HIGH-FIDELITY CFD SIMULATIONS OF MICROFLUIDIC DEVICES

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ABSTRACT

Current state-of-the-art Computational Fluid Dynamics (CFD) techniques are applied to two microfluidic devices. Flow simulations in a bistable microfluidic amplifier and a micropump with dynamic valves were performed with CFD-ACE, an advanced CFD code. The bistable amplifier simulations showed good agreement with experiments in steady-state and switching modes and hysteresis behavior. Preliminary simulations of the flow in a micropump with dynamic valves are in progress and flow rectification is correctly predicted. An advanced, integrated, CAD environment for MEMS involving 3D geometry models/meshing, fluids/structures solver and visualization tools is proposed.

INTRODUCTION

Advances in the CFD techniques coupled with the speed and capabilities of the computer hardware has made it possible to use these techniques for complex flow problems with good confidence and fast turnaround times. The work reported here is a demonstration of use of CFD techniques to microfluidic devices. The eventual aim of the present effort is to develop a virtual computational environment (VCE) for multi-disciplinary analyses of microfluidic devices. It will contain virtual model "assembly tools", advanced analysis techniques, graphics driven menus for quick problem set-up and parallel processing capability to provide a powerful tool that can be used in the design and optimization process of microfluidic devices.

CODE DESCRIPTION

The simulations were performed using CFD-ACE, an advanced CFD code developed at CFDRC[1]. This code uses a finite-volume, pressure-based methodology for integration of the Navier-Stokes equations on body-fitted coordinate (BFC) grids. The code has an implicit, structured grid, multi-domain solution capability. The physical and numerical models include high order spatial and temporal discretization, selection of boundary types, turbulence models, and a moving grid algorithm. This code has been validated using a variety of benchmark, and experimental flow problems. Currently it is being applied to microfluidic device simulations.

SIMULATION RESULTS

1. Bistable Wall Attachment Amplifier

This device was described by Vollmer et.al.[2], and can be used as a fluidic amplifier or as an actuator/switch. A description of the problem and grid used is shown in Figure 1. Working gas at supply pressure P_s is fed to the supply nozzle which forms a jet. Position of this jet is controlled by application of control pressure P_c at one of the control ports. The jet pressure at the output port is used

Figure 1. Flow domain, boundary conditions and computational grid for the amplifier.

to actuate or drive other micro-devices. The amplifier shows a hysteresis behavior during switching due to the Coanda effect at the walls as shown in Figure 2, where pressure P_o at the output port opposite to the control port is plotted as a function of P_c in the increasing and decreasing mode.

Figure 2. Switching behavior of Bistable amplifier [2]. The dashed lines indicate the predicted switching behavior.

Simulation were performed to a) predict the steady-state jet at stable positions and calculate the output jet pressures, and b) vary P_c in the hysteresis region to see if the observed hysteresis behavior is predicted. Both items are needed to give a successful demonstration result.

1.1 Problem Description: An 18-domain, 2-D, BFC structured grid, with 15K cells was generated; the grid and boundary conditions are shown in Figure 1. The jet width was set at 32 microns. Nitrogen gas was the working fluid with density=1.15 kg/m³ and dynamic viscosity=17.8 mPa-s. The supply pressure P_s was 33 hPa(gage). The control pressure P_c was applied at control port No. 2 (Figure 1), and all other ports were kept at 0 Pa (gage). The flow was assumed

to be laminar and with constant fluid properties.

1.2 Results of Simulations : Steady state jet results in terms of the horizontal velocities are shown in Figures 3a and 3b where the P_c was set to ± 15 hPa to generate stable jets. The simulations used quiescent flow initial conditions. Comparison with Figure 2 shows that the jet positions are consistent with the experimental data. The maximum calculated jet pressure P_o at the output port is 75 hPa, which compares with an experimental passage-average value of 40 hPa. Two series of steady-state runs were performed next to simulate the switching behavior and hysteresis loop (Figure 2). These runs consisted of (a) series A where starting from the solution for $P_c = 15$ hPa, the control pressure was decreased to -12 hPa, and (b) series B where $P_c = -15$ hPa at start and was increased to +12 hPa. In both cases, the converged solution at the previous higher/lower P_c setting was used as the initial condition for the next run. Results of the series A are shown in Figures 4a through 4d. The jet starts out exiting in output port No. 1 for $P_c = 15$ hPa, and is seen to stay in that position till P_c is dropped to -6 hPa; further lowering of P_c then moves the jet from the upper to lower output port. A symmetrical trend was seen in the series B runs (results not shown) where P_c was increased from -15 hPa to 12 hPa. The predicted switching pressures are between ± 6 hPa and ± 12 hPa which compare with P_c values of ± 12 hPa seen in Figure 2. Time-dependent simulations of the switching sequence also showed similar behavior.

2. Micropump Simulations

One class of micropumps use dynamic valves with diffuser shaped inlet/exit channels to provide a net fluid motion from inlet to exit. One such geometry was described by Gerlach and Wurmus [3] with high diffuser angles, and relies on flow separation in the diffusing direction to generate flow rectification.

2.1 Problem Description : A 7 mm. square pump chamber with rectangular inlet and outlet sections with 70 degree diffuser section angles was used, with a deforming top wall. A 3-domain grid with 18000 cells was generated and a 'solids model' of the pump is shown

Figure 3. Steady-State, Stable jet configurations. P_c applied at the lower control port.

Figure 5. 'Solids model' of the micropump [3].

in Figure 5.

2.2 Simulation Results : Preliminary time-dependent simulations were carried out at a frequency of 3 KHz. The deformation amplitude is unknown, and needs to be matched with one experimental data point. After this anchoring, additional parametrics can be worked out. A typical velocity plot through the cross-section in the pump is shown in Figure 6, which shows the flow separation in the inlet diffuser during the pumping part of the cycle.

CONCLUSIONS

These simulations demonstrate the ability of CFD-ACE code to treat the complex geometries of the microfluidic devices considered here and provide reasonably accurate results of complex problem of the bistable amplifier. Additional validation problems and demonstration problems including simulations in microvalves are underway to establish the usefulness of the advanced CFD techniques in the analyses and designs of microfluidic devices.

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REFERENCES

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Figure 4. Dynamic Switching behavior of the amplifier, horizontal velocities.

Figure 6. Velocity in pump cross-section during 'down-stroke'.