Modeling of Micro Flows Using Perturbation Method

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Abstract A new method for modeling micro flows is presented in this research. The basis of this method is the development of governing continuum equations on fluid dynamics using perturbation expansion of the velocity, pressure, density and temperature fields in dependence of Knudsen number. In the present work, we use three-term perturbation expansions and reach three order of equations O(1), O(Kn), O(Kn^2). Required boundary conditions (BC) for solving each order of these equations are obtained by substitution of the perturbation expansions into the general boundary conditions for the velocity slip and temperature jump. This set of equations is discretized in two-dimensional state on a staggered grid using the finite volume method. A three-part computer program has been produced for solving the set of discretized equations. Each part of this code, solve one order of the equations with the SIMPLE algorithm. Incompressible slip micro Poiseuille and micro Couette flows are solved either analytically or numerically using the perturbation method (PM). Good agreement is found between analytical and numerical results in the low Knudsen numbers, whereas numerical results deviate from analytical results by increasing the Knudsen number. The results of perturbation method are also compared with the results obtained from different slip models.

Keywords: Micro Flow, Perturbation Method, Slip Flow, Micro Poiseuille, Micro Couette

1. Introduction

Based on the Knudsen number, the flow regime is divided into four categories: the continuum regime (Kn < 0.001), the slip flow regime (0.001 < Kn < 0.1), the transition regime (0.1 < Kn < 10) and the free molecular regime (Kn > 10).

Micro-Electro-Mechanical-Systems (MEMS) refer to devices that have characteristic length between 1mm and 1μm. MEMS devices operate in a wide range of flow regimes covering the continuum, slip, and transition flow. Application of these systems is rapidly increased in the industry and medicine. Because the obvious difficulties associated with testing and validating these devices experimentally, numerical analysis is an alternative for investigating the flow inside a micro channel or a more complex geometry. The use of molecular modeling is more efficient going from the continuum regime to the free molecular regime. Inversely, the use of continuous modeling is useful and easier going from the free molecular regime to the continuum regime (Karniadakis et al., 2005; Gad-el-Hak, 2006).

Over the last two decades, many investigations have been performed about continuum simulation of micro flows. In most of them, first and second order slip models have been used for the velocity slip and temperature jump on the wall. For example, Chen et al, (1998) have investigated gas flow in micro channels in the slip regime using the Navier-Stokes equations and first order boundary conditions. Dongari et al, (2007) have investigated gas flow in micro channels using the Navier-Stokes equations and second order boundary conditions. An important challenge which exists in this type of simulations is the type and accuracy of applied slip model.

In the present work, micro flows are simulated using perturbation method which is a continuum method. Required boundary conditions are obtained by substitution of perturbation expansion of the velocity and temperature fields into the general and high order slip boundary condition formula (Karniadakis et al., 2005). Therefore, if perturbation expansions with sufficient terms are used, it will be expected to more accurate results in comparison with other continuum methods. We start with the isothermal incompressible flows and use three-term perturbation expansions of the velocity and pressure fields in the perturbation method.

2. Governing Equations and the Slip BC

In the slip flow regime, the Navier-Stokes equations with slip boundary conditions govern the flow. The Navier-Stokes equations consist of continuity equation, momentum equations and energy equation.

Based on kinetic theory of gases, first order boundary conditions for the velocity slip and temperature jump have been proposed by Maxwell and Smoluchowski (Kennard, 1938). Based on this theory, high-order boundary conditions can be derived by an approximate analysis of the gas motion in the isothermal conditions (Karniadakis et al., 2005). These boundary conditions for two-dimensional flows in the nondimensional form have the form:

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v}\left[Kn\left(\frac{\partial U}{\partial n}\right)_s + \frac{Kn^2}{2}\left(\frac{\partial^2 U}{\partial n^2}\right)_s + \cdots\right] \quad (1)$$

$$T_s - T_w = \frac{2-\sigma_T}{\sigma_T}\left[\frac{2\gamma}{\gamma+1}\right]\frac{1}{\Pr}\left[Kn\left(\frac{\partial T}{\partial n}\right)_s + \frac{Kn^2}{2}\left(\frac{\partial^2 T}{\partial n^2}\right)_s + \cdots\right] \quad (2)$$

where n and s are the normal and tangential direction to the wall. General second-order slip condition has the nondimensional form:

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v}\left[C_1 Kn\left(\frac{\partial U}{\partial n}\right)_s - C_2 Kn^2\left(\frac{\partial^2 U}{\partial n^2}\right)\right]_s \quad (3)$$

where C_1 and C_2 are the slip coefficients. Typical values of the slip coefficients developed by different investigators are shown in Table 1 (Karniadakis et al., 2005; Gad-el-Hak, 2006).

