Modeling and design optimization of a novel micropump

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ABSTRACT

The purpose of this paper is to give an overview about the design process of a new–type micropump. Four different coupled physical domains must be considered. The coupling effects on the pysical level are modeled using only commercially available finite element tools. From these simulations, a lumped network model is constructed and assigned with parameters, in order to optimize the design of the system. Based on the simulation results, the first prototype of the pump was fabricated and tested. It proved, that the investigated pumping effect can be used for microfluidic applications.

Keywords: finite–element modeling, coupled simulation, network modeling, micropump

INTRODUCTION

Microfluidic systems are recently gaining more and more attention from many research laboratories. Micropumps form the active part of such systems, as they have to supply the exact amount of liquid which is needed for the various applications. The most critical element in such pumps is the realization of the valves, in order to achieve a pumping effect. Some very sophisticated solutions use passive check valves (e.g. [1], [2]) for this purpose. A more simple but very reliable alternative is the concept of dynamic valves, as introduced by STEMME [3] and GERLACH [4]. Here, the direction of flow is determined by the design in terms of diffuser–nozzle elements. Another type of dynamic valve was suggested in [5], using the dynamic temperature change in two narrow fluid channels to achieve a net flow. The advantage of this principle is the truely bi–directional pumping behavior, which is determined by the electronic control circuit.

From the new principle of operation, it was decided to develop a first prototype of the micropump. Since there was no practical experience with this type of pumping effect, the whole design was based entirely on modeling and simulation. However, the behavior of the system strongly depends on four different physical domains, which are tightly coupled with each other. Some of the coupling effects can not even be modeled by conventional simulation software, especially electromechanical coupling and fluid–structure interaction. The intention of this paper is therefore to show the problems which occur in such a design process and to demonstrate a possible solution strategy.

THE CONCEPT OF DYNAMIC THERMAL VALVES

The operation principle of a dynamic valve type micropump is shown in figure 1. Rather than a static flow rectification characteristics, the valves show a direction–dependent flow resistance, which is only present in the dynamic mode, i.e. during pumping. The larger the difference of this resistance in both directions, the higher the efficiency of the pump.

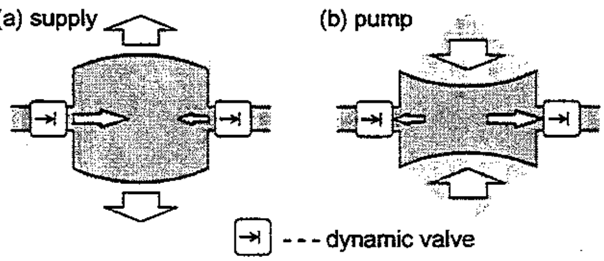

Figure 1: Concept of dynamic valve

The ratio of pressure drop to volume flow in a narrow channel with rectangular cross section can be expressed by the viscous flow resistance:

$$R_{visc} = \eta(T) \cdot \frac{Po \cdot l \cdot (w+h)^2}{2 \cdot (w \cdot h)^3} \qquad (1)$$

where the viscosity η is a function of temperature T. The geometric dimensions of the channel l, w and h as well the POISEUILLE constant Po of the cross section [6] might be considered as constant.

From the physical effect, that the viscosity of liquids strongly depends on the temperature (see figure 2), the flow resistance of a narrow fluid channel can thus be controlled by controlling the temperature of the fluid in the channel. If the thermal time constants are small enough, the process of heating and cooling can be synchronized with the movement of the pump membrane. Theoretically, a pumping effect should be observed in such a case.

