Simulation of Electronic Control in Electroosmotic Flow Channels

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Abstract - An algorithm and simulator for electronic control in electroosmotic flow channels is presented. Using this simulator accurate simulation of a complex interconnection of channels can be performed. In addition, various flow control schemes can be evaluated for their effectiveness.

I. Introduction

The interest in microfluidics emerged in the late 1980s with experiments of U.S., Canadian and Swiss scientists, who moved chemical solutions through networks of microfabricated channels etched on a sheet of glass [1]. Although the first microfluidic devices were rather simple, the present day devices and microfluidic systems can be very complex. Examples include biomedical analysis, environmental monitoring, automotive applications and process control [2]. A unique application is the use of electrophoresis chips for high-speed DNA genotyping as described in [3]. In this case, an interconnection of electroosmotic devices in a capillary array electrophoresis chip is used to demonstrate the rapid analysis of biological samples.

In any complex design problem, there is a need for computational prototyping tools whereby devices or systems can be simulated before fabrication. Although the state-of-the-art in integrated circuit design is very advanced, computer-aided design tools for microfluidic systems are still in a stage of infancy. Recently, there has been a focus on simulation of microfluidic systems using coupled circuit and flow simulators [4]. In this paper, we present a coupled circuit (SPICE3) and electroosmotic solver (EOFLOW) that allows accurate simulation of a complex interconnection of channels. In addition, we demonstrate several examples of how the simulator can be effective in designing control strategies for electroosmotic flow.

The paper is organized as follows. In Section II a brief description of EOFLOW is provided. The coupling of this solver with SPICE3 including appropriate boundary conditions is described in Section III. Flow control examples and a complex simulation example are provided in Section IV. Finally, conclusions are given in Section V.

II. EOFLOW

EOFLOW is a new simulation program for electroosmotic fluid transfer as described in [5]. Three basic microfluidic structures: straight-, T- and cross-channels (shown in Figure 1) can be simulated in EOFLOW.

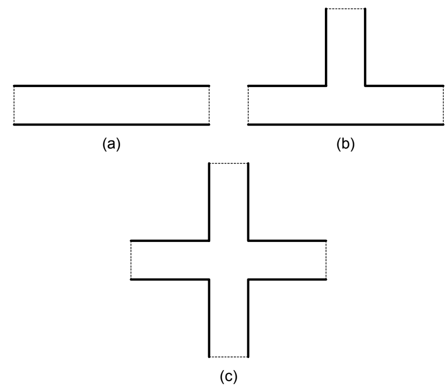

Figure 1 Types of channels used in EOFLOW. (a) Straight channel, (b) T channel, (c) cross channel.

A combination of these can be used to construct complicated structures. Transient responses of these devices (distribution of potentials within a device and the flow rate through the outlets with time) can be simulated for any voltage excitations applied at the outlets. EOFLOW uses a semi-implicit integration method with fixed time steps during transient simulation.

III. Coupling Of EOFLOW To SPICE

SPICE3 [6] is a very well established tool for large systems simulations. It solves a system of nonlinear differential algebraic equations. Although initially developed for electrical circuit simulations, SPICE is also suitable for microfluidic system simulations. In flow problems, satisfying the conservation laws with appropriate boundary conditions results in a set of equations similar to that for electrical circuits. For this reason SPICE3 is an excellent framework for simulating different types of systems.

The accuracy of a simulator depends on the quality of models used for the devices. For this reason coupling of the electrical simulator with detailed physics based device simulators results in an accurate simulator. Furthermore, an interconnection of devices can be simulated in conjunction with the control electronics. This is an important aspect of coupling EOFLOW with SPICE3. The following subsections address the boundary conditions and the coupling algorithm.

A. Boundary Conditions

The set of boundary conditions for an example interconnection of three cross channel microfluidic devices is shown in Figure 2.

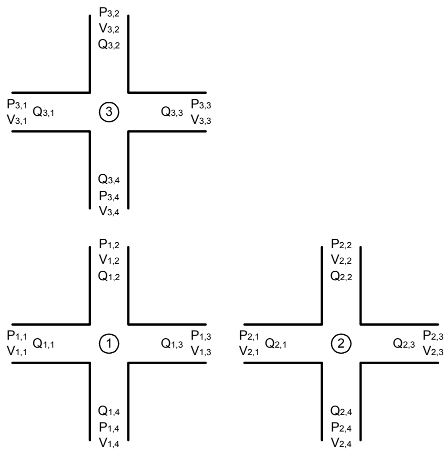

Figure 2 Boundary conditions that have to be matched for an interconnection of channels.

