A Compact Model for Flowrate and Pressure Computation in Micro-fluidic Devices

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ABSTRACT

A compact model to compute flowrate and pressure in micro-fluidic devices is presented. The micro-fluidic flow can be driven by either an applied electric field or by a pressure gradient or both. In the proposed compact model, the complex fluidic network is simplified by using an electrical circuit. The compact model can predict the flowrate, pressure distribution and other basic characteristics in microfluidic channels quickly with good accuracy when compared to detailed numerical simulations.

Keywords: Compact model, electrokinetic flow, pressure driven flow, Micro-fluidic devices.

1 INTRODUCTION

Integrated microfluidic systems with a complex network of fluidic channels are routinely used for chemical and biological analysis and sensing. The use of detailed numerical simulations based on partial-differential equations can be very expensive and prohibitive for microfluidic system designers. Compact models, which are simplified models - yet accurate enough to capture the basic physical characteristics, can be enormously useful for system designers to quickly evaluate new design concepts. Once the design concept is selected, detailed numerical simulations can be performed to obtain extensive and more accurate flow characteristics.

In this paper, we report on the development of a compact model for microfluidic devices that use electric field and/or pressure gradient as driving forces. The compact model also accounts for the pressure generated in micro-fluidic channels because of non-uniform ζ-potential on the channel walls. Numerical results indicate that the compact model can be several orders of magnitude faster compared to detailed numerical simulations without sacrificing too much accuracy.

2 COMPACT MODEL DEVELOPMENT

The derivation of a compact model for an electric field driven fluid flow is described in this section. The approach can be extended in a straight-forward manner when the flow is driven by other type of forces e.g. a pressure gradient or a combined pressure gradient and an electrical field. The compact model is composed of two parts - namely, the electrical part and the fluidic part.

2.1 Compact Model: Electrical Part

For micro-fluidic devices that rely on electrokinetic force for fluid flow, the electric field must be solved first. In the case of an electroosmotic flow, the potential field due to an applied potential can be computed by solving the Laplace equation

$$\nabla^2 \Phi = 0 \tag{1}$$

where Φ is potential. To solve equation (1) on a complex geometry, the network of channels is represented by a number of straight channels and each straight channel is further represented as a resistor. For example, for the fluidic network shown in Figure 1, the electrical part of the compact model is represented by the circuit shown in Figure 2. Assuming that the potential drops linearly in each straight channel and that the channel walls are well-insulated, the applied potential field in the entire network is obtained by solving the circuit problem. In most micro-fluidic devices, the channel width is much smaller compared to the length of the channel. Hence, the assumption employed above is justified in most part of the fluidic network, except near channel intersections.

2.2 Compact Model: Fluidic Part

The flow field in micro-fluidic devices is usually governed by the Stokes equation [1]

$$\mu \nabla^2 \mathbf{u} - \nabla P + \mathbf{F} = 0 \tag{2}$$

$$\mathbf{F} = \varepsilon \nabla \Phi \nabla^2 \Psi \tag{3}$$

where Ψ is the potential induced by the ζ-potential on the channel walls. The Stokes equation can be greatly simplified by considering the flow characteristics in micro-fluidic channels. In the compact model development, we assume that (1) the flow is fully developed and (2) the electrokinetic force term, stated in equation (3), can be represented by a slip velocity at the wall given by the Helmholtz-Smoluchowski equation [2]

$$u_{slip} = -\varepsilon \zeta / \mu \nabla \Phi \tag{4}$$

The first assumption is justified because the channel length is usually much longer compared to the channel width and the flow is fully developed in most part of the fluidic network. The second assumption is justified because typically the electrokinetic force exists only within a short distance (a few nanometers) from the wall. Based on these assumptions, the velocity profile across the channel is a function of only the slip velocity and the pressure gradient

$$u_{streamwise} = \frac{1}{2\mu}\frac{dp}{dx}\left(y^2 - \frac{h^2}{4}\right) + u_{slip} \tag{5}$$

where x denotes the stream-wise direction of the channel, y denotes the transverse direction across the channel and h is the channel width. With u_{slip} easily obtained from equation (4), the problem is reduced to computing the pressure distribution in the fluidic network. Usually pressure is strongly coupled with the velocity in an incompressible flow, however, for the Stokes flow, one can obtain a Poisson equation for the pressure after taking the divergence of equation (2):

$$\nabla^2 P = \nabla \cdot \mathbf{F} \tag{6}$$

Equation (6) decouples the solution of pressure from the solution of velocity. Equation (6) implies that pressure in a fluidic system can arise from two sources - the first is due to the applied pressure at the entrance and exit of the channel and the second is the induced pressure due to the non-uniform electrokinetic force that arises when the ζ-potential on the channel wall is non-uniform. When the electrokinetic force is divergence free, the only source of pressure is from boundary condition and equation (6) is reduced to a Laplace equation.

