Proceedings of the ASME 2010 3rd Joint US-European Fluids Engineering Summer Meeting and 8th International Conference on Nanochannels, Microchannels, and Minichannels
FEDSM-ICNMM2010
August 1-5, 2010, Montreal, Canada

FEDSM-ICNMM2010-30252

NUMERICAL SIMULATION OF MIXING IN MICROCHANNELS WITH ROUGH SURFACE

Dayong Yang
School of Environmental & Chemical Engineering, Nanchang University, Nanchang Jiangxi, 330031, China

ABSTRACT

Electroosmotic flow is widely used to transport and mix fluids in microfluidics. Aiming at the parallel-plate microchannel with sinusoidal surface roughness, this paper solved the governing equations using the finite element method and the effects of roughness height and frequency on mixing efficiency are investigated. The simulation results indicate that the mixing efficiency increases with the roughness height and frequency, which is approximately proportional to the roughness height. The results can provide valuable insights into the efficient mixing in microfluidics with rough surface and the optimal design of microchannel.

NOMENCLATURES

L	length of the microchannel (m)
H	half height of the microchannel (m)
D	height or dimension of the microchannel (m)
E	electrical field strength (V/cm)
p	pressure (N/m^2)
e	charge of a proton (C)
k_B	Boltzmann constant (Jk^{-1})
T	temperature (K)
$n_\infty(c)$	ionic concentration (M)
z_0	valnece term of ion
u	velocity (mm/s)
E_x	applied electrical field strength (V/cm)
ψ	local EDL potential (V)
ρ_e	net charge density (Cm^{-3})
ρ_f	density of the fluid ($kgms^{-3}$)
ε_0	permittivity of vacuum ($C^2J^{-1}m^{-1}$)
ε_r	dielectric constant of the solution
μ	dynamic viscosity of the fluid ($kgms^{-1}$)
ζ	zeta potential (V)
λ	Debye layer thickness (nm)
k	Debye-Hückel parameter (nm^{-1})
Mi	mixing efficiency (%)
D_i	diffusion constant (cm^{-2} sec^{-1})
k	relative roughness height (%)
a	roughness element frequency (π)

1 INTRODUCTION

Lab-on-a-chip (LOC) devices are frequently required to have an effective mixing capability[1]. The Reynolds number in such devices are small enough not to induce a turbulent mixing, thus the mixing operation are relied upon diffusive mixing[2]. Several studies are made in recent past on enhanced microfluidic mixing devices based on active mixers[3], using time dependent electric-field, or passive mixers[4] under a steady electric field (DC).

Generally, the microchannel surface may exhibit certain degrees of roughness generated by the manufacturing techniques or by adhesion of biological particles from the liquids. The reported surface roughness ranges from 0.1 to 2 µm, which may have an important effect on the flow and mixing in microchannels[5]. Some studies are made on the EOF[6] and micromixing in rough mcirochannels based on the finite volume method (FVM)[7] and the lattice Boltzmann method (LBM)[8]. All the above studies just deal with the mixing in microchannels with a group of rectangular roughness. Actually, the surfaces possess random roughness textures and the rectangular roughness can hardly describe the real rough surface adequately. However, the numerical simulation of EOF and micromixing in a randomly rough channel is extremely difficult and expensive[9]. This paper focuses on EOF and micromixing in microchannels with sinusoidal structured roughness, which is closer to the real roughness than the rectangular one. The effects of roughness height and frequency on mixing efficiency are also investigated.

2 GOVERNING EQUATIONS

Electroosmotic transport can be described by the Poisson equation and the incompressible Navier-Stokes equations. The model includes:

$$\nabla^2 y = -\frac{r_e}{e_r e_0} \tag{1}$$

$$r_e = -2 z_0 e n_\infty \sinh\left(\frac{z_0 e y}{k_B T}\right) \tag{2}$$

$$r_f(\frac{\partial u}{\partial t}+u\cdot\nabla u)=-\nabla P+m\nabla^2 u+r_e E \qquad (3)$$

$$\nabla\cdot u=0 \qquad (4)$$

where ψ is the electrical potential induced by the zeta potential in the electric double layer (EDL), ε_r is the dielectric constant of the solution, ε_0 is the permittivity of vacuum, and ρ_e is the net charge density per unit volume in Eq. (1), which meet the Eq. (2) with the ψ. In Eq. (2), n_∞ and z_0 are the bulk ionic concentration and the valence of ion in the symmetric electrolyte solution, respectively, e is the charge of a proton, k_B is the Boltzmann constant and T is the temperature.

