# Modelling free jet ejection on a system level – an approach for microfluidics

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## ABSTRACT

Fast simulation of complex microfluidic systems requires consideration of network simulations based on lumped models as an alternative to standard computational fluid dynamic (CDF) simulations. In this paper we describe an analytical model of an orifice, capable of handling free jets and droplet ejection. It is intended to be used as a multi-purpose model for simulations of microfluidic systems (e.g. ink-jet print heads or micro dispensers). The approach is based on distinction between different fluidic states occurring during operation. Whether the orifice is self-priming by capillary forces or ejecting a liquid jet driven by a certain pressure for example, different formulas are used to describe the flow. Though the used formulas are adopted from standard fluidic theory good agreement is found between simulations and experiments performed to validate the model.

***Keywords***: lumped model, microfluidic system, system simulation, fluid jets, droplet

## 1 INTRODUCTION

Modelling of free surface flows is – due to its complexity – usually a domain for full CFD-simulations. This field of research has been topic of a large number of publications (cf. [1] and references therein). Several numerical solvers, that can deal with this kind of problems (e.g. CFDRC´s ACE+, Flow-3D etc.), are now commercially available. Nevertheless in certain situations a simplified analytical approach can lead to satisfying results [2,3], while requiring much less computational resources. Based on fluidic network theory [4] it is possible to perform system simulation quickly, once suitable models are built. In the past however most approaches to describe a free jet or droplets ejected from an orifice within fluidic network theory have been extremely simplified and very specific [3].

Since an engineering approach to micro fluidics requires highly flexible and combinable models, we present a lumped model of a circular orifice which is intended for use as a general purpose model in network simulations of microfluidic systems (e.g. micro dispensers, ink jet print heads). This model, presented here for the first time, is compatible with models described in [5] and [6].

## 2 APPROACH

The system under consideration is a simple circular orifice of diameter $d$ and length $l$. At one end (**top)** models for capillaries, reservoirs, valves etc. can be connected. No further consideration of free surface flow is done at this point. Those effects are accounted for only on the other side (**bottom)**, which serves as an outlet for a free jet or droplet. To be able to find a suitable analytical model for this system, several assumptions have been made. First it is assumed that the flow is completely laminar. This is a common assumption in microfluidics, where typical Reynolds numbers are less than 300. A further assumption is the incompressibility of the fluid. Stationary friction, inertia, gravity and capillarity are considered by simple textbook models, according to the common assumptions for small Weber numbers (less than 70 in our case).

The key to building analytical models is to find the different modes of operation of the device and the formula describing each one of them. For the considered geometry the flow through the orifice can be specified by six separate equations, valid for different states of operation, like shown in Table 1.

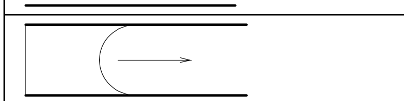
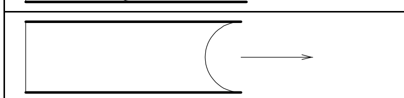
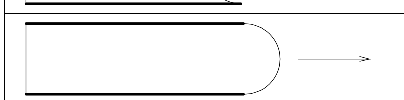
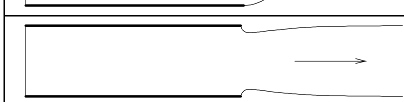
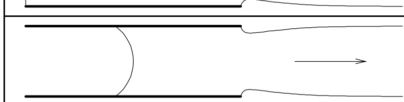
| Illustration | State |
|---|---|
|  | State 1: *empty* |
|  | State 2: *filling* |
|  | State 3: *full* |
|  | State 4: *overfilled* |
|  | State 5: *eject* |
|  | State 6: *depleting* |

Table 1: States of the flow through the orifice

For each of the states depicted in Table 1 standard fluid-mechanical formulas (taken from [4,7,8]) are used to calculate flow and pressure loss.

| Variable | Unit | Description |
|---|---|---|
| $p$ | Pa | Pressure loss due to flow |
| $q$ | m³/s | Flow through the orifice |
| $R_{fluid/air}$ | Pa s/m³ | Fluidic resistance of air |
| $R_{fluid}$ | Pa s/m³ | Fluidic resistance of fluid |
| $p_{inert}$ | Pa | Pressure loss due to inertia |
| $p_{cap}$ | Pa | $p_{cap} = \frac{4 \cdot \sigma \cdot \cos(\theta)}{d}$, (cf. [8]) |
| $p_{grav}$ | Pa | Pressure loss due to gravity |
| $p_{meniscus}$ | Pa | Counter pressure induced by meniscus |
| $A$ | m² | Cross section of the orifice |
| $\rho$ | kg/m³ | Density of the fluid |
| $\mu$ | – | Scaling factor, see below for details |
| $fill$ | $\in [0,1]$ | Relative fill level of the capillary filling orifice |
| $overfill$ | $\in [0,1]$ | Relative fill level of the overfilled orifice |

Table 2: Variables used for equations.

