Computational Design Analysis for In-Plane Microfluidic Valves

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ABSTRACT

Simulations of fluid flow across in-plane microvalves were performed using an advanced multi-physics commercial software system and compared with experimental data. Model validation required careful consideration of leakage pathways left by fabrication artifacts. Following model validation, the effects of leakage pathways caused by variations in sealant thickness were explored. These results were used to predict the effect of leakage gap thickness on the ratio of flow resistances across the open and closed valves. The effects of structural modifications on the valve performance were also explored in this study.

Keywords: Unidirectional Microvalves, CFD-ACE+, Flow Resistance

1 INTRODUCTION

The traditional trial-and-error experimental approach towards the design optimization of microfluidic components is costly and often requires extensive physical prototyping and testing. This method is being currently replaced in the microfluidics community by more cost-effective CAD-based approaches, which enable rapid virtual testing and provide valuable insight into the function of individual components. This paper describes the application of CAD tools, developed at CFD Research Corporation, for computational design studies on in-plane, free-floating, uni-directional silicon microfluidic valves being developed and tested at UC Berkeley as part of a novel micromixing system [1-3].

The in-plane microvalves and interconnecting microchannels are etched in 75 µm thick SOI and released by an etch of the 2 µm underlying oxide. The release process provides a 2 µm clearance for in-plane valve movement within the channel and also creates leakage pathways by undercutting the sidewalls of the channels by approximately 6 µm. The release process also produces 2 µm leakage pathways extending 6 µm into the silicon bulk material underside of the valve. Additional leakage pathways result from the gaps left by layers of epoxy used to seal the channel to a glass cover. These leakage pathways are approximately 2 µm in height and extend approximately 20 µm on each side of valve. The major objective of this study was to evaluate the effect of changes in the fabrication process and in the valve design for optimization of pressure-flow characteristics and reduction of leakage flow.

2 METHOD OF APPROACH

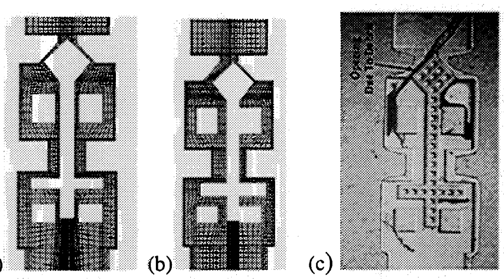
Modeling was performed with the CFD-ACE+ multi-physics software suite [4], which includes grid generation (CFD-GEOM), data visualization (CFD-VIEW), graphical problem setup (CFD-GUI), and coupled fluidic, thermal, mechanical, electrostatic, and magnetic physical model solvers (CFD-ACE+). Simulation of the dynamic valve function represents a classical solid/fluid interaction problem. However, the valve remains in either the fully open or fully closed configuration during a major portion of the mixing cycle. Therefore, we chose to evaluate valve functionality under these static conditions as a first step.

Fluid flow was modeled as 3-D, steady-state, incompressible, Newtonian flow. The flow domain included the upstream and downstream microchannels, valve housing, leakage zones created by fabrication artifacts, and the solid valve. The macro tubing and connectors used to measure pressure drop across the open/closed valves were not considered in the simulations.

Models of the valves included fabrication and sealing artifacts, which produced leakage paths around the actual valves. Three-dimensional models were generated in CFD-GEOM by first creating 2-D faces representing zones of solid and fluid. The faces were extruded in the third dimension in increments which represented leakage dimensions and dimensions of the channel containing the microvalve. Leakage gap dimensions were 2 x 6 µm in the bulk material under the plane of the valve, and 2 x 20 µm in the epoxy material above the plane of the valve, while the plane of the valve was 75 µm in height. Following extrusion, various 3-D zones were assigned appropriate volumetric properties of the fluid or the solid. This method of model generation allowed a continuum of cells throughout the model even though various layers of the model represented different materials.

A body-fitted structured mesh was used to sub-divide the flow domain into discrete computational cells (see

Figures 1a, 1b). To ensure grid-independence of the solutions, simulations were performed with both coarse (~ 70,000 cells) and fine grids (~ 500,000 cells). The valves were modeled in an idealized, centered, well-seated position (Figure 1a). Because the closed valves tend to settle in various positions, a simulation of the closed valve in an off-axis position (Figure 1b), based on photographs taken during experimental evaluations (Figure 1c), was also performed. Input velocities which correspond to the flow rates (Q for open valves = 100, 200, 300 μL/min, Q for closed valves = 5, 10, 20 μL/min) used in the experimental testing were used as boundary conditions during the analysis.

