Simulation Toolkit for Micro-Fluidic Pumps Using Lumped Models

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ABSTRACT
Simulation of micro pumps is complicated by the interaction of the fluidic and mechanical domain. The fluid structure interaction (FSI) essentially determines the dynamics of micro pumps and therefore has to be taken into account. Mesh based approaches are in this context very time consuming, though very accurate. However to perform parameter variations and optimizations usually simplified analytical and numerical models have to be set up. To speed up model development and parametrical variations of single pump elements, a modular approach where FSI has been taken into account within a system simulation is used. The system simulation is based on lumped models, combined in the multiphysics simulator SABER [1]. A simulation toolkit based on various lumped models is used for the simulation of two different micro-pump layouts well known from literature. Furthermore a concept for a three finger peristaltic pump is proposed based on simulation results.

Keywords: lumped models, micro pumps, valves, system simulation

1 INTRODUCTION
A large variety of different micro-pumps has been reported during the last decades [2]. They differ in layout and actuation. The various components of micro pumps like channels, valves, membranes, etc. can be modeled separately by lumped models. The lumped models of the components can be combined in a system simulation to model a complete micro pump. The use of such a modular approach for the pump simulation provides several advantages: Compared with mesh-based simulations the simulation with lumped models allows parametrical studies and optimization within fraction of time. Additionally the modular approach allows fast redesign and substitution of parts. In the following a toolkit is presented consisting of different elements like channels, diffusers, actuators and valves. Finally the toolkit is applied to simulate some exemplary micro pumps.

2 LUMPED ELEMENTS
Micro pumps reported in literature [2] differ in several aspects, for example geometry and working principle. Following the classification of [3] the two pumps considered as examples in this paper [4], [5], [6] belong to the category of reciprocating displacement pumps. Both pumps are diaphragm pumps that differ in their valve types and actuation principles. In the following lumped models for the various components are derived and models for the two pump types are presented.

2.1 Capillaries
In micro fluidics usually laminar Poisseuille flow can be anticipated. Thus well known analytical formulas can be found in the literature [7] to model fluidic channels. These formulations can be applied for circular and rectangular channels and have already been reported as lumped models for SABER in [8]. They implement the fluidic resistance as well as the fluidic inductance whereas the compressibility is not considered.

2.2 Valve types
To cover the typical reciprocating diaphragm micro pumps, the two most commonly used valve types have been chosen: nozzle-diffuser valves and flap type valves.

For conical nozzle-diffuser elements in general the flow resistance coefficient $\xi$ is written as:

$$\xi = \frac{\Delta p}{\rho v^2/2} \quad (1)$$

This coefficient varies with the pressure drop $\Delta p$ over the nozzle-diffuser element, the fluid density $\rho$ and the mean flow velocity $v$ at the narrowest part of the element. It is different in forward and backward direction [9]. Thus a flow directing capability is given by the ratio of the flow resistance coefficient in the negative direction (nozzle) and the positive direction (diffuser). With increasing flow also the flow directing capability increases.

These elements are used in the pump example modeled first. It is described in detail in [4] and depicted in Figure 1.

The valve is implemented as lumped model with the input parameters of the smallest diameter, the nozzle-

Figure 1: Nozzle-diffuser pump with the inlet on the left side and the outlet on the right in a) supply mode and b) pump mode causing a net-flow towards the right side.
diffuser length and the opening angle \( \alpha \) within the limits of \( 5^\circ < \alpha < 40^\circ \). Depending on the flow direction the pressure loss over the element is calculated by using equation (1), (6) and (10) of reference [9].

As second example the pump reported in [5] is chosen, cf. Figure 2. This pump type uses passive flap valves. These valves typically consist of a flexible diagram or flap and a valve seat. These valves are open in flow direction and closed if the flow is in reverse direction. Nevertheless some leakage of this valve types is often reported and in most cases caused by particles that prohibit a complete sealing.

