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Static and dynamic flow simulation of a KOH-etched microvalve using the finite-element method

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Abstract

In this paper, we present the simulation of the flow rate through a KOH-etched microvalve, which is part of an electrostatically actuated micropump. It is realized by a coupled simulation of liquid flow and structural displacement of the valve using the finite-element method (FEM). For this purpose, a new simulation method is developed to calculate the solid motion inside a liquid by a fluid-structural coupling. Thus the static and dynamic behaviour of the valve can be simulated in good agreement with measurements. In addition, an analytical model of the valve is developed, which allows the explanation of static as well as complex dynamic effects. In combination with analytical approaches, the simulations of the valve can be integrated into system simulations of a micropump. The results are of basic importance for the understanding and optimization of bidirectional silicon micropumps.

Keywords: Microvalves; Micropumps; FEM simulation; Fluid flow simulation; System simulation

1. Introduction

At the moment great efforts are being directed to the development of micromechanical components and their employment in microsystems [1]. Applications for them can be found in medicine, where drug-delivery systems are planned for implantation, as well as in the field of chemical analysis systems [2,3]. In both cases, the advantages of micromechanics are the small lateral dimensions, which are realized by the integration of actuators, sensors and the electronics on the same chip.

The main components of micro fluid systems are micropumps and most of them are of the reciprocating type. They usually consist of an actuation unit and two passive check valves (or diffuser/nozzle elements [4]). Different principles are used as driving mechanisms. Among them are piezoelectric, thermopneumatic and electrostatic drives [5–7]. Flap or membrane valves are normally used for the definition of the flow direction of the fluid.

These pressure-controlled check valves are very important for the behaviour of a micropump. Due to their static and dynamic properties, they basically determine the flow rate of the pump. The following simulations and measurements relate to the flap valve that is used in the electrostatically driven micropump published in Ref. [7]. It consists of a thin flap with a length of 1700 μm, a width of 1000 μm and a thickness of 15 μm. In the state of rest, the flap closes a square valve seat with a length of 400 μm and a width of 5 μm.

By means of a simulation of the static and dynamic properties of the valve, the geometric dimensions and transient behaviour can be optimized. With the finite-element method (FEM), the exact transient behaviour of the valve can be simulated, which up to now cannot be determined by measurements because of the small dimensions and the high frequencies of the valve motion. The results contribute to the understanding of the complex dynamic behaviour of the pump.

2. Static finite-element simulation of the valve

For the numerical modelling of the valve, we use the commercial FEM program ANSYS/FLOTRAN®. Besides a lot of other features, the program includes mechanical and fluid-mechanical simulation, which are both necessary for the calculation of the valve.

In a first approach, we simulated the static flow rate by a non-iterative combination of structural and fluid flow calculation as has been done before [8,9]. For the geometry of the model, the exact lateral dimensions of the valve were as described above. In a first step we calculate the structural displacement of the flap in a two-dimensional model of the valve (Fig. 1) including large deflection and stress stiffening.

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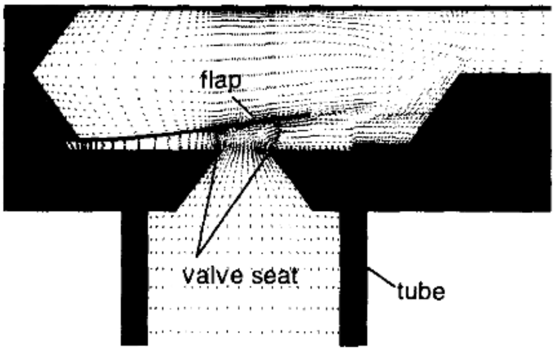

Fig. 1. FEM simulation of the velocity distribution inside the flap valve at a pressure difference of 30 000 Pa: model, 10 000 elements.