**State 1: *empty***

The orifice is completely empty, only air flows. As inertial effects are neglected, pressure loss occurs only by the fluidic resistance with respect to air.

$$q = \frac{p}{R_{fluid/air}} \tag{1}$$

**State 2: *filling***

In this case the fill level of the orifice is variable, while **top** leads fluid and **bottom** leads air. Therefore other effects like capillarity, gravity and inertia also affect the flow. The equation describing the flow of liquid is:

$$q = \frac{p - p_{cap} - overfill \cdot p_{grav} - p_{inert}}{fill \cdot R_{fluid}} \tag{2}$$

**State 3: *full***

When the fill level of the capillary reaches the state where the meniscus has reached the **bottom** end of the orifice (state 3 – shown in Table 1) capillary pressure no longer affects the flow. In this case the variable *fill* equals one, while the variable *overfill* is still smaller than one. As the shape of the meniscus now changes another pressure loss called $p_{meniscus}$ appears. This counter pressure is a function of the fill level of the device, that can be calculated by modelling the meniscus as a sector of a sphere of variable radius, calculating the surface pressure of this sector and integrating the pressure over the radius yields the counter pressure. This nonlinear formula is too complex to be solved by the simulator, but it can be very well approximated by a sine-function:

$$\mathrm{p_{meniscus}} \cong \mathrm{p_{cap}} + \mathrm{p_{cap}} \cdot \sin\left(\pi \cdot \frac{\mathrm{d} \cdot (1 + \mathrm{overfill}) + 3 \cdot 1 \cdot (\mathrm{overfill} - 1)}{2 \cdot \mathrm{d}}\right) \tag{3}$$

The formula for the flow in this case then reads:

$$q = \frac{p - p_{inert} - overfill \cdot p_{grav} + p_{meniscus}}{R_{fluid}} \tag{4}$$

**State 4: *overfilled***

This state only serves as a separator between the ***full*** and the ***eject*** state. It has the function of a threshold for the pressure. Flow at this point is zero ( $p = 2 \cdot p_{cap}$ ).

**State 5: *eject***

At the moment when the pressure at the orifice reaches the level needed for ejection ( $p > 2 \cdot p_{cap}$ ), the ejection starts. As the orifice is completely filled neither capillary pressure nor meniscus counter pressure have to be implemented here. But the jet by itself causes a pressure loss, which can be described by the Toricelli formula [7]:

$$p = \frac{\rho \cdot q^2}{2 \cdot A^2 \cdot \mu^2} \tag{5}$$

Whereas $\mu$ is a factor depending on the nozzle geometry (cf. [7]), that is mainly determined by the jet contraction. Therefore it is possible to extract this factor from one single measurement or CFD-simulation. The flow in this case can be described through the following formula:

$$q = \frac{A \cdot \mu^2}{\rho} \cdot \left( A \cdot fill \cdot R_{fluid} - \left(A^2 \cdot fill^2 \cdot R_{fluid}^2 + 2 \cdot \rho \cdot \left(-p + overfill \cdot p_{grav} + p_{inert}\right) \cdot \mu^{-2}\right)^{\frac{1}{2}} \right) \tag{6}$$

**State 6: depleting**

Here the fill level of the orifice decreases during ejection. This is mainly the same situation as above, but capillary pressure here again has to be taken into account due to depletion from the other end (**top**).

$$\mathrm{q} = \frac{\mathrm{A} \cdot \mu^2}{\rho} \cdot \left( \mathrm{A} \cdot \mathrm{fill} \cdot \mathrm{R_{fluid}} - \left(\mathrm{A}^2 \cdot \mathrm{fill}^2 \cdot \mathrm{R_{fluid}^2} + 2 \cdot \rho \cdot \left(-\mathrm{p} + \mathrm{p_{cap}} + \mathrm{overfill} \cdot \mathrm{p_{grav}} + \mathrm{p_{inert}}\right) \cdot \mu^{-2}\right)^{\frac{1}{2}} \right) \tag{7}$$

# 3 VALIDATION

Validation of the described model can be performed by experiments or by CFD-simulations. Two types of validation will be done here: Comparison of the dosage volumes dispensed by a simple pressure driven dispenser - termed static validation - and comparison of the time dependent flow during jet ejection of the same device – called dynamic validation. As measuring flows at such small dimensions is a very complicated task, experimental validation has been carried out only for the static case. The validation of the dynamic behavior will be based on CFD-simulation using CFDRC's ACE+ solver [9]. The network simulation has been performed using Avant!'s SABER simulator [10] in all cases.

