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A High Order Modification on the Analytic Solution of 2-D Microchannel Gaseous Flows

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ABSTRACT

A new analytic solution of the Navier-Stokes equations for two-dimensional microchannel flows is presented. The solution is based on the concept of the continuum approach using the Chapman-Enskog method, but built upon the proposal to introduce a hyperbolic tangent function of Kn number in the power series of the distribution function and slip boundary condition. The solution of the Navier-Stokes equations is extended successfully to the transition flow regime. The analytic solutions are compared with results of the DSMC in both slip flow and transition flow regimes. Satisfactory agreements on the velocity profiles and pressure distributions have been achieved.

NOMENCLATURE

D	molecular diameter
F	velocity distribution function
H	height of microchannel, m
K	Boltzmann constant
Kn	Knudsen number
L	length microchannel
N	number density
P	pressure, Pa
R	gas constant
Re	Reynolds number
T	temperature, K
u	velocity component in the x-direction, m/s
v	velocity component in the y-direction, m/s
Φ	pressure ratio (= p_{in}/p_{out})
ε	ratio of height to length in microchannel, perturbation quantity
λ	mean free path
μ	dynamic viscosity, $\mathrm{kg/m \cdot s}$
ρ	density, kg/m^3
σ	tangential momentum accommodation coefficient

Superscripts and Subscripts

0, 1	zero- or first-order variables for perturbation
in, out	variable at inlet and outlet
~	non-dimensional variable
-	mean value

1. INTRODUCTION

Micro-Electronic-Mechanical-System (MEMS) is a rapidly emerging technology in which micron-scaled devices are fabricated. Unique features of MEMS, such as the large ratio of surface area to volume and the micron order scales, highly influence the dynamic properties which dominate the system performance (Andraw, et al. 1992 and Hosaka et al. 1995). Effectively modelling the flow in microchannel becomes an important step of understanding the fluid behaviors in the micro system. Unfortunately some limitations of underlying assumptions which are commonly employed in the study of fluid dynamics became the barriers to apply the results into micro scale world. For example, although the macro scale channel flow have been well studied, the results cannot be used for the flow in microchannel directly. With the development of MEMS, the scales of many devices have reached microns or sub-micron orders in magnitude. Assumptions used to develop the analytical solutions under standard circumstances are broken down. Therefore, it is necessary to construct a new theoretical framework to meet the requirements in the micro system applications.

To achieve the goals, many previous studies of gaseous flow in microchannel have been conducted such as Harley et al. (1995), Arkilic et al. (1997), Pong et al. (1994), Beskok and Karniadakis (1993), and Piekos and Breuer (1996). The work of Harley et al. (1995) focused on the experimental and theoretical investigations of subsonic, compressible flow in micro size, long conduits. Their numerical simulations indicated that the pressure may be assumed to be uniform and the transverse velocity can be neglected. Consequently, the 'locally fully developed' (Van de Berg et al. 1993) approximation leads to results which are in agreement with those resulting from Navier-Stokes equations. Arkilic et al. (1997) solved the full two-dimensional, time-invariant Navier-Stokes equations for compressible fluid flow in long microchannels analytically using perturbation method. The boundary condition for the solution consists of the first-order correction of the nonzero wall velocity. The velocity predictions are in agreement with the direct simulation Monte Carlo (DSMC) simulations at low Knudsen number.

It is known that Navier-Stokes equations are the first order approximation of the Chapman-Enskog solution for the Boltzman equation (Chapman and Cowling, 1970) and are accurate to O (Kn). Because all the results of the continuum approximation are derived under the Chapman-Enskog method. The validity of the results are limited by Knudsen number.

In the present study, we propose a high order modification on the analytic solution of microchannel gaseous flow. The solution is based on the concept of the continuum approach using the Chapman-Enskog method, but built upon the proposal to introduce a hyperbolic tangent function of Kn number in the power series of the distribution function and the slip boundary condition. The results are compared with predictions using the method of direct simulation of Monte Carlo (DSMC) in both slip flow and transition flow regimes.