As can be observed from Figure 2 at each of the interconnection nodes the flow rates, voltages, and fluid pressures of two devices should be identical. Referring to the example in Figure 2 the following conditions should be satisfied:

$$V_{1,3} = V_{2,1},\ \ V_{1,2} = V_{3,4};\ \ Q_{1,3} = Q_{2,1},\ \ Q_{1,2} = Q_{3,4}$$
$$P_{1,3} = P_{2,1},\ \ P_{1,2} = P_{3,4}$$

where *V, Q* and *P* are potential at the in/outlet, flow rate through the in/outlet and pressure at the in/outlet, respectively. SPICE3 is used to force these device constraints during a simulation.

B. Coupling EOFLOW to SPICE3

EOFLOW is embedded in SPICE3 as a subroutine as shown in Figure 3. SPICE3 provides the electrical simulation engine and the framework for interconnecting several devices. The microfluidic devices are treated as a model in the SPICE3 framework.

Each distributed model of a fluidic device calls EOFLOW. The time stepping scheme used has been described in [4]. Since EOFLOW runs with larger time steps than SPICE3, synchronization timepoints are determined by EOFLOW and transferred to the SPICE3 numerical engine. At every synchronized timepoint SPICE3 supplies the terminal voltages to EOFLOW and in return obtains the values of the derivatives of the flow rate through the i^{th} edge with respect to the voltage applied to the j^{th} outlet. Symbolically, $g_{ij} = \partial Q_i / \partial V_j$, (where Q_i, $i = 1,...,4$ is the flow

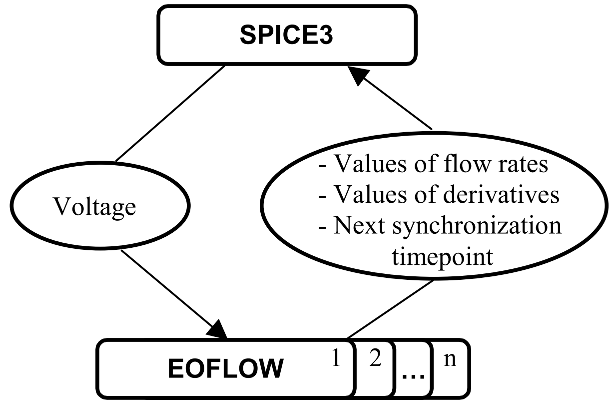

Figure 3 Simulator block diagram.

rate through the i^{th} edge, and V_j, $j = 1,...,4$ is the voltage applied to the j^{th} edge) for every microfluidic element. The SPICE3 transient analysis lumped element representation of a cross channel is shown in Figure 4. The dependence of the flow rates on the applied voltages is modeled as voltage controlled current sources. The g_{ij} are the parameters for these controlled sources.

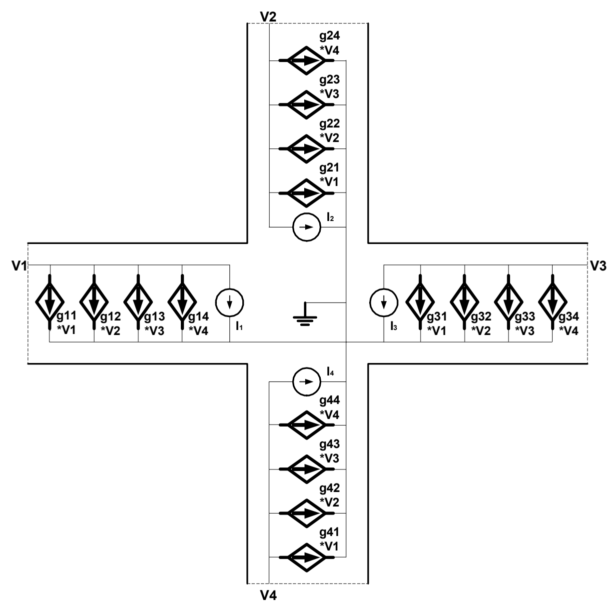

Figure 4 SPICE3 model for cross channel.

