Simulation of Flow in Structurally Programmable Microfluidic Channels

V. B. Makhijani*, A. J. Reich*, A. Puntambekar**, C. Hong** and C. Ahn**

*CFD Research Corporation, 215 Wynn Drive, #501
Huntsville, AL, USA, vbm@cfdrc.com, ajr@cfdrc.com
**Dept. of Electrical & Computer Engineering and Computer Science,
University of Cincinnati, Cincinnati, OH,
puntamap@email.uc.edu, chong@ececs.uc.edu, chong.ahn@uc.edu

ABSTRACT

This paper describes the simulation of liquid filling in a structurally-programmable microfluidic delivery system being developed as part of a disposable biochip for clinical diagnostics. Flow control in the system is achieved by using passive valves and adjusting channel dimensions. The computational model, based upon the Volume-of-Fluid method, takes into account surface tension effects. When liquid filling is simulated under constant flow rate conditions, the model predicts sequential filling similar to that seen in experimental studies. Progressively increasing pressure surges are needed to push the liquid front through successive passive valves. Simulations indicate that surface tension and surface wettability are critically important for achieving flow control functionality in the system. The filling process under a sufficiently large constant pressure head is predicted to be quite different, and indicates that discrete (increasing) pressure bursts are needed to achieve the desired flow control functionality in the system.

Keywords: CFD-ACE+, Hydrophobic Filling, Flow Control

1 INTRODUCTION

A computational model has been developed to simulate liquid filling in a network of microchannels within a structurally programmable microfluidic system (sPROMs). This is an innovative system that is being developed at the University of Cincinnati as part of a disposable biofluidic chip for clinical diagnostics. It does not require moving parts and provides a passive control modality to the biochip system. Flow control in the network is accomplished through the placement of flow restrictions along the flow direction (or passive microvalves) of unequal dimensions in certain channels and through the adjustment of channel dimensions [1]. The system works on the principle that the pressure drop of the channels is small compared to the pressure drop across the passive microvalves [1,2]. This allows the valves to mainly control the flow sequence. By changing the locations of the passive valves and/or their sizes relative to the channels, it is possible to program the fluid delivery sequence of the system. Additional details on the working of the system are provided in Reference 1.

Analytical expressions have been previously used to predict the individual pressure drops required to fill different channels in the network and to push the liquid through the different microvalves [1]. However, analytical models cannot be used to predict the time sequences of the filling process in the individual channels, which is an important aspect of flow control in the biofluidic chip.

The computational fluid dynamics approach was therefore used to develop a high-fidelity numerical model, which simulates liquid filling in the structurally programmable system under different modes of liquid pumping. The two-phase flow model is based upon the Volume-of-Fluid (VOF) method in which the motion of the liquid-air interface is computed at different time instants during the filling process. The model accounts for surface tension at the liquid-air interface as well as the liquid-wall physicochemical interactions. The eventual aim of this approach is to use the computational model for design analysis and optimization of the microfluidic system to achieve the desired level of flow control.

2 METHOD OF APPROACH

CFD Research Corporation's (CFDRC's) advanced multi-physics and multi-scale commercial software package, CFD-ACE+, which is ideally suited for simulation of biophysicochemical processes in bioMEMS and biomicrofluidic devices, was used for the simulations. As a first approximation, the filling process was simulated in two-dimensions (2-D). The objective of these preliminary simulations was to characterize and understand the important physical parameters that govern the mechanics of fluid flow in the system under different modes of liquid pumping. Because the channel width is uniform throughout the fluidic network, it is unlikely to influence any of the trends predicted by the model. Details of the computational model are presented in the following sections.

2.1 Geometry and Mesh Generation

A CAD model of the multiplexer device, generated using AUTOCAD (Autodesk, Inc., San Rafael, CA), was used to define the computational flow domain geometry.

The CAD model was imported into CFDRC's geometric modeling and mesh generation software package, CFD-GEOM, to create a 2-D model of the domain along the length of the channels. A body-fitted structured Eulerian mesh of approximately 2600 cells was generated for the channel network geometry as shown in Figure 1.