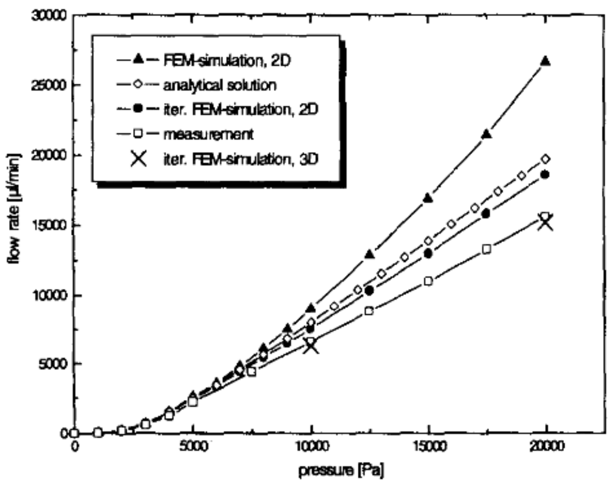

Fig. 2. FEM simulation, analytical simulation and measurement of the flow rate through a KOH-etched flap valve.

As a simplification, we assume a constant pressure inside the valve seat and a zero pressure on the outside.

In a second step, we use these geometric results as an input for the fluid-mechanical model. It consists of two-dimensional four-node elements with three degrees of freedom (two velocities and the pressure). The achieved flow rate of the 2D model has to be multiplied by the whole length of the 3D valve seat (1600 μm) to get the three-dimensional result. By repetition with different pressures, a characteristic line is created, which corresponds to the pressure-dependent static flow rate of the valve (Fig. 2, ▲).

A comparison with measured results shows a difference of up to 50% for high pressures and large displacements of the flap. The reason for this is the real pressure distribution under the flap, which does not agree with the assumed constant pressure (see Fig. 4). In the area behind the small gap between flap and valve seat, a low pressure exists, which is the result of the removal of fluid in the diffuser. This low pressure reduces the displacement of the flap and the flow rate with it.

To consider the effect, a new iterative simulation method was developed. It transfers the pressure distribution underneath the flap, which is the result of the fluid flow simulation, back to the structural model as boundary condition for the next structural simulation. For this purpose, a new algorithm, which allows an automatic meshing of the fluid model, using the geometry of the displaced flap, was implemented into ANSYS. After some iterations, the structural displacement and pressure distribution reach an equilibrium. When a model with 10 000 elements and 10 iterative steps for the static convergence is used, the results of the coupled 2D simulation show better agreement with the measurement (Fig. 2, ●).

In a third approach, a 3D model of the valve with its exact lateral dimensions was calculated in an iterative solution, too. By taking into account that over 60 000 elements are necessary to get convergence, it would require too much time to simulate the whole characteristic of the valve. Hence only flow rates at pressure differences of 10 000 and 20 000 Pa were calculated and both results show an excellent correspondence with the measurements (Fig. 2, ×).

Only at low pressure differences ($p < 5000$ Pa) can the influence of the low-pressure region be neglected and the displacement of the valve y shows a linear dependence on the pressure p (Fig. 3):

$$F = pA = k_1 y \tag{1}$$

where A is the area within the valve seat (1.6×10^{-7} m^2) and k_1 a constant factor similar to a spring constant. In our example its value is about 65 N m^{-1} (Fig. 3).

At high pressure differences, the influence of the low pressure increases and the pressure-dependent displacement of the flap becomes non-linear. Nevertheless, the displacement can be described analytically in good agreement with the

