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发散形通道内的稳定电渗流动

王小章¹, 王朝晖², 蒋庄德¹

(1. 西安交通大学 机械工程学院, 陕西 西安 710049;

2. 西安交通大学 机械制造系统工程国家重点实验室, 陕西 西安 710049)

摘要:电渗流通过外加电场来驱动液体通过微小通道,同时由于焦耳热效应的存在,也会在流体及通道表面形成热传导现象。应用计算流体力学方法,对矩形发散形微通道内电渗流流动所产生的流场、温度场进行了数值模拟和研究。由于流体的介电常数、电导率、粘性、热导率等属性依赖于温度的变化,焦耳热效应产生的温度场会改变流体的多种属性,并进而影响到流动速度、压力分布等。计算结果表明,焦耳效应在微管道芯片上产生了一个非均匀的热梯度场,并同时影响液体流动。热梯度场的存在均匀截面通道内可以提高液体的流动速度,但在发散形通道内却不能产生相似的效果,此时的出口速度和体积流速都明显下降,分别达到约16%和60 $\mu\text{l}/\text{min}$ 。焦耳热效应同时通过降低流速和流动压力减弱了发散形管道的电渗流泵送性能。

关键词:电渗流;发散形通道;焦耳热效应;计算流体力学

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Steady electroosmotic flow in diverging microchannels

WANG Xiao-zhang¹, WANG Chao-hui², JIANG Zhuang-de¹

(1. School of Mechanical Engineering, Xi'an Jiaotong University, Xi'an 710049, China ;

2. State Key Laboratory for Manufacture Systems Engineering,

Xi'an Jiaotong University, Xi'an 710049, China)

Abstract: The electroosmotic flow drives a fluid passing through microchannels by an applied electric field, which also induces heat transfers both in the fluid and channel walls because of a Joule-heating. Using the Computing Flow Dynamics(CFD) technique, a flow field and a temperature field in diverging channels are numerically investigated with a 3-D microchip model. Due to the temperature-dependent physical properties of the fluid including viscosity, relative dielectric constants, electric conductivity, and thermal conductivity, the induced temperature gradient imposes great influence on flow behaviors of channels. The results suggest that a nonuniform gradient thermal field is formed in a microchip by the Joule heating and it affects the flow field severely. This gradient thermal field has increased the flow velocity in uniform cross-section channels but can not do it similarly in diverging channels, so that the outlet velocity and volume flow rate have decreased by 16 % and 60 $\mu\text{l}/\text{min}$, respectively. Moreover, the Joule heating also weakens the pumping performance of diverging channels by decreasing the flow velocity and pressure.

Key words: electroosmotic flow; diverging channel; Joule heating; Computing Flow Dynamics(CFD)

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1 Introduction

Microfluidic systems and Lab-on-a-chip devices have attracted a tremendous interest in the last decade, since they bring novel applications into reality in many areas such as chemical process, propulsion, power generation, electronic chip cooling, and biological industries. Electroosmotic Flow (EOF) is one of the most important ways, which controls the fluid transport by applying an electric field and drives fluid to pass through microchannels without a pressure difference between the inlet and the outlet. It is widely employed to drive and manipulate fluid in microchips, such as liquid pumping, species dielectrophoresis separating, sample injecting, and mixing^[1-4], because EOF involves no moving mechanical parts and generates a perfect plug-like flow profile. Although it is investigated extensively both in numerical and experimental methods, there still remain challenges to fully understand EOF in microchannels and design microfluidic devices successfully, for instance, electroosmotic flow in nonuniform cross-section channels.

In this paper, the ‘whole-chip’ approach is taken to study the characteristics of electroosmotic flow in diverging microchannels using Computer Flow Dynamics(CFD) technique. The microchip with a diverging channel is designed to study the flow field and temperature field induced by electroosmotic flow. The temperature field induced by the Joule heating effect, which couples closely with the flow field and electrical field, is investigated by taking into account the temperature-dependent properties of fluid. The flow field influenced by the temperature field is also investigated to reveal the influence of heat generation and heat transfer in the microchip. In addition, the pumping performance of different channels are also compared by the numerical results.

