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A GENERAL SLIP BOUNDARY CONDITION OF FLUID FLOW ON SOLID SURFACES

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SCHOOL of MECHANICAL and AEROSPACE

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ABSTRACT

In view of advancement in MEMS and biological technology, enormous interest has moved into microfluidics. Flows often behave differently at small length scales than macroscopic situation, which have serious implications for microfluidic devices. The goal of this research is to derive a shear-dependent slip model that derived from microscopic view, which can be applied to describe the flow behavior at micro-scale and nano-scale.

It is found that tangential momentum accommodation coefficient (TMAC) as used in Maxwell's model is not enough to describe the interaction of the gas and wall. The friction and restitution coefficient are introduced to account for the different type of gas molecules interaction with the wall. The value of TMAC is also demonstrated to be influenced by incident angle and tangential velocity of gas molecules. The shear-dependent slip model indicates that the slip velocity depends nonlinearly on the shear rate, but not as a linear function of the shear rate as previously assumed. By comparing with linearized Boltzmann equation solution and experimental results, the slip model agrees well and can be applied in a wide range of flow regimes. In addition, it is validated that the shear-dependent slip model can describe the nonlinearity of slip velocity and shear rate observed in liquid flow. The roughness effects and properties of the interface are also discussed. The fitting values of the parameters in the slip model are essentially consistent with the assumption in the derivation. In general, the shear-dependent slip model offers us a comprehensive understanding for the phenomena in microfluidics.

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List of Symbols

Symbols

A	coefficient defined in Eq.(4-6)
A_1, A_2	slip coefficients in second-order slip model
b	slip length
b_g	slip coefficient
B	coefficient defined in Eq.(4-6)
c	mean molecular speed
d	channel height
D	inverse Knudsen number
e	restitution coefficient in normal direction
f	fraction of diffuse reflection
f^*	correction factor
J	impulse
Kn	Knudsen number

L	channel length
L_c	characteristic length
m	molecular mass
Ma	Mach number
n	number density
P	pressure
Q	mass flow rate
R	gas constant
Re	Reynolds number
T	temperature
u	velocity vector in stream-wise direction
u_0	bulk velocity
v	velocity vector in normal direction
W	channel width
x, y	coordinate system

λ	the mean free path
ρ	density
σ	tangential momentum accommodation coefficient
σ_{s-d}	tangential momentum accommodation coefficient defined in Eq.(4-7)
ω	rotation speed
β	tangential restitution coefficient
τ	shear stress
Π	pressure ratio
γ	shear rate
ε	coefficient defined in Eq. (3-29)
ε_0	coefficient defined in Eq.(3-44)
ε_1	coefficient defined in Eq.(3-44)

Subscript

ave	average
i	incident
r	reflected
s	slip
t	tangential direction
w	wall
s-d	shear-dependent

Abbreviations

AFM	Atomic Force Microscope
DSMC	Direct Simulation Monte Carlo
EDDA	Emission Detection of Doppler-shifted Absorption
FDA	Fluorescent Doppler Anemometry
MEMS	Micro-Electro-Mechanical-Systems
RELIEF	Raman Excitation plus Laser-Induced Electronic Fluorescence

Chapter 1 Introduction

1.1 Introduction

With the advent of mini fabrication, Micro-Electromechanical system (MEMS, the devices with characteristic length less than 1mm but more than $1\mu\text{m}$, Gad-el-Hak, 1999) have attracted considerable attention for last few decades. Several kinds of microfluidic devices, such as micro flow sensors, micro pumps and micro mixers have been created based on this technology. However, the behaviors of micron size devices are different from that of macro-scale devices. The physical principles of devices have not been investigated as thoroughly as that in macro scale systems. It is important to effectively model flow behaviors at small scales to produce well-behaved micro devices. Size effects and slip boundary conditions have been explored to explain discrepancies observed in fluid flows between macro-scale and micro-scale devices. The flow mechanisms behind are still elusive and more efforts are needed to fully understand the ambiguity.

1.2 Some Basic Concepts

1.2.1 Gas Flow Characteristics at Microscopic Length Scales-Rarefaction

Several factors cause the flows difference at microscopic length scales and macro scales. In general, surface tension, friction force play an important role at micro length scales, while inertia force, gravitational force dominate at macro length scales (Madou,1997). The disparities are evident when the characteristic length reaches to the sub-micron scale. The

fundamental continuum assumption is not applicable when the characteristic length approaches the mean free path of gas.

Knudsen Number

The Knudsen number (K_n) is the most fundamental parameter to describe non-continuum effects in gases. It is defined as:

$$K_n = \frac{\lambda}{L_c} \quad (1.1)$$

where λ is the mean free path of a gas molecule. The parameter expresses the distance traveled by the molecules between collisions and is written as:

$$\lambda = \frac{1}{\sqrt{2}\pi d_g^2 n} \quad (1.2)$$

where d_g is the molecular diameter of gas, n is number density.

