Simulation of a micro dispenser using lumped models

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ABSTRACT

In this paper the modelling of a micro dispenser by system simulations according to fluidic network theory is reported. The dispensing device under consideration (the so called "Nano-Jet" dispenser) is described in detail in [1]. In this device the dispensing process is triggered by the displacement of a diaphragm. Upon this actuation a free jet of liquid in the volume range of 10 nl to 100 nl is ejected from the orifice of the device. Thus the system is in some sense similar to an ink-jet print head except the fact, that a liquid jet is generated rather than droplets and a much larger volume is delivered. To set up a system model for the sketched device first a lumped model for a circular plate is derived which accounts for all essential features of fluid structure interaction (FSI) in the system. Then the plate model is combined with lumped elements of a fluidic channel and a nozzle to yield the system model of the dispenser. The results obtained with the system model are compared to experimental data in terms of ejected volume and influence of system parameters.

Keywords: system modelling, lumped model, microfluidic systems, micro dispenser, circular plate

1 INTRODUCTION

Simulation of micro pumps, ink jet print heads and micro dispensers is an important topic in microfluidics. This task is complicated by the interaction of various physical domains. The fluid structure interaction (FSI) essentially determines the dynamics in these systems and therefore has to be taken into account. Mesh based approaches combining computational fluid dynamics (CFD) and finite element methods (FEM) for solid-state simulation are in this context very time consuming, though very accurate. However to perform parameter variations and optimizations usually simplified analytical and numerical models have been set up [2,3]. Such models can also be constructed from lumped elements within the framework of fluidic network theory [4]. An approach similar to the circuit simulation used successfully in electronic circuit design.

The system simulation of microfluidic systems however lacks of a sufficient number of suitable lumped models, which can be combined to whole systems. Elementary models (resistors, inductors etc.) are described in textbooks (cf. [4]), some more elaborated models can be found sometimes in the literature [5,9]. However whole system simulations based on the network approach are rarely found in the literature due to the fact, that important effects often cannot be accounted for.

In this paper we derive a lumped model for a circular plate, which can be used for example to model the diaphragm of a micro pump. The model considers the elasticity of the plate itself as well as pressure changes inside a volume of liquid confined below the plate. Thus, the considered plate model is able to convert a force or displacement into a pressure or flow (if a fluidic outlet is connected). By this the mechanical domain in the system simulation can be linked to the fluidic domain. And therefore FSI – occurring in micro pumps as well as in the considered dispensing device – can be accounted for. By performing simulations of the micro dispenser described in [1] the applicability of the model is demonstrated.

2 APPROACH

The model for a circular plate with radius R_{pl} and thickness h is derived by solving the relevant differential equation known from elastic-theory. In the considered case of a plate loaded with a force in the middle and a homogeneous pressure from below an analytical solutions is possible.

2.1 Plate Model

To determine the flux and potential variables in the different domains (mechanical and fluidic domain) needed by the network-simulator the deflection line of the plate has to be used. Having this relation it is easy to calculate the central deflection $w(0)$ from the applied force. By integration and differentiation, the volume change (i.e. the fluidic flow) can be obtained as a function of pressure. In this calculation it is assumed, that below the circular plate a certain volume of incompressible fluid is confined. By changing the bending line the volume of this confinement can be altered which results in a flow. The magnitude of the confined volume however is of no importance and thus arbitrary and not considered further.

For the case of a circular plate loaded with a specific load profile, a differential equation is given by Timoshenko [6].