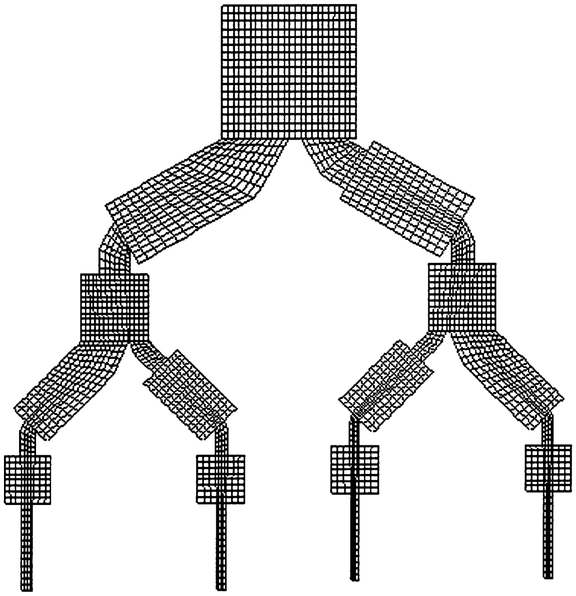

Figure 1: Geometric model and body-fitted structured mesh

2.2 Numerical Methodology

CFD-ACE+ was used to model the fluid flow as 2D, transient, incompressible, Newtonian, two-phase flow. The fluids used were air and water. CFD-ACE+ utilizes a modular approach to performing coupled, multi-disciplinary simulations. This approach allows the user to invoke the necessary physical models for flow, heat transfer, mass transfer, biochemistry, electrokinetics, electrostatics, electromagnetics and structural dynamics. The flow simulation module within CFD-ACE+ solves the Navier-Stokes equations using the finite volume method. CFD-ACE+ uses a pressure-based, strongly implicit algorithm for solving the Navier-Stokes equations for all flow speeds, and can handle 2D planar, axisymmetric, and 3D formulations [2]. The code has the capability to solve the governing equations on unstructured mixed element grids including tetrahedral, hexahedral, pyramid, and prism cells.

The unsteady motion of the liquid front was computed using the free surface module in CFD-ACE+, which is based upon the Volume-of-Fluid (VOF) method [3]. This module can simulate the fluid dynamics of two incompressible, immiscible fluids with arbitrary interface shapes and surface tension, with or without deforming solid boundaries. The module can handle both Newtonian and non-Newtonian fluid viscosities, and can also solve for heat transfer within the flow domain. In the VOF technique, an additional mass conservation is solved for the second fluid, and volume fraction of the second fluid is tracked using a scalar parameter. Mixture properties in each computational cell are computed based on weighted averages using the volume fraction. The two-fluid interface is reconstructed based on the distribution of volume fraction. CFD-ACE+ uses both a lower-order as well as a higher-order method for interface reconstruction.

2.3 Boundary and Initial Conditions

A fixed inlet velocity was prescribed at the boundary for the constant mass flow rate simulations. The inlet velocity was computed based upon a flow rate of 10 μl/min for the 3-D inlet structure geometry (1 mm width, 25 μm height). For the fixed pressure head flow simulations, a fixed pressure boundary condition of 2 kPa was used at the inlet. A zero exit pressure value was used for both cases. For the case with surface tension, a 110 degree contact angle (slightly hydrophobic) was prescribed at all the walls. Surface tension at the air-water interface was taken as 0.0725 N/m.

2.4 Parametric Studies

Simulations were performed under both fixed mass flow rate and fixed pressure head conditions to investigate and characterize liquid flow patterns in the microfluidic system. Simulations were also performed with, and without, consideration of surface tension effects to assess the effect of this parameter on the liquid filling patterns.

3 RESULTS AND DISCUSSION

3.1 Fixed Mass Flow Rate Simulations

Figure 2 shows model predictions of liquid filling in the microfluidic system for the case when surface tension effects were considered. The simulations show a sequential filling of the microchannels based upon the individual resistances of the passive microvalves. Experimental flow visualization studies at the University of Cincinnati with a syringe pump have shown similar sequential filling patterns in such types of networks as reported, for example, in reference [1].

The model predicts progressively increasing pressure spikes at the system inlet as the liquid front continues to break through each successive passive valve that it encounters in its flow path. Once the front has broken through a passive valve, based on the current geometry of the channels, the inlet pressure reduces to a lower value corresponding to the pressure drop required to maintain laminar flow through a channel of constant cross-sectional area. The inlet pressure then stays almost constant until the front reaches the next valve. The flow directionality is a direct result of the relative resistances the liquid front has to overcome at any given instant along the two branches of the network during the filling process.