In Eqs. (3)-(4), u is the velocity vector, μ is the viscosity, ρ_f is the density of the fluid, ρ_e is the local net charge density, E is the electrical field strength and P is the pressure applied to the microchannels.

The objective of this paper is to investigate the surface roughness effect on a fully developed electroosmotic flow and the mixing within a long channel whose height is 10 μm. The strong fluid resistance effect is induced by the periodic roughness symmetrically on the channel wall, shown in Fig.1. The channel is L in length and D in width. The roughness is designed to be sine wave and the function is $h(x)=0.5k\sin(ax)$, h is the height of the roughness, the relative roughness height $k=h/D$, and a is the frequency of the roughness element on the channel wall, describing the roughness element density. Then the equations above could be simplified into two-dimensional mathematic models.

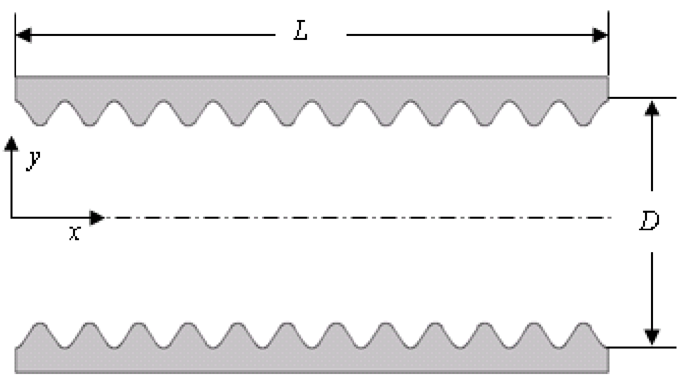

Fig. 1 Schematic of the microchannels with sinusoidal surface roughness.

Substituting Eq. (2) into Eq. (1) leads to the nonlinear Poisson-Boltzmann equation with the coordinates shown in Fig.1.

$$\frac{\partial^2 y}{\partial y^2}=\frac{2z_0 e n_\infty}{e_r e_0}\sinh(\frac{z_0 e y}{k_B T}) \qquad (5)$$

Fully developed flows and the zero pressure gradients are assumed in microchannels, in addition, for sufficiently small Reynolds number (for the channel sizes considered in this work *Re~0.1* or smaller), the Eq. (3) as described above could be simplified into

$$0=m\frac{\partial^2 u}{\partial y^2}+r_e(y)E_x \qquad (6)$$

Defining Debye-Hückel parameter $k=\lambda^{-1}=(2z^2e^2n_\infty/e_r e_o k_B T)^{1/2}$, and λ is the EDL thickness, which is named as Debye length depending strongly on the ionic concentration and the temperature in the bulk of the fluid.

The corresponding boundary conditions follow:

$$y=0,\frac{\partial y}{\partial y}=0,\quad y=\pm\frac{D}{2}(1-h), y=z \qquad (7)$$

$$y=0,\frac{\partial u}{\partial y}=0,\quad y=\pm\frac{D}{2}(1-h), u=0 \qquad (8)$$

where, h and ζ are the roughness element height and zeta potential on microchannel wall, respectively.

When two liquids with different concentrations flow into the microchannel from the upper and lower part, the species transport in the fluid system can be described by the diffusion-convection equation[10]:

$$\frac{\partial c}{\partial t}+u\cdot\nabla c=D_i\nabla^2 c \qquad (9)$$

where c and D_i are the concentration and diffusion constant of the species, respectively.

For analysis of the mixing efficiency quantitatively, the following equation is introduced[11]:

$$M_i=(1-\frac{\int_A|c_i-c_\infty|dA}{\int_A|c_0-c_\infty|dA})\times 100\% \qquad (10)$$

Here c_i is the concentration in element i of the cross-section; c_0 is the initial concentration at the entrance; c_∞ is the concentration at infinity; M_i is the mixing index, which equals unity to denote complete mixing. The concentration is normalized to unit for the upper inlet but zero for the lower one.

3. RESULTS AND DISCUSSION

To simulate the EOF in 2D microchannels, we applied a 2D-computation code COMSOL Multiphysics 3.5 (COMSOL Inc.) based on the finite element method (FEM). The non-uniform grid was used to discretize the domain in microchannels in view of the large difference in dimension between the EDL thickness and channel width, i.e., the extremely small grid was used in the near-wall region, and the coarser comparatively was used in the bulk flow region. And every case was examined before the analysis of the EOF to insure the convergence of the result.