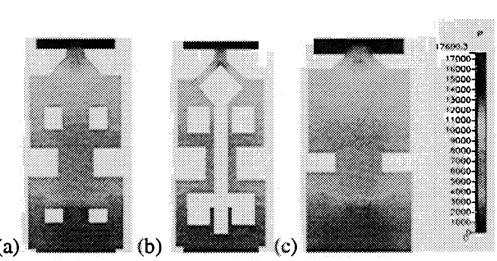


(a) (b) (c)

Figure 1: Geometric model and body-fitted structured mesh for the valve in: (a) idealized centered position, and (b) off-axis position. The physical off-axis valve is shown in (c).

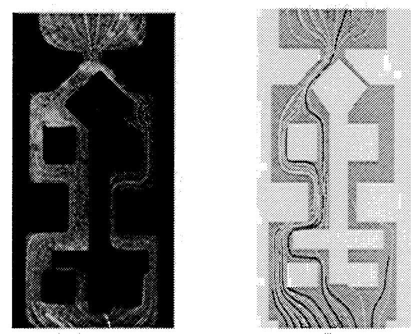
3 MODEL VALIDATION

Model validation was performed by comparing the simulation results for flow across the fully open and fully closed valves with corresponding experimental data in both the centered idealized and off-axis positions. Figure 2 shows the changes in pressure gradients across the 2 μm gap left beneath a valve by the oxide release etch, across the mid-section of a valve, and across the 2 μm gap left by the layer of epoxy sealant. For ease of viewing, the solid objects (silicon) in each view have been blanked, leaving only the fluid visible. Experimental and numerical flow traces across the valve in an off-axis position are compared in Figure 3.



(a) (b) (c)

Figure 2. Pressure gradients along the plane of the valve (a) in the leakage gap beneath the valve, (b) through the valve mid-plane, and (c) in the gap over the valve. (flow rate = 200 μL/min; valve in idealized open position; leakage gap above valve = 2 μm)



(a) (b)

Figure 3. Experimental (a) and simulated (b) flow traces across the valve in the off-axis position.

The valve resistance is defined as the ratio of pressure drop across the valves and volumetric flow rate across the valves ($R_v = \Delta P/\Delta Q$). The average resistance of the open valves was measured to be 103 Pa/(μL/min) while the simulations predicted an average resistance of 87.7 Pa/(μL/min) for the idealized open position. Similarly, the average resistance of the closed valve was found to be 11,377 Pa/(μL/min), while simulations with the valve in the off-axis position predicted a resistance of 11,790 Pa/(μL/min). Since the simulations exclude the pressure drop across the tubing and various connectors which attach the syringe pump and the pressure gauge to the system, an electrical analog model was used to factor out these effects from the experimental data. In the electrical model, the total resistance across the microvalve system is given as:

$$R_{total} = R_{in} + R_v + R_{out} \quad (1)$$

where R_{in} is the resistance of the tubing and connectors leading from the syringe pump to the microchannel/valve, R_v is the resistance of the microchannel/valve, and R_{out} is the resistance of the tubing and connectors leaving the microchannel/valve. Since the resistance of the tubing and connectors is expected to remain constant regardless of valve orientation (assuming material compliance is very small), the difference in total system resistance for the valve in the closed and open positions can be expressed as:

$$R_{total\_open} - R_{total\_closed} = (R_{in} + R_{v\_open} + R_{out}) - (R_{in} + R_{v\_closed} + R_{out}) = R_{v\_open} - R_{v\_closed} \quad (2)$$

The experimentally-measured differential resistance of the valve was found to be 11,308 Pa/(μL/min), while the simulated differential resistance was predicted to be 11,859 Pa/(μL/min), which is within 4% of the experimental data.

4 RESULTS AND DISCUSSION

4.1 Effect of Fabrication Artifacts

The effect of fabrication artifacts on the trans-valvular flow resistance was investigated by conducting simulations with simple valves (without any fabrication artifacts) in the open and closed positions. The only flow paths for the simple closed valve was through the 2 μm clearance within the channel. Figure 4 shows the pressure gradient across the mid-plane of simple closed valve and the idealized closed valve with fabrication artifacts at a flow rate of 5 μL/min. The simulations clearly show a large effect of the fabrication artifacts on the pressure drop across the closed valve (~3X). This difference is much smaller in the open valve simulations. All subsequent simulations presented here include gaps caused by fabrication artifacts.