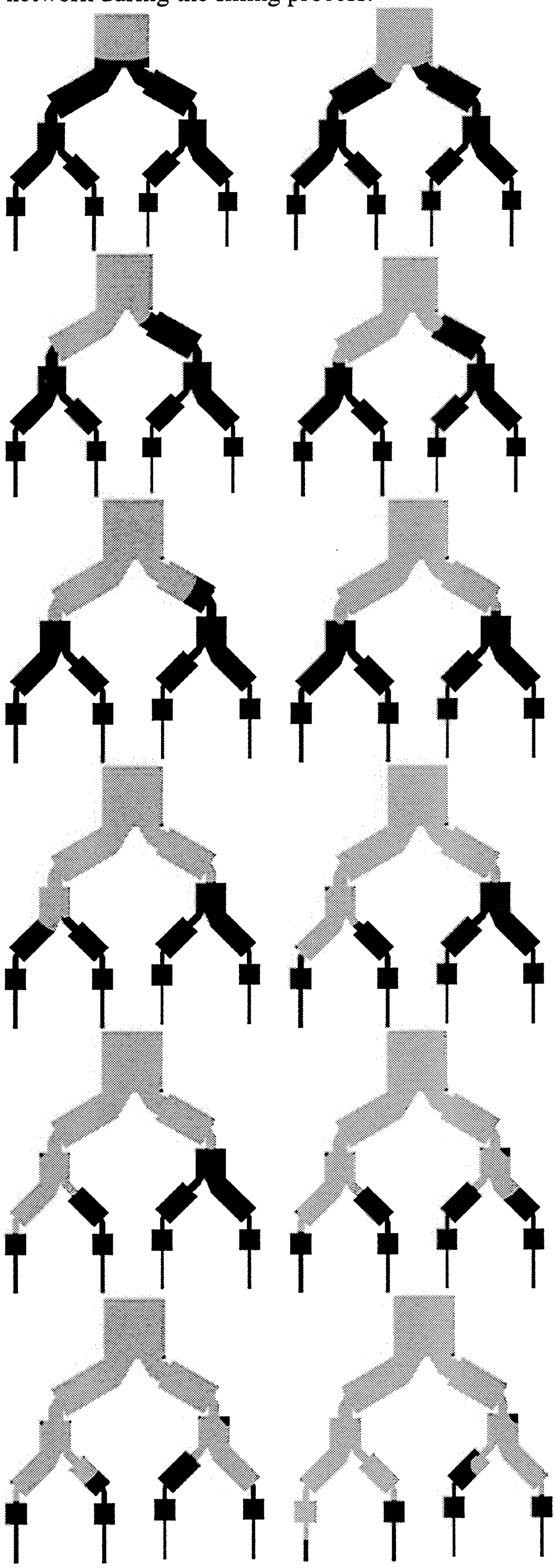

Figure 2: Sequential liquid filling in the microchannel network (left to right and top to bottom) under fixed inlet mass flow rate (with surface tension effects considered).

3.2 Effect of Surface Tension

The test case shown in Figure 2 was rerun with the surface tension turned off in the model. The results of this simulation are shown in Figure 3. In the absence of surface tension, the channel filling does not occur in a sequential manner. These results clearly indicate that surface tension and surface wettability are as important as the geometry of the microchannel network in achieving the desired flow control functionality in the system.

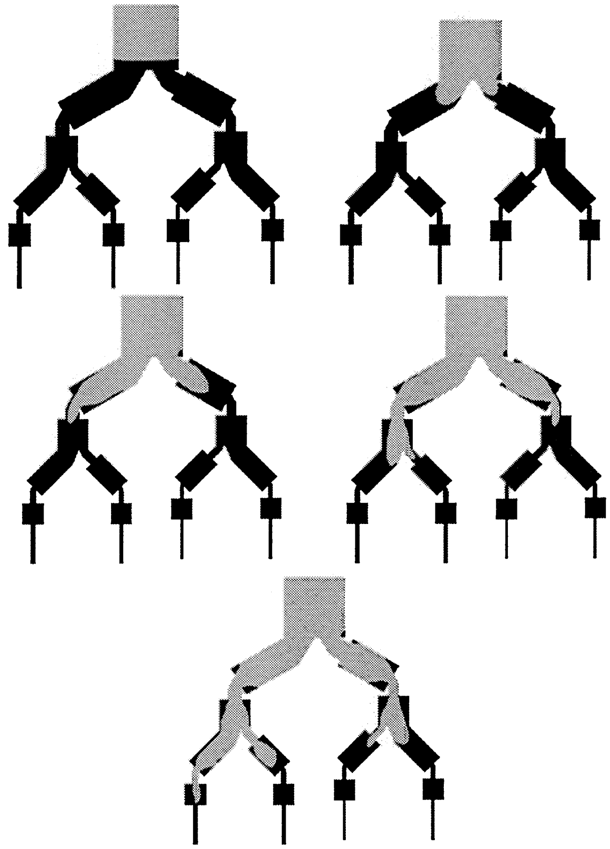

Figure 3: Liquid filling in the microchannel network (left to right and top to bottom) under fixed inlet mass flow rate (without consideration of surface tension)