## 3.1 Model description

The system used for validation consists of a fluid-filled reservoir of diameter 1.5mm and depth 425µm comprising an orifice of 100µm length. If an air pressure pulse is applied to the top of the device fluid is ejected (as described in [11]). The flow through the device and thus also the dosage volume depends on the pressure pulse, the geometrical shape and the physical properties of the fluid. The real system – used for measurements – contains several reservoirs as depicted in figure 1.

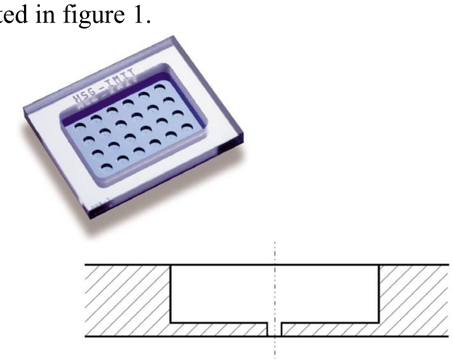


Figure 1: Photograph of the real device and cross section of one single reservoir with orifice.

As each reservoir is unaffected by the others, the real system can be simulated by considering only a single capillary (cf. network model in figure 2). As dosage medium DMSO has been assumed.

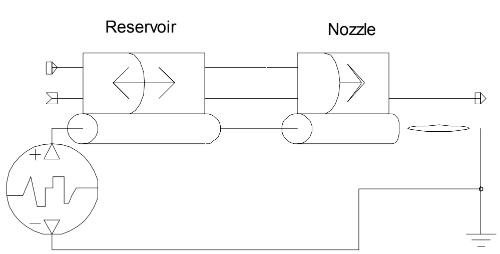



Figure 2: System model used for network simulation.

## 3.2 Static validation

Since the measured results strongly depend on the experimental setup, it is necessary to characterize the actually applied pressure pulse beforehand. Such pressure measurements have been carried out to be used in the simulations as depicted in figure 3.

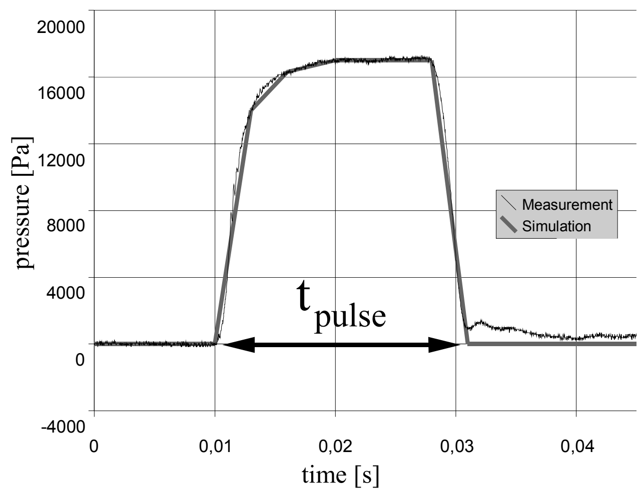



Figure 3: Typical pressure pulse as measured and an approximation of it used for network simulation.

Applying the measured boundary conditions to the system simulation the results of experiment and simulation agree very well as shown in figure 4. The agreement is not only good in the linear regime of pressure variation, but also striking for different nozzle diameters.

A calibration of the model at only one specific point ($d$=50µm, P=20kPa, $t_{pulse}$=10 ms, highlighted in figure 4) has been sufficient to obtain this good agreement. The resulting factor µ=0.905 is of the same order of magnitude as determined from a photo of the jet contraction (µ=0.91, cf. figure 5). Thus the calibrated value of the jet contraction µ corresponds nearly to its ab initio value!