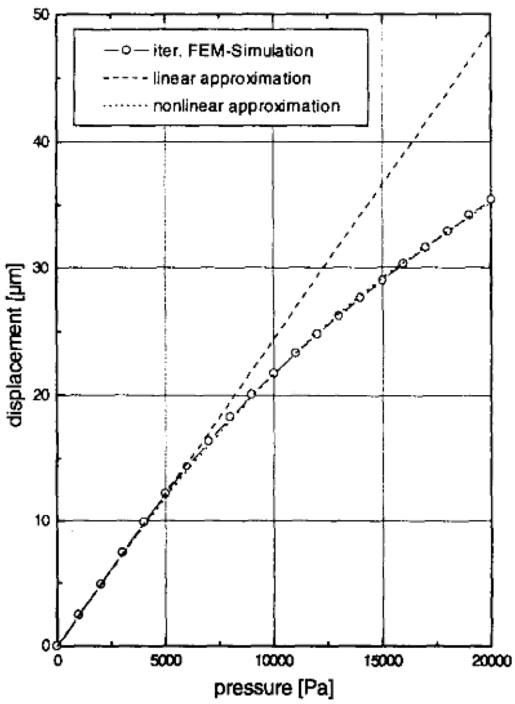

Fig. 3. FEM simulation of the pressure-dependent displacement of the valve

FEM simulation, including the linear behaviour at low pressures (Fig. 3):

$$F = pA = k_1 y + k_2 y^2 + k_3 y^3 \qquad (2)$$

where k_1 is again the linear factor of Eq. (1) and k_2 and k_3 are factors describing the non-linear behaviour with values of 1.55×10^5 N m^{-2} and 2.5×10^{10} N m^{-3} (determined by comparison of Eq. (2) and the FEM simulation in Fig. 3). This non-linear behaviour is not a material effect, but a result of the difference between the real pressure distribution and the calculated force F, which is the product of the pressure difference over the valve p and the area A.

3. Analytical model of the static flow rate

As an alternative to time-consuming FEM simulations, an analytical model was developed for the calculation of the static flow rate of the microvalve. By means of this model, design parameters of the valve can be optimized very fast, depending on the outer demands. Furthermore, this model can be used for an integration into more complex systems, like the simulation of the dynamic behaviour of the valve, a model for the whole micropump or a microsystem.

Static fluid flow in the gap between flap and valve seat can be described by the extended Bernoulli equation [10]:

$$p_1 + \alpha\frac{\rho}{2}v_1^{\,2} = p_2 + \alpha\frac{\rho}{2}v_2^{\,2} + (p_e)_{1-2} \qquad (3)$$

p_1, v_1 and p_2, v_2 are pressure and velocity at the beginning and the end of the gap. α is a coefficient related to the flow profile and $(p_e)_{1-2}$ describes the pressure losses because of fluid friction. This friction includes laminar friction as well as vortex losses.

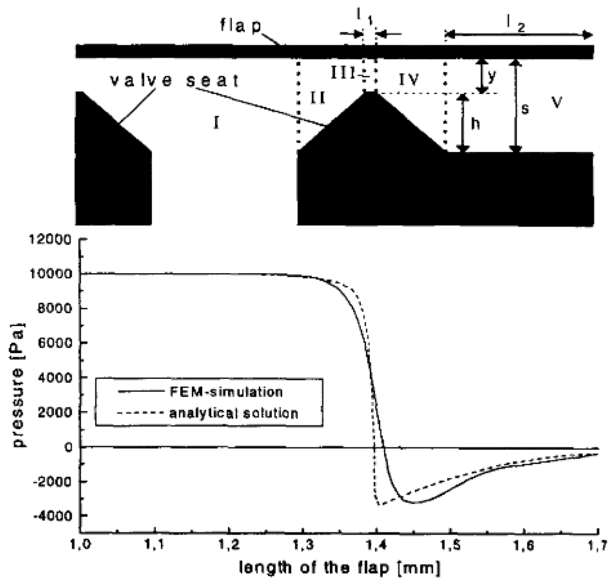

Fig. 4. Schematic view of the valve opening and simulated pressure distribution under the flap, including low-pressure region