For the fluidic network shown in Figure 1, the pressure at all inlets and outlets is set to zero. However, there is a sudden change of ζ-potential at point E i.e. ζ-potential on all the channel walls to the left of E is ζ_1 and the ζ-potential on all the channel walls to the right of E is ζ_2. Thus, the solution of pressure is governed by the Laplace equation in most of the channel region except near point E. It is important to point out that the variation of the pressure across the channel is ignored as the pressure is also assumed to drop linearly within each segment of the channel system.

To compute the pressure in the entire network shown in Figure 1, a circuit model as shown in Figure 3 is set-up. The constant current source, P_{source}, at point E, accounts for the pressure induced due to the change in the wall ζ–potential at point E. P_{source} is computed by using mass conservation principle. Since we assume that the pressure is linearly distributed in channel regions A-E and E-B, the velocity profile across these two channel regions can be expressed as:

$$u_{AE} = \frac{1}{2\mu}\frac{P_A - P_E}{\Delta X_{AE}}\left(y^2 - \frac{h_{AE}^{\,2}}{4}\right) + u_{slip,AE} \tag{7}$$

$$u_{EB} = \frac{1}{2\mu}\frac{P_E - P_B}{\Delta X_{EB}}\left(y^2 - \frac{h_{EB}^{\,2}}{4}\right) + u_{slip,EB} \tag{8}$$

The pressure in the channel A-E-B can be expressed as:

$$\frac{P_A - P_E}{\Delta X_{AE}} + P_{source} = \frac{P_E - P_B}{\Delta X_{EB}} \tag{9}$$

Mass balance at point E yields an analytical expression for P_{source} at that point:

$$P_{source} = f(u_{slip,AE}, u_{slip,EB}, h_{AE}, h_{EB}, P_A, P_E, P_B) \tag{10}$$

It is straightforward to set up a node equation for each intersection point between channels. Once the pressure at the points A, B, C, D and E is obtained, the pressure gradient along the channel, the velocity profile and the flow-rate at any cross-section (except near the intersections) can be computed analytically by using equations (5), (7) and (8).

3 RESULTS AND DISCUSSION

Both full simulation (two-dimensional) and compact model analyses have been done for the fluidic network shown in Figure 1. The channel width (W) is taken to be 50nm and two cases for the Debye length (λ_D) are investigated: λ_D = 1.25nm and λ_D = 2.5nm. A potential of 0.1 V is applied at ports 0, 1, and 2 and a potential of 0.06V is applied at port 3. All other ports are grounded. The pressure at all channel entrances is set to zero. The ζ-potential on the channel walls on the left half (all channel walls to the left of the dashed line in Figure 1) and on the right half of the fluidic network is -10mV and -30mV, respectively.

The full simulation involves the solution of Laplace equation for the applied potential field, the Poisson-Boltzmann equation for the ζ-potential field and the Stokes and the continuity equations for fluid flow. The compact model involves only the solution of the circuit problem shown in Figure 2 and Figure 3. A typical full simulation takes about 15 minutes while the compact model needs only a few microseconds. Figure 4 shows a comparison of the pressure gradient along line *O-A-C-5*. It is clear that the compact model is able to predict the pressure gradient very well in most parts of the channel except for positions near the intersection of two channels. This is because the assumptions made in the compact model are no longer valid near the intersections. Figure 5 shows the scaled error in the flow-rate at different positions of the network and the compact model provides a solution that is within 8% accuracy when λ_D/W is 5% and within 3% accuracy when λ_D/w is 2.5%. From Figure 4 and Figure 5, it can be observed that the compact model gives better results when the λ_D/W ratio is small. This is because as the λ_D/W ratio decreases, the slip velocity model becomes more accurate. The compact model proposed in this paper can be expected to provide better accuracy results for microfluidic networks as λ_D/W ratio is typically in the order of 10^{-4}.