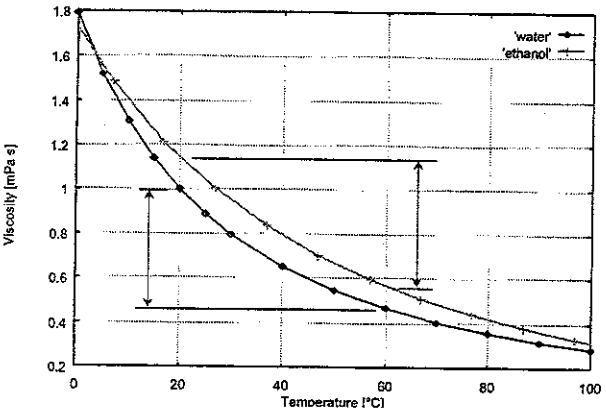

Figure 2: Viscosity of water and ethanol as a function of temperature

PROTOTYPE DESIGN

The final design of the pump is shown in figure 3. The whole structure consists of one silicon substrate with pyrex glass anodically bonded on top of it. A pump membrane (anisotropically etched into the back side of the substrate) with bulk PZT fixed to it creates the driving pressure in the pump chamber due to the piezoelectric actuation. Pump chamber and fluid channels are etched into the front side of the chip. Inlet and outlet channel comprise a narrow part in order to give high flow resistance. Boron doped heating resistors are located on top of the narrow parts, to form the dynamic thermal valves. The thermal valves are the most critical point in the design as well as for fabrication. A photo of such a valve is shown in figure 4.

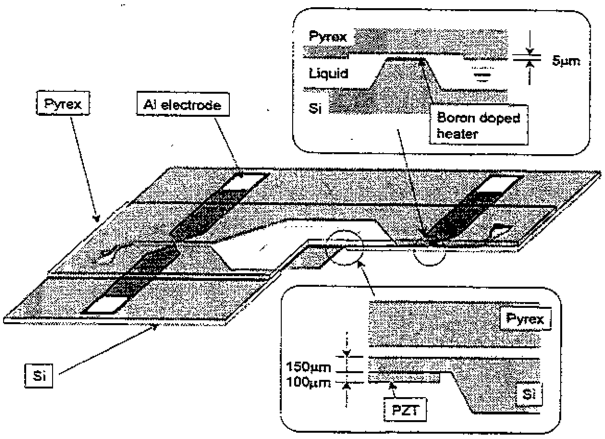

Figure 3: Final pump design

Although presented at the beginning of this paper, the final design is the result of the simulation and optimization process. The main questions which had to be answered can be summarized as follows:

1. What are the optimum geometry parameters to yield high volume flow, high temperature difference and small mechanical and thermal time constants?

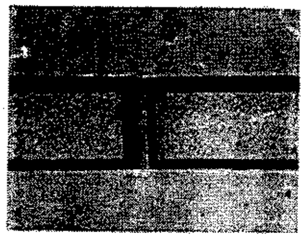

Figure 4: Photograph of thermal valve

2. What is the optimum pulse sequence to control membrane actuation as well as the two heating resistors?

Since there are too many geometry parameters, the optimization must be focussed on a few of them only.

DESIGN STRATEGY

The design cycle might be regarded as a bottom–up process, starting from the detailed geometry and material data, as obtained either from process simulation, data sheets or measurements. As a first step, the involved physical effects must be investigated. Four different physical domains have to be considered, as shown in figure 5.

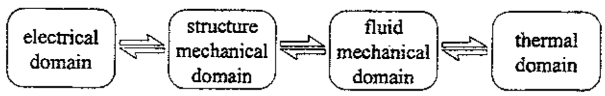

Figure 5: Coupled physical domains

It becomes obvious, that the domains are more or less coupled with each other. Hence, they can not be modeled independently. Mainly, three types of coupling must be considered: electromechanical coupling (for the piezoelectric actuation of the pump membrane), fluid–structure coupling (volume displacement of the pump membrane) and thermo–fluiddynamical coupling (temperature distribution in the flow channel). Each coupled effect will be investigated seperatly within the following section, focussing only on a limited part of the whole system. The finite element program ANSYS was used as simulation tool [7].

In general, the described method makes it possible to simulate the whole system on the pysical level within one simulation run. However, this would require such a hugh hardware performance, that it could only be solved by supercomputers. Therefore, the interaction of the whole system is modeled on a higher abstraction level, using lumped network elements. In order to enable design optimization, the design variables which are to be optimized must be visible at this level. For this purpose, parameter dependencies in terms of data tables or regressional functions must be obtained from the finite element simulations.