2. THEORETICAL ANALYSIS

To classify the flow regimes from continuum flow to free molecular flow, a non-dimensional number known as the Knudsen number (Kn) is introduced. The Knudsen number is defined as the ratio of the mean free path to the characteristic dimension, i.e.

$$Kn = \frac{\lambda}{H} \tag{1}$$

where, λ is the mean free path, and H is the flow characteristic dimension. The Knudsen number reflects the degree of rarefaction of a gas in the studies of rarefied phenomena. A simple expression derived for an equilibrium gas modeled as hard spheres is

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n} \tag{2}$$

where, d is the molecular diameter and n is the number density of gas. For an ideal gas, the state equation is given by

$$p = \rho RT = nkT \tag{3}$$

where, p is the pressure, ρ is the density, n is the number density, R is the specific gas constant, k is the Boltzmann constant, and T is the thermodynamic temperature. Upon substituting equations (2) and (3) into (1), the Knudsen number is inversely proportional to the product of the pressure and the characteristic dimension

$$Kn = \frac{kT}{\sqrt{2}\pi d^2 pH} \tag{4}$$

As shown in equation (4), on one hand, low pressure and normal characteristic dimension can lead to high Kn, for example the gas flow in space, where the rarefied gas dynamics applies. On the other hand, tiny characteristic dimension and normal pressure also can lead to the same result, such as the gaseous flow in microchannels, which is the rarefied phenomena discussed in the present study.

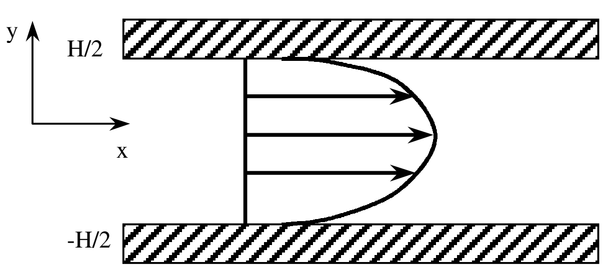


Figure 1 Geometry for micro channel analysis

The geometry for microchannel flow is given in Figure 1. We assumed the flow between two infinite parallel plates be compressible, time-independent and isothermal. The continuity equation is given by

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \tag{5}$$

The Navier-Stokes equations, ignoring body forces and bulk shear viscosity, are

$$\rho\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{1}{3}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 v}{\partial x \partial y}\right)\right) \tag{6}$$

$$\rho\left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{1}{3}\left(\frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 u}{\partial x \partial y}\right)\right) \tag{7}$$

where, u and v are the streamwise and wall-normal components of velocity, μ is the molecular viscosity. To solve the equations, Arkilic et al. (1997) recast the governing equations into non-dimensional form. The non-dimensional continuity equation can be written as

$$\varepsilon\frac{\partial(\tilde{p}\tilde{u})}{\partial \tilde{x}} + \frac{\partial(\tilde{p}\tilde{v})}{\partial \tilde{y}} = 0 \tag{8}$$

The non-dimensional Navier-Stokes equations can be written as

$$\mathrm{Re}\,\tilde{p}\left(\varepsilon\tilde{u}\frac{\partial \tilde{u}}{\partial \tilde{x}} + \tilde{v}\frac{\partial \tilde{u}}{\partial \tilde{y}}\right) = -\frac{\varepsilon\,\mathrm{Re}}{\gamma M^2}\frac{\partial \tilde{p}}{\partial \tilde{x}} + \varepsilon^2\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{u}}{\partial \tilde{y}^2} + \frac{1}{3}\left(\varepsilon^2\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \varepsilon\frac{\partial^2 \tilde{v}}{\partial \tilde{x}\partial \tilde{y}}\right) \tag{9}$$

$$\mathrm{Re}\,\tilde{p}\left(\varepsilon\tilde{u}\frac{\partial \tilde{v}}{\partial \tilde{x}} + \tilde{v}\frac{\partial \tilde{v}}{\partial \tilde{y}}\right) = -\frac{\mathrm{Re}}{\gamma M^2}\frac{\partial \tilde{p}}{\partial \tilde{y}} + \varepsilon^2\frac{\partial^2 \tilde{v}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{v}}{\partial \tilde{y}^2} + \frac{1}{3}\left(\frac{\partial^2 \tilde{v}}{\partial \tilde{x}^2} + \varepsilon\frac{\partial^2 \tilde{u}}{\partial \tilde{x}\partial \tilde{y}}\right) \tag{10}$$

where, all terms represented by (~) are non-dimensional variables which are in the following manner: velocities (u,v) are normalized by the area-averaged streamwise velocity at the channel exit (u_{out}), the streamwise coordinate x by the channel length L, the wall normal coordinate y by the channel height H, the density ρ and pressure p by the channel outlet conditions ρ_{out} and p_{out}, $\mathrm{Re} = \rho_{out}u_{out}H/\mu$, is the Reynolds number which is constant at the outlet, M is the outlet Mach number based on u_{out}, and $\varepsilon = H/L$ is the ratio of the channel height to its length.