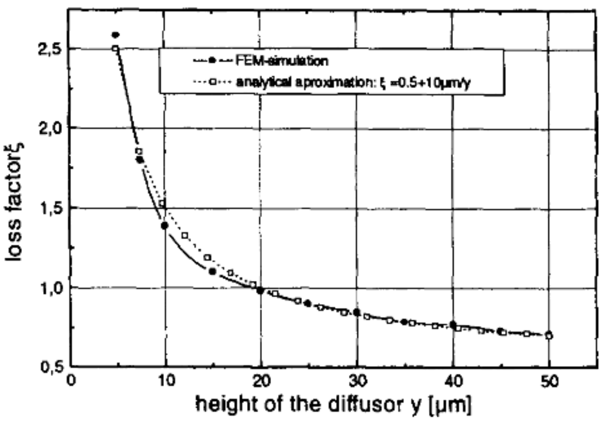

Fig. 5. Loss coefficient of the gap opening of the valve.

The geometry of the valve gap can be separated into five sections (Fig. 4). Sections I and II show decreasing cross section. Friction losses can be neglected and only acceleration losses have to be considered.

Eq. (3) simplifies to

$$\Delta p_{\rm I} = \frac{\alpha\rho\Phi^2}{2b^2}\frac{1}{s^2} \qquad \Delta p_{\rm II} = \frac{\alpha\rho\Phi^2}{2b^2}\left(\frac{1}{y^2} - \frac{1}{s^2}\right) \qquad (4)$$

where Φ is the flow rate, h the height of the valve seat, y the pressure-dependent displacement of the flap and b the length of the valve seat in the third dimension.

Sections III and V are gap shaped, and only laminar friction has to be considered:

$$\Delta p_{\rm III} = \frac{12\eta l_1 \Phi}{by^3} \qquad \Delta p_{\rm V} = \frac{12\eta l_2 \Phi}{bs^3} \qquad (5)$$

where $l_{1,2}$ are the lengths of the gaps.

In section IV, the fluid flow takes on a very complex structure. Because of the large opening angle of the diffuser, the liquid removes from the wall and forms vortexes. So the pressure loss is composed of acceleration and friction losses:

$$\Delta p_{\rm IV} = \frac{\alpha\rho\Phi^2}{2b^3}\left(\frac{1}{s^2} - \frac{1}{y^2}\right) + (p_e)_{1-2} \qquad (6)$$

An approximation for the friction loss in the diffuser is

$$(p_e)_{1-2} = \xi\frac{\rho\Phi^2}{2b^2y^2} \qquad (7)$$

assuming that the pressure loss is proportional to the kinetic energy of the fluid. ξ is a loss coefficient which depends on the lateral dimensions. It normally has to be determined by an empirical solution [11]. In our case, we determined the loss coefficient by simulating a diffuser with different dimensions, using FEM fluid simulation. The result is a characteristic line of the loss coefficient ξ of the diffuser which approximates the flow in section IV including vortices and removing effects at the boundary walls (Fig. 5):

$$\xi = 0.5 + \frac{10\ \mu\text{m}}{y} \qquad (8)$$

where y is the height of the diffuser.

Adding up these results, the flow rate Φ through the valve can be calculated as a function of the total pressure difference p and the height of the gap opening y:

$$p=\sum_{i=1}^{v}\Delta p_i(\Phi,y)\Rightarrow\Phi(p,y)$$

$$=\frac{-\frac{12\eta}{b}\left(\frac{l_1}{y^3}+\frac{l_1}{s^3}\right)+\sqrt{\frac{144\eta^2}{b^2}\left(\frac{l_1}{y^3}+\frac{l_2}{s^3}\right)^2+\frac{2\rho}{b^2}\left(\frac{\alpha}{s^2}+\frac{\xi}{y^2}\right)p}}{\frac{\rho}{b^2}\left(\frac{\alpha}{s^2}+\frac{\xi}{y^2}\right)} \tag{9}$$

To calculate the pressure-dependent flow rate through the valve, it is necessary to derive a connection between pressure p and flap displacement y. For this, Eq. (1) or Eq. (2), which are the result of the static FEM simulation, can be used.