$$\frac{\partial}{\partial r}\left(\frac{1}{r}\cdot\frac{\partial}{\partial r}\left(r\cdot\frac{\partial}{\partial r}w(r)\right)\right)\equiv\frac{l(r)}{D} \quad (1)$$

variable	equals	unit
r	radial distance from the center of the plate	m
$w(r)$	deflection of the plate at r	m
$l(r)$	load per unit length at r	N/m
D	plate constant	Nm
E	Young's modulus of the plate's material	Pa
h	thickness of the plate	M
ν	Poisson's ratio of the plate's material	-
$p(r)$	pressure at r	Pa
p	pressure resulting from the fluid below	Pa
F	force applied by the piezo-actuator	N
R_c	radius of the contact region	m
R_p	radius of the pestle's hemisphere	m
E_{eff}	effective Young's modulus between plate and pestle	Pa
E_p	Young's modulus of the pestle's material	Pa
$w_{in}(r)$	deflection of the plate for $r \le R_c$	m
$W_{out}(r)$	deflection of the plate for $r > R_c$	m
R_{pl}	radius of the plate	m
V	volume of fluid under the plate	m³
q	flux of fluid in or out of the plate	m³/s
V_d	Cumulative dosage volume	m³
$\sigma_r(r)$	radial stress within the plate at r	Pa

Table 1: Variables used in the calculations

Following the definition of Timoshenko [6] for plate properties and the Hertzian formulas for a sphere-plane contact as given by Dubbel [7] we define:

$$D = \frac{E \cdot h^3}{12 \cdot (1-\nu^2)} \quad (2)$$

$$l(r) = (2\pi \cdot r)^{-1} \cdot \int_r 2\pi \cdot p(r) dr \quad (3)$$

$$R_c = \sqrt[3]{1.5 \cdot (1-\nu^2) \cdot F \cdot R_p \cdot E_{eff}^{-1}} \quad (4)$$

$$E_{eff} = 2 \cdot E \cdot E_p \cdot (E + E_p)^{-1} \quad (5)$$

For the considered problem of a circular plate loaded with pressure from below and force from above, we can establish a piecewise defined load function.

$$p(r) = \begin{cases} p + \dfrac{F}{\pi \cdot R_c^2} & \forall\, r \le R_c \quad (= inner\ region) \\ p & \forall\, r > R_c \quad (= outer\ region) \end{cases} \quad (6)$$

With these formulas and definitions, the differential equation (1) can be solved piecewise for both regions:

$$w_{in}(r) = \frac{p \cdot r^{4r}}{64 \cdot D} + \frac{F \cdot r^4}{64\pi \cdot R_c^2 \cdot D} + \frac{r^2}{2} \cdot C_2 + C_3 + C_1 \cdot \ln(r) \quad (7)$$

$$w_{out}(r) = \frac{p \cdot r^4}{64 \cdot D} - \frac{F \cdot r^2}{8\pi \cdot D} + \frac{F \cdot r^2 \cdot \ln(r)}{8\pi \cdot D} + \frac{r^2}{2} \cdot C_5 + C_6 + C_4 \cdot \ln(r) \quad (8)$$

The integration constants C_i can be found using the boundary conditions arising in the problem, such as the equality of inner and outer solution and their derivatives at their common boundary and the defined position and stress of the plate at the outer boundary and in the centre:

$$\begin{aligned} &w_{out}(R_{pl}) \equiv \tfrac{\partial}{\partial r} w_{out}(R_{pl}) \equiv \tfrac{\partial}{\partial r} w_{in}(0) \equiv 0,\ w_{in}(R_c) \equiv w_{out}(R_c), \\ &\tfrac{\partial}{\partial r} w_{in}(R_c) \equiv \tfrac{\partial}{\partial r} w_{out}(R_c),\ \tfrac{\partial^2}{\partial r^2} w_{in}(R_c) \equiv \tfrac{\partial^2}{\partial r^2} w_{out}(R_c)) \end{aligned} \quad (9)$$

Using these constraints, both the inner and outer solutions can be matched to yield the complete bending line.

