

Full Coupling Simulation of a Membrane Micropump

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ABSTRACT

This paper presents full coupling simulation of a whole micropump: three-dimensional (3-D) numerical simulations are carried out with consideration of interaction between electro mechanics and solid mechanics, solid mechanics and fluid mechanics. The simulation of a membrane micropump with diameter 6 mm, driven by PZT disc is implemented using *CFD-ACE+*, the commercial software from *CFDR*. A series of transient simulations are carried out under the excitation of Sine-wave voltage 70V and at the frequencies 8, 50, 100, 200 and 500 Hz respectively. The deflections of membrane, the detailed fluid fields and the pump performance curves are shown. Computational effort required for the case studies is discussed. The present simulation shows that computational CPU time increases with the increasing electrical driving frequency. The 3-D coupling simulation is acceptable for design and analysis in the lower actuating frequency region, i.e. $f \leq 50$ Hz for the present micropump model. In higher frequency region, extensive CPU time is required.

Keywords: Drug delivery device, MEMS, membrane micropump, CFD simulation, piezoelectric pump.

1 INTRODUCTION

PZT (lead (*Plumbum*) Zirconate Titanate) actuated membrane micropumps with diffuser valves are promising for a variety of applications in micro-electro-mechanic systems (*MEMS*), micro chemical assays and drug delivery systems due to their operation-reliability, delivery-accuracy, simplicity for fabrication, and applicability for the fluid flow with particles. The operation of the micropumps is a complex process as it involves the knowledge of electro mechanics, solid mechanics and fluid mechanics. Some research progress has been made on pump principles and performances [1-8]. The simulations of the whole pumps reported are mostly based on lumped-mass models [4], simplified dynamic system model [5] and simplified analytical models [6-8], etc. So far, accurate, flexible and broadly applicable model is still unavailable for micropump design and analysis due to its complex coupling nature. The low Reynolds number (*Re*) characteristics of the laminar fluid flow within the micropump components causes further errors if the

evaluation of the components are based on the analytical methods or testing data for high *Re* turbulent flow. To prevent such drawbacks, it is ideal to carry out 3-D simulations of whole micropump in order to show the flow fields in details and take full coupling effects into consideration. Generally it is regarded as impractical to use full coupling simulation for micropump design or analysis, due to the possible extensive computational effort required. In the present work, we want to know whether it is practical under some conditions. Our 3-D numerical simulations of a membrane micropump with diameter 6 mm are carried out using the *CFD-ACE+*, the commercial package from *CFDRC*, with the consideration of interaction between electro mechanics and solid mechanics, solid mechanics and fluid mechanics. The PZT membrane micropump is excited by Sine-wave voltage 70V and frequencies 8, 50, 100, 200 and 500 Hz. The 3-D coupling simulations are also significant for the evaluation of other simplified system models such as lumped-parameter models.

2 THE PUMP MODEL AND SIMULATIONS

The pump geometry and the meshes are shown in Fig. 1, where the micropump is made of Silicon Nitride (*Si3N4*) with pump diameter 6mm, height 0.6mm and the membrane thickness 0.05mm. PZT disc is 5mm in diameter and 0.05mm in thickness.

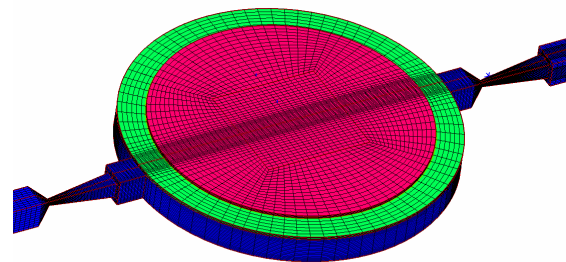


Figure 1: Micropump geometry and meshes

The other computational parameters are given as follows.

- Diffuser throat: $0.04\text{mm} \times 0.04\text{mm}$.
- Inlet & outlet channels: $0.5\text{mm} \times 0.5\text{mm}$.
- Pump flow rate: $\dot{q} \geq 33\text{ nL/s}$ or $3 \times 10^{-8}\text{ L/s}$.

- Operation voltage:

$$V = V_0 \sin(360 \cdot f \cdot t) \quad (1)$$

where $V_0 = 70$ Volts. Higher voltage may cause some problems for practical applications, such as heat dissipation and operation safety.