Yet the displacement of the flap can be analytically calculated as well. Using Eq. (9) together with Eqs. (4)–(7), the lateral pressure distribution underneath the flap can be calculated (Fig. 5). This pressure distribution $p(x)$ can be used to determine the displacement of the flap using the differential equation for a cantilever beam [12]:

$$y''(x)=\frac{-M(x)}{EI_y}\quad M(x)=\int_0^l p(x)b\mathrm{d}x \tag{10}$$

where M is the torque, E the Young modulus of the silicon, I_y the moment of inertia, b the width and l the length of the flap. The static flow characteristic of the valve can be calculated by an iterative numerical solution which is similar to the iterative FEM simulation explained earlier. The final results of the FEM as well as the iterative analytical simulation are nearly identical (Fig. 3). Both take the significant influence of the low pressure in the diffuser region into account. It reduces the displacement of the flap and the flow rate of the valve with it.

4. Simulation of the dynamic behaviour of the valve

To understand the high-frequency behaviour of micropumps, we used a transient FEM analysis. For it we combined transient structural simulations of the valve, including the damping property of the liquid, with a transient flow simulation [13]. For a coupled fluid-structural simulation with ANSYS, some additional modules have to be integrated into the FEM program. Considering the physical effects between both models, each transient simulation step has to be carried out in two sub-steps:

- transfer of the velocity of the solid structure to the fluid model
- transfer of fluid pressure and fluid friction to the solid model

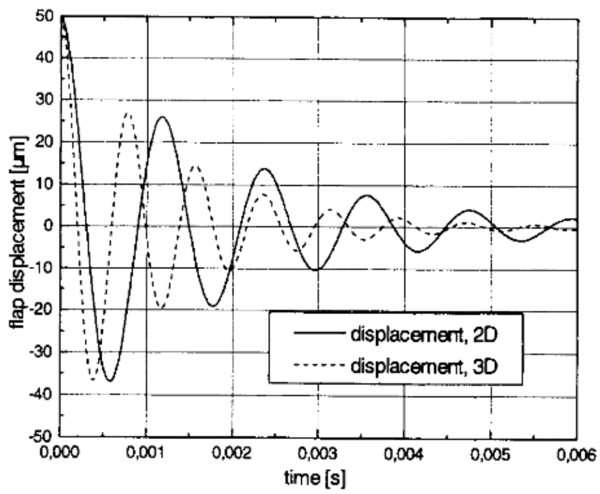

Fig. 6. 2D and 3D FEM simulations of a freely oscillating flap inside the fluid (water) using fluid-structural coupling.

Each transient step consists of two calculations, a mechanical simulation of the flap and, with the geometrical results as boundary condition, the simulation of the fluid flow. The transfer of the velocity and pressure data takes place at those nodes of the FEM mesh that are located at the boundary of the solid and fluid model.

As a first example, we simulated the dynamic behaviour of a flap freely oscillating in the surrounding fluid without any valve seat. The vacuum resonance frequency of the flap is 6000 Hz. The model consists of a 2D flap which has an initial displacement of 50 μm. Each oscillation of the flap needs about 100 transient simulation steps to consider the fluid-structural coupling. Because of the large damping of the fluid, the resonance frequency decreases to 830 Hz (Fig. 6).

The same simulation has been done for a 3D model of the flap. The 2D and 3D results are quite similar to each other, except for the resonance frequency. The fluid flow in a 3D model not only occurs over the top of the flap but also over both side edges. The fluid resistance decreases and the damping influence is smaller. Due to this, the resonance frequency of a 3D model is 1200 Hz.