The interface with SPICE3 depends on the time integration algorithm used in the physical device solver. In this case, EOFLOW uses a semi-implicit time marching method. An implicit scheme is used for the viscous term in the Navier-Stokes equation [5], [7] and an explicit scheme is used for the convective term. Because of this integration method a system of linear equations is solved at each time step instead of a system of nonlinear equations. As a result the values of the derivatives (g_{ij}, $i,j = 1,...,4$) are constant at a particular time point regardless of the applied voltages. Therefore, every iteration of the Newton method uses these values without the need for recalculations. Moreover, the values of the g_{ij} change slowly in time, which allows their reuse during time stepping. In every N time steps the values are recalculated and compared with the values that have been previously used. If the error is less than 0.1% the value of N is doubled. If the value of the error is between 0.1% and 1% the value of N is kept the same. Finally, if the value of error is more than 1% the value of N is divided by two. This allows for EOFLOW/SPICE3 coupling to be computationally efficient.

IV. Simulation Results

In this section, we apply the coupled SPICE3/EOFLOW simulator to different types of problems. We demonstrate the usefulness of the simulator in determining an appropriate flow control strategy. Also, a complex interconnection of channels is simulated to show the versatility of this simulator.

A. Control Systems for Flow

Microfluidic systems consisting of cross channel pipes and control electronics (Figures 5 and 6) were simulated. The intent of the control loop is to reduce the vertical velocity so that flow spreading can be avoided. Zero flow rates are obtained through the vertical channels by automatically adjusting the voltages applied to the vertical channels. The block diagram of the system with a proportional type controller is shown in Figure 5, whereas an integral type of controller is shown in Figure 6.

The dynamic behavior of the controlled potentials and flow rates and the streamlines, for these systems are shown in Figures 7, 8, 9 and 10, respectively. As shown in Figures 7 and 9, it is not possible to stabilize the flow rate at the given level in a reasonable amount of time when using a proportional control system.

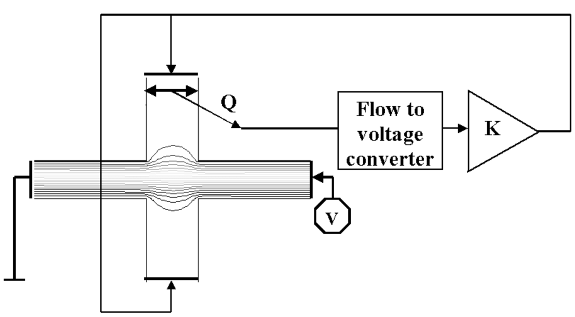

Figure 5 Block diagram of the proportional control system.

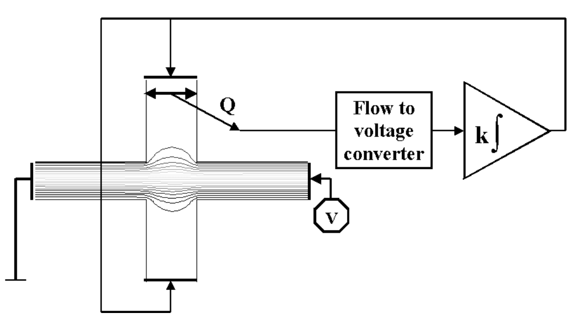

Figure 6 Block diagram of the proportional-integral control system.

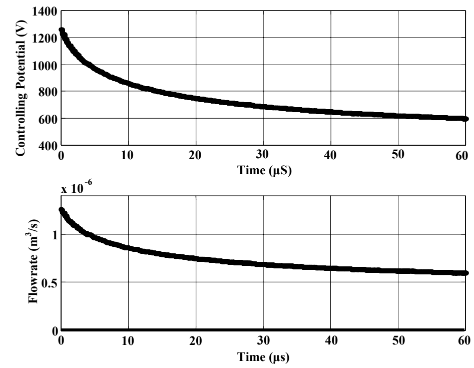

Figure 7 Dynamic behavior of controlled potentials and flow rate for the electroosmotic system with proportional control.

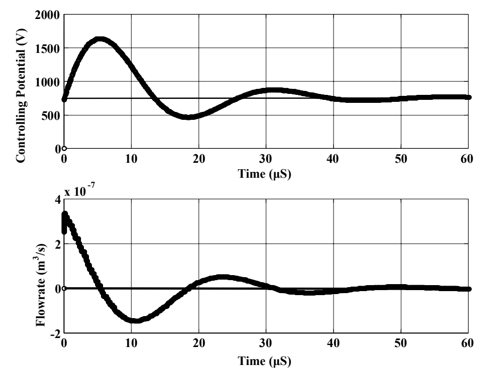

Figure 8 Dynamic behavior of controlled potentials and flow rate for the electroosmotic system with proportional-integral control.

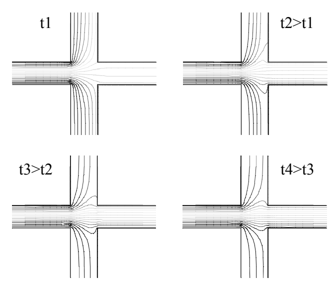

Figure 9 Dynamic behavior of streamlines for the electroosmotic system with proportional control.