- Operation frequencies $f = 8, 50, 100, 200$ and 500 Hz.

- Fluid density: $\rho = 997$ kg/m.
- Fluid dynamic viscosity: $\mu = 8.55 \times 10^{-4}$ kg/m-s.
- Reference pressure: $P = 10^5$ Pascal.
- Reference temperature: $T = 300$ K.

Commercial software CFD-ACE+ is applied to simulate the transient flow in the micro pump, with couplings between driving voltage and PZT material, PZT material and membrane, the membrane and fluid.

To simulate solid deformation and stress, Finite Element method (FEM) with structured elements is adopted. The discrete algebraic equations are solved by direct method. For fluid flow field, Finite Difference Method (FDM) is chosen. In the simulation model shown in Fig. 1, the total grid node used is about 70789, FEM volume is 9588 and the total cells are 62564. Auto re-mesh option is used. In all the case studies, the total mesh numbers are fixed. The coupling frequency is set to be unit so that the information is updated every iteration.

The total number of time steps is set as 500 for simulation of 1.25 periods. Therefore, for one period T , 400 time steps are used ($N=400$). The time step shown in table 1 is determined by

$$\Delta t = 1 / (f \cdot N) \quad (2)$$

The solution at the first 0.25 period (the first 100 time steps) may not be accurate because the initial flow field in the pump is specified as constant pressure and zero velocities. The discrete algebraic equations are solved by numerical iteration at every time step.

$f(\text{Hz})$	8	50	100	200	500
$T(s)$	0.125	0.02	0.01	0.005	0.002
$\Delta t(s)$	3.125×10^{-4}	5×10^{-5}	2.5×10^{-5}	1.25×10^{-4}	5×10^{-5}

Table 1: Frequencies, periods, time steps and iterations

The average flow rate of micropump is dependent on the actuating electric voltage V_0 , frequency f , and pressure rise through the micropump ΔP . Here, $\Delta P = P_{out} - P_{in}$, where P_{in} and P_{out} are the pressures at the entrance and the exit of the pump. Therefore, we have

$$\dot{q} = F(V_0, f, \Delta P) \quad (3)$$

The effects of the electric frequency to the average flow rate of the micropump are investigated under the following conditions with zero pressure differences $\Delta P = 0$. The effects of both frequencies and pressure differences $\Delta P \neq 0$ are also carried out to show the pump performance.

2 RESULTS AND DISCUSSIONS

A series of transient coupling simulation of the micropump are carried out.

Typical convergent history of the iteration within a time step is presented in Fig.2, where U , V , and W are the residuals of velocity components in the x, y and z directions respectively; P and Del_max are the fluid pressure and the maximum deformation of the solid membrane. The number of iteration is determined such a way that it will be big enough to make the normalized residuals less than 10^{-3} , i.e. $|R_U / U| \leq 10^{-3}$. Therefore a convergent solution is guaranteed at each time step.

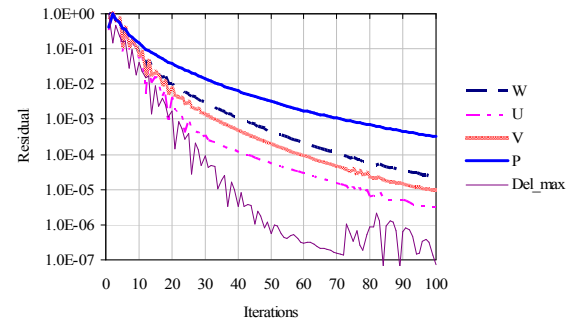


Figure 2: Convergence History

2.1 Flow fields and membrane deflections

The simulation results are shown in Fig.3-5. The velocity distribution in the supply phase is given in Fig. 3. The fluid is flowing into the pump chamber from both inlet and outlet, because electrically actuated PZT disc moves up together with the membrane in the moment.