$$w(r) = \begin{cases} \dfrac{p \cdot (r - R_{pl})^4}{64 D} + \dfrac{F \cdot (2r^2 + R_c^2) \cdot \ln\left(\frac{R_c}{R_{pl}}\right)}{16\pi \cdot D} + \dfrac{F(4 R_c^2 \cdot R_{pl}^4 + R_{pl}^2 \cdot (r^4 - 3 R_c^4) - 2 r^2 \cdot R_c^4)}{64\pi \cdot D \cdot R_c^2 \cdot R_{pl}^2} & \forall\, r \le R_c \\ \dfrac{(r - R_{pl})^2 \cdot ((r - R_{pl})^2 \cdot \pi \cdot R_{pl}^2 - 2F \cdot (R_2^4 + 2 R_{pl}^2))}{64\pi \cdot D \cdot R_{pl}^2} + \dfrac{F \cdot (2r^2 + R_c^2) \cdot \ln\left(\frac{r}{R_{pl}}\right)}{16\pi \cdot D} & \forall\, r > R_c \\ \dfrac{F \cdot \left(R_{pl}^2 + R_c^2 \cdot \ln\left(\frac{R_c}{R_{pl}}\right)\right)}{16\pi \cdot D} + \dfrac{\pi p \cdot R_{pl}^4 - 3 \cdot F \cdot R_c^2}{64\pi \cdot D} & \forall\, r = 0 \end{cases} \quad (10)$$

Equation (10) has been evaluated for various limiting cases of simpler load-profiles (e.g. $F \to 0$ or $p \to 0$ etc.). The results obtained by straight-forward calculation are consistent with formulas given by Timoshenko [6], Dubbel [7] or Roark [8]. Correct integration of the bending-line (cf. figure 1) across the two regions results in the volume of fluid under the plate.

$$V = \int_0^{R_{pl}} \int_0^{2\pi} w(r)\, d\theta\, dr = \frac{\pi p \cdot R_{pl}^6 + F(15 R_{pl}^4 + 9 R_c^2 \cdot R_{pl}^2 - 23 R_c^4)}{192 D} \quad (11)$$

The time-derivative of the volume gives the flux q of fluid into or out of the volume below the plate. Having this flux and the central deflection $w(r=0)$ from (10) each of the system-variables F, $w(0)$, p, q can be uniquely determined, provided two of them are given by a boundary condition from the network simulator. For simulation the formulas (10) and (11) have been implemented as MAST-template.

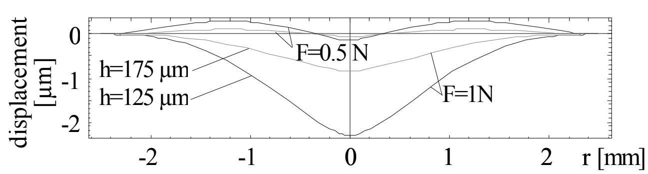

Figure 1: Bending lines for various forces and plate thickness at a fixed pressure $p=100\ kPa$, material: silicon

Having obtained an analytical solution for the bending line, it is also possible to determine the stress in the system. It is straight-forward to predict for example the minimum required thickness by comparing maximum stress within the plate with the tensile strength for the plate material. Based on the formulas given in [7] the radial stress for example reads:

$$\sigma_r(r) = \frac{6}{h^2}\left(\frac{\partial^2}{\partial r^2} w(r) + \frac{\nu}{r}\frac{\partial}{\partial r} w(r)\right) \qquad (12)$$

2.2 System model of the dispenser

The investigated system model (cf. figure 2) of the nano liter micro dispenser described in [1] consists - apart from the circular plate model derived in section 2.1 - of an ideal position source modelling the piezo-actuator. The actuator drives the microfluidic dosage chip, which consists of a rectangular capillary model given by [5] for the inlet channel and a model for the nozzle taken from [9]. An integrator serves for detection of the dispensed liquid volume V_d according to:

$$V_d = \int q\, dt \qquad (13)$$

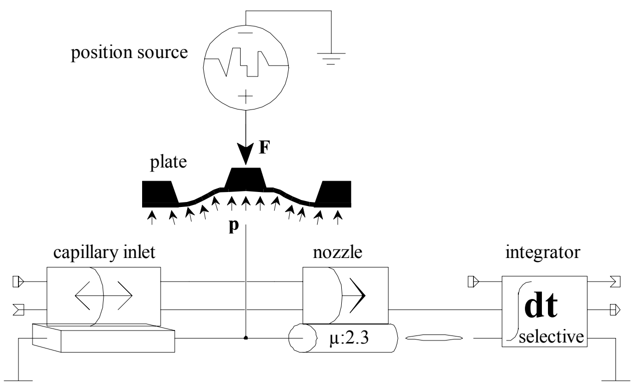

Figure 2: Sketch of the simulation set-up including the plate model described in section 2.1