The Chapman-Enskog theory (Chapman and Cowling, 1970) provides a solution of the Boltzmann equation for a restricted of problems in which the distribution function of f is perturbed by a small amount from the equilibrium Maxwellian form. The Navier-Stokes equations are the first-order approximation of the Boltzmann equation using the Chapman-Enskog method. It is assumed the velocity distribution function (f) can be expressed in the form of the power series

$$f = f^{(0)} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \ldots \tag{11}$$

where the first term $f^{(0)}$ is the Maxwellian distribution for an equilibrium gas. When Knudsen number is small enough, its order is same as that of ε. The velocity distribution function can be written in the term of Kn

$$f = f^{(0)} + Knf^{(1)} + \mathrm{O}(Kn) \tag{12}$$

Under this assumption, the compressible Navier-Stokes equations are derived as the first order solution of the Boltzmann equation and are accurate to O(Kn).

The problem arises when the continuum approximation is extended to the transition flow regime, where the Knudsen number is close to or even greater than 1. Obviously, the fundamental assumption of the Chapman-Enskog method breaks down. The physical process of the micro flow tells that as Kn > 1, there will be significant effect from the Knudsen layer. The Knudsen layer is a very thin layer (about one to a few mean free paths) next to the wall. As Kn $\rightarrow \infty$, that is, the Knudsen layer covers the channel entirely, it will become a diffusion process and the "slip" velocity depended on the shear stress on the wall will be finite.

Therefore we look for a function of Kn number, which should satisfy two necessary conditions. Firstly, it should be at the same order as Kn when it is small. Secondly, the function should asymptotically be unity as Kn $\rightarrow \infty$. So we propose a small quantity, $\tanh(Kn)=\frac{e^{Kn}-e^{-Kn}}{e^{Kn}+e^{-Kn}}$, to replace Kn in the power series of the velocity distribution function. It is of the same order of magnitude as Kn and ε when Kn number is small. But, it will approach unity asymptotically as Kn $\rightarrow \infty$. The velocity distribution function can be written in terms of tanh(Kn)

$$f = f^{(0)} + \tanh(Kn) f^{(1)} + \mathrm{O}(\tanh(Kn)) \tag{13}$$

The Navier-Stokes equations accurate to O (tanh(Kn)) can also be obtained with this assumption, and its format is not changed. Meanwhile the boundary condition for the Navier-Stokes equations accurate to O (tanh(Kn)) consisted of the first order wall slip velocity can be given by

$$\left.\tilde{u}\right|_{wall} = \frac{2-\sigma}{\sigma}\left(\tanh(Kn)\right)\left.\frac{\partial \tilde{u}}{\partial \tilde{y}}\right|_{wall} \tag{14}$$

When the Kn is small enough, tanh(Kn) and Kn are in same order. The above equation can be replaced by

$$\left.\tilde{u}\right|_{wall} = \frac{2-\sigma}{\sigma} Kn \left.\frac{\partial \tilde{u}}{\partial \tilde{y}}\right|_{wall} \tag{15}$$

The analytical solution with this boundary condition has attained by Arkilic et al. (1997). Using the proposed hyperbolic tanget function tanh(Kn), we have actually approximated micro channel gaseous flow with n-order solution.

Using the perturbation method, the $\tilde{x}$ -momentum equation can be written as

$$\frac{\varepsilon \mathrm{Re}}{\gamma M^2}\frac{d\tilde{p}_0}{d\tilde{x}} = \frac{\partial^2 \tilde{u}_0}{\partial \tilde{y}^2} \tag{16}$$

where the subscript '$_0$' is used to denote the zero order variables for perturbation method. With symmetry conditions, slip flow boundary conditions and equation (4), equation (16) can be integrated twice with respect to $\tilde{y}$ and obtain

$$\tilde{u}_0(\tilde{x},\tilde{y}) = \frac{\varepsilon \mathrm{Re}}{8\gamma M^2}\frac{d\tilde{p}_0}{d\tilde{x}}\left(1-4\tilde{y}^2+4\frac{2-\sigma}{\sigma}\left(\tanh\frac{Kn_{out}}{\tilde{p}_0}\right)\right) \tag{17}$$