3. Perturbation Method

Every macroscopic properties φ of the flow can be written with an asymptotic expansion as a function of the Knudsen number (Karniadakis et al., 2005; Qin et al., 2007):

Table 1
Coefficients for first and second-order slip models.

Author	C_1	C_2
General	1.0	-0.5
Maxwell(1879)	1.0	0.0
Schamberg(1947)	1.0	5π/12
Albertoni et al.(1963)	1.1466	0.0
Deissler(1964)	1.0	9/8
Cercignani(1964)	1.1466	0.9756
Sreekanth(1969)	1.1466	0.14
Hisa and Domoto(1983)	1.0	0.5
Cercignani(2003)	1.1466	0.647

$$\varphi = \varphi_0 + Kn\,\varphi_1 + Kn^2\varphi_2 + Kn^3\varphi_3 + O(Kn^4)$$
$$\varphi = u, v, w, P, T, \rho, \ldots \quad (4)$$

where φ_0 corresponds to the no-slip flow, φ_1 is the first order correction, φ_2 is the second order correction, φ_3 is the third order correction of the φ, and so on. Increasing the Knudsen number, i.e., going from transition to free molecular flow regime, higher corrections of the φ become important.

We consider three-term perturbation expansions, i.e., two-correction perturbation expansions of the velocity and pressure fields:

$$\boldsymbol{u} = \boldsymbol{u_0} + Kn\,\boldsymbol{u_1} + Kn^2\,\boldsymbol{u_2} + O(Kn^3) \quad (5)$$

$$P = P_0 + Kn\,P_1 + Kn^2 P_2 + O(Kn^3) \quad (6)$$

Now, we substitute these expansions into the 2D incompressible Navier–Stokes equations and also into the high-order boundary conditions for the velocity slip, e.g., equation (1). Next, we rearrange the terms as a function of their Knudsen number order and obtain different orders of Kn dependence equations and boundary conditions.

Conservation equations of mass, momentum and slip boundary conditions of order O(1) yield:

$$\frac{\partial u_0}{\partial x} + \frac{\partial v_0}{\partial y} = 0 \quad (7)$$

$$\rho\left[\frac{\partial u_0}{\partial t} + \frac{\partial (u_0 u_0)}{\partial x} + \frac{\partial (v_0 u_0)}{\partial y}\right] = -\frac{\partial P_0}{\partial x} + \frac{\partial}{\partial x}\left(\mu\frac{\partial u_0}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial u_0}{\partial y}\right) + S_{C_u} + S_{P_u}u_0 \quad (8)$$

$$\rho[\frac{\partial v_0}{\partial t}+\frac{\partial(u_0v_0)}{\partial x}+\frac{\partial(v_0v_0)}{\partial y}]=-\frac{\partial P_0}{\partial y}+ \frac{\partial}{\partial x}\left(\mu\frac{\partial v_0}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial v_0}{\partial y}\right)+S_{C_v}+S_{P_v}v_0 \quad (9)$$

$$u_0\big|_s=u_w \quad (10)$$

Conservation equations of mass, momentum and slip boundary conditions of order O(Kn) yield:

$$\frac{\partial u_1}{\partial x}+\frac{\partial v_1}{\partial y}=0 \quad (11)$$

$$\rho[\frac{\partial u_1}{\partial t}+2\frac{\partial(u_0u_1)}{\partial x}+\frac{\partial(v_1u_0)}{\partial y}+\frac{\partial(v_0u_1)}{\partial y}]= -\frac{\partial P_1}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u_1}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u_1}{\partial y}\right)+S_{P_u}u_1 \quad (12)$$

$$\rho[\frac{\partial v_1}{\partial t}+\frac{\partial(u_1v_0)}{\partial x}+\frac{\partial(u_0v_1)}{\partial x}+2\frac{\partial(v_0v_1)}{\partial y}]= -\frac{\partial P_1}{\partial y}+\frac{\partial}{\partial x}\left(\mu\frac{\partial v_1}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial v_1}{\partial y}\right)+S_{P_v}v_1 \quad (13)$$

$$u_1\big|_s=\frac{2-\sigma_v}{\sigma_v}L_c(\frac{\partial u_0}{\partial n})\bigg|_s \quad (14)$$