Consider the microchannels with a width $D=10\mu m$, a length $L = 5D$, the relative roughness height $k=0\sim0.1$ leading to a $h=0\sim1\mu m$, roughness element frequency $a=1\sim5\pi$, means the roughness intervals vary from $2\sim0.4\mu m$. Applied electrical field strength along the x direction $E_x=200V/cm$, and the other parameters including: the dynamic viscosity $\mu=0.9\times10^{-3}Nsm^{-2}$, density $\rho_f=1.0\times10^3\ kgm^{-3}$, the dielectric constant of the solution $\varepsilon_r=80$, the permittivity of vacuum $\varepsilon_0=8.854\times10^{-12}C^2J^{-1}m^{-1}$, the Boltzmann constant $k_B=1.38\times10^{-23}JK^{-1}$, the charge of a proton $e=1.6\times10^{-19}C$, the temperature $T=298K$, zeta potential on the channel wall $\zeta=-100mV$. The concentration in the upper inlet is unit and for the lower one is zero.

3.1. Validation of the EOF

EOF in smooth microchannels is modeled based on FEM numerically first when the relative roughness height is k=0 or the roughness element frequency is a=0. Figure 2 represents the dimensionless EOF velocity profiles in smooth microchannels with the width much larger than the EDL thickness. The linearized Possion-Boltzmann(LPB) result[12] is also provided to compare with the numerical solution, which validates the accuracy of the FEM in this paper. It's easy to find that the plug-like EOF is generated and the velocity in the bulk flow region is the maximum and constant for different EDL thickness, which agrees well with the Smoluchowski equation.

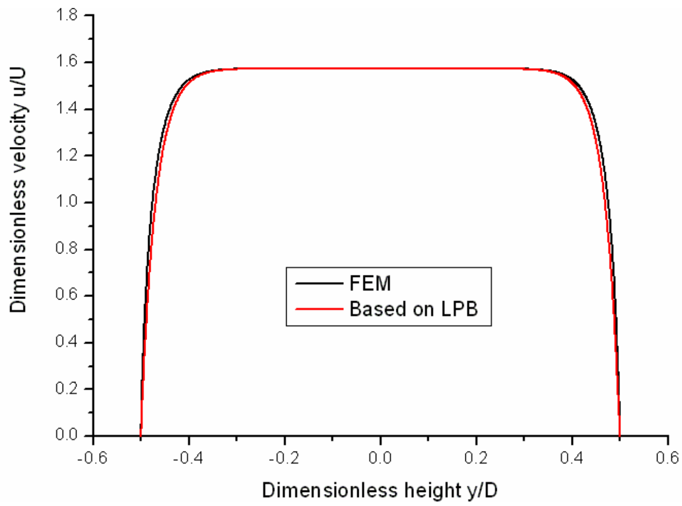

Fig. 2 Dimensionless velocity profiles in smooth microchannels.

3.2. Effect of the roughness element height

Supposing the roughness element frequency is invariable, the liquids flow from inlet to outlet after the convection and diffusion in microchannels. Fig. 3 is the concentration field distribution in rough microchannels, the relative roughness height *k=0.05*. Fig. 4 shows the concentration profiles at inlet and outlet of the microchannels, the horizontal coordinate is the dimensionless distance along the channel width and the vertical one is the concentration. It's easy to be found that the concentration in the rough channel is more uniform than that in the smooth one. This is because the EOF velocity is lower in rough microchannels in the presence of the roughness, thus the time of flow and the diffusion is extended.

Figure 5 shows the mixing efficiency of different crosses-section in microchannels with different relative roughness height *k*, the horizontal coordinate is the ratio of the channel length and width, and the vertical one is the concentration based on the Eq. (10). The results indicate that the mixing efficiency is higher when the roughness height is higher or the mixing length is longer. Fig. 6 shows the mixing efficiency at the outlet changing with the roughness height in microchannel. The results indicate that the mixing efficiency increases with the roughness height, which is approximately proportional to the roughness height. The mixing efficiency can be increased 20% when the comparative roughness element height is 10% at the 5 times of the outlet to the width of the channel, which means the mixing length can be decreased for the rough microchannels.