2 Format descriptions

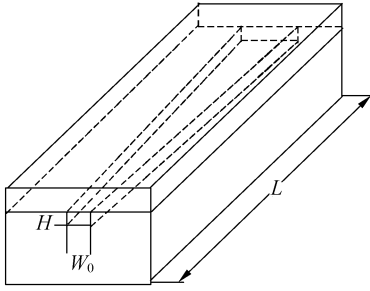
Electroosmotic flow mainly is formed by the interaction of the applied electric field and the induced charge inside an electric double layer. The developed mathematical model includes the Poisson-Boltzmann equation and the Navier-Stokes equations^[5]. The Poisson-Boltzmann equation describes the electric field in microchannels, whereas general Navier-Stokes equations govern the flow driven by electroosmotic force. The corresponding governing equations can be found in references^[5-7]. The Joule heating brings the heat transfer between fluid and channel walls and generates a temperature gradient both in the fluid and a microchip. The heat generation and heat transfer can be described by an energy equation by taking into account of the heat source and the thermal conductivities of working fluid:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \cdot \nabla(\bar{v} \cdot T) = \nabla k \cdot \nabla T + (\mu \rho_e + E\sigma)^2 / \sigma, \quad (1)$$

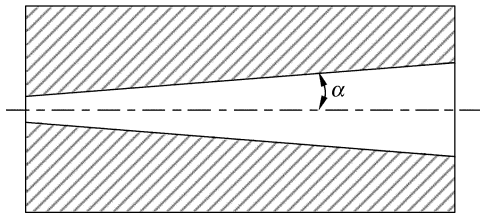
$$\rho_w C_{pw} \frac{\partial T_w}{\partial t} = k_w \cdot \nabla T_w, \quad (2)$$

where \bar{v} , E are the flow velocity and applied electrical field; C_p , k , μ , σ are the heat capacity, thermal conductivity, viscosity, and electric conductivity of fluid; ρ_w , C_{pw} , k_w , T_w are the density, heat capacity, thermal conductivity, and temperature of channel wall, respectively. The last term in the right side of Eq. (1) is due to the Joule heating effect, which includes two parts, conducting and convection current. The conducting current is due to the applied electric field and the convection current is caused by the net charged density moving with the fluid. Here, we consider a microchip with a diverging rectangular microchannel, as shown in Fig. 1. This microchip has dimensions in a length of 2 mm, a width of 0.8 mm, and a thickness of 2.0 mm, and is comprised of a lower substrate and a upper cover. The thickness of substrate and upper

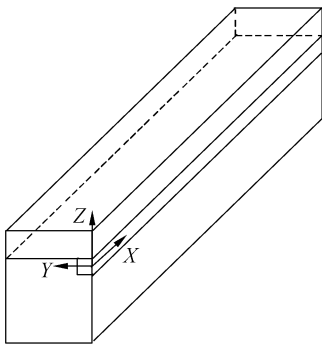
cover is 1.5 mm and 0.5 mm, respectively. The diverging channel is machined on the substrate with inlet width W_0 50 μm , height H 40 μm , and diverging angle 3° . Because of the symmetry of microchips, only a half chip is considered in the numerical computation (as shown in Fig. 1 (c)).



(a) Geometry of microchip with a diverging channel



(b) Schematics of diverging channel



(c) Half microchip as computational domain

Fig. 1 Schematics of microchip with diverging channel

The working fluid is KCl water solution in all calculations, whose physical and electric properties are: density $\rho = 1\,000\text{ kg/m}^3$, dynamic viscosity $\mu = 0.001\text{ Ns/m}^2$, and relative dielectric con-

stant $\epsilon_r = 78.5$, heat capacity $C_p = 4\,180\text{ J/kg} \cdot \text{K}$, and thermal conductivity $k = 0.61$. The microchannel chip is assumed to make from poly(dimethylsiloxane) (PDMS) by microfabrication technologies. The PDMS material has a density of $1\,030\text{ kg/m}^3$, a heat capacity of $1\,100\text{ J/kg} \cdot \text{K}$, and a thermal conductivity of 0.18 . The temperature of the fluid is $T = 293\text{ K}$ and the strength of the external electric field is $E = 10\,000\text{ V/m}$. The zeta potential of the channel wall is selected as -50 mV , and the Helmholtz-Smoluchowski velocity is selected as reference, which equals to $3.87 \times 10^{-4}\text{ m/s}$ in this paper, to get the dimensionless form of the computed results. Due to the temperature-dependent physical properties of fluid including viscosity, relative dielectric constant, electric conductivity, and thermal conductivity, this temperature gradient imposes great influence on electroosmotic flow in channels. The temperature-dependent properties used in this paper are listed as below^[7-9]:

Dynamic viscosity:

$$\mu = 2.76 \times 10^{-6} \exp(1\,713/T), \quad (3)$$

Dielectric constant:

$$\epsilon_r = 305.7 \exp(-T/219), \quad (4)$$

Electric conductivity:

$$\sigma = 0.129(1 + 0.02(T - T_0)), \quad (5)$$

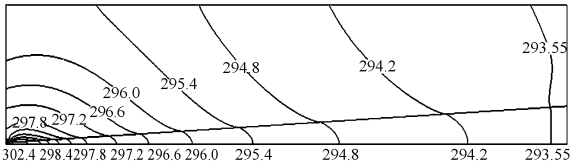
Thermal conductivity:

$$k = 0.61 + 0.001\,2(T - T_0). \quad (6)$$

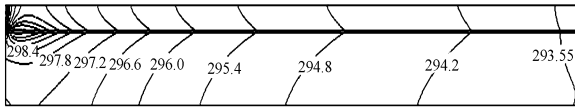
3 Results and discussion

3.1 Temperature field

Fig. 2 presents the steady temperature field induced by the Joule heating and the thermal transfer between fluid and channel walls. The applied external heat transfer boundary condition for the chip outer surfaces is the ambient temperature 293 K and the convection thermal conduct coefficient between the chip and the surrounding air is $10\text{ W/m}^2 \cdot \text{K}$. Fig. 2 (a) shows the temperature field at the mid-height plane of the diverging channel ($z = 0$), which implies



(a) Temperature profile of mid height plane of channel ($z=0$)



(b) temperature profile of symmetric plane ($y=0$)

Fig. 2 Steady temperature field of the microchip with a diverging angle of 3°

that the temperature gradient is nonuniform along the channel centerline. Fig. 2 (b) plots the temperature distribution at the symmetric plane ($y=0$), which also indicates the non-uniformity of the temperature field. This nonuniformity can also be seen from Fig. 3 which displays the Joule heating induces temperature increasing and dropping along the channel centerline. From Fig. 3, it is clear that the temperature reaches the maximum value near the inlet ($x/H=30$) and gradually decreases to the ambient temperature. This temperature field is quite different from the nearly uniform profile in a uniform cross-section channel, and can be used for isoelectric focusing application using temperature-dependent pH value buffer solution^[10].

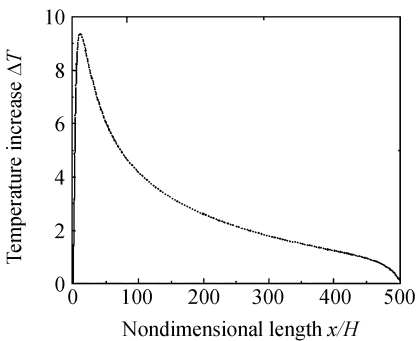


Fig. 3 Temperature increase along channel centerline with Joule heating

3.2 Effects on EOF velocity

The Joule heating induces the temperature field and influences the EOF velocity in microchannels. Fig. 4 compares the velocity profiles of u with and without the Joule heating at the mid- x plane and outlet. We can see that EOF velocity u profile at the mid- x plane with the Joule heating is slightly larger than that without the Joule heating, but it is reversed at outlet. The velocity u at outlet becomes a concave profile, as fluid near the divergence walls flows faster and the bulk more slowly than that without the Joule heating. It works so because the induced temperature gradient changes the properties of working fluid, which in turn alters the velocity profiles. The increase of temperature diminishes the fluid viscosity according to Eq. 15. This variation makes the momentum in EDL diffuse into fluid bulk more difficultly and the center velocity of fluid slow down. Combining with the diverging channel shape, the concave profile comes up. The concave profile can also be explained by the negative pressure gradient in a diverging channel (as shown in Fig. 6).

Fig. 5 plots the comparison of the streamwise velocity distribution curves along the channel centerline with and without the Joule heating, which illustrates that the two distribution curves have the same varying trend along the centerline and only differ in quantities. The Joule heating drops the streamwise velocity of EOF at the inlet

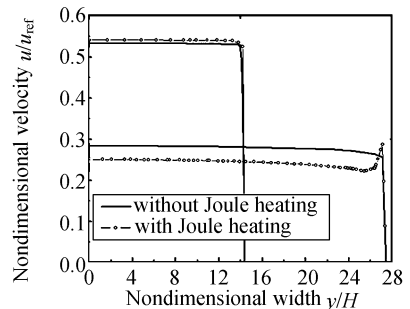


Fig. 4 Comparison of u profile with and without Joule heating at the mid- x -plane and outlet of channel