The Knudsen number can also be related to the Reynolds number and the Mach number, which are important parameters used in fluid mechanics. The relationship between viscosity and the mean free path of gas is:

$$\frac{\mu}{\rho} = \frac{1}{2} \lambda u_{avg} \quad (1.3)$$

where u_{avg} is the mean speed and is expressed as:

$$u_{avg} = c \sqrt{\frac{8}{\pi\gamma}} \quad (1.4)$$

Combining Eq. (1.3) and (1.4) (Gad-el-Hak, 2006), the Knudsen number is given by:

$$K_n = \sqrt{\frac{\gamma\pi}{2}} \frac{Ma}{Re} \quad (1.5)$$

where

$$Re = \frac{\rho u_{avg} L_c}{\mu} \quad (1.6)$$

Re is the Reynolds number based on the characteristic length and average velocity in a micro device. Ma is the Mach number and is given by:

$$Ma = \frac{u_{avg}}{c} \quad (1.7)$$

Flow Regimes Classification

Gas flows can be classified into several flow regimes according to Knudsen number (Gad-el-Hak, 2006). This classification is based on empirical information and the range can be variable depending on the geometry of the problem. (as illustrated in Figure 1-1)

- $K_n < 0.001$: the flow is considered as the continuum flow regime. The Navier-Stokes equation with the no slip boundary condition is valid for this regime.
- $0.001 < K_n < 0.1$: the flow is considered as the slip flow regime. The Navier-Stokes equation with an appropriate slip model is adopted.
- $0.1 < K_n < 10.0$: the flow is considered as the transition flow regime. The Direct Simulation Monte Carlo (DSMC) method, the Burnett equation or the Boltzmann equation with appropriate slip boundary conditions is used.
- $10.0 < K_n$: the flow is considered as the free molecular flow regime. The molecular motion must be analyzed with the kinetic theory. Either the Boltzmann equation or the DSMC is used.

In the case of MEMS devices involving gas flow, the characteristic length of a micro-device

is usually of the order $10^1 \mu\text{m}$, and the Knudsen number ranges from 0.001 to 0.1. Therefore gas flows in the MEMS devices are usually treated as in the slip flow regime which means the Navier-Stokes equation and appropriate slip boundary can be applied in micro-channels for most studies (Harley et al. 1995; Arkilic et al. 2001; Zohar et al. 2002).

Figure 1-1. The regime of Knudsen number

Tangential Momentum Accommodation Coefficient

TMAC is an important parameter to describe the degree of slip of gas molecules at the gas/solid boundary. It is defined as:

$$\sigma = \frac{u_{t,i} - u_{t,r}}{u_{t,i} - u_{t,w}} \quad (1.8)$$

where $u_{t,r}$ is the average reflected tangential velocity of gas molecules, $u_{t,i}$ is the average incident tangential velocity of gas molecules and $u_{t,w}$ is the average tangential velocity of the surface. TMAC is a parameter describing the average tangential momentum exchange between gas molecules and wall (Arkilic et al. 2001). When $\sigma = 0$, the case is called specular reflection. When $\sigma = 1$, a diffuse reflection happens. In this case, the

molecules transfer all the tangential momentum to the wall, which is likely to occur for rough surface (Karniadakis and Beskok, 2002).

The value of TMAC depends on the solid material, gas type and surface roughness (see Table 1-1). The experiments showed the value was to be between 0.2-1. The upper limit is typical of most surface, while the lower limit is for very smooth surface. In most engineering work, the surface is normally rough enough to assume diffuse reflection, and the value of TMAC is often set to 1. With improvements in fabrication techniques, the roughness of surface can reach to several nanometers and the assumption of diffuse reflection is not applicable in this case.

Table 1-1 TMAC for several gases and surfaces (Arkilic et al. 1996; Fain 1981; Seidel and Steinheil 1974).

Gas	Surface Material	Range of TMAC
Air	Al	0.87-0.97
Air	Iron	0.87-0.93
Air	Bronze	0.88-0.95
He	Polished copper	0.65-0.95
He	Glass	0.70-0.80
Nitrogen	Si	0.81-0.95
Argon	Si	0.65-0.98

1.2.2 Flow Characteristics at Microscopic Length Scales-Compressibility

Compressibility is another important characteristic that is frequently detected in many experiments conducted within micro-channels. In compressible flows, the density changes appreciably throughout the flow field. The Mach number (as defined in Eq. (1.7)) is the parameter for estimating compressibility. Compressibility becomes more detectable in the flow with large temperature or large pressure change.

