Coupled Fluid-Thermal-Structural Simulations In Microvalves And Microchannels

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ABSTRACT

This paper presents the results of high-fidelity, 3-D simulations of coupled flow, heat-transfer and structural mechanics simulations of microchannels, micropumps, microvalves, and time-accurate simulations of a microoscillator. In each of these cases, the simulated results were compared with experimental and/or other published data, with excellent agreement. These results demonstrate the capabilities, accuracy and speed of the simulation tools for predictions of coupled, complex multi-physics processes in MEMS devices and their utility during the design phases of these devices for optimization and performance prediction.

INTRODUCTION

Microfluidic systems use microchannels and microvalves, to move and control fluid flow. Processes in these elements require a number of different capabilities in the simulation software such as treatment of rarefied/non-continuum flows [1,2], and multi-physical capabilities such as coupled fluid-structures-thermal analysis [3-6]. Fluid-structures problem treatment has been done using loosely coupled, commercial flow and structures codes [3,5]. Codes coupled in such manner may lead to convergence difficulties in some problems. Recently a new simulation environment, CFD-ACE+MEMS [7], has been developed by CFD Research Corporation (CFDRC) for high-fidelity multi-physics simulations of MEMS. The package uses state-of-the-art numerical techniques coupled with user-friendly grid generation and problem setup and execution interfaces. With the multi-physical capabilities, ease of use and rapid turnaround times, such a package can be a great asset in the design process of MEMS devices.

The present paper presents details of simulations of several microfluidic devices performed using CFD-ACE+MEMS for demonstration and validation of the software. These include compressible flow in microchannels [1], coupled flow-structures simulations of a passive check-valve[5], time-accurate flow in a microfluidic oscillator[8], and transient fluid-structures simulations of a beam-actuated micropump[3]. Although computational simulations of the check-valve and the beam micropump, performed with loosely-coupled codes have been performed[3], simulations of the microchannel and micro-oscillator have not been previously reported. In all cases, present results were compared with available experimental and/or published data to ascertain the accuracy and validity of the predictions.

MICROFLUIDICS DESIGN TOOL

The design tool, CFD-ACE+MEMS consists of a fluid+thermal solver, CFD-ACE+, which is used to solve flow, thermal and other coupled physics such as electrostatics [7]. The structural mechanics solutions are handled by FEM-STRESS, a finite-element code, which is coupled implicitly with CFD-ACE+ for predictions of mechanical and thermal stress-strains in solid parts.

The flow and thermal solver, CFD-ACE+ uses a pressure-based algorithm on an unstructured/hybrid/adaptive mesh system to integrate the Navier-Stokes flow equations[9]. Salient features of the solver relevant to MEMS problems include high-order spatial and temporal accuracy, steady and transient compressible and incompressible flows, accurate incompressible and compressible flows, moving grid formulation, conjugate heat transfer, VOF method for free-surface flows with surface tension, a variety of turbulence models and slip wall formulation. CFD-ACE+ is implicitly linked to CFD-FEM-STRESS, which is an advanced dynamic solver for fluid-structure-thermal electrostatic interaction, and multidisciplinary analysis including thermoelasticity, solid-fluid interaction, electrostatic actuators. Current capabilities include 1, 2 and 3-D elements, shell elements, first and second order accuracy, nonlinear elements, and a comprehensive contact model. Pre- and post-processing is done via CFD-GEOM (grid generation), CFD-GUI (problem setup) and CFD-VIEW (graphical post-processing).

MEMS SIMULATIONS RESULTS

Compressible Flow in a Microchannel [1]

Microchannel flow and heat transfer is of interest in MEMS as well as microelectronic cooling applications. The present case deals with compressible flow of nitrogen in a microchannel as described in Ref 1. The channel size was 1.25x40x3000 microns, with pressure taps along the channel length (Figure 1). The flow was generated by a pressure differential across the channel. The measured pressures showed nonlinear variation along the channel length. ACE+MEMS was used to simulate the flow on a 4x12x200 grid. Slip-wall formulation was used at the walls. Flow at five different pressure differentials was simulated and computed pressure distributions along the channel are plotted in Figure 2. Also shown are the experimental results; the dotted lines show the reference linear pressure variation. Computed results show an excellent agreement with experimental data, indicating the accuracy of the numerical method. Such high fidelity simulations can be used to generate simpler models for such flows without the necessity of expensive experiments.