The whole design approach can be summarized as follows:

1. Modeling of coupled physical phenomena using finite element simulation
2. Extraction of fixed parameters (no optimization!) and variable parameters (which are to be optimized!) from the finite element simulation
3. Construction of lumped system model and parameter optimization

At each modeling level, the designer has to verify its simulation model. Especially for fluid and thermal simulation, this is still an unsolved problem. The proposed approach will be demonstrated next.

INVESTIGATION OF COUPLED PHYSICAL PHENOMENA

Piezoelectric coupling

The three-dimensional model of the membrane bimorph is shown in figure 6. The square shape of the membrane results from the anisotropical etching process. The geometry of the bulk PZT is mostly determined by the providing company. The remaining geometry parameters are thickness and lateral length of the silicon membrane.

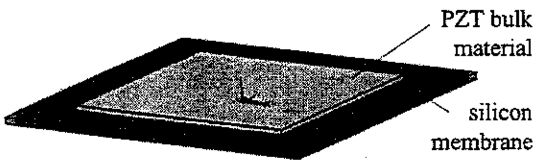

Figure 6: FEM-model of pump membrane

For model verification, the static and dynamic displacement of bimorph membranes was measured by a laser interferometer. The simulated displacement was up to four times larger than the measured value. This effect is due to several reasons, mainly the quality of the mechanical contact between the PZT material and the silicon membrane. Based on this measurements, the simulation model can be considerably improved.

Fluid-structure interaction

The purpose of simulating the fluid-structure interaction between membrane displacement and fluid flow in the pump chamber is to give a conclusion about the following concerns:

1. What is the dynamic behavior of the membrane bimorph under fluidmechanical load?
2. Is it possible to describe this coupled behavior by lumped circuit elements?
3. What are the mechanical time constants for the fluid flow in the channels?

The problem can not be solved by one finite element program itself. Instead, two different solvers must be coupled with each other. The programs ANSYS and FLOTRAN have been used to model the membrane and the fluid, respectively. Nodal results in terms of displacement and pressure must be transfered between both programs. The equilibrium state between the two models can only be found by an external iteration loop, whose realization is left to the user. The iteration process must be repeated for each time step. Therefore, the simulation becomes extremely time-consuming. The whole process is scetched out in figure 7.

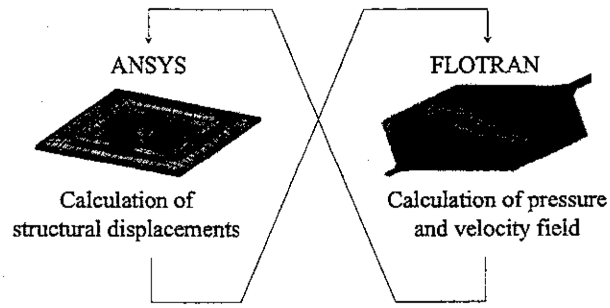

Figure 7: Simulation of fluid-structure coupling

The main problem with this kind of coupled simulation is the convergence of the external iteration algorithm. The most simple approach are relaxation-based methods, such as the GAUSS-SEIDEL-algorithm used by ULRICH [8]. However, it can be shown that this method fails to converge for strongly coupled problems, as they are present in most cases if liquids are the considered