Substituting the above equation into the continuity equation and integrating once with respect to $\tilde{y}$, the wall-normal component of velocity can be derived as

$$\tilde{v}_1 = \frac{\varepsilon \mathrm{Re}}{8\gamma M^2}\frac{1}{\tilde{p}_0}\left[\frac{1}{2}\frac{d^2(\tilde{p}_0^2)}{d\tilde{x}^2}\left(\tilde{y}-\frac{4}{3}\tilde{y}^3\right)+4\tilde{y}\frac{2-\sigma}{\sigma}\left\{\left(\frac{\partial\tilde{p}_0}{\partial\tilde{x}}\right)^2\tanh\left(\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\right)\right.\right.$$

$$\left.\left.+\tilde{p}_0\frac{\partial^2\tilde{p}_0}{\partial\tilde{x}}\tanh\left(\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\right)-\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\left(\frac{\partial\tilde{p}_0}{\partial\tilde{x}}\right)^2\left(1-\tanh\left(\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\right)\right)\right\}\right] \tag{18}$$

Evaluating this at the wall, where the wall-normal velocity must be zero at the wall, results in an equation for pressure

$$\frac{\mathrm{d}^2(\tilde{p}_0^2)}{\mathrm{d}\tilde{x}^2}+12\left\{\left(\frac{\partial\tilde{p}_0}{\partial\tilde{x}}\right)^2\tanh\left(\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\right)+\tilde{p}_0\frac{\partial^2\tilde{p}_0}{\partial\tilde{x}}\tanh\left(\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\right)\right.$$

$$\left.-\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\left(\frac{\partial\tilde{p}_0}{\partial\tilde{x}}\right)^2\left(1-\tanh\left(\frac{\mathrm{Kn}_{out}}{\tilde{p}_0}\right)\right)\right\}=0 \tag{19}$$

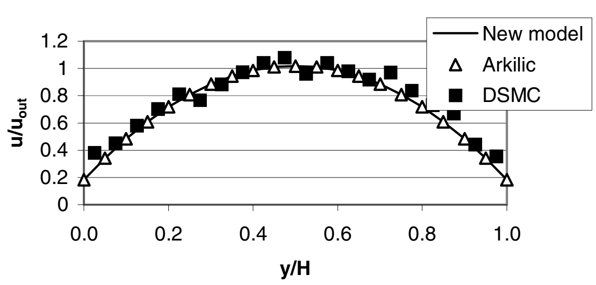
Assuming the momentum accommodation coefficient is unity and using the fact that $\tilde{p}_0$ = 1 at the outlet ($\tilde{x}$ = 1) and $\tilde{p}_0$ is specified by the inlet to outlet pressure ratio, Φ, at the inlet ($\tilde{x}$ = 0). Although the direct analytical expression of the pressure distribution cannot be shown, the numerical solution of it and its differential with respect to $\tilde{x}$ can be obtained.

To validate the new continuum based slip model, the DSMC simulations were performed for microchannel flows. A DSMC code (Xue *et al*. 2000) was developed based on the method proposed by Bird (Bird, 1994). DSMC is a particle-based numerical modeling technique. It computes the trajectories of a large number of particles and calculates macroscopic quantities by sampling particle properties. In the simulation, the computational domain is divided into a net of cells, each particle is positioned into the cell with a velocity and an internal energy. This is similar to the molecular dynamics method. The computation proceeds in small discrete time step Δt, over which the motion of the particles and their interactions are uncoupled. Within one time step, all particles are first advanced according to their individual velocity. Then in each cell, a certain number of statistical collisions are computed by the no-time-counter (NTC) method, which is proposed by bird (1994) as a generalized scheme for DSMC.

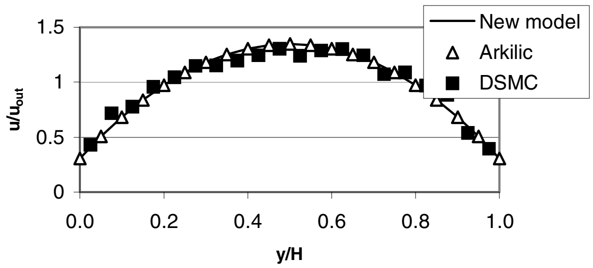
The DSMC simulation is performed in a physical space of 30 μm × 1.12 μm, which is divided into 300 × 20 sampling cells. Each cell consists of 2 collision sub-cells. Twenty particles are located in one collision sub-cell. The total number of simulated particles is about 2.4×10^5. The total number of samples ranges from 1.3×10^4 ~ 5.0×10^6 depending on the different Kn number. The calculations were carried out on a Cray J916 supercomputer.