Conservation equations of mass, momentum and slip boundary conditions of order O(Kn^2) yield:

$$\frac{\partial u_2}{\partial x}+\frac{\partial v_2}{\partial y}=0 \quad (15)$$

$$\rho[\frac{\partial u_2}{\partial t}+2\frac{\partial(u_0u_2)}{\partial x}+\frac{\partial(u_1u_1)}{\partial x} +\frac{\partial(v_2u_0)}{\partial y}+\frac{\partial(v_0u_2)}{\partial y}+\frac{\partial(v_1u_1)}{\partial y}]= -\frac{\partial P_2}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u_2}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u_2}{\partial y}\right)+S_{P_u}u_2 \quad (16)$$

$$\rho[\frac{\partial v_2}{\partial t}+\frac{\partial(u_2v_0)}{\partial x}+\frac{\partial(u_0v_2)}{\partial x} +\frac{\partial(u_1v_1)}{\partial x}+2\frac{\partial(v_0v_2)}{\partial y}+\frac{\partial(v_1v_1)}{\partial y}]= -\frac{\partial P_2}{\partial y}+\frac{\partial}{\partial x}\left(\mu\frac{\partial v_2}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial v_2}{\partial y}\right)+S_{P_v}v_2 \quad (17)$$

$$u_2\big|_s=\frac{2-\sigma_v}{\sigma_v}\left[L_c\frac{\partial u_1}{\partial n}+\frac{L_c^2}{2}\frac{\partial^2 u_0}{\partial n^2}\right]_s \quad (18)$$

where L_c is the characteristic length and S is the source term. Equation (10), (14) and (18) are written for the horizontal wall and for the vertical wall, the v component of velocity is used in these equations.

4. Discretization and Solution Algorithm

Different orders of produced equations are discretized in two-dimensional state on a staggered grid using the finite volume method. In the micro and nano flows the cell Reynolds is small due to the small length scales of the micro device rather than very small velocities. Therefore, diffusion has an important role. The diffusion terms are discretized with a central difference scheme. Different order of velocities is needed on the cell faces to discretize the convective terms. These velocities are also interpolated centrally.

Overall algorithm of the solution includes three steps: the first step is the solution of the O(1) equations with the O(1) boundary conditions. The second step is the solution of the O(Kn) equations with the O(Kn) boundary conditions. This step's boundary conditions are obtained by fitting the first step's fields on the walls. The third step is the solution of the O(Kn^2) equations with the O(Kn^2) boundary conditions. This step's boundary conditions are also obtained by fitting the first and second step's fields on the walls.

A three-part computer program has been produced for solving this set of equations. Each part of this code solves one order of the equations with the SIMPLE algorithm. The velocity and pressure fields of the slip flow are obtained by corresponding perturbation expansions.

5. Micro Poiseuille Flow

5.1 Flow specifications

An incompressible slip micro Poiseuille flow is considered in isothermal conditions for Nitrogen gas at T=298K and P=1atm. The channel has a length of L=5μm and a height of H=1μm. The flow at the inlet is assumed to be a uniform flow with U_{in}=0.1 m/s (Fig. 1). Hence, the Knudsen number is Kn=0.06 and the Reynolds number is Re=0.007. We also assume σ_v=1 for the present study.

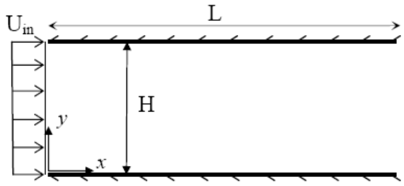

Fig. 1. Channel geometry for micro Poiseuille flow.