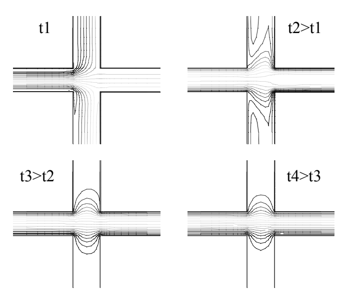

Figure 10 Dynamic behavior of streamlines for the electroosmotic system with proportional-integral control.

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For an integral control system the flow rate can be stabilized in less than 60 µS as shown in Figures 8 and 10. Thus, an integral control system provides a better performance for this application.

B. Complex System Simulation Results

As an example of a complex system consider a mesh of 10 × 10 interconnected cross channel pipes as shown in Figure 11. Voltage sources with different amplitudes and frequencies were connected to each outlet.

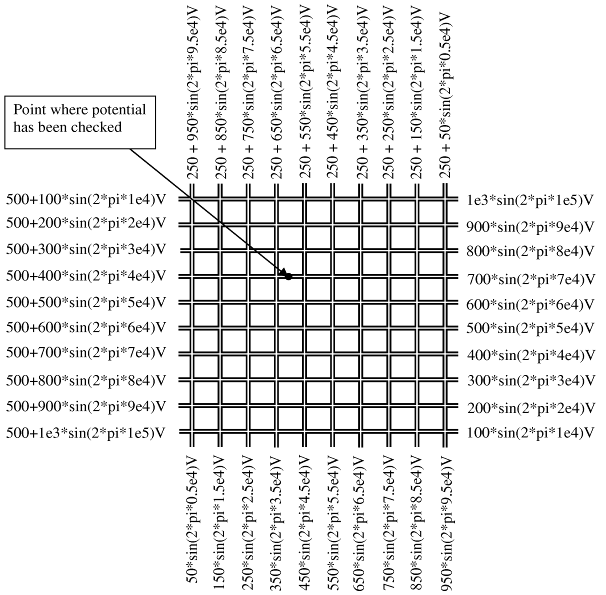

Figure 11 10 × 10 cross channel mesh simulated with voltages at the outlets.

This example shows that the voltage at any interconnection point can be readily simulated. Furthermore, the computational efficiency of the coupling algorithms when a large number of interconnected microfluidic devices need to be simulated is demonstrated. The response (frequency-domain spectrum) is shown at a point near the center of the mesh in Figure 12. The resulting output signal contains harmonics corresponding to the input frequencies as expected.

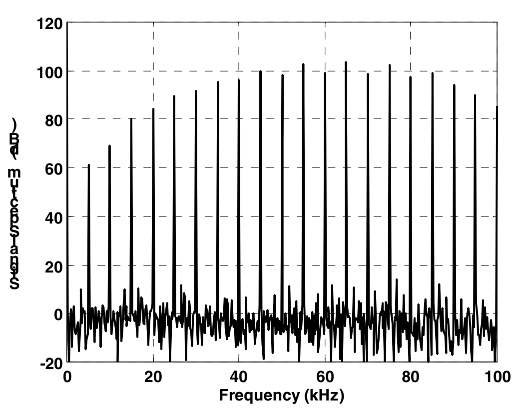

Figure 12 Spectrum of the output signal.

The computational time is an important issue for this type of simulation. One EOFLOW calculation for a device with 2370 nodes takes about one minute on a Sun Solaris with UltraSparc 440 MHz processor. At every time point each device requires four simulations for the cross channel to calculate the derivative values. For a transient simulation up to 300 µS each device is evaluated at approximately 1000 time points. Based on this approximation the simulation would require $100*1000*4 = 400000 \text{ min} \approx 9$ months. Taking into account that the derivatives and flow rates change slowly with time and reusing previously calculated values, based on the techniques described in Section III.B, helps reduce this time to 48 hours. The simulation time could be decreased further by evaluating the devices in parallel. In this case, the 100 devices can be simulated simultaneously on different machines, whereby the total simulation time can be reduced to a few hours.

V. Conclusions

A new approach for the simulation of electroosmotic systems has been developed. SPICE3 is combined with a flow solver EOFLOW to enable simulation of a complex network of interconnected channels. Furthermore, various electronic control options for flow can be evaluated. A system consisting of one hundred microfluidic elements was simulated to demonstrate the versatility of this simulator.

Acknowledgement

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