The oscillation of the flap inside the fluid can be approximated by the basic differential equation of a driven mechanical oscillator [14]:

$$m\ddot{y}+d\dot{y}+ky=F \tag{11}$$

The spring constant k can be taken from the static displacement of the valve and is equal for the 2D and 3D models (65 N m^{-1}). The solution of Eq. (11) neglecting an external force ($F=0$) leads to a damped harmonic oscillation:

$$y=a_0\exp(-dt/2m)\cos\left(\sqrt{\frac{k}{m}-\frac{d^2}{4m^2}}t\right) \tag{12}$$

A comparison of this formula with the FEM simulation (Fig. 6) results in a damping constant $d=0.00259$ for the 2D model and $d=0.00200$ for the 3D model. The effective masses m are 2.36×10^{-6} kg and 1.02×10^{-6} kg, respec-

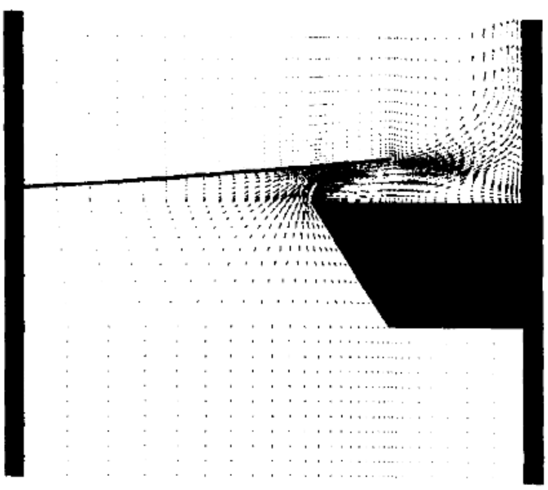

Fig. 7. Simplified 2D FEM model for a transient simulation of the valve, including the valve seat.

tively. These effective masses are much bigger than the real mass of the silicon valve flap, which is 1×10^{-9} kg. The effective mass includes the mass of the surrounding fluid, which has to be accelerated during a motion of the flap. With these three coefficients, k, d and m, together with the differential equation of the oscillator, Eq. (11), the transient behaviour of the flap can be analytically described.

As a second more complex calculation, we did a coupled transient simulation of the valve, including the valve seat. A simplified model was generated to decrease the time of calculation (Fig. 7). This is necessary because of the large number of transient time steps that are required to consider the influence of the valve seat. The valve seat itself has been simulated by contact elements, which prevent a penetration of the flap. As actuation, we assumed a sinusoidal pressure of different frequencies and a maximum amplitude of 2500 Pa. The results show the influence of the resonance frequency of the valve on the simulated flow rate. At a frequency of 200 Hz, which is much smaller than the resonance frequency of 1660 Hz (twice as much as for the free flap, because of the influence of the valve seat), the valve shows a quasistatic behaviour (Fig. 8). The driving pressure and displacement of the valve are in phase. At a frequency of 2500 Hz, the behaviour changes, basically because of a phase shift between the actuation and displacement of the valve, which results in a negative flow rate. This valve behaviour has a basic influence on the dynamics of the micropump.

The dynamic behaviour can also be derived by an analytical solution. The displacement of the valve can be calculated in a numerical way, solving Eq. (11). In doing so, the actuating force F is the product of the area of the valve seat A and the sinusoidal pressure p. The spring constant k again was simulated by a static FEM simulation and has a value of 155 N m^{-1} for this model. The area A of the flap, at which the pressure works, is 1.4×10^{-6} m^2. The damping constant and the effective mass are taken from the coupled FEM simulation of the freely oscillating 2D flap. The fluid flow through the valve gap is calculated by Eq. (9). The results show a good agreement with the FEM simulation (Fig. 8), but have been