3.3 Fixed Inlet Pressure Simulations

In the fixed inlet pressure test case (with surface tension turned on), a sufficiently large value (2000 Pa), which was larger than the highest pressure drop encountered by the liquid front in the fixed mass flow rate simulations, was used. The motion of a liquid plug of length equal to the length of the common inlet channel in the system was modeled. The idea was to try and understand the behavior of the liquid plug in the system when being propelled by a steady pressurized source of air that maintains a constant pressure head at the channel inlet.

Figure 4 shows that the motion of the liquid plug in the microchannel network under a sufficiently large fixed pressure head is fundamentally quite different. As expected, because the pressure head is so large, the liquid front is able to simultaneously overcome the flow resistances at two competing geometric constrictions in the system. Hence, the plug almost "blasts through" both branches of the channel network, and the sequential filling seen in Figure 2 is not seen for the present case. (The motion of the plug, however, is asymmetric, and seems to push through the left branch faster than the right branch. This can be attributed to the higher flow resistance "programmed" into the right branch of the current system, which results in a similar flow bias in fixed flow rate case – see Figure 2.) The model predictions, therefore, indicate that a series of discrete pressurized bursts of air, at progressively increasing pressure levels, are needed in order to achieve sequential flow control under this mode of liquid pumping.

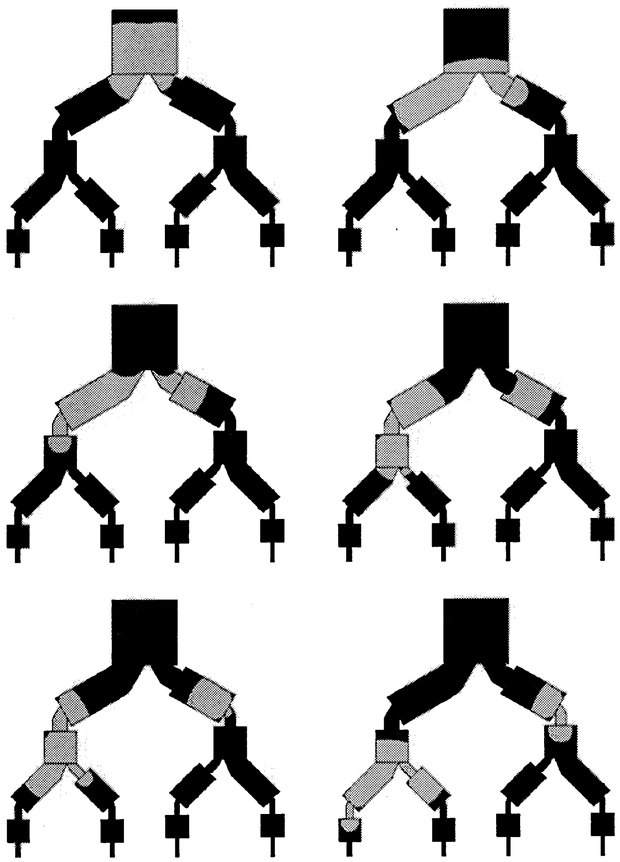

Figure 4: Transport of a liquid plug in the microchannel network under the influence of a sufficiently high constant pressure head (with consideration of surface tension).

4 CONCLUSION

This paper demonstrates the application of an advanced computational fluid dynamics model for the design analysis of a structurally-programmable fluidic system, which can be used for passive flow control in disposable microfluidic biochip systems. The model was used to study the effects of surface tension and the mode of fluid pumping (fixed flow rate versus fixed pressure head) on the liquid filling process in the system. Simulation results provided valuable insight and enabled characterization of the important physical parameters that govern the fluid mechanics of the microchannel system. Further studies are currently underway to investigate and characterize the effects of variations in the channel geometry on the system functionality.

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