Compared with the microscopic length scales, the judgment whether to take the compressibility into account is simple in macroscopic length scales. If the local Mach number is less than 0.3, the flow can usually be considered as incompressible flow. This criterion is not valid at microscopic length scale even when the Mach number is much smaller than 0.3. For instance, the fluid density will change due to strong wall heating or cooling in heat transfer fields. The flow should be regarded as compressible flow at low velocities because of considerable density change. Another situation is that pressure may be considerably changed due to viscous dissipation rather than inertia force at low Mach number in micro-channels (Gad-el-Hak, 2006).

Nonlinear pressure distribution was also observed by some experimentalists (Pong et al. 1994; Arkilic et al. 1997). This phenomenon was attributed to the compressible effect. The non-linear distribution becomes apparent when the pressure ratio increases. On the other hand, the curvature in the distribution can be reduced due to rarefaction effect, which is most apparent in strongly rarefied flow.

1.3 Objectives and Scope of study

With the improvement of mini fabrication, the study of fluid flow was extended to the Micro-electromechanical System (MEMS) where no-slip condition is no longer valid. One method to solve this problem is using traditional Navier-Stokes equations combined with appropriate slip boundary conditions; the other is the use of Boltzmann equation which is considered as the equation governing all flow regimes. The latter is too computationally difficult for most engineering work. The determination of slip boundary is the main obstacle we encountered, especially in high Knudsen number flow regime. This forms the motivation of this thesis.

The objective of this research is to establish a new analytical slip model that accounts for fluid molecular effects. Surface roughness, properties of materials and shear rate are all the intrinsic factors that influence the slip velocity. The nonlinear function of shear rate and slip velocity is indicated. The newly proposed slip model provides a mathematical relationship between surface roughness, material properties, shear rate and fluid molecular effects, and also a physical interpretation of the experimental results obtained by earlier experimentalists, in which the slip length was found to be dependent on shear rate.

The thesis is organized into six chapters. Chapter 1 presents introductory remarks on gas flow characteristics at micro scales. Rarefaction, compressibility and some basic concepts are covered. In chapter 2, the literature relevant to this research is reviewed. Slip models, experimental works at micro-channels and existing micro-flow models are introduced. In chapter 3, we analyze the weakness of Maxwell's scattering model and put forward the new

scattering model. In chapter 4, the new slip model is proposed. Based on the newly proposed slip model, slip velocity and flow rate are compared with that obtained by Boltzmann equation and other slip models. According to the study on several experimental results at micro-channels, the shear-dependent slip model is testified to be consistent with the phenomena observed in these experiments. In chapter 5, it is demonstrated that the shear-dependent slip model is also applicable to micro-scale fluid flows that involve liquids. In addition, techniques used in the measurement of slip velocity at the liquid/solid interface are briefly reviewed. The conclusion and recommendation for future work are given in chapter 6.

Chapter 2 Literature Review

2.1 Slip Models for Gas Flow

Velocity slip for gas flow was first proposed by Kundt and Waburg in 1875 (Goodman et al. 1976). The experiment was conducted with a disk oscillating in a low pressure gas at constant temperature, the decay of the oscillation amplitude of disk is found slower than that predicted by conventional theory. They explained this phenomenon by the slip effect at the gas-solid surface. Later, Maxwell (1879) proposed the most famous slip model. He assumed the slip velocity on the fluid/solid boundary can be expressed as:

$$u_s = u_g - u_w = \frac{2 - \sigma}{\sigma} \frac{1}{\rho \left(\frac{2RT_w}{\pi} \right)^{\frac{1}{2}}} \left(\frac{\partial u}{\partial y} \right) + \frac{3}{4} \frac{P_r (\gamma - 1)}{\gamma \rho R T_w} (-q_s) \quad (2-1)$$

where σ is the tangential momentum accommodation coefficient, T_w is the wall temperature, y is the direction normal to the wall, P_r is the Prandtl number, γ is the ratio of specific heats, and q_s is the heat flux in the direction normal to the surface.

Burgdorfer (1959) proposed that the slip velocity is a function of the molecular velocity at the distance that one mean free path away from the wall. The slip velocity is expressed as:

$$u_s = u_g - u_w = f_v \frac{2 - \sigma}{\sigma} \lambda \left(\frac{\partial u}{\partial y} \right) \Big|_{wall} \quad (2-2)$$

where f_v is a numerical constant which is often regarded as 1.

The slip model proposed by Maxwell can be considered as the first-order slip model.

This model provides us a method to calculate the velocity and mass flow rate for isothermal and local fully developed flows with an analytical solution between plane plates or in cylindrical ducts with simple geometry.

The analytical results, obtained by using the first-order slip boundary condition have shown a relatively accurate result in the slip flow regime ($K_n < 0.1$). This has been