3 RESULTS

Simulations of the system model sketched in figure 2 have been carried out using the Avant! SABER simulator [10] to achieve appropriate results, the nozzle model [9] had to be fitted with the orifice parameter μ at a single point (cf. figure 5). With this calibration, all other simulations and validations have been performed.

As a first test various simulations with different plate thickness (i.e. different plate-constants) were conducted. The results showed that thinner plates need much less force from the piezo actuator and produce a smoother flow and pressure profile. It is expected, that thinner plates produce a more reproducible jet, because pressure oscillations (which can cause satellite droplets) are suppressed (cf. figure 3). It seems to be a unique feature of the dispensing system, that even large changes in the thickness do not affect the dosage

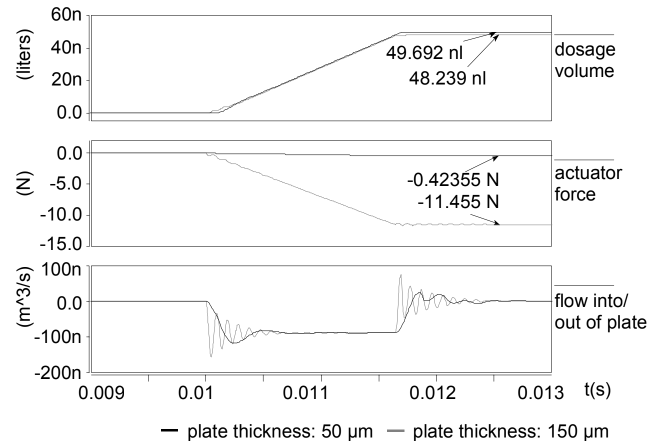

Figure 3: Characteristics for different plates thickness

volume (cf. figure 3 and 4). This shows the robust design of the real dispenser.

Using the radial stress from (12), it is now possible to optimise the design for the dispenser by minimizing the plate thickness i.e. the applied force, taking into account a maximum stress restriction for the membrane.

Analysing the values from figure 4 shows a linear relationship between the applied force and the plate stiffness. It is a remarkable feature of the model, that though the force needed to create a certain central deflection is a linear function of the plate constant the pressure is not! This is due to the fact, that the model accounts for the back bending of the plate due to the pressure from below (cf. figure 1).

As a further test of the plate model, flux and potential boundary conditions have been tested on both the mechanical and fluidic pins. Using the output from one simulation as boundary condition for a comparative run gives equivalent results (e.g. applying a force-source delivers the same result as using a position source with corresponding values). Since the model implements the bending line, it is even possible to obstruct any flow out of the volume under

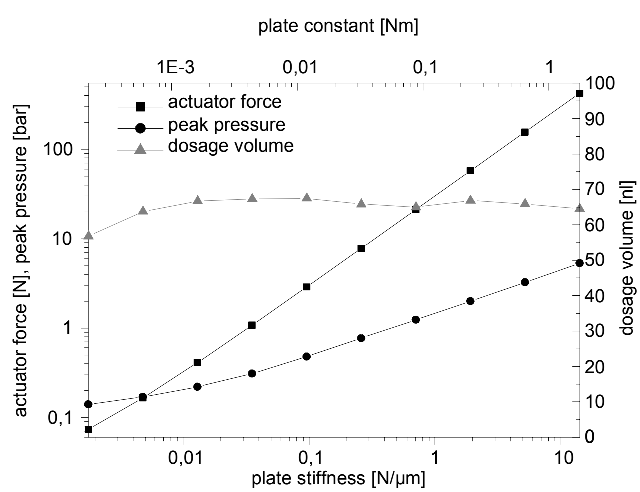

Figure 4: linear dependency of actuators force on the plate stiffness for plates thickness 25...500 µm