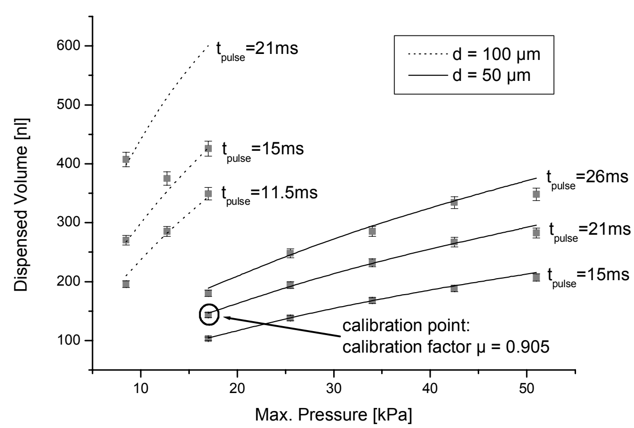



Figure 4: Dispensed volume at various pressure and orifice diameter. Measured (symbols) and simulated (lines) values.

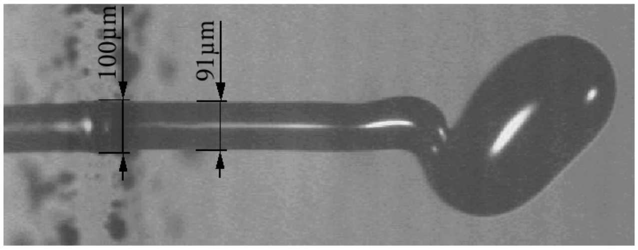



Figure 5: Photograph of the jet-ejection to determine the jet-contraction $\mu$ visually.

### 3.3 Dynamic validation

For comparison with CFD-simulations the flow through the orifice as a function of time has be considered. The simulations have been performed with a 2D-model (according to the cross-section shown in figure 1) using CFDRC's ACE+ software. For actuation a constant pressure starting at t=0 has been assumed, the dispensed medium has again been DMSO. The network simulations for comparison have been performed using a pressure pulse with a rise time of 1µs. (A rise time is required by the SABER simulator for the PWL source.) Since the considered time scale is of the order of magnitude of several microseconds the pressure pulse in this case can also be considered as constant.

The results of the simulations for various values of the pressure head and two orifice diameters (50µm and 100µm) are displayed in figure 6. Though there is an systematic deviation between the simulation results (the CFD simulation underestimates the flow) the characteristic features of flow are visible in both simulations: The time until a constant flow is reached is similar in both simulations. Also the shape of the curve is comparable, though there seems to be an artifact in the compact model of the orifice which causes a peak in the flow a short time after ejection (not present for 50µm orifice). This might be caused by the abrupt change in the driving pressure.

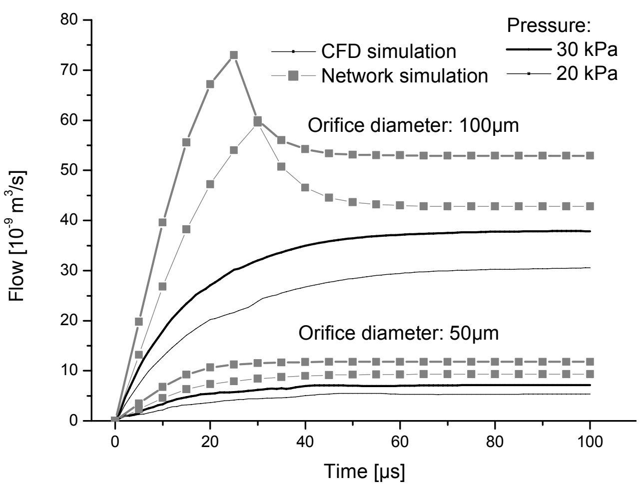



Figure 6: Flow through the orifice for various conditions determined by CFD- and network simulations respectively.

The CFD-simulations also exhibited some irregularities which could not be clarified up to date: After approximately 10µs one heavy peak (not displayed in figure 6!) has been observed in all CFD-simulations. Because the convergence has been normal at these points, this behavior can only be attributed to the unphysical boundary condition or some restrictions of the code. Due to this fact no final conclusion can be drawn. There might be some inherent limitation of the model, but it is also possible that the CFD-simulations have not worked properly. A further investigation is necessary at this point.

## 4 CONCLUSION

We have presented a compact model for a circular orifice which is intended to be used in network simulations of microfluidic systems (at small Weber numbers). The comparison with experiments showed excellent agreement as far as dispensed volumes are concerned. The comparison of the flow through the orifice with CFD-simulations revealed some quantitative deviations which might originate from both, the CFD-model or the compact model. Further investigations are needed to clarify this point.

## 5 ACKNOWLDEGMENTS

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