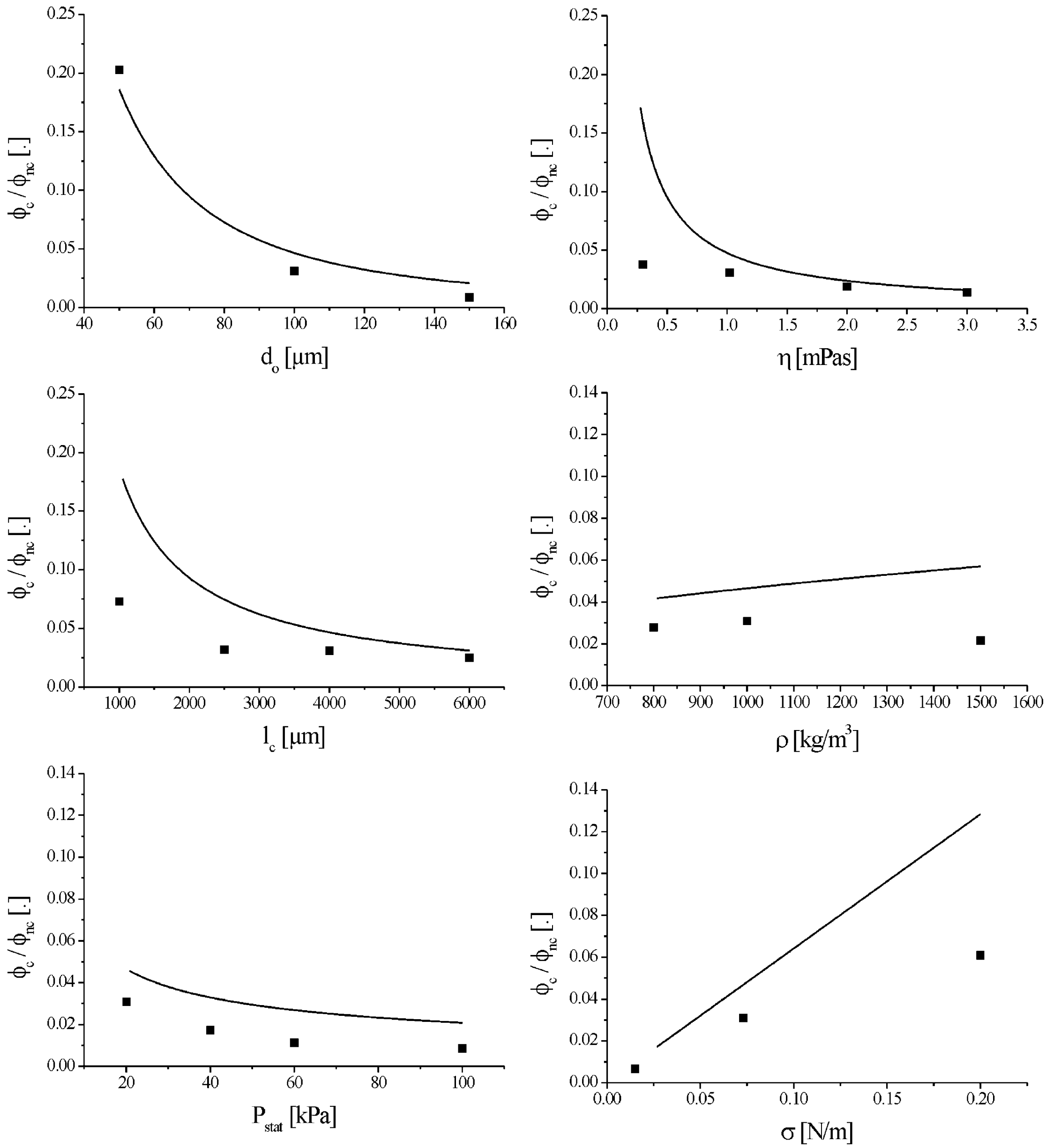

Fig. 8. Relative flow through the connection channel as function of various system parameters as calculated with the analytical model (line) and CFD-simulations (squares).

connection channel the dosage volume is higher than the volume initially contained in the nozzle chamber. It is lower than the anticipated volume if a significant residual volume remains in the nozzle chamber. Both of these effects are unwanted, because they create a dependence of the dosage volume on actuation parameters and liquid properties. The flow through the connection channel depends essentially on the viscosity, while the residual volume is influenced very much by surface tension. Finally the reduction of the spray effect also requires a negligible residual volume: If only few liquid is contained in the nozzle at jet tear off only a little spray is generated by the inevitable high speed gas flow after jet tear off. Summarising all these statements following design rules can be given to optimise the performance.