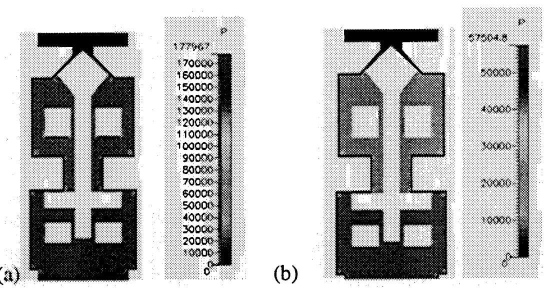

(a) (b)

Figure 4. Pressure gradient (Pa) along the mid-plane of the closed valves (a) without, and (b) with the fabrication artifacts (Q = 5 μL/min)

4.2 Effect of Leakage Gap Dimensions

Parametric simulations were performed to study the effects of changes in the leakage gap dimensions caused by changes in the thickness of epoxy layers used to seal the top to the microchannels. For the idealized position of the valves, the gap distances above both open and closed valves were varied from 2 – 10 μm in increments of 2 μm. A constant inlet flow velocity, which corresponds to a constant flow rate of 5.051 μL/min, was prescribed in the simulations. As expected, Figures 5 and 6 show that the pressure drop across both the closed and open valves, respectively, decrease as the thickness of the epoxy layer increases. The effects of gap distance on the pressure gradients are obviously greater with the closed valve than with the open valves.

4.3 Effect of Fabrication-Related Modification

The effect of fabrication-related modification on the valve function was studied by simulating a modified valve which included the addition of oxide bumps in the 2 μm area beneath the valve. Figure 7 shows a 3-D model of a structurally modified valve along with an unmodified valve for comparison. These oxide bumps might be fabricated by masking strips of oxide before the release process and carefully monitoring the release process to ensure that some of the oxide remains. A 5.051 μL/min flow rate simulation showed an increase in pressure from 57.5 kPa across the mid-plane of the unmodified valve to 74.7 kPa across the mid-plane of the modified valve (Figure 8). These results provided a guide for optimization of leakage pathways.

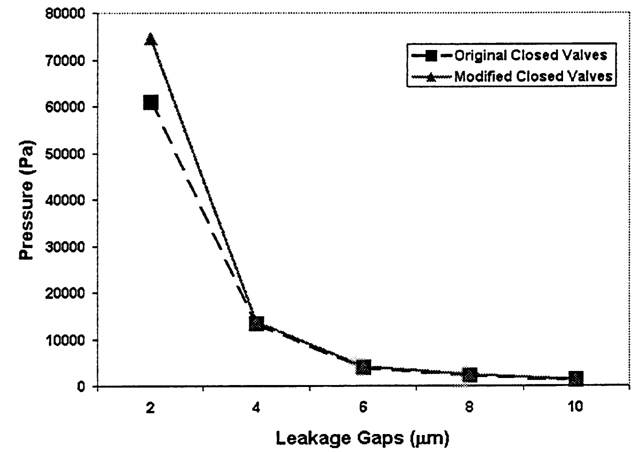


Figure 5. Effects of leakage gap distance on pressure drop for the idealized closed valve position (Q = 5.05 μL/min).

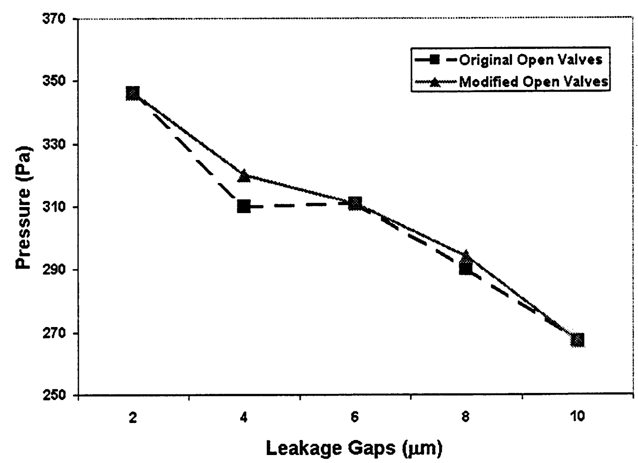


Figure 6. Effects of leakage gap distance on pressure drop for the idealized open valve position (Q = 5.05 μL/min).