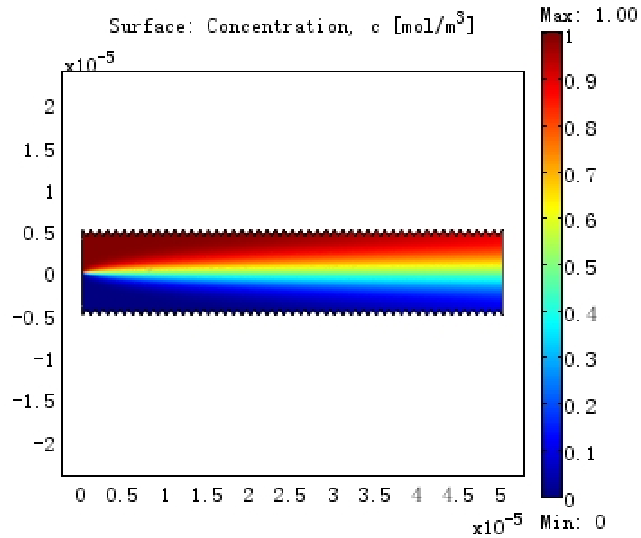

Fig.3 Liquid concentration in rough microchannel

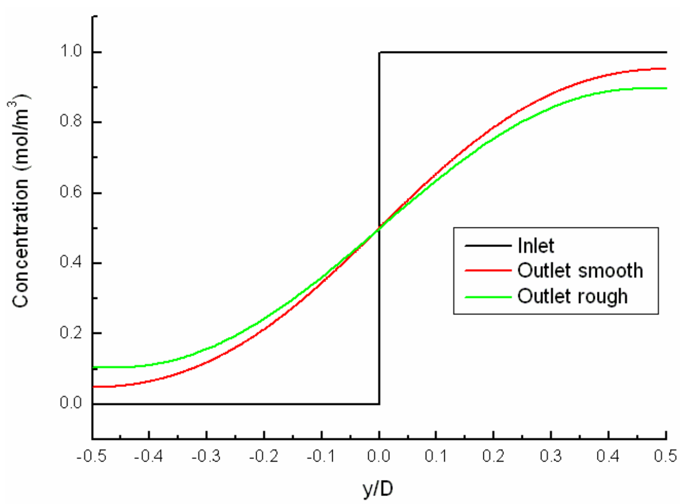

Fig. 4 Liquid concentration profiles in microchannels

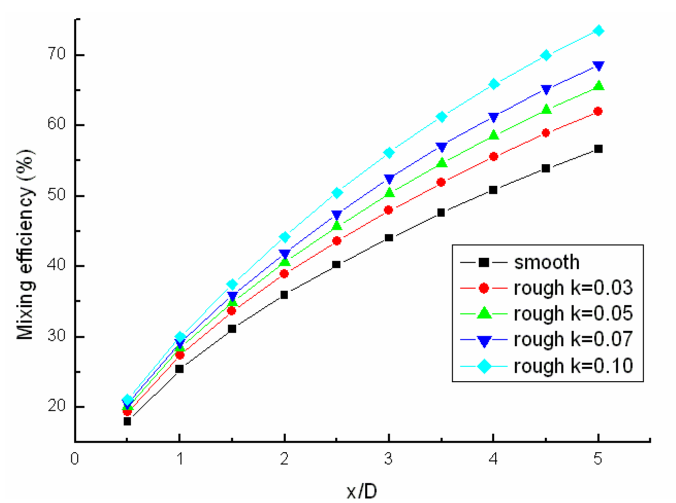

Fig. 5 Mixing efficiency of different crosses-section in microchannels

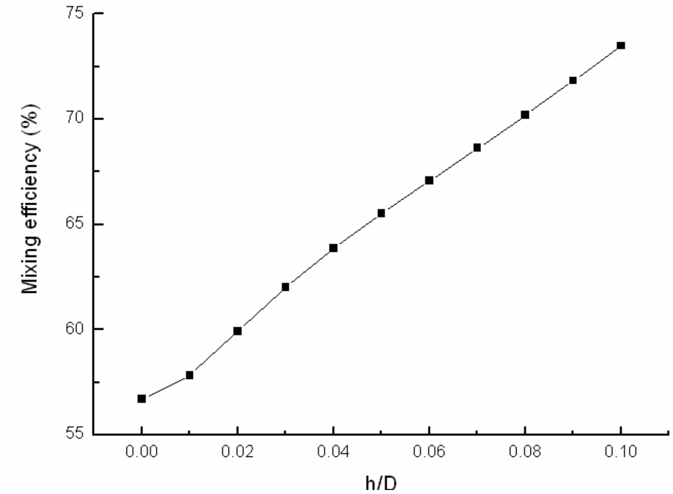

Fig. 6 Mixing efficiency vs. roughness height

3.3. Effect of the roughness element frequency

Supposing the roughness height is invariable. Fig. 7 shows the mixing efficiency in the outlet of 2 times of width changing with the roughness frequency, the horizontal coordinate is the roughness element frequency in rough microchannls. It can be found that the mixing efficiency increases with the frequency and the trend becomes slower. This is because the rough surface is close to smooth one when the frequency is smaller, and the EOF resistance is lower, thus the mixing time is closer to that in smooth channel. And the EOF resistance increases with the frequency, so the flow and mixing time is longer. When the frequency is larger, roughness element has less relatively influence on the EOF.