As there is no general analytical description that models a flap valve, waning from the geometrical parameters and the material data, the lumped model flap-valve is based on a diode model with two fit factors, well known from the electrical domain:

\[
\Phi = a \cdot \left( e^{b \cdot p} - 1 \right)
\]  

(2)

The factors \( a \) and \( b \) of (2) define the interrelation between the pressure \( p \) and the volumetric flow \( \Phi \). They have been determined by fitting the curve to the points of a lookup-table, extracted from Figure 3a) of reference [6]. This is a limitation to the model, due to the fact that the flow-pressure pairs of the specific flap-valve have to be provided resulting from measurement or fully coupled FEM-simulations.

As depicted in Figure 3 there are several actuation principles for reciprocating membrane micro pumps. In case of the nozzle-diffuser pump in our example, a piezo disc actuator is used. It is mounted onto the membrane by an adhesive layer, cf. Figure 3a). The flap valve pump in our second example is actuated by an external pneumatic system like displayed in Figure 3e).

All those actuation principles launch their force into a membrane that induces the volume displacement in the pump chamber. Depending on the actuation principle, either a source element (force or displacement) provided by the network simulator can be used directly or a transducer element has to be applied in between like for example a piezo-beam [10].

The actuators are connected to the lumped model of a membrane with circular shape. This membrane model of the toolkit has already been presented by the authors in [11]. The membrane is displaced in its center by a certain force/displacement and loaded from below by a counter pressure. Since it is a quasi static model it is only valid for actuation frequencies much smaller than the plates resonance frequency.

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2.4 Capacitive elements

To receive a more uniform flow in simulations it has been suggested in [6] to add elastic elements into the system. This pressure and flow signal smoothing can be realized by implementing fluidic capacities like diaphragms or flexible tubes.

As lumped model, the capacity is implemented as a gas bubble, following the law of Boyle-Marriotte at constant temperature. The input parameter is just the initial gas volume at normal pressure.

2.5 Toolkit elements

The applied toolkit provides all the lumped models listed in Table 1. The additional lumped models which are required are provided by the standard library of the simulator. For the simulations the different lumped elements are interconnected as shown in Figure 4 and 6. The signals passed along the interconnections for the fluidic parts are pressure and flow. To track the total flow into and out of the system integrator elements are used.
<table>
<thead>
<tr>
<th>Element</th>
<th>Input parameters</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channels</td>
<td>dimensions</td>
<td>![Channels_icon]</td>
</tr>
<tr>
<td>Nozzle-diffuser elements</td>
<td>diameter at input, length, opening angle</td>
<td>![Diffuser_icon]</td>
</tr>
<tr>
<td>Flap valve</td>
<td>fit factors $a$, $b$ for $\Phi = a \cdot (e^{b \cdot p} - 1)$</td>
<td>![Flap_icon]</td>
</tr>
<tr>
<td>Membrane</td>
<td>diameter, thickness, Youngs-Moduls, poisson-number</td>
<td>![Membrane_icon]</td>
</tr>
<tr>
<td>Pneumatic actuation</td>
<td>transient pressure profile, dead volume</td>
<td>![Actuation_icon]</td>
</tr>
<tr>
<td>Fluidic capacitance</td>
<td>bubble volume at normal pressure</td>
<td>![Capacitance_icon]</td>
</tr>
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Table 1: Input parameters of the toolkits elements used to rebuilt the pumps using the network simulator SABER [1]

3 MODEL SETUP

For both pump examples there have been attempts to describe the system either by analytical formulations or model it with mesh-based simulation tools [4], [6].

To validate our toolkit approach, the mentioned pumps are modeled and the simulation results are compared to the experimental data of [4], [5], [6]. To rebuild the pumps the different elements of the toolkit are interconnected. As depicted in Figure 4a) the nozzle-diffuser pump therefore consists of the nozzle-diffuser elements and the membrane in between. The membrane is driven by an ideal position source that models the piezo's displacement and driving frequency. A spring and a mass can be added from the simulator toolkit to model the actuators transient behavior. Since the experimental setup does not allow a flow measurement directly at the pumps inlet or outlet, two capillaries have to be added in the real pump as well as in the simulation model. The fluid parameters (viscosity, density etc.) as well as other global parameters are defined in an include file which inherits its values to all components.