5.2 Analytical solution using the PM

For the fully developed flow, $v=0$, $u=u(y)$ and $P=P(x)$. Therfore:

$$v_0 = v_1 = v_2 = \cdots = 0 \tag{19}$$

$$u_0 = u_0(y),\quad u_1 = u_1(y),\quad u_2 = u_2(y),\ \ldots \tag{20}$$

$$P_0 = P_0(x),\quad P_1 = P_1(x),\quad P_2 = P_2(x),\ \ldots \tag{21}$$

Hence, different orders of tangential momentum eguations are simplified and can be easily solved with their velocity slip boundary condition. In the incompressible flow, the slip does not change the flowrate. In other words,

$$\dot{m} = \dot{m}_0\,,\ \dot{m}_1 = \dot{m}_2 = \cdots = 0 \tag{22}$$

As a result, the velocity corrections in terms of the average velocity are:

$$u_0(y) = -6u_m[(\frac{y}{H})^2 - \frac{y}{H}] \tag{23}$$

$$u_n(y) = (-6\frac{2-\sigma_v}{\sigma_v})^{n-1} \times (n-1+6\frac{2-\sigma_v}{\sigma_v}) \times u_m \times \left\{6[(\frac{y}{H})^2 - \frac{y}{H}]+1\right\} \quad ,\ n \geq 1 \tag{24}$$

The final slip velocity profile is produced by substituting these velocities into the perturbation expansion of the velocity:

$$u(y) = \sum_{i=0}^{\infty} u_i(y)(Kn)^i = (\frac{-6u_m}{[1+6\frac{2-\sigma_v}{\sigma_v}(Kn-Kn^2)]}) \times \left[(\frac{y}{H})^2 - \frac{y}{H} - \frac{2-\sigma_v}{\sigma_v}(Kn-Kn^2)\right] \tag{25}$$

5.3 Numerical solution using the PM

A three-part computer program has been produced for solving the set of discretized equations. Each part of this code solves one order of the equations with the SIMPLE algorithm. A uniform 75×30 staggered grid is employed for the present study. The boundary conditions at the channel inlet are:

$$u_1(y)\big|_{x=0} = u_2(y)\big|_{x=0} = 0 \tag{26}$$

$$u(y)\big|_{x=0} = u_0(y)\big|_{x=0} = U_{in} \tag{27}$$

In figs. 2, 3 and 4, nondimensional and fully developed form of the no-slip velocity and the velocity corrections are compared with those analytical in the middle section of the channel ($x=L/2$).

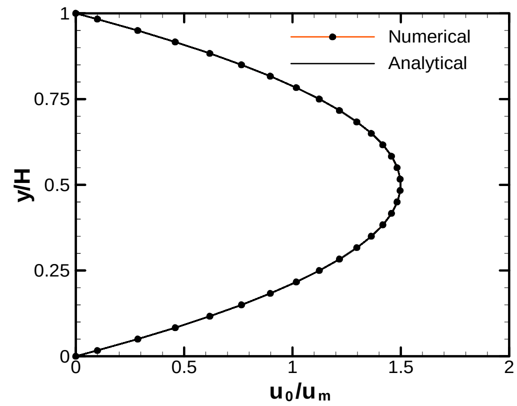

Fig. 2. The no-slip velocity or u_0.

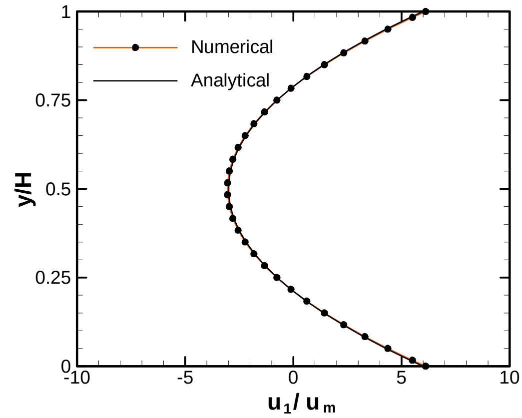

Fig. 3. First order correction of the velocity or u_1.

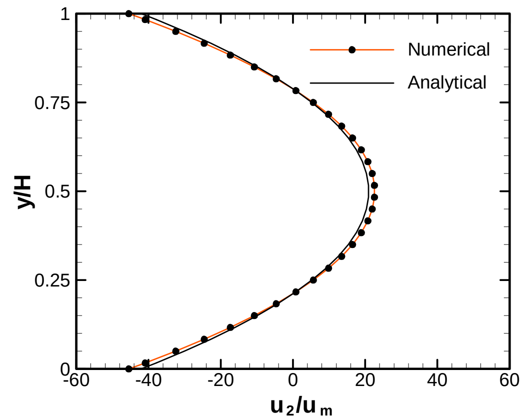

Fig. 4. Second order correction of the velocity or u_2.