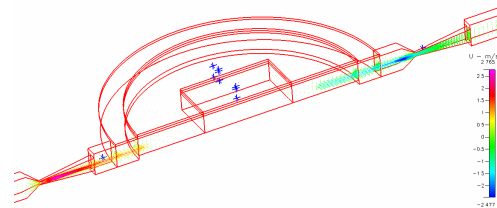


Figure 3: Velocity field

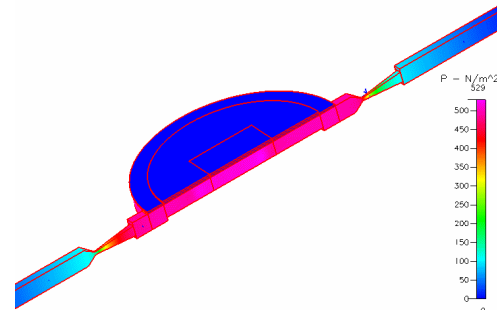


Figure 4: Pressure contour

The pressure contour in a pump phase is shown in Fig. 4, where the pressure inside the chamber is high because the membrane moves downwards in the moment.

The membrane deflections in a supply phase are shown in Fig. 5, where the PZT disc and the membrane are moving upwards. The maximum membrane is located at the central part of membrane.

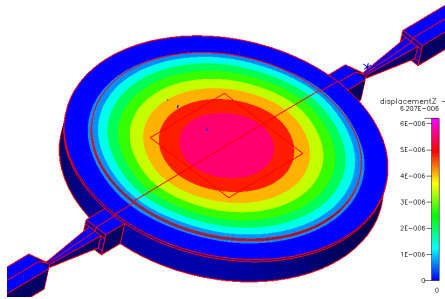


Figure 5: Membrane deflections

2.2 Pump flow rates and performances

The instant flow rates at frequency $f = 50$ is given in Fig.6, where the positive values represent that fluid flows into the pump chamber through the inlet or the outlet, and the negative values mean that fluid flows out of the pump through the inlet and the outlet. It shows that the flow into or out of the pump chamber varies with time and actuating voltage periodically. The flow period is same as the actuating voltage period, as expected.

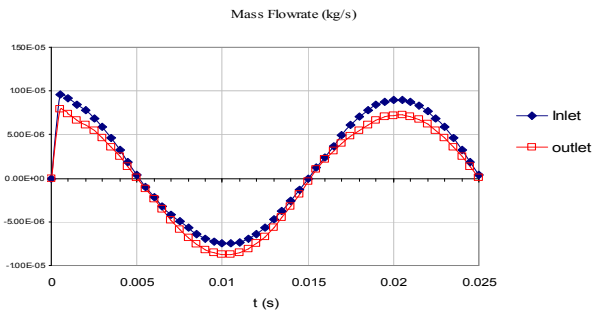


Figure 6: The time history of flow rate at inlet and outlet ($f = 50$ Hz, $\Delta P = 0$)

The pump principle can be demonstrated by the curves in Fig.6. The maximum flow rate values of the inlet and the outlet are different. For the inlet, the maximum positive value is larger than the maximum absolute negative value in the same period. In the contrary, for the outlet, the maximum absolute negative value is larger than the maximum positive value. Comparing the flow rate through the inlet and through the outlet, the maximum inflow through inlet is larger than the maximum inflow through the outlet. There is much more inflow through the inlet than that through the outlet at the supply phase, and there is much less outflow through the inlet than that through outlet at the pump phase. The overall effect of each complete period leads to an average net from inlet through the pump to outlet.

The average mass flow rate is obtained by numerical integration over one period of flow rate shown in Fig. 6 for the frequency $f = 50$ Hz. Fig.7 shows the relationship between the averaged flow rates and actuating frequencies under zero pressure head $\Delta P = 0$, where the horizontal dashed line corresponding to the desired operational

volume flow rate $q = 33.3 \text{ nL/s}$. The results indicate that the average flow rate increases with increasing frequencies and reaches its maximum value at $f_0 = 200$ Hz. The average flow rate decreases beyond frequency 200 Hz. Therefore, the operating frequency should be chosen to be less than 200 Hz. In the practical application, the pump operating condition can be determined using overall pump performance curves Fig. 8, according to the desired flow rate and pressure head.