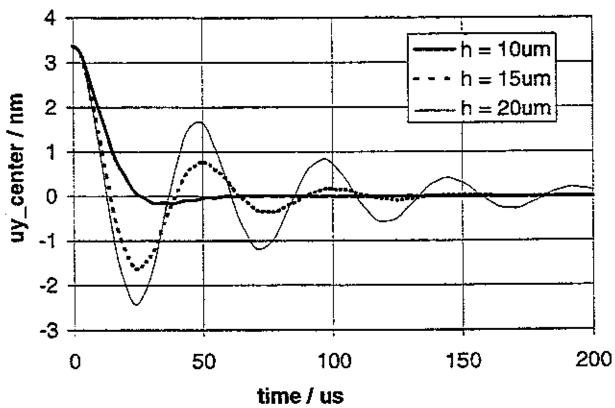

Figure 8: Simulated membrane displacement

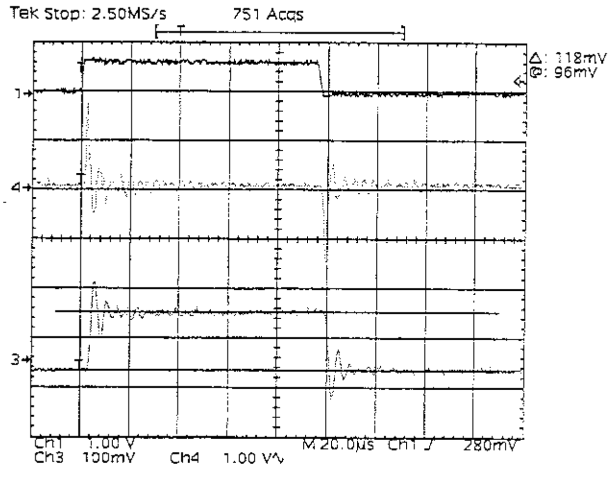

Figure 9: Measured response of membrane velocity (middle) and displacement (bottom) to an applied voltage pulse (top)

fluid instead of gases [9]. An algorithm with better convergence stability is the NEWTON–iteration, whose application for the simulator coupling is currently under investigation.

For the construction of a lumped network model, the transient simulation was carried out for air as the fluid medium in the pump. Because of calculation time, only two–dimensional models were used. The results of the simulation can therefore only qualitatively be compared to measurements. Figure 8 shows the transient simulation of the membrane center deflection for three different values of the channel height h. Figure 9 gives the measured behavior of velocity and displacement at the membrane center obtained by laser interferometry.

Thermal flow simulation

The third type of coupling is the interaction between thermal and flow behavior of the heated channel. This effect can be simulated using conventional CFD software packages such as FLOTRAN. The overall goal of the finite element analysis can be summarized as follows:

1. to investigate the influence between the thermal condition of the channel and its flow behavior
2. to evaluate the required amount of heating power
3. to determine the thermal time constant for heating and cooling

A view of the finite element model is given in figure 10. The structure of the channel (as shown in figure 4) was simplified to a two–dimensional model. The critical point is the proper treatment of the thermal boundary conditions. If the silicon chip is connected to a heat sink body (with ideal thermal contact), a constant temperature at the bottom of the chip might be a valid

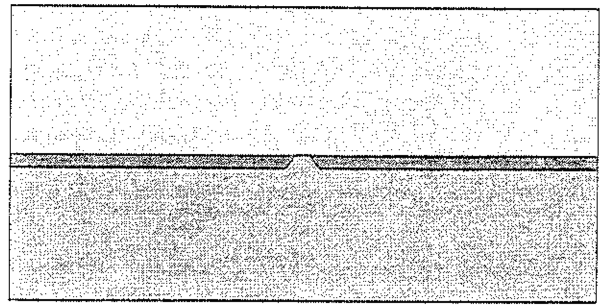

Figure 10: FEM model of the channel

assumption for the time range of several ms. However, if a constant thermal convection coefficient is chosen instead, the maximum temperature difference decreases dramatically. Therefore, maintaining a constant temperature at the bottom of the silicon chip is a necessary requirement.

To investigate the influence between flow and temperature distribution in the channel, static calculations were carried out. The result of a static analysis is shown in figure 11. The dynamic behavior of the heating and cooling process must be determined by a transient simulation. The simulated temperature as a function of time at three different points of the channel is plotted in figure 12.