Good agreement is found between the analytical and numerical results of the perturbation method. In fig. 5, the nondimensional u_0, u_1 and u_2 velocities are compared together at the middle section. Also in fig. 6, the slip velocity, no-slip velocity and correctional velocities are compared at the middle section of the channel.

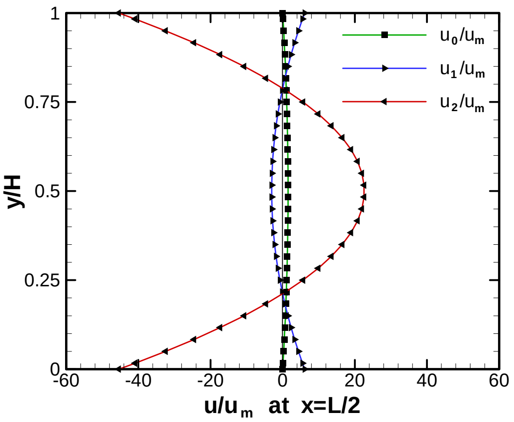

Fig. 5. Comparison of u_0, u_1 *and* u_2 at middle section.

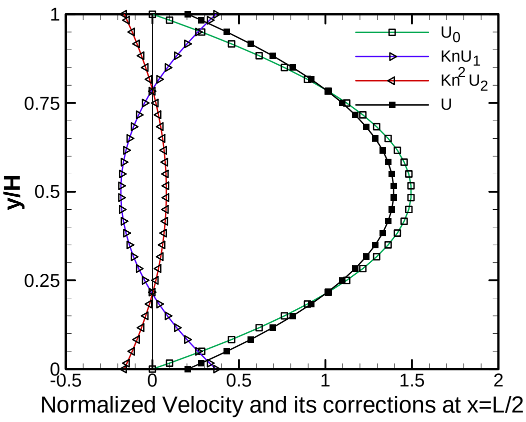

Fig. 6. The nondimensional slip velocity, no-slip velocity and correctional velocities at middle section for Kn=0.06.

5.4 Comparison with other slip models

If we use the boundary condition of equation (3) in the analytical perturbation method, an analytical solution is obtained as follows:

$$u(y) = \frac{-6u_m}{[1+6\dfrac{2-\sigma_v}{\sigma_v}(C_1Kn+2C_2Kn^2)]} \times \left[(\frac{y}{H})^2 - \frac{y}{H} - \frac{2-\sigma_v}{\sigma_v}(C_1Kn+2C_2Kn^2) \right] \quad (28)$$

where C_1 and C_2 are the slip coefficients. In fig. 7, the slip and no-slip velocities obtained by the perturbation method (PM) and slip velocities obtained by the equation (28) are compared together at the middle section. Good agreement is still found between the results. For a better comparison between the PM results and the results produced by different slip models, in fig. 8, normalized slip velocities at the channel walls are shown versus the Knudsen number. If we use one correction, or first order perturbation expansions ($\varphi = \varphi_0 + Kn\varphi_1$), the slip velocity is overpredicted than its real limit by increasing the Knudsen number. Also, If we use two correction, or second order perturbation expansions ($\varphi = \varphi_0 + Kn\varphi_1 + Kn^2\varphi_2$), the slip velocity is underpredicted as compared to its real limit by increasing the Knudsen number.

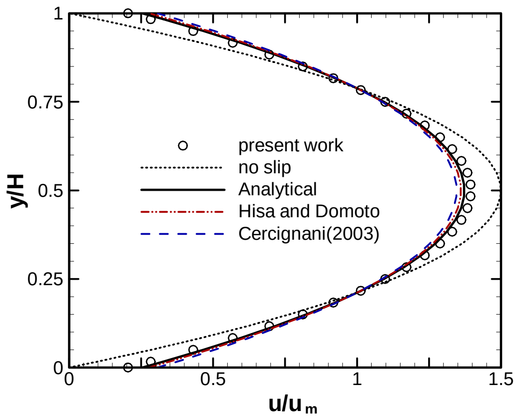

Fig. 7. Slip and no-slip velocities at the middle section of the channel for Kn=0.06.

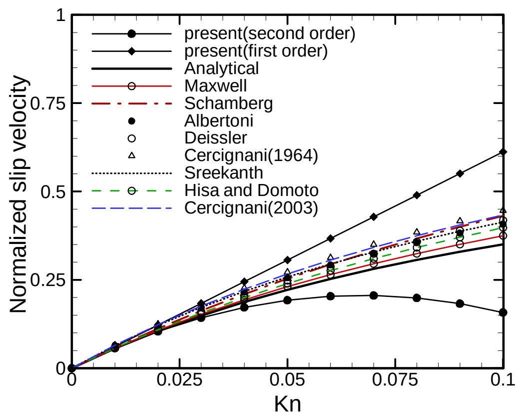

Fig. 8. Normalized slip velocity with the average velocity versus Kn for the micro Poiseuille flow.

However, numerical results of the PM deviate from its analytical results by increasing the Knudsen number. This reveals that more corrections are needed in the perturbation method by increasing the Knudsen number.

6. Micro Couette Flow

6.1 Flow specifications

An incompressible shear-driven slip flow is considered between two parallel plates in isothermal conditions. The fluid is Nitrogen gas at T=298K and P=1atm. The channel has a length of L=5μm and a height of H=1μm. The top surface moves with U_{in}=0.1 m/s (Fig. 9). Hence, the Knudsen number is Kn=0.06 and the Reynolds number is Re=0.007. We also assume σ_υ=1 for the present study.

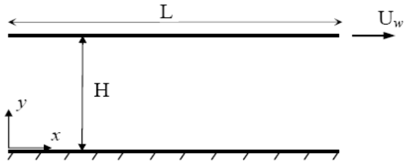

Fig. 9. Channel geometry for micro Couette flow.

6.2 Analytical and Numerical solution using PM

In this problem, *v=0*, *u=u(y)* and *P* is constant. Similar to the previous problem, the velocity corrections can be written in terms of the U_w as following:

$$u_0(y) = U_w(\frac{y}{H}) \quad (29)$$

$$u_n(y) = (-\frac{2-\sigma_v}{\sigma_v})^n \times 2^{n-1} \times U_w \times (\frac{2y}{H} - 1) \quad , \quad n \geq 1 \quad (30)$$

The final slip velocity profile is obtained by substituting these velocities into the perturbation expansion of velocity:

$$u(y) = \sum_{i=0}^{\infty} u_i(y)(Kn)^i = U_w \left[\frac{\frac{y}{H} + \frac{2-\sigma_v}{\sigma_v} Kn}{1 + 2\frac{2-\sigma_v}{\sigma_v} Kn} \right] , \; Kn < \frac{1}{2\frac{2-\sigma_v}{\sigma_v}} \quad (31)$$

For numerical solution of this problem with the PM, we employ the previous uniform 75×30 staggered grid. In fig. 10, the slip velocity, no-slip velocity and correctional velocities are compared in nondimensional form. Very good agreement is found between the analytical and numerical results.

Considering the skin friction coefficient

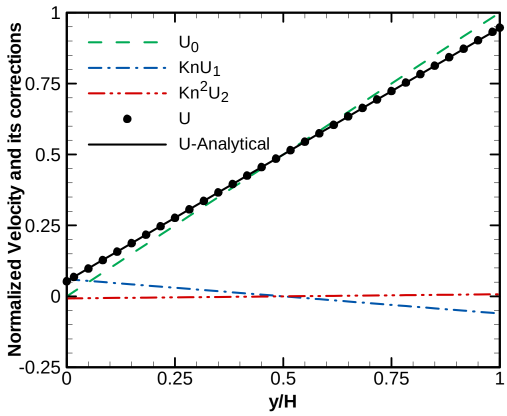

Fig. 10. The slip velocity, no-slip velocity and correctional velocities of the micro Couette flow for Kn=0.06.

$C_f = \tau_w/(0.5 \times \rho U_w^2)$, there can be written the below relations:

$$(C_f Re)_{no\,slip} = 2 \quad (32)$$

$$(C_f Re)_{slip} = \frac{2}{1 + 2\frac{2-\sigma_v}{\sigma_v} Kn} \quad (33)$$

In fig. 11, analytical and numerical results of the PM for the skin friction coefficient are compared.

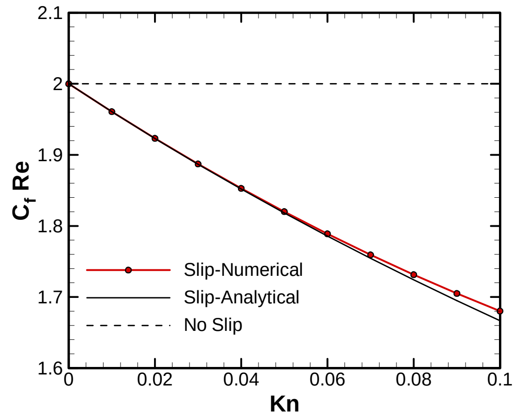

Fig. 11. Variation of skin friction coefficient as a function of Kn for the micro Couette flow.

In the shear-driven micro flows, the compressibility effects become important for large temperature fluctuations or at high speeds. So, the two-correction perturbation method is adequate for isothermal micro Couette flow in the slip flow regime.

7. Conclusions

In the present paper, micro flows are simulated using the perturbation method. At the beginning of this work, two dimensional incompressible flows are investigated. We used three-term perturbation expansions of the velocity and pressure fields in order to obtain three order of equations O(1), O(Kn), O(Kn^2) and their boundary conditions.

This set of equations is discretized in two-dimensional state on a staggered grid using the finite volume method. A three-part computer program has been produced for solving the set of discretized equations. Each part of this code solves one order of the equations with the SIMPLE algorithm.

Incompressible slip micro Poiseuille and micro Couette flows are solved either analytically or numerically using the Perturbation Method (PM). Good agreement is found between analytical and numerical results. These results are also compared with the results obtained from different slip models. In micro Poiseuille flow, numerical results agree with analytical results almost for (Kn < 0.03). In micro Couette flow, numerical results agree with analytical results almost for (Kn < 0.15). In both case, numerical results of the perturbation method deviate from analytical results by increasing the Knudsen number. This reveals that more corrections are needed in the perturbation method by increasing the Knudsen number.

Additional considerable studies on the micro flows using the perturbation method will be published in the near future. For example, the Karniadakis and Beskok's slip model (Karniadakis et al. 2005) is developed both analytically and numerically. We also have studies on the rarefaction, compressibility and thermal creep.

8. Nomenclature

BC	boundary conditions
C_f	skin friction coefficient
C_1	first slip coefficient
C_2	second slip coefficient
H	channel height, m
Kn	Knudsen number (= λ/H)
L_c	characteristic length, m
O	order
P	pressure, Pa
Pr	Prandtl number
PM	Perturbation Method
Re	Reynolds number
S	source term
T	temperature, °K
u, v, w	velocity components, m/s
U	nondimensional velocity
u	velocity vector, m/s
$\dot{m}$	Mass flow rate, kg/s
	Greek
γ	ratio of specific heats
λ	mean free path of gas molecules, m
μ	first coefficients of viscosity, kg/(m.s)
ρ	density, kg/m^3
σ_T	energy accommodation coefficient
σ_v	momentum accommodation coefficient
τ_w	wall shear stress, N/m^2
	Subscript
C	Constant part of source
in	channel inlet
m	average
P	indicates slope of source
s	slip and streamwise direction
w	wall
0	corresponding to no-slip
1	first-order correction
2	second-order correction
n	*n*th-order correction and normal direction

9. References

Chen, C. S., Lee, S. M. and Sheu, J. D., 1998. Numerical analysis of gas flow in microchannels. Numerical Heat Transfer A-33, 749–762.

Dongari, N. and Agrawal, A., 2007. Analytical solution of gaseous slip flow in long microchannels. International Journal of Heat and Mass Transfer, 50, 3411–3421.

Gad-el-Hak, M., 2006. MEMS: introduction and fundamentals. CRC Press, New York.

Karniadakis, G., Beskok, A. and Aluru, N., 2005. Microflows and Nanoflows- fundamentals and simulation. SpringerScience and Business Media, Inc., New York.

Kennard, E. H., 1938. Kinetic theory of gasses. McGraw-Hill Book Co. Inc., New York.

Qin, F. H., Sun, D. J. and Yin, X. Y., 2007. Perturbation analysis on gas flow in a straight microchannel. Physics of fluids 19, 027103–14.