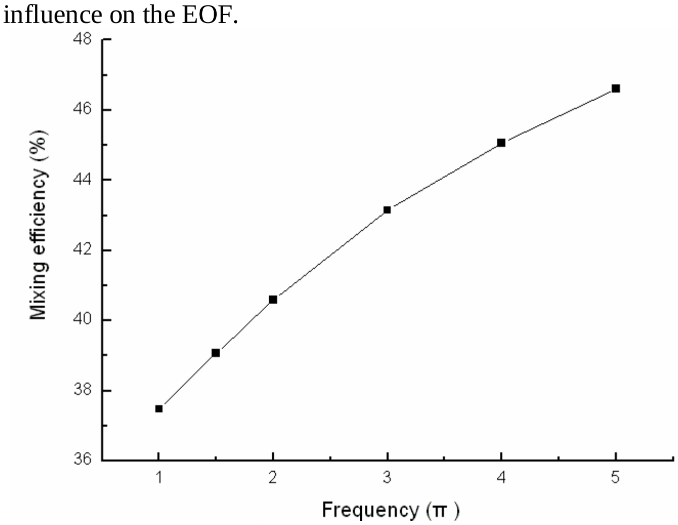

Fig. 7 Mixing efficiency vs. roughness frequency

4. CONCLUSIONS

The EOF and mixing in rough microchannels were modeled by using FEM based on the non-uniform grid. The effects of sinusoidal roughness height and frequency on mixing efficiency were also discussed. The results indicate that the mixing efficiency increases with the roughness height and frequency, which is approximately proportional to the roughness height. The mixing efficiency can be increased 20% when the comparative roughness element height is 10% at the 5 times of the outlet to the width of the channel, which means the mixing length can be decreased for the rough microchannel. The results can provide valuable insights into the efficient mixing in microfluidics with rough surface and the optimal design of microchannel.

ACKNOWLEDGMENTS

This work was supported by the Grants from the National Natural Science Foundation of China (Grant No. 50730007).

REFERENCES

[1] V Hessel, H Lowe, F. schonfeld. Micromixers-a review on passive and active mixing principles, Chem. Eng. Sci., 2005, 60: 2479-2501

[2] C. Zhang, , D. Xing, Y Li. Micropumps, microvalves, and micromixers within PCR microfluidic chips, Biotechnol. Adv., 2007, 25: 483-514

[3] S. Qian, H. H. Bau. A chaotic electroosmotic stirrer. Anal. Chem., 2002, 74: 3616-3625

[4] C.-C. Chang, R-J Yang. Electrokinetic mixing in microfluidic systems, Microfluid and Nanofluid, 2007, 3: 501-525

[5] Y. Hu, C. Werner, D Li. Electrokinetic transport through rough microchannels. Anal. Chem., 2003, 75: 5747-5758

[6] H.A. Stone, A.D. Stroock, A Ajdari. Engineering flows in small devices microfluidics toward a lab-on-a-chip, Annu. Rev. Fluid Mech. 2004. 36:381-411

[7] Y. Hu, X. Xuan, C. Werner, et al. Electroosmotic Flow in Microchannels with Prismatic Elements. Microfluid and Nanofluid, 2007, 3:151-160

[8] D. Wang, J. L. Summers, Gaskell Philip H. Modelling of electrokinetically driven mixing flow in microchannels with patterned blocks. Computers and Mathematics with Applications, 2008, 55: 1601-1610.

[9] A. S. Rawool, S. K. Mitra, S G Kandlikar. Numerical simulation of flow through microchannels with designed Roughness. Microfluid and Nanofluid, 2006, 2: 215-221

[10] S. H. Wong, M. C.L. Ward, C.W Wharton. Micro T-mixer as a rapid mixing micromixer, Sensor Actuat B-Chem., 2004, 100: 359-379

[11] J.-T. Yang, W.-F. Fang, K.-Y Tung. Fluids mixing in devices with connected-groove channels. Chem. Eng. Sci., 2008, 63: 1871-1881

[12] P. Dutta, A. Beskok, T. Warburton. Numerical simulation of mixed electro-osmotic/pressure driven microflows, Numer. Heat Transfer, Part A, 2002, 41: 131-148.