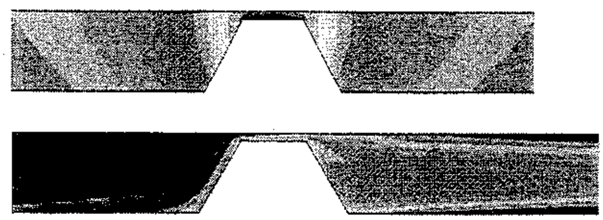

Figure 11: Temperature distribution in the channel with zero flow (top) and maximum flow (bottom)

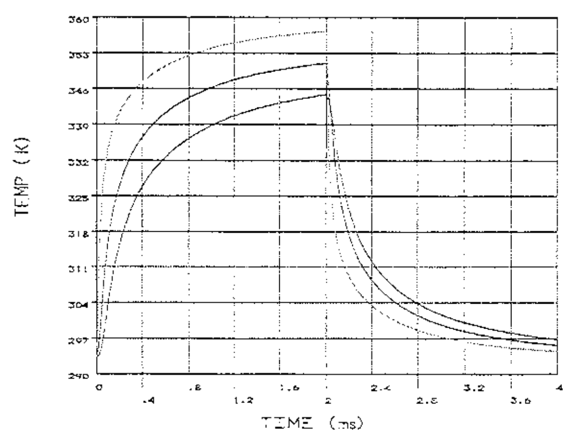

Figure 12: Time history for heating and cooling at three different points of the channel

network type	electrical	fluidic	thermal
through quantity	current	volume flow	heat flow
across quantity	voltage	pressure	temperature
capacitor element	electrical capacity	volume compliance	thermal capacity
inductor element	electrical inductance	fluidic mass	(not defined)
resistor element	electrical resistance	viscous flow resistance	thermal resistance

Table 1: Definition of concentrated network variables and elements

From the finite element simulations, several conclusions can already be drawn without considering the entire system:

1. A constant temperature at the bottom of the silicon chip is important for obtaining a stable temperature difference. The amount of heating power produced by the resistors must be compensated by a heat sink body.
2. The geometrical size of the heated area has to be as small as possible, in order to minimize both the thermal time constant as well as the total heating power required to achieve a certain temperature difference. (The limiting fact is the fabrication technology as well as the required volume flow.)
3. The height of the channel should be as small as possible, to prevent a large temperature gradient in the channel in vertical direction. (This is limited by the high risc of blocking which is given by a too narrow channel.)

CONSTRUCTION OF A PARAMETERIZED SYSTEM MODEL

Since only two different finite element solvers were used in the last section to model the coupling mechanism between four different physical domains, the entire system could be simulated (in principle) by coupling two finite element solvers. However, even if the necessary calculation effort could be handled by a supercomputer, the simulation time would not allow to investigate more than a few parameter settings. Therefore, there are two major goals for simulating the entire system:

1. investigation of the working behavior of the pump
2. to find an optimum parameter set within limited time

The first step towards a lumped model is to decide which concentrated variables will be used to describe each subsystem. As in the electrical domain, where voltage and current are commonly used in terms of network variables, generalized KIRCHHOFF's networks represent a powerful tool to model subsystems with different physical domains. The choice of "through" and "across" quantity as well as the resulting network elements are given in table 1.

Piezoelectric pump membrane

It can be seen from table 1, that there is no mechanical network defined. This is not necessary, since the pump membrane is modeled as a four–terminal transducer element, which forms the interface between electrical and fluidic network. The electrical characteristics of the piezoelectric actuator can be described by its capacitance C_{el}. The mechanical behavior in the static case is determined by the volume compliance, which is defined as the ratio between volume displacement dV and pressure change dp at constant electrical voltage v:

$$C_V = \left. \frac{dV}{dp} \right|_{v=const} \qquad (2)$$

The value of C_V can easily be determined by a static FEM analysis.

In the dynamic case, the membrane is characterized by its first eigenfrequency f_0, which can be calculated by a FEM modal analysis. From f_0, the value of the fluidic mass M_V, is given by the relation

$$M_V = \frac{1}{C_V\,(2\pi f_0)^2} \qquad (3)$$

The coupling between electrical and fluidic network is caused by the piezoelectric effect. Two linear transducer coefficients are introduced in order to describe the interaction:

$$k_{v-p} = \left. \frac{dp}{dv} \right|_{q=0} \qquad (4)$$

$$k_{q-i} = \left. \frac{di}{dq} \right|_{v=0} \qquad (5)$$

Both coefficients can be determined by a static FEM analysis.