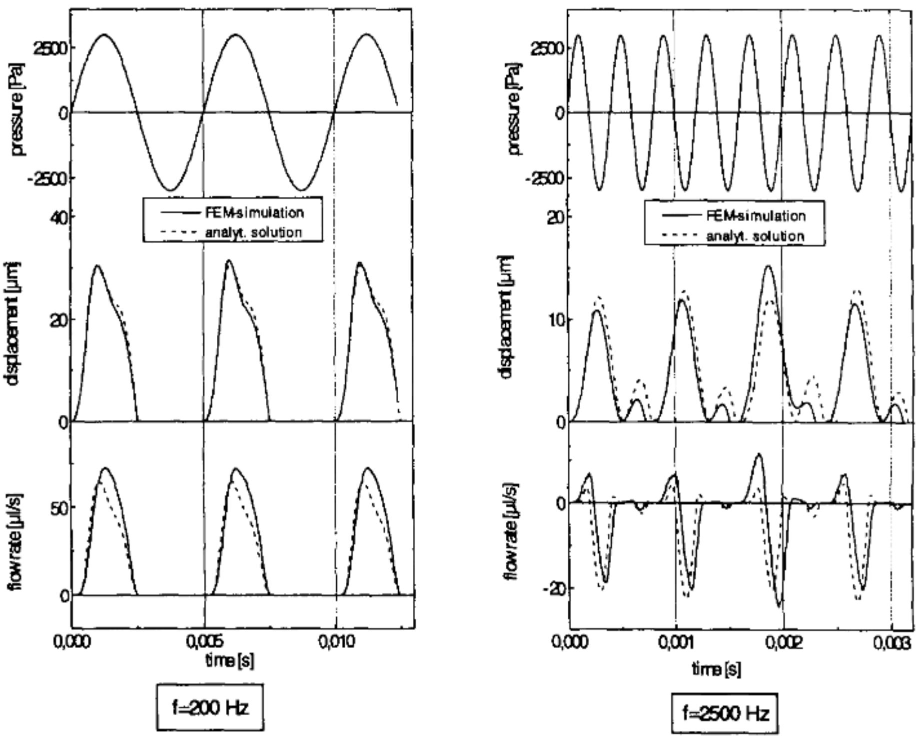

Fig. 8. Coupled fluid-structural simulation of the valve: driving pressure, displacement of the flap and flow rate through the valve at driving frequencies of 200 and 2500 Hz.

calculated much faster. Differences can be explained by the use of Eq. (9), which was simulated for static flow. Its use in a dynamic simulation produces an inaccuracy, since acceleration effects are neglected. For an exact simulation, the acceleration of the fluid in the valve opening has to be considered in the analytical solution. However, as can be seen from Fig. 8, the transient flow can be approximated by Eq. (9), derived for static flow, up to driving frequencies of some thousand hertz. This simulation method shows how to calculate more complex dynamic models by a combination of FEM simulation and analytical solutions.

5. Simulation of a bidirectional micropump

Up to now the fluid simulation of a whole micropump has been too complex a model for a coupled FEM analysis. The method of choice is a combination of an analytical solution with the results of the FEM simulation.

Reciprocating micropumps consist of an actuation unit and two passive check valves. Using an analytical approach, they can be described by three differential equations. The transient pump chamber pressure of an electrostatic micropump can be calculated by a differential equation [15,17]:

$$\dot{p}=\frac{\Phi_{iv}(p,y_{iv})-\Phi_{ov}(p,y_{ov})}{(\mathrm{d}V_0(p)/\mathrm{d}p)-(\mathrm{d}V_{gas}(p)/\mathrm{d}p)} \quad (13)$$

where iv = inlet valve and ov = outlet valve.

This equation can be derived from the continuity equation and includes the inlet and outlet flows Φ_{in} and Φ_{out}, the volume of the pump chamber V_0 and the volume of gas bubbles V_{gas}. For the calculation of the fluid flow, we use Eq. (9). The pressure-dependent volume displacement of the actuation membrane has been simulated by a static FEM simulation.