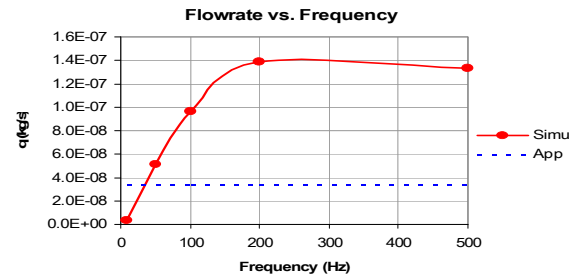


Figure 7: The pump performance-flow rate vs. frequency at zero pressure head ($\Delta P = 0$)

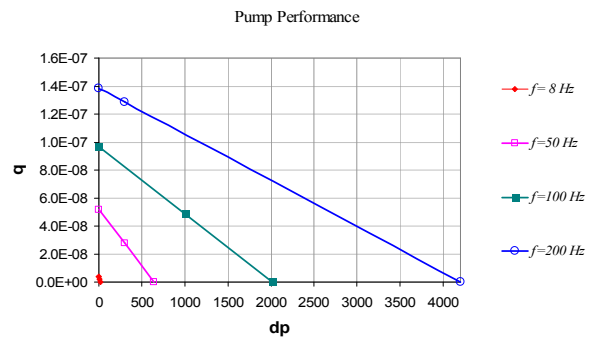


Figure 8: The pump performance-flow rate q vs. pressure difference ΔP and frequency f

The overall pump performances, the effects of pressure differences and frequencies on mass flow rates are shown in Fig. 8, all based on the full coupling simulation results. The simulations are carried out at $f = 8, 50, 100, 200$ Hz respectively, and with different pressure heads $\Delta P > 0$. The curve in Fig. 7 shows that the pump application frequency should be less than 200 Hz. Therefore the time consuming case studies for $f = 500$ Hz at non-zero pressure heads are dropped. With the pump performance curves like in Fig. 8, user can choose the driving frequency to obtain desired pressure head and delivery flow rate.

2.3 Computational effort

The computational effort is a critical concern for application of full coupling simulation to practical micropump design and analysis. The CPU time for 3-D full coupling simulation of a micropump is affected by many factors, such as geometry, material properties, meshes, numerical methods (FD, FEM, iteration methods) and parameter selection (time steps, relaxation factors, accuracy), operational conditions (voltage, frequency and pressure head), etc. In the present simulation, we try to fix the most of the affecting effectors and evaluate the effects of operational parameters, namely the actuating frequency f and pressure head ΔP on simulation CPU time. We want to know whether it is affordable to simulate the whole pump for design and analysis.

In all the present simulations, design parameters, meshes, numerical methods and actuating voltage are fixed. Time step Δt is chosen in such a way that there are 400 time steps in a complete period for any frequency, as shown in expression (2) and table 1. In this case, the computational effort should depend on the pressure head ΔP and frequency f .

It is found that with fixed frequency f , the CPU time is nearly same for different pressure heads ΔP . Therefore the effects of pressure heads can be ignored, if the present coupling simulation routine is adopted.

In contrary, the simulation CPU time shows that the actuating frequency plays a very important role in computational effort. It is found that with the increasing frequency and decreasing time step, the relaxation smaller factors must be chosen to obtain the convergent solutions with the desired accuracy. The smaller relaxation factors lead to more iterations for computational stability and convergence. The iterations required for accuracy, together with the total computational efforts are shown in table 2 and Fig. 9.

$f(\text{Hz})$	8	50	100	200	500
Iterations	50	60	80	300	1000
CPU	100 hrs 4 days	118 hrs 5 days	198 hrs 8 days	636 hrs 26.5 days	2133 hrs 89 days

Table 2: The frequency, iterations and CPU time

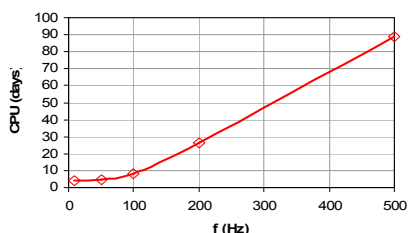


Figure 9: CPU time vs. frequency

It is found that 4 -5 days are required to carry out a case study at a frequency less than 50 Hz. At the critical frequency $f_0 = 200$ Hz, 26.6 days are required. Beyond the

critical frequency, the computational effort is extensive. It may take about three months to obtain the simulation results for frequency $f = 500$ Hz.

3 CONCLUSIONS

A series of transient coupling simulations of a PZT membrane micropump are carried out under the excitation of Sine-wave voltage 70V and at the different frequencies 8-500Hz respectively. The deflections of membrane, the detailed fluid fields and the pump performance curves are shown. The present simulation shows that computational CPU time increases with the increasing electrical driving frequency. The 3-D coupling simulation is acceptable for design and analysis in the lower actuating frequency region, i.e. $f \leq 50$ Hz for micropump model. In higher frequency region, extensive CPU time is required.

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