4.4 Effect of Leakage Gap Above Valve

The valves are designed to function as a part of a micromixing system, where they either block or open specific fluidic pathways depending upon the flow direction. Therefore, minimization of the ratio of the open to closed flow resistances of the valves is important from the point of view of design optimization. Flow simulations were performed for both the unmodified and the structurally modified open and closed valves in the idealized positions for the 2-10 μm range of leakage gap distances. A constant inlet flow velocity, which corresponds to a volumetric flow rate of 5.051 μL/min, was used in the simulations. The ratios of the valve resistances were plotted against the gap distances to illustrate the trends. Figure 9 shows that the resistance ratio is lowest in valves that contain only a 2 μm gap above the valve and is seen to increase as the gap distances increases. In addition, the structurally modified valves provide a slightly reduced resistance ratio when compared to the structure of the original valves. Studies such as these can be used to design valves with improved functionality.

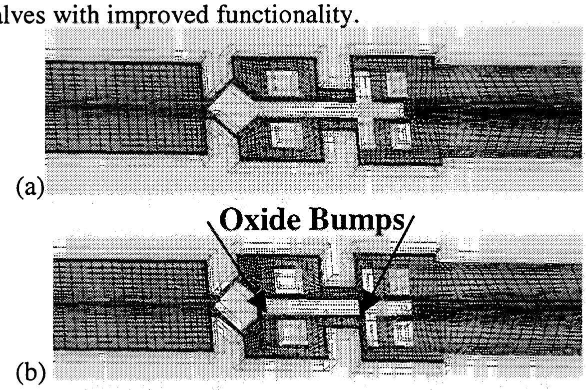


Figure 7. 3-D views of (a) idealized closed valve, and (b) modified closed valve.

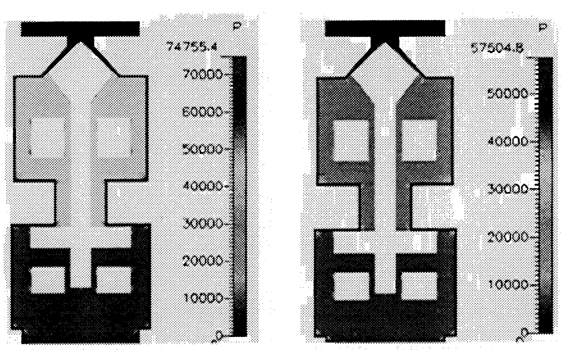


Figure 8. Pressure gradient (Pa) across mid-plane of (a) structurally-modified, and (b) original valve, in idealized closed position. (Q = 5 μL/min, 2 μm leakage gap).

5 CONCLUSIONS

Modeling of in-plane, uni-directional silicon microfludic valves, developed and tested at UC Berkeley, was conducted with the CFD-ACE+ multi-physics software suite. Experimental data were used to validate the 3-D models of valves in the open and closed positions. After an electrical analog model was used to factor out the effect of macro-tubing and connectors on the pressure drop across the valves, the experimental resistance of the valves was found to be in good agreement with the simulation data. Following validation, the effects of fabrication artifacts and structural modifications to the valve (variations in leakage gap above valve due to different sealant thicknesses and addition of oxide bumps in gaps beneath the valve) on the flow resistance of the valves were explored. The ratio of flow resistances for the open and closed valves was shown to monotonically decrease with a decrease in leakage gap distance for both the original valve and the structurally modified valve. Also, the corresponding flow resistance ratios for the modified valve configuration were slightly lower than for the original valve. Simulations are currently underway to further explore the effect of variations in valve geometry on its function within the micromixer system.

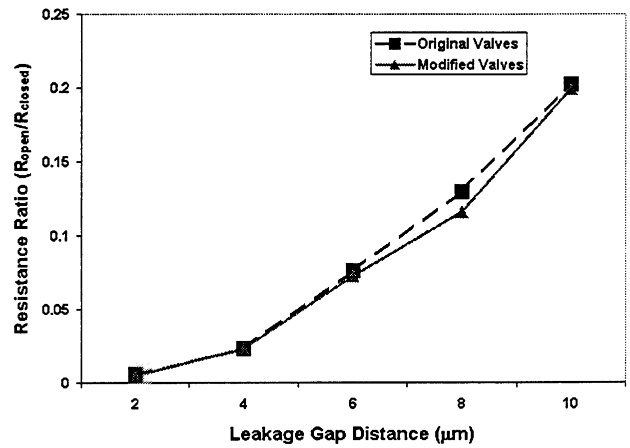


Figure 9. Effects of leakage gap distance on the ratio of open to closed valve resistances for the original and modified valve geometry (Q = 5.05 μL/min).

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