Microfluidic Oscillator [8]

An SEM picture of a microfluidic oscillator is shown in Figure 3; the solids model and surface computational mesh is shown in Figure 4. The inlet port is supplied with pressurized gas, which forms a jet past the throat area. This jet is unstable and flips and attaches to one side wall. This energizes the corresponding bypass loop which generates high pressure at the jet base which causes it to flip over to the other side. This generates self-sustained oscillations of the jet, the frequency of which depends on the geometry and gas flow rate. The jet produces an oscillatory pressure differential across the outlet ports that can be used to drive a tool. A 3-D multi-block grid with 14K cells was built for this geometry. Compressible flow of nitrogen was simulated with no-slip and adiabatic walls. The exhaust port flow was vented to the atmosphere through small diameter tubes. The flow is fully turbulent in the jet region, and nearly laminar in the rest of the flow domain and a 2-layer k-ε turbulence model was used to handle this unique flow behavior.

Simulations were carried out at supply pressures of 90 and 140 kPa. The computed and experimental data are shown in Table 1. As seen, the flow rates are somewhat underpredicted, however the predicted frequencies match well with the experimental data. A sequence of plots of the jet velocity over one cycle of oscillation are shown in Figures 5a-d where the motion of the jet is clearly seen.

Membrane Pump by A. Klein [3]

Micropumps are needed to move fluids in microfluidic systems. The typical micropump involves interaction of a driven flexible structure with the working fluid. Schematic of a membrane pump described by A. Klein [12] is shown in Figure 6. The membrane is actuated by a piezoelectric layer, and results in a constant pressure at t=0 across the membrane.

Typical computational results are shown in Figure 6. At t=0, the actuator pressure causes the membrane to move down and squeezes the fluid out of the chamber. The fluid viscosity generates pressure that resists the membrane motion, and slows down deformation rate. When the membrane reaches the lowest point, the elastic deformation energy causes it to rebound and move upward. The upward motion increases the chamber volume and sucks fluid from the inlet and induces negative fluid pressure near the membrane, which resists the membrane motion. Due to this interaction, the fluid damps the structural dynamics. The mid-point displacement of the membrane is shown in Figure 7, which matches well with the computational results from Klein [3]. When the chamber contains no fluid (vacuum), the membrane oscillates with constant amplitude (zero damping). With air as the working fluid, the standard fluid-damped exponential amplitude decay behavior is seen which is more pronounced with water. Water also changes the oscillation frequency, and important effect, due to its fluid inertia. The computed results show excellent agreement with the reported results.

Flow Simulation of a KOH-etched Microvalve [5]

A 3D KOH-etched flap valve was simulated using the ACE+MEMS code. It is the same valve as analyzed and tested by Ulrich and Zengerle [5]. 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 covers a square valve seat with a length of 400 µm and a width of 5 µm. In the simulation, the flap was modeled using shell elements, with a Young's Modulus of 200 GPa, and Poisson ratio of 0.3. The working fluid was air. Figure 8 shows the 3D flow field when the valve is fully open at a pressure of 10,00 Pa. The corresponding flow rate with pressure are shown in Figure 9, which matched rather well with the experiments.

SUMMARY AND CONCLUSIONS

Numerical results of several different MEMS Microchannel, microvalves, and oscillators were obtained using CFD-ACE+MEMS, a multi-physics, high-fidelity simulation software developed for MEMS performance prediction and design optimization. The fluidic simulations of microchannels and micro-oscillators demonstrate the versatility of the software, and the capability of the physical models to treat specific situations encountered in MEMS devices including slip-walls, compressible flow effects, and the special turbulence models needed to treat widely different turbulence behavior possible in a single device. The coupled fluid-structures simulations again show the versatility of the codes in handling different types of flow-structures problems including dynamic interaction in the micropump and the steady, 3-D interactions in the microvalves. These examples demonstrate the capabilities of the code in dealing with complex, multi-physics problems encountered in MEMS devices. With the advances in modeling and computational power, it is certain that the high-fidelity simulation tools will find a definite place in the design environment of MEMS for performance prediction and optimization of new devices and help reduce the cost and cycle time of development of new MEMS devices.