Eq. (13) has to be extended by two differential equations describing the dynamics of the valves [13]. For this, we use the basic differential equation of a driven mechanical oscillator:

$$\begin{aligned} m\ddot{y}_{iv}+d\dot{y}_{iv}+ky_{iv}&=F_{iv}\\ m\ddot{y}_{ov}+d\dot{y}_{ov}+ky_{ov}&=F_{ov}\end{aligned} \quad (14)$$

The spring constant k is taken from the static valve simulation. With it, the damping factor d and the effective mass m can be derived from the 3D FEM simulation of the freely oscillating flap. By a numerical solution of this system of coupled differential equations, we simulated the frequency-dependent pump rate of the micropump [13].

For low frequencies, the model results in the well-known quasistatic behaviour of minaturized diaphragm pumps (Fig. 9). The pump rate can be increased with higher driving frequency. At frequencies above 1200 Hz, the flow rate decreases and becomes negative for frequencies higher than the resonance frequency of the valves. This is due to the phase shift between actuation and valve displacement. As a result, the pump can be used as a bidirectional micropump. The direction of the fluid transport can be chosen by varying the driving frequency.

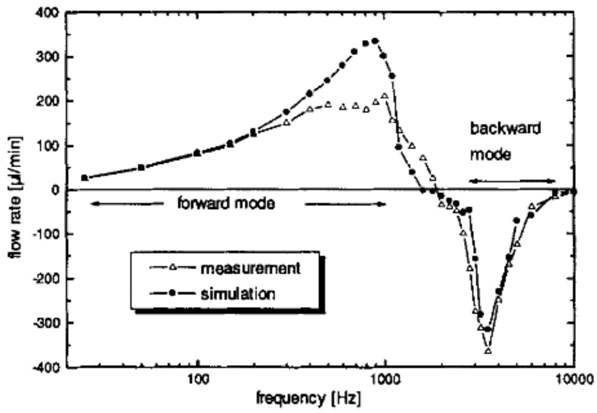

Fig. 9. Frequency-dependent pump rate of a bidirectional micropump.

The simulated results show very good agreement with the measurement of the electrostatic actuated micropump published in Ref. [16] (Fig. 9). Differences can be explained by inertia effects of the fluid in the tubes and by the approximation of the 3D system by a 2D model.

6. Conclusions

We presented FEM simulations and analytical calculations of the static and dynamic behaviour of a KOH-etched silicon check valve. It has been shown that, for the flow characteristic of the valve, the detailed pressure distribution around the valve seat has to be taken into account. The influence of the low pressure in the diffuser region of the valve has been considered in an iterative solution.

Furthermore, we investigated the transient flow through the valve by means of a coupled fluid-structural FEM analysis and compared the results with an analytical model of the valve dynamics. It has been shown that, at operation frequencies higher than the resonance frequency of the flap valve, the flow changes its direction. This is due to the phase shift between the flap opening and the actuation pressure. On the basis of these results, the working principle of a bidirectional micropump [16] can be simulated in good agreement with the measured results.

Acknowledgements

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Biographies

Jörg Ulrich was born in 1967 and received his diploma in physics from the Technical University of Munich, Germany, in 1994. From 1993 to 1994 he worked during his diploma thesis on the simulation of a micropump at the Fraunhofer-Institut für Festkörpertechnologie in Munich. Since 1994 he has been working for his doctorate at Siemens AG, Zentrale für Produktion und Logistik, in Munich, Germany, on FEM simulation of microfluidics and micromechanics.

Roland Zengerle was born in 1965 and received his diploma in physics from the Technical University of Munich, Germany, in 1990. From 1991 to 1995 he worked on the development of micro-actuators at the Fraunhofer-Institut für Festkörpertechnologie in Munich. He obtained his doctoral degree from the Universität der Bundeswehr in 1994. Since July, 1995, he has been leading the microfluidics department at the Hahn-Schickard-Institut für Mikro- und Informationstechnik in Villingen-Schwenningen, Germany. His current research topics include microactuators, minaturized fluid systems and integrated chemical-analysis systems.