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SUB-GRID MODELING OF ELECTROKINETIC EFFECTS IN MICRO FLOWS

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Introduction

Advances in micro-fabrication processes have generated tremendous interests in miniaturizing chemical and biomedical analyses into integrated microsystems (Lab-on-Chip devices). To successfully design and operate the micro fluidics system, it is essential to understand the fundamental fluid flow phenomena when channel sizes are shrink to micron or even nano dimensions. One important phenomenon is the electro kinetic effect in micro/nano channels due to the existence of the electrical double layer (EDL) near a solid-liquid interface. Not only EDL is responsible for electro-osmosis pumping when an electric field parallel to the surface is imposed, EDL also causes extra flow resistance (the electro-viscous effect) and flow anomaly (such as early transition from laminar to turbulent flow) observed in pressure-driven microchannel flows.

Modeling and simulation of electro-kinetic effects on micro flows poses significant numerical challenge due to the fact that the sizes of the double layer (10 nm up to microns) are very thin compared to channel width (can be up to 100's of μm). Since the typical thickness of the double layer is extremely small compared to the channel width, it would be computationally very costly to capture the velocity profile inside the double layer by placing sufficient number of grid cells in the layer to resolve the velocity changes, especially in complex, 3-d geometries. Existing approaches using "slip" wall velocity and augmented double layer are difficult to use when the flow geometry is complicated, e.g. flow in a T-junction, X-junction, etc. In order to overcome the difficulties arising from those two approaches, we have developed a sub-grid integration method to properly account for the physics of the double layer. The integration approach can be used on simple or complicated flow geometries. Resolution of the double layer is not needed in this approach, and the effects of the double layer can be accounted for at the same time. With this approach, the numeric grid size can be much larger than the thickness of double layer. Presented in this report are a description of the approach, methodology for implementation and several validation simulations for micro flows.

Description of the Sub-Grid Modeling

To enable simulations without resolving the double layer, its effects on the flow can be modeled using the concept of a ζ potential near the wall. A body force term, resulting from the interaction of the ζ potential and the applied pressure drop, is added to the fluid momentum equations, written as:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}\rho u_j u_i = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{i,j}}{\partial x_j} + \rho_e E_i \qquad (1)$$

The last term of equation (1) represents the electrokinetic effect. For streaming potential induced by the applied pressure,

$$\lambda_0 E_i = -u_i \rho_e , \tag{2}$$

and the local electric charge density, ρ_e, is governed by the Poisson equation

$$\nabla^2 \zeta = -\frac{\rho_e}{\varepsilon\varepsilon_0} . \tag{3}$$

In the above equations, ρ is the fluid density, u_i the Cartesian velocity components, p the pressure, $\tau_{i,j}$ the stress tensor, ε the fluid permittivity, δ=1/κ the Debye thickness of the double layer, and λ_0 the bulk fluid conductivity. Under equilibrium situation, the ion distribution can be described by the exponential function, then equation (3) becomes the well-known Poisson-Boltzmann equation. For small surface charge situation investigated in this study, the linearized form of the Poisson-Boltzmann equation can be used. Equation (3) thus becomes:

$$\nabla^2 \zeta = \kappa^2 \zeta \tag{4}$$

with BCs': $\begin{cases} \zeta = \zeta_0 , & y = 0 \\ \zeta = 0 , & y = \infty \end{cases}$

ζ is the potential field inside the electrical double layer and ζ_0 is the zeta potential.

Equations (3) and (4) will be used to substituted into the last term of equation (1) for the electrokinetic effect. (We would combine ε and ε_0 into one single symbol ε in the following formulation.) Considering the nature of ζ potential, we analytically integrate the equation (4) combining with the boundary conditions, along a local wall normal direction to obtain the distribution:

$$\varsigma = \varsigma_0 e^{-\kappa y} \tag{5}$$

Where, y is normal distance to the wall, and ζ_0 is the value of ζ potential at the wall. The electrokinetic source term defined in equation (1) is only applied in a very narrow region near the wall. We analytically integrate it while neglecting the impact of ζ potential outside the double layer, with assumption that the velocity profile within the double layer to be linear, and the application of Grahame equation [1] relating surface potential to surface charge density, σ, the source term becomes

$$\vec{S} = \frac{1}{\lambda_0} \sigma^2 \kappa \frac{1}{4} (1 - 3e^{-2}) A u_c \tag{6}$$

Where, V is grid volume near the wall, A is the area of the wall face (see figure 1). The vector S denotes the momentum source contributions due to the streaming potential effect in different directions. The shear stress on the wall is calculated as:

$$\vec{\tau}_w = -\frac{1}{\lambda_0} \frac{1}{4} \frac{\sigma^2}{\dfrac{e^2}{e^2 - 3} \delta} u_c \tag{7}$$

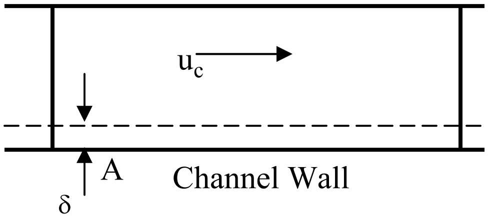

Figure 1. Integration Grid Volume.