4.1. Design rules

4.1.1. Influence of connection channel and nozzle size

It has been mentioned before, that in order to obtain good accuracy the orifice diameter, the resistance of the connection channel and the driving pressure should be "sufficiently large" to reduce the residual flow. To quantify this statement we consider the relative flow as obtained with the analytical approximations (2) and (6):

$$\phi_{\mathrm{rel}} = \frac{\phi_{\mathrm{c}}}{\phi_{\mathrm{nc}}} \approx \frac{P_{\mathrm{cap}}}{R_{\mathrm{c}} A_{\mathrm{o}}} \frac{1}{\sqrt{(2/\rho) P_{\mathrm{stat}}}} \tag{9}$$

In the framework of the presented approximations the channel resistance, the orifice diameter and the driving pressure

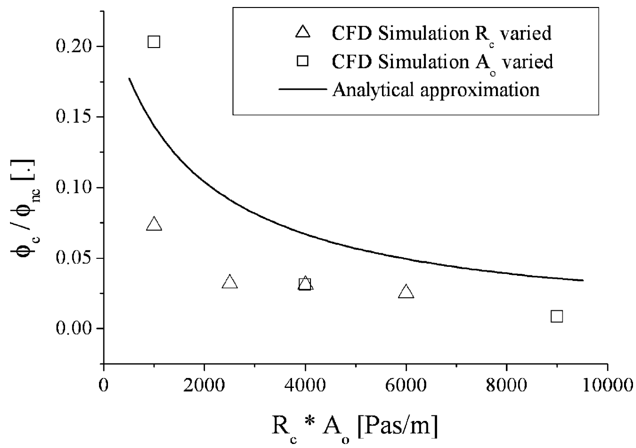

Fig. 9. Relative flow as given by formula (9) compared to CFD-simulations.

can be designed explicitly according to formula (9) to compensate for a given capillary pressure which drives the refilling process. The value of P_{cap}/R_c defines a capillary driven flow rate responsible for the refilling of the nozzle channel. This flow rate must be much smaller than the flow rate through the nozzle. In other words, the time scales for jet ejection and for capillary refilling have to be sufficiently separated to minimize the relative flow. In particular formula (9) states that this separation of time scales can be achieved in principle for any design by simply selecting a suitable high driving pressure P_{stat}.

In order to verify the simplifications made within the analytical formulas it is illustrative to plot ϕ_c/ϕ_{nc} according to formulas (9) over $R_c{*}A_o$ like displayed in Fig. 9. This curve can be compared with CFD-simulation where once the orifice area A_o and the other time the channel resistance R_c are varied. If the approximation according to formula (9) would be exact the CFD-results obtained in both cases had to be identical. Fig. 9 highlights that this is definitively not the case, but the approximation holds quite well in terms of providing an upper estimate for the relative flow. In the considered parameter range the capillary forces are indeed dominating the flow through the connection channel. Therefore the design rule to adapt channel resistance and orifice area according to the capillary pressure holds quite generally. As a rule of thumb it can be stated that the fluidic resistance of the connection channel should be at least five times greater than the resistance of the nozzle, keeping in mind that especially the orifice area is of importance and not its length (which also enters into the resistance).

To illustrate the importance of a proper layout of the connection channel, the dispensing dynamics of a pathological example of a dispenser is given in Fig. 10. If the resistance of the connection channel is not sufficiently large (e.g. due to a large cross section and small length), the time scales for refilling and dispensing are not separated. Fast refilling takes place during the dispensing and the nozzle is never depleted. After an initial decent the liquid meniscus rises again and finally reaches the upper end of the nozzle chamber. From this point on the jet is supplied completely from the connection channel. Thus the dosage volume is not limited by the volume initially contained in the nozzle chamber and the dispensing continues as long as the pressure is applied. The dispensed volume as a function of time does not reach a plateau like in the proper case shown in Figs. 4 and 5 which makes the dispensing less accurate and strongly dependent on the driving pressure.