Figure 6 shows a schematic plot for a fluidic mixer. Three types of fluids (A, B and C) are driven from reservoirs 1, 2 and 3 to reservoir 4. Because of the different fluid properties, the ζ-potential at channel walls is also different as shown in Figure 6. A problem of practical importance would be to investigate how the mixing ratio of different fluids changes with the applied potential at different reservoirs. Doing a full simulation for such a problem would be very time-consuming, however, by using the compact model developed here, the solution can be obtained within a few seconds. Shown in Figure 7 is the electrical circuit to compute the pressure in the fluidic network. Figure 8 shows the mixing ratio of fluid A and fluid B when the potential at reservoir 1 is varied and the potential at reservoir 2 is fixed and the flowrate at location *Xc* (see Figure 6) is fixed. The mixing ratio of fluid A to fluid B is defined as the ratio of flowrate of fluid A at location X_A to flowrate of fluid B at location X_B. Observe that the mixing ratio varies with the applied potential at reservoir 1 and the mixing ratio can be negative for certain applied voltages. A negative mixing ratio means that the fluid is flowing into reservoir 2 instead of from reservoir 2.

Though the compact model developed here is based on the assumption that the flow and potential is two-dimensional, the development of a compact model for three-dimensional flow and potential problems involves the same steps detailed here.

4 CONCLUSION

A compact model to compute the flowrate and pressure distribution in micro-fluidic devices is presented. The compact model can analyze the flow rate and pressure distribution in a fluidic network driven by electrokinetic force, and/or applied and induced pressure. The results obtained from the compact model are in good agreement with full simulation results. Compared to the full simulation, the compact model involves negligible computational cost. Because the fluidic network is represented as electrical circuit in the compact model, the compact model can be easily integrated into readily available circuit analysis software.

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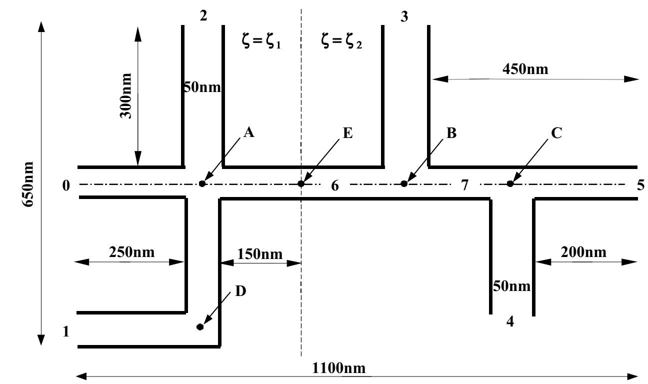

Figure 1. A typical micro-fluidic channel system.

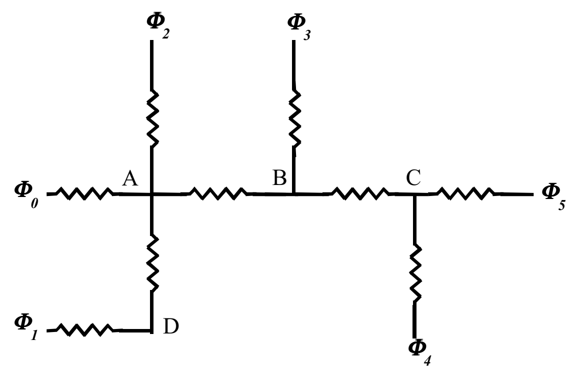

Figure 2. A circuit model to compute the potential for the channel system shown in Figure 1.

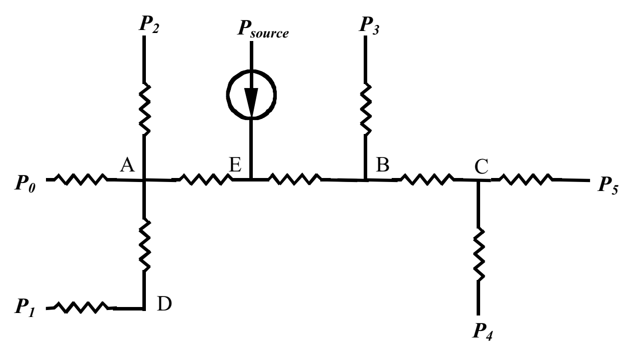

Figure 3. A circuit model to compute the pressure distribution for the channel system shown in Figure 1.