In deriving equation (7) we used the relation $\delta = 1/\kappa$. u_c is cell center velocity of grid near the wall and u_w is the wall velocity. The wall velocity is zero for a stationary wall. This definition of the effective distance essentially reduces the apparent wall shear stress, calculated based on the available information during calculations (i.e. u_c, u_w and δ).

The above equations were implemented into ESI-Group's CFD-ACE+ v2004 "Electro" module. Due to the sub-grid model nature, the grid system near the wall should be carefully constructed such that the first cell away from wall should cover the EDL thickness.

Results and Discussion

The model was first compared to the benchmark test case of rectangular microchannel flow of Ren at al. [2]. Detailed channel dimensions and testing conditions were described in [2]. The model prediction and the experimental data are shown in Table 1. As discussed in [1], the electro-viscous effect would be significant when the ionic concentration of the solution is smaller the $5x10^{-3}$ M. As stated in [2], the data for KCl aqueous solution of 10^{-2} M was taken to be the case without EDL effect. As can be seen from Table 1. The model predictions compared well (within 5%) with the experimental data.

	No EDL	No EDL	With EDL DIUF H2O	With EDL DIUF H2O
dP/dx (10^6Pa/m)	**Re,** pred.	**Re,** exp.	**Re,** pred.	**Re,** exp.
2	1.01	~1.05	0.79	~0.82
3	1.50	~1.45	1.20	~1.25
4	1.98	~1.90	1.58	~1.62

Table 1. Prediction and experimental data [2] comparison.

The second test case involved a T-junction micro flow on the Caliper N145 chip. The present model predicts up to about 40% deduction in flow rate when EDL effect is accounted for, as seen in Figure 2. Due to the uncertainties introduced by the dye in the experimental procedure for obtaining velocity data [3], the comparison is qualitative and the model shows correct trend for this complex micro fluidics system.

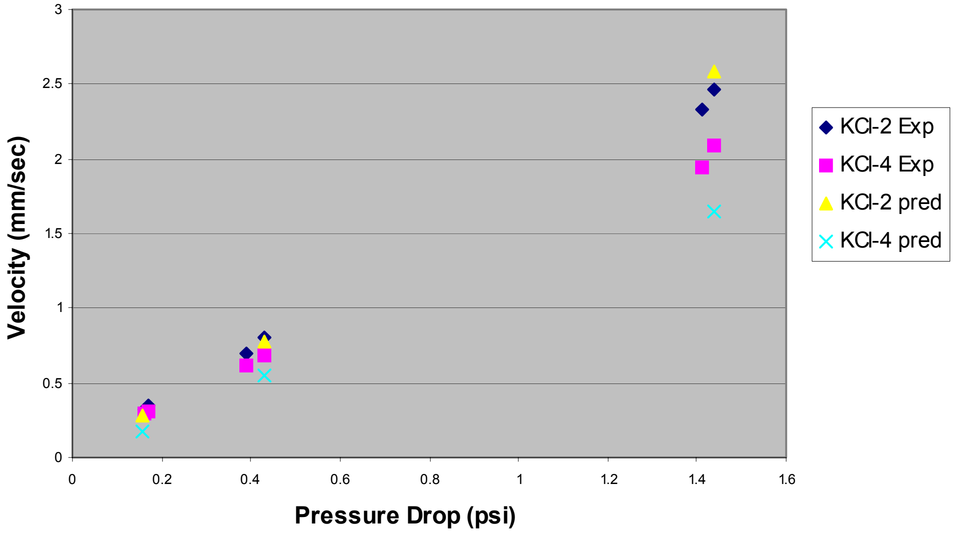

Figure 2. Prediction and data comparison for Caliper N145 chip.

Conclusion

A sub-grid model was developed to account for electro-viscous effect in lab-on-chip microfluidics system. The model was successfully implemented into CFR-ACE+, and validation study was performed. The present model predicts straight micro channel flow well and qualitatively predicts T-junction flow correctly. The electro-viscous effects were found to be quite significant and reduce flow rate (up to 40% in T-junction flows), when compared to the classical laminar theory. Further refinement of the model to account for realistic velocity profile and non-linear Boltzmann distributions within EDL are desirable. Further validations with carefully designed complex micro flow experiments are also recommended.

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References

[1] Hunter, R. J. (2001), *Foundation of Colloidal*, 2nd ed., Oxford University Press.
[2] Ren, L, Qu, W. and Li, D. (1996), "Interfacial Electrokinetic Effects on Liquid Flow in Microchannels," Int. J. Heat and Mass Transfer, vol. 44, pp. 3125-3134.
[3] Hunterhower, H. (2004), "Study to Aid Computer Modeling of Lab-on-Chip Technologies," Presentation at NASA-Marshall Space Flight Center, USRP Summer Program, July, 21.