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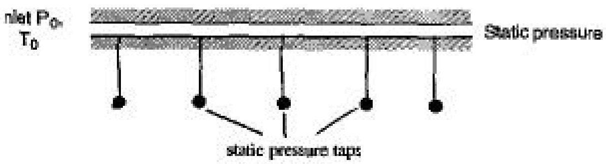


Figure 1. Schematic of the microchannel flow domain

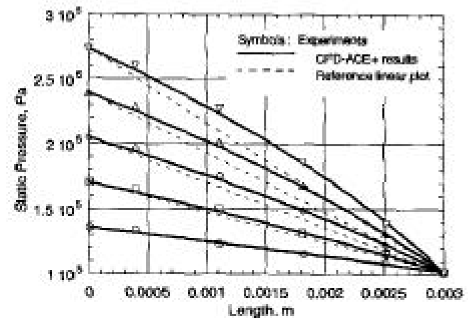


Figure 2. Computed and experimental pressure distributions in the microchannel at different supply pressures

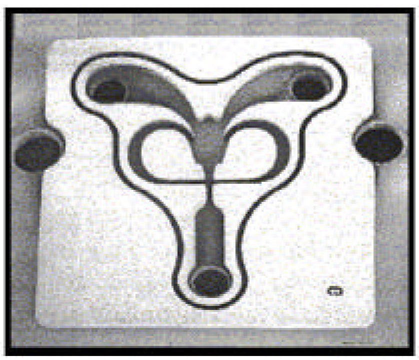


Figure 3. A SEM picture of the microfluid oscillator [8]

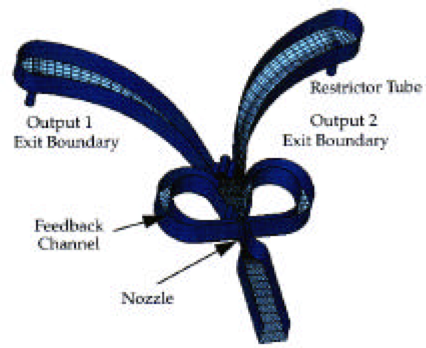
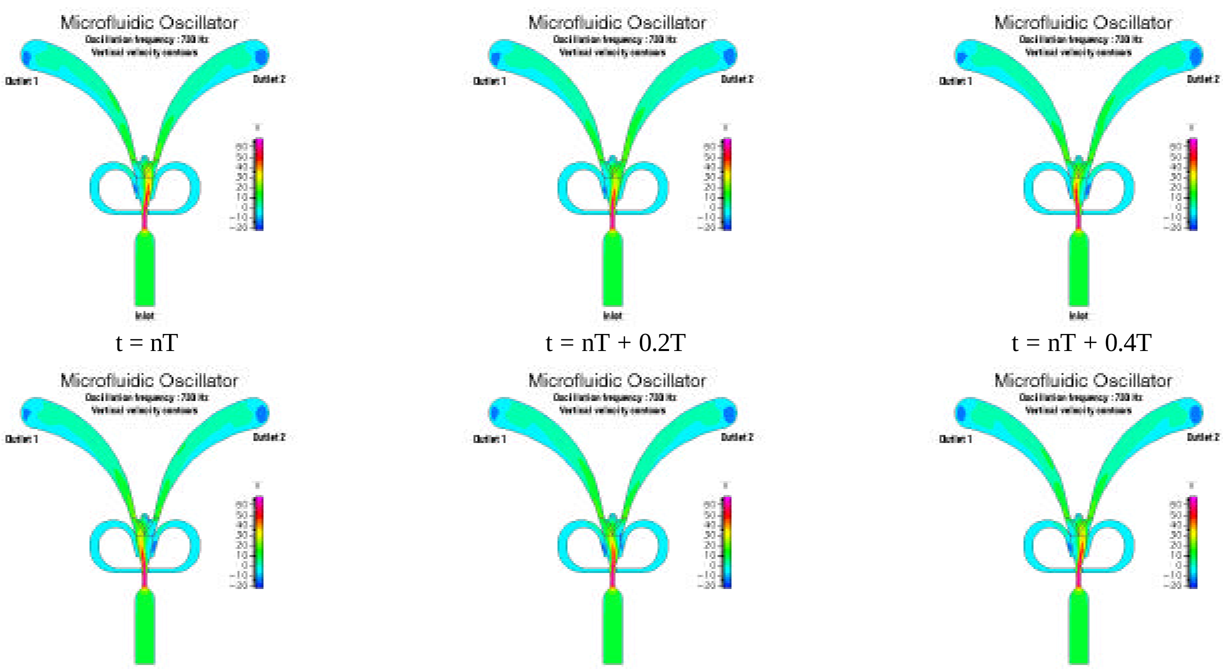