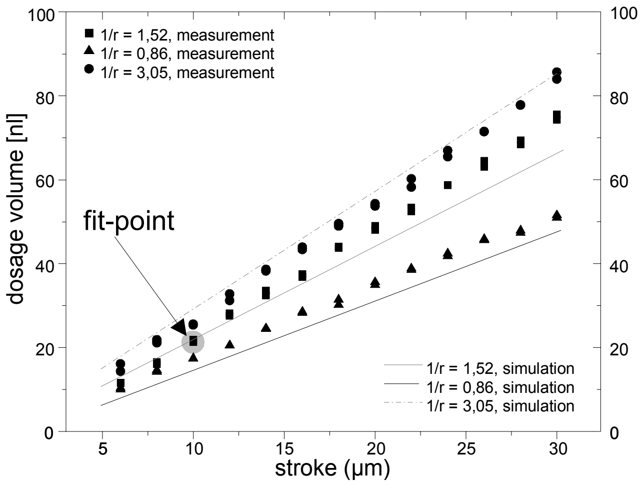

Figure 5: Comparison between simulation and measurement on dosage lines for different chip types

the plate and perform a displacement on the plate. This results in a increasing pressure under the plate and a bending line with constant volume under it. This behaviour for example cannot be accounted for by a piston/plunger model where the piston is connected to a spring with variable stiffness!

The best test for evaluating the complete system model of the dispenser is the comparison of the dosage volume with measured data. Especially the dosageline i.e. the dispensed volume as function of the central membrane displacement is of interest. The dosage line depends on the design of the microfluidic dosage chip as discussed in detail in [1]. The relative resistance defined as the ratio of the fluidic resistance of the capillary inlet channel to the nozzle channel mainly determines the slope of the dosage line. The results of the simulation versus the measurements for different values of the relative resistance 1/r are shown in figure 5. Obviously the influence of the relative resistance on the slope of the dosage line is reflected correctly by the simulations. They have been performed by calibrating the compact model for the nozzle [9] at one single point (cf. highlighted point in figure 5). The obtained parameter $\mu=2.3$ describes the fluidic characteristics of the nozzle mainly represented by the jet contraction.

Though the simulations and measurements agree quite well quantitatively as far as the dosage line is concerned there is still some room for improvements: First of all the value of the fitted nozzle parameter can not be interpreted in terms of jet contraction. A parameter $\mu>1$ would represent a diffuser nozzle, while in real experiments a jet contraction of about 0.9 is observed. One reason for this behaviour could be, that the resistance of the capillary inlet channel is not modelled correctly. If it is too low compared to the nozzle this would require an unphysical value for μ as observed in the current calibration. Another reason could be that the resistance of the inlet channel scales with p (cf. [5]) while the resistance of the nozzle scales with p^2 (cf. [9]). This implies a non constant value for 1/r, which might cause the mentioned artifact. This could also explain the observation, that the simulations predict shorter ejection times than observed in experiments. This means that the pressure below the membrane is underestimated due to the fact that the resistance of the supply channel is underestimated (scales with p instead of p^2).

4 CONCLUSIONS

We have presented a compact model for a circular plate to be used for system simulations of microfluidic systems like micro pumps or micro dispensers including fluid structure interaction. The model has been tested by comparison with textbook formulas in limiting cases. The essential feature of the model is, that it includes the back bending of the membrane due to a counter pressure. This is reflected by a non-linear relationship between the plate stiffness and the resulting pressure, while the required force scales linearly.

Using this model a system simulation of the "Nano-Jet" dispenser has been carried out. Good agreement has been found between simulation and experimental results on first glance. However some inconsistencies relates to the used capillary and nozzle models require a more thorough investigation of the system model before a final conclusion on its performance can be drawn.

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