The modular constitution of the second example is shown in Figure 4b). Two lookup-table elements generate the driving pulse as provided in Figure 5 of reference [6]. The first lookup-table generates the pressure pulse as given in [6] while the second lookup-table converts this pressure into a displaced volume leading to a generated flow, see figure 5 in [6]. Capacitive elements following the ideal gas law model the pressure-smoothing-elements (PSE's) applied for modeling in [6]. The parameters for the two flap valves were extracted from the experimental data from [6] as well as the dimensions of the attached capillaries.

Figure 4: Model setup of a) the nozzle-diffuser pump [4] with a piezoelectric actuation and nozzle-diffuser valves [9] and b) the flap valve pump [6] with a pneumatic actuation.

4 RESULTS

The actuation of the nozzle-diffuser pump of [4] was modeled in the system simulation by a sinusoidally driven displacement source (cf. Figure 4a)). The parameters for the displacement source were obtained from experimental data like follows: By fitting the simulated flow rate of pump type A to the experimental results reported for a stroke of $9.2 \ \text{mm}$ at 100 Hz in [4] an "equivalent stroke" of $6.5 \ \text{mm}$ in the system simulation was determined at which the flow rate could be reproduced. This number corresponds well to the displacement values also applied in [4] for simulating the pump. Based on this fit point all other operation conditions at strokes between 3.9 $\text{mm}$ and 9.6 $\text{mm}$ at a driving frequency of 100 Hz could be reproduced for pump types A and B without adapting any other parameters. The deviation from experimental results concerning the flow rate was in any case smaller than 15 %. However, the frequency dependence of the flow rate could not be reproduced correctly. This might be caused by the different implementation and size of the fluidic capacities or by limitations of the membrane models transient behavior.

For the flap valve pump the dynamic behavior (Figure 5) as well as the maximum overall flow rate can be reproduced well by the simulation. The simulated flow rate of 380 $\text{l/min}$ is 5% lower than the experimental data of...
400 µl/min given in [6]. Compared to Figure 8 in [6] the peaks indicating the switching of the valves are more distinctive.

Figure 5: Results of the flow characteristics for a pneumatic actuation of the flap valve pump driven by a pump frequency of 10 Hz.

Figure 6: Setup for an peristaltic pump with the elements of the toolkit.

Figure 7: Driving profile and resulting flow characteristics for two pump cycles of a three-finger peristaltic pump.

5 EXAMPLE FOR FAST PUMP DESIGN

As shown in the previous sections it is possible to rebuilt known micro pumps with the toolkit with reasonable accordance to the experimental results. This encourages to design, test and optimize new micro pumps with the aid of the toolkit. Figure 7 shows a possible pump design for a three-finger peristaltic micro pump with no flow directing elements (valves). The flow direction and pumping is determined by the inductance and resistances of the connected system and the consecutive stimulation of the three membranes.

The simulation result of this pump design is depicted in Figure 8. It is obviously possible to gain a net flow of 120 µl/min at a pump rate of 167 Hz. The actuator stroke is chosen to be 30 µm resulting in a maximum force of 0.5 N.

The toolkit would now allow an easy addition of further pump fingers or flow directing elements such as the valves or diffusers shown. This could be used to gain higher flow rates with the final design.

6 CONCLUSIONS AND OUTLOOK

It has been demonstrated with two examples that micro pumps can easily be simulated by lumped models. The system models have been verified by the experimental results of well-known micro pumps and are in good agreement. This encourages to enlarge the toolkit in the future to cover more pump types (e.g. with ball-valves) or even to model complete micro fluidic systems, e.g. by combining a pump with a micro mixer [12] and sensor models. This will allow for a fast design of lab-on-a-chip or other micro fluidic systems.

REFERENCES