Figure 4. Solids model with boundary condition for the micro-oscillator



t = nT   t = nT + 0.2T   t = nT + 0.4T

t = nT + 0.6T   t= nT + 0.8T   t = (n+1)T

Figure 5. Distribution of vertical velocity at different time instances to show the positions of the jet during one typical cycle of the oscillator

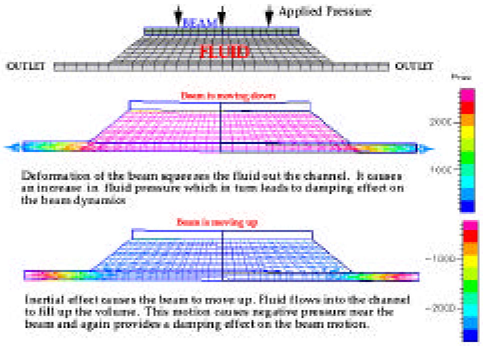


Figure 6. Problem definition and computed results for the vibrating beam micropump

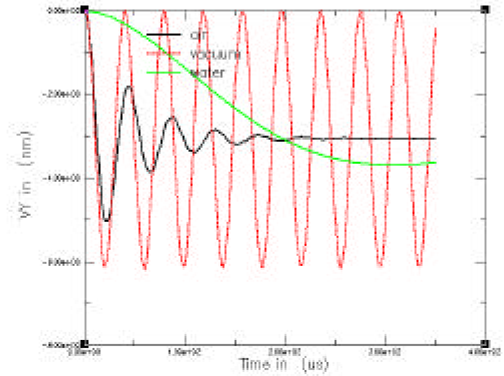


Figure 7. Computed time history of the beam center position under different clamping conditions

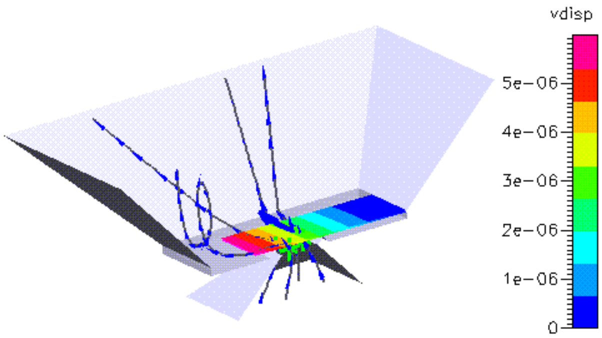


Figure 8. Coupled fluids-structures solution in the flap valve. Shown are typical particle traces.

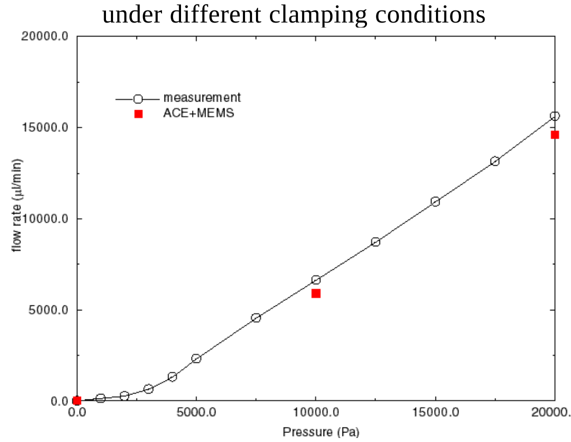


Figure 9. Predicted and experimental values of flow rates through the flap valve at different pressures