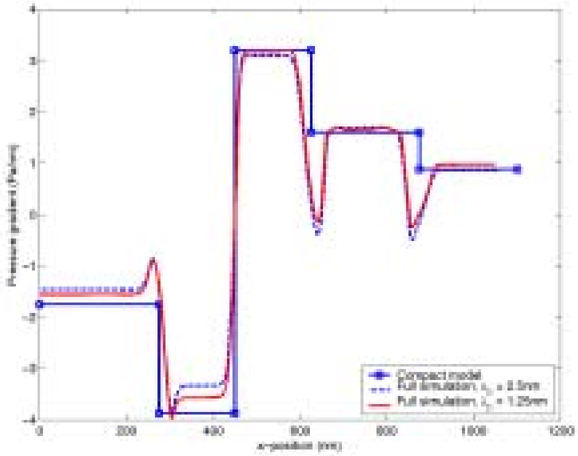

Figure 4. Comparison of pressure gradient along line *0-A-C-5* shown in Figure 1

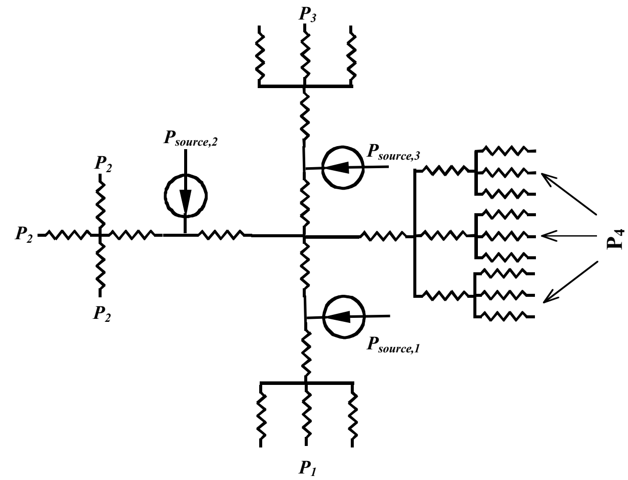

Figure 7. Electrical circuit to compute pressure in the fluidic network shown in Figure 6

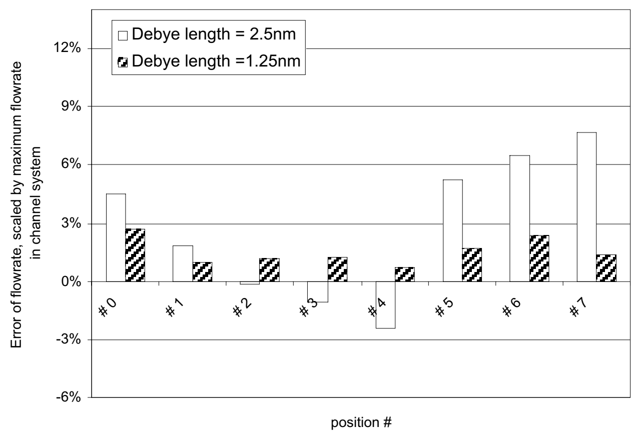

Figure 5. Scaled error of flowrate computed by the compact mode at positions shown in Figure 1

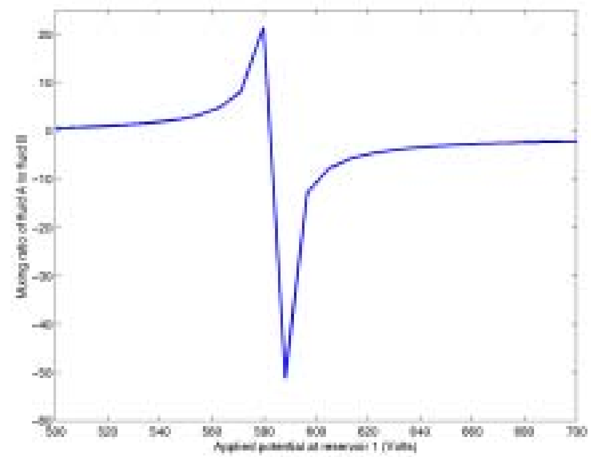

Figure 8. Variation of mixing ratio of fluid A and fluid B with different applied potential at reservoir 1.

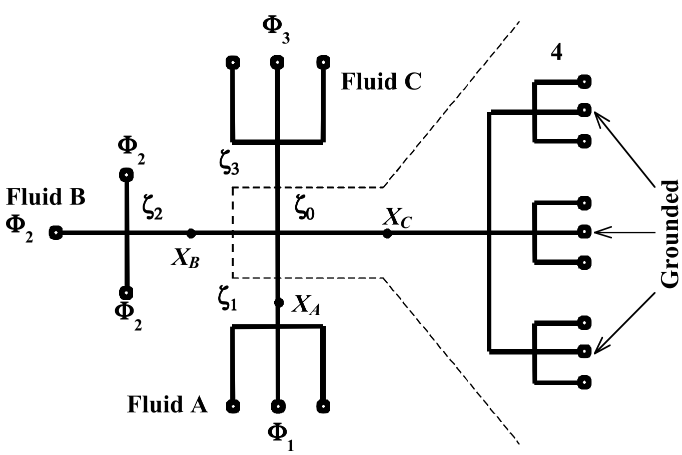

Figure 6. Schematic view of a fluidic mixer. The dotted line indicates the region where ζ-potential on channel wall is ζ_0.