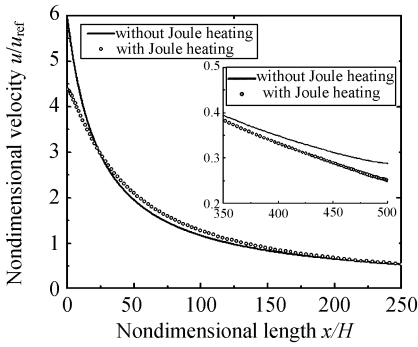


Fig. 5 Distribution of u profile along channel centerline with or without Joule heating. The inset figure shows the distribution from $x = 1.22$ mm to 2.0 mm.

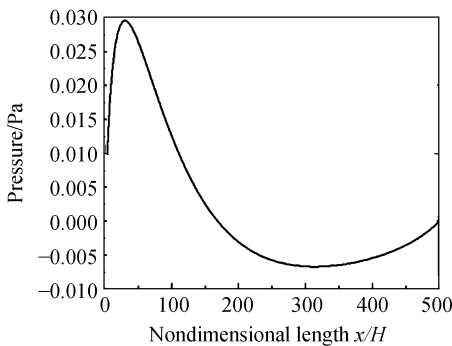


Fig. 6 Pressure distribution in divergent channel with Joule heating

and outlet of the diverging channel, although it increases the velocity u to a larger quantity in a portion of microchannel. This mainly attributes to the nonuniform electric field induced by temperature field in microchannel. According to Eq. (6), the temperature gradient formed in a chip changes the electric field strength in fluid and in turn the electroosmotic driving force varies. The expansion of channel cross-section is another factor contributing to the decrease of u velocity. The non-uniform electric field and the increasing channel width vary EOF velocity and keep the continuity of the flow. As a result, the EOF velocity with the Joule heating drops further along the channel centerline than that without Joule heating. The decrease of velocity can also be ex-

plained by the concave profile at the outlet.

3.3 Effects on pumping performance

Since the temperature increases and gradient forms in the microchip, the pumping performance is also changed. From section 3.2 we know that the EOF velocity drops due to the temperature gradient, so does the volume flow rate in the diverging channel. The computed volume flow rate is $10 \mu\text{l}/\text{min}$ with the Joule heating effect, comparing to the $69 \mu\text{l}/\text{min}$ without the Joule heating. The pressure profile changes severely along the channel centerline in Fig. 6, whose maximum value decreases and the asymmetric profile vanishes completely with a negative pressure portion appearing in the back half of channel ($140 < x/H < 500$). This negative pressure gradient is formed because of the Joule heating and the continuity of flow field, which also contributes to the formation of the concave profile at the outlet of channel.

4 Conclusions

Electroosmotic flow attracts extensively study and is widely used in Lab-on-a-Chip or Micro total Analysis System (μTAS) devices. In this paper, EOF in diverging microchannels is investigated using CFD techniques. The flow field and the induced temperature field are numerically simulated using a 3D microfabricated chip model with a diverging channel. Because of the applied electric field and conductivity of working fluid, the Joule heating is generated in the bulk flow and it forms a temperature field in a microchip, which also couples closely with the electric field and flow field through the temperature-dependent properties of fluid. This temperature field can increase EOF velocity in uniform cross-section channel but doesn't work similarly in a diverging channel, which drops the streamwise ve-

locity of EOF at the inlet and outlet of the diverging channel, although it increases the velocity u in a portion of microchannel. The Joule

heating also weakens the pumping performance of diverging channel by decreasing the flow velocity and pressure.

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Authors' biographies:



WANG Xiao-zhang (1975 —), male, Ph. D candidate of the School of Mechanical Engineering, Xi'an Jiaotong University, his researches focus on precious metrology and BioMEMS applications. **E-mail:** jlab@mail.xjtu.edu.cn

JIANG Zhuang-de(1955—), male, professor of the School of Mechanical Engineering, Xi'an Jiaotong University, his researches focus on precious instruments and metrology, electrical-optic test, Microelectromechanical Systems (MEMS), and nanotechnology. **E-mail:** zdjiang@mail.xjtu.edu.cn

WANG Chao-hui(1968—), male, associate professor of the Department of Instrument and Science, Xi'an Jiaotong University, his researches focus on precious instruments and metrology, electrical-optic test, and BioMEMS applications. **E-mail:** chhw@mail.xjtu.edu.cn