4.1.2. Dosage rate

The dosage rate (or repetition rate) of a DWP device is mainly limited by the capillary refilling time, i.e. the time it takes capillary forces to refill the nozzle via the connection channel. This refilling time can be approximated by

$$t_{refill} = \frac{R_c}{P_{cap}} V_d \approx \frac{R_c}{P_{cap}} V_{geom} \tag{10}$$

Reducing the refilling time by decreasing R_c/P_{cap} contradicts the requirement set by (9) to reduce the residual flow. Here a trade off is required which also involves the orifice diameter determined by d_o. Unfortunately the orifice diameter cannot be increased arbitrarily since the capillary forces at the orifice need to be able to prevent the device from dripping, and therefore the orifice cannot be “too large”. Which size of orifice is indeed affordable is a very complex problem depending on liquid properties, orifice geometry and surface properties; parameters which are difficult to control. Therefore it is best practice to fix a certain orifice geometry at defined surface properties which prevents dripping reliably and then design the nozzle to hold a certain volume (i.e. fix h_{nc} and d_{nc}). The connection channel finally can then be optimised according to (9).

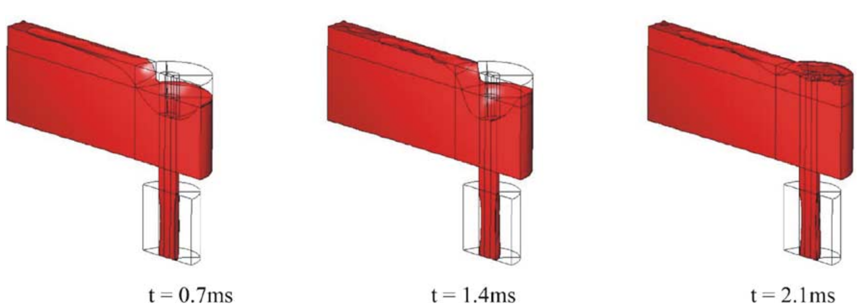

Fig. 10. CFD-simulation of a design with an insufficient resistance of the connection channel leading to a refilling of the nozzle chamber during dispensing.

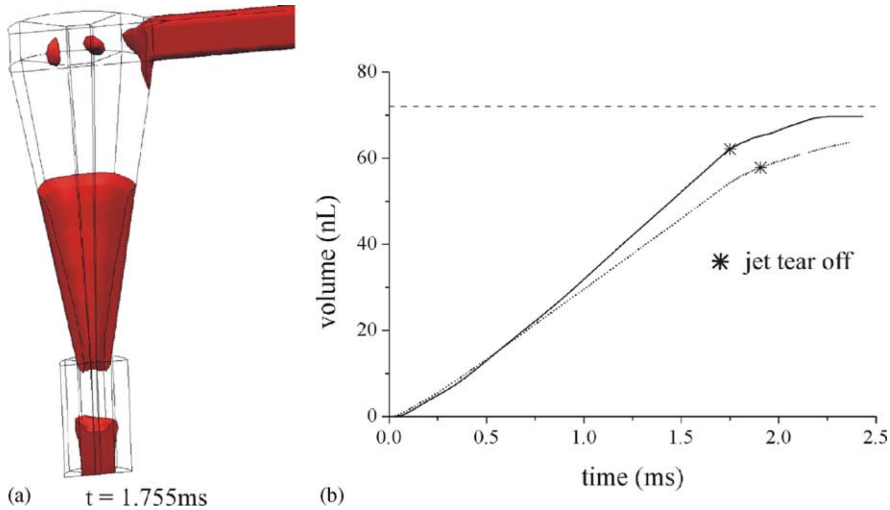

Fig. 11. (a) Simulated rest volume of the optimised design at jet tear off. (b) Integral flow through the nozzle for the optimised design and a design according to Table 1 (doted line).

4.1.3. *Jet quality and residual volume*

The optimisation of the jet quality is the most complex problem in designing a dispenser according to the DWP method since it can only be handled by a full CFD treatment. The CFD calculations are complicated due to the two phase flow including surface tension and the large density difference between the dispensed liquid and the driving gas (typically air) of about a factor of 1000. An exact analysis therefore is out of scope of this paper. Nevertheless some basic design rules can be given which reduce the spraying after jet tear of and improve the jet quality.