The resulting network model of the membrane can be seen in figure 13 as part of the system model.

Thermal dynamic valve

The effect of the dynamic valve is described by electrical, thermal and fluidic network elements, as can be

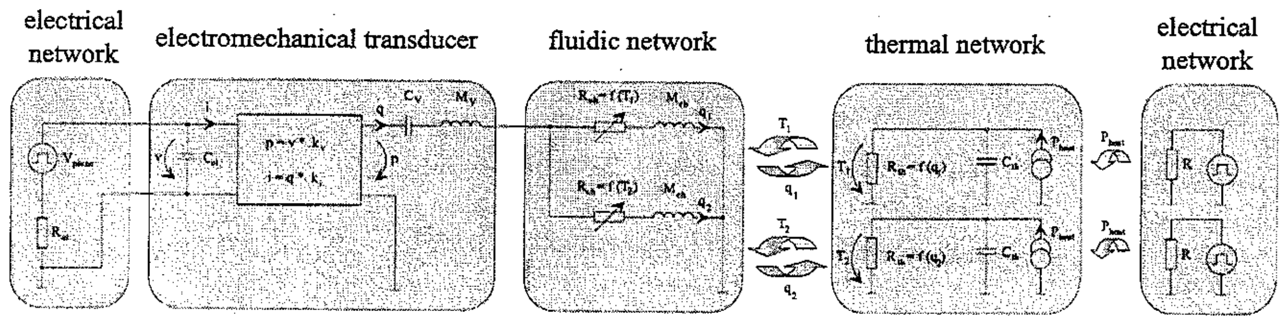

Figure 13: Network model of the micropump

seen from figure 13. The electric resistance R of the boron doped heater elements causes the heating power $P_{heat} = v^2/R$ (with v as the applied voltage) to be generated. In the thermal network, this value is induced as a current source. From multiple steady–state thermal FEM analysis, the thermal resistance R_{th} is determined as a function of the volume flow q. The value of the thermal capacity C_{th} can be estimated from the transient thermal simulation (see figure 12).

The fluidic network elements represent the viscous flow resistance of the channel R_{ch} (as a function of the channel temperature) and the fluidic mass of the channel. Both values must be determined from the finite element models.

Parameter optimization

In order to enable design optimization, it must be decided which design parameters are considered to be "fixed" and which are "variable" (i.e. they are to be optimized). For the variable parameters, the network quantities which were determined from the finite element models must be derived as functions of those parameters.

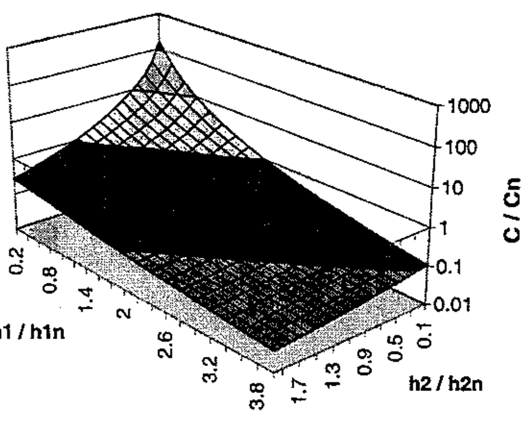

Figure 14: Membrane compliance C_V as a function of membrane thickness h_1 and PZT thickness h_2 (normalized to C_n, h_{1_n} and h_{2_n})

To demonstrate the approach, the thickness of the membrane (h_1) and the thickness of the PZT (h_2) were chosen as variables. The resulting values for C_V, M_V, k_{v-p} and k_{q-i} are to be represented as functions of them, as demonstrated in figure 14.

CONCLUSION

A micropump based on the coupling effects between four different physical domains was investigated. Since no commercial simulation software can handle all the necessary coupling mechanisms within one model, they were modeled seperately using finite element solvers. The behavior of the whole system is described by a lumped network model, whose parameters are determined by FEM analysis.

The micropump has already been fabricated and tested successfully. It has proved the efficiency of a design procedure, which is based on modeling and simulation.

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