3. RESULTS AND DISCUSSIONS

The analytical solutions of the Navier-Stokes equations indicate that the streamwise velocity profile is parabolic in shape, which changes slowly along microchannels with the pressure drop.



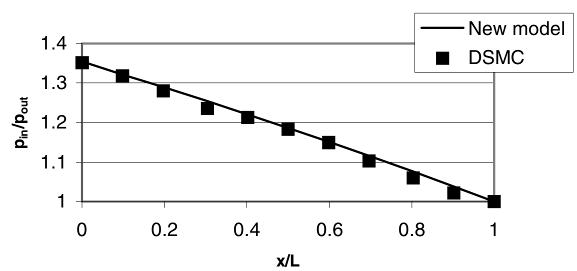
(a) at $x/L = 0$



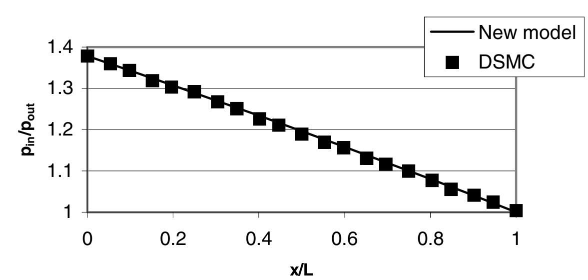
(b) at *x/L* = 1

Figure 2 Velocity profiles at Kn = 0.0743 and Φ = 1.354

Figure 2 shows the streamwise velocity distribution at two cross sections $x/L = 0$ and $x/L = 1$ at Kn = 0.0743. The analytic solutions by Arkilic et a. (1997), which were based on the Navier-Stokes equations with the first-order slip boundary condition accurate to *O*(Kn), are plotted for comparison. From Fig. 2, it is seen that the two analytically predicted velocity profiles are consistent and in excellent agreement with the results of DSMC. This is expected since the proposed hyperbolic tangent function, tanh(Kn), is as accurate as Kn number when Kn number is less than 0.1. The pressure distribution along the microchannel is also calculated analytically and is compared with the prediction of the DSMC, as shown in Fig. 3. Owing to the change of the gas density along the microchannel, the pressure distribution is nonlinear with negative curvature. The analytic solution coincides well with the DSMC prediction up to about Kn = 0.2.



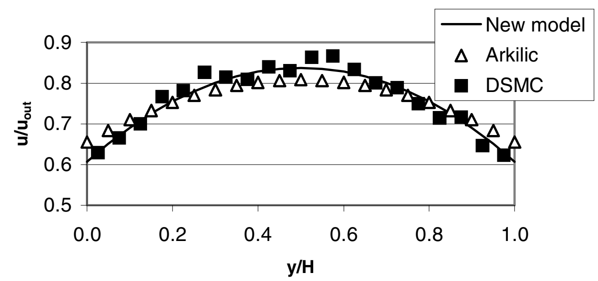
(a) at Kn = 0.0743 and $\Phi = 1.354$



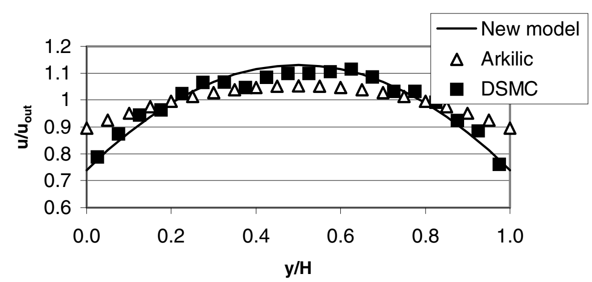
(b) at Kn = 0.224 and $\Phi = 1.38$

Figure 3 Pressure distribution along the micro channel

Testing and evaluation of the new continuum based slip model on microchannel flows in the transition flow regime is the prime objective of the present study. At Kn = 1.41, the predicted velocity profiles at two cross-sections of microchannels are plotted in Fig. 4. The analytic results by Arkilic et al. (1997) and numerical predictions by DSMC are superimposed in Fig. 4 for comparison. It is clear that the Arkilic's predictions are deviating from the DSMC outputs, but the velocity profiles predicted by equation (16) performs well compared with the DSMC simulations. This trend can also be found in the comparisons of the streamwise central line velocity distributions obtained by the two analytical results and DSMC, as shown in Fig. 5. At Kn = 0.0743, the analytic solutions and the results of the DSMC are consistent. The deviation of Arkilic's analytic solutions starts at Kn = 0.2, where flow in the microchannel enters the transition flow regime. The present analytic solutions, however, follow closely the results of DSMC even at Kn = 1.411. The new model has successfully extended the valid prediction flow regime of the continuum approximation to the transition flow regime. The analytic solutions are further investigated in the transition flow regime at higher Kn number.