First of all the rest volume of liquid contained in the nozzle at jet tear off has to be as small as possible. The fewer liquid is contained in the nozzle when the high speed gas flow sets in the less can be transported by the spray. To reduce the rest volume obviously a more streamlined nozzle geometry is required. Second the pressure difference between nozzle and ambient needs to be as small as possible at jet tear off to achieve lower gas flow rates. And finally the pressure must be switched off as soon as possible after jet tear off, to reduce the gas flow to a minimum. This requirement however is very hard to meet since the flow rate through the nozzle is especially sensitive to viscosity. Thus different liquids take different times to accomplish the dispensing process. A time controlled pressure pulse with fixed duration might therefore influence the accuracy and media independent performance if the switching time is set too short. In this case the nozzle might not be depleted completely. On the other hand, if it is set too long the spraying is not sufficiently reduced.

4.2. *CFD-simulation of an improved design*

Based on the design rules given in the previous section an improved design of a DWP dispenser has been developed. The improved design consists of a tapered cylindrical nozzle with orifice diameter of 100 μm which is usually sufficient to prevent dripping of water or DMSO based solutions from silicon orifices. The geometrical volume of the nozzle has been set to 72 nL and the product of $R_c * A_o$ corresponds to 4 Pa s/m. The devices has been simulated by CFD at a constant driving pressure of 20 kPa using water as dispensing liquid. The results of the simulation are displayed in Fig. 11. The graphs reveal that the flow is slightly accelerated compared to the reference case (cf. Table 1) and that the rest volume is reduced by approximately 5 nL. Thus less liquid is transported by the spray. Furthermore the geometric limit (dashed line) is almost reached. Therefore less liquid remains in the nozzle chamber when the pressure is switched off and the dispensed volume corresponds better to the geometrical volume than for the reference design with a sudden contraction in the nozzle.

5. Summary

The dispensing dynamics of a DWP-type nanodispenser was analysed in detail using CFD-simulations and analytical considerations. A CFD model of the dispenser was developed and validated by comparison with experimental data. Based on the CFD model the working principle of the DWP method has been proven and a parameter study has been performed. It turned out that the dosage volume is greatly independent of liquid properties and actuation parameters if the system is properly designed.

Design rules have been deduced how to construct and operate the dispenser to achieve better performance. In this context the main optimisation potential is related to the residual flow during dispensing and the spraying of liquid after jet tear off which degrades the jet quality. The reason for this spraying is the rest volume contained in the nozzle chamber which is driven out of the nozzle by the high speed air flow after jet tear off. An optimised design with reduced rest volume and therefore better jet quality was proposed.

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Biographies

Peter Koltay studied physics at Universities of Freiburg (Germany) and Budapest (Hungary) and obtained his PhD from the University of Freiburg 1999 for his work on solar cells and photovoltaic modules. End of 1999 he joined the laboratory of Prof. Zengerle at the Institute for Microsystem Technology (IMTEK) of the University of Freiburg. There he is heading the pL & nL dispensers group and the group fluidic simulation. His research interests are especially related to the development of microfluidic liquid-handing devices for various life-science applications as for example micro dispensers, modelling of free surface flows and simulation of microfluidic devices by system simulation and computational fluid dynamic simulation.

Jan Kalix studied Physical Engineering at the University of Applied Science in Münster, Germany. He wrote his diploma thesis at the Institute of Microsystem Technology (IMTEK) at the University of Freiburg about the DWP dispensing process. At the moment he takes part for the Master's Program in Computer Science at the University of Hagen. His main interests are microfluidics and computational fluidic dynamics.

Roland Zengerle holds the chair in MEMS applications at the Institute of Microsystem Technology (IMTEK) at the University of Freiburg, Germany. In addition he works in close cooperation with the Institute for Micro- and Information Technology of the Hahn-Schickard-Society. His research is focused on microfluidics and covers topics like miniaturized and autonomous dosage systems, nanoliter & picoliter dispensing techniques, lab-on-a-chip systems, micro reaction technology as well as micro- and nanofluidics simulation. He co-authored more than 120 technical publications and 20 patents. He serves on the International Steering Committee of the IEEE-MEMS conference, on the European Technical Programme Committee of the Transducers 2005 conference as well as on the technical program committee of the bi-annual actuator conference. He is the European editor of the newly launched Springer Journal of Microfluidics and Nanofluidics.