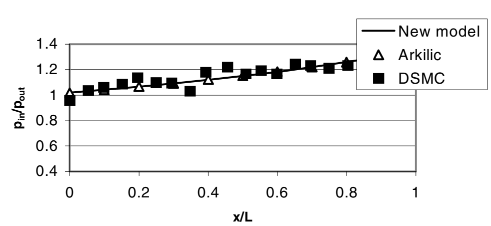


(a) at *x/L* = 0

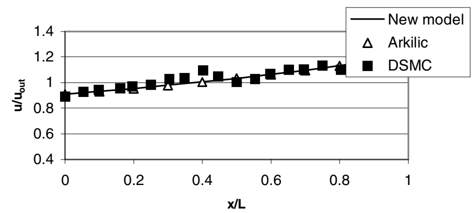


(b) at *x/L* = 1

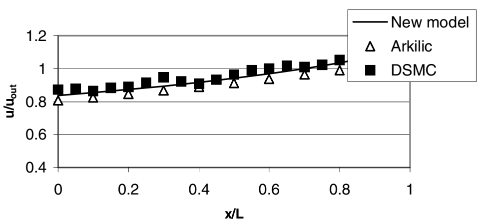
Figure 4 Velocity profiles at Kn = 1.41 and *Φ* = 1.542



(a) Kn = 0.0743

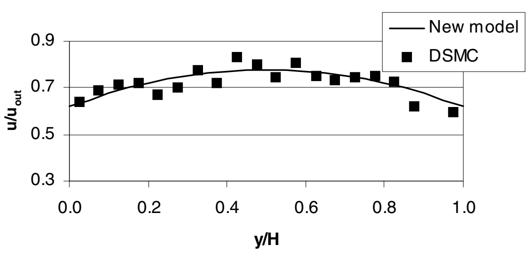


(b) Kn = 0.224

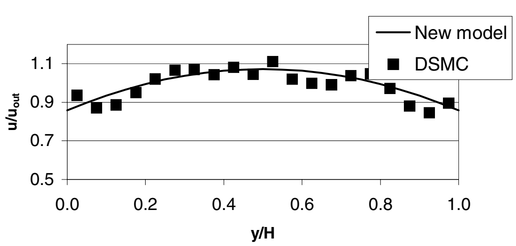


(c) Kn = 1.411

Figure 5 Streamwise central line velocity distributions



(a) at *x/L* = 0



(b) at *x/L* = 1

Figure 6 Velocity profiles at Kn = 3.44 and *Φ* = 1.38

Figure 6 depicts the velocity profiles predicted by the new model and DSMC at Kn = 3.44. Although there are statistical fluctuations appeared in the results of DSMC, the agreements between the two methods are satisfactory. The statistical flucturation is an inherent feature of the low-speed DSMC (Piekos and Breuer, 1996). It tends to be more significant as the Kn number increases. Unfortunately, there is no effective way to eliminate it completely under the present algorithm of DSMC. It should be noted that no analytic solutions can be obtained when the previous analytic model with first-order slip boundary condition accurate to O(Kn) is applied in this case. Since Kn number is the coefficient of the slip velocity, where it exceeds 1, the slip velocity will be unrealistically over-predicted, which will lead to the eventual divergence of the results. With the modification on the continuum approximation and adopting the slip velocity boundary condition accurate to O (tanh(Kn)), the valid range of the continuum approximation is widened to the entire transition flow regime.

4. CONCLUSION

In the present study, we proposed a hyperbolic tangent function of Knudsen number to approximate the velocity distribution function in the Chapman-Enskog method to solve the Boltzmann equation. The concept is implemented on the platform of the Navier-Stokes equations and the slip boundary condition, which are accurate to O(tanh(Kn)).

The Navier-Stokes equations and the slip boundary condition accurate to O(tanh(Kn)) are applied to two-dimensional, compressible, and isothermal microchannel flow. The analytic solutions are obtained using a perturbation method. The results are compared and evaluated from the slip flow regime to the transition flow regime with the computational results of DSMC. It is shown that the present analysis can give satisfactory prediction on the velocity profiles and pressure distributions of microchannel flows up to the transition flow regime. The new continuum based slip model has extended the upper Knudsen number limits of continuum approaches, which is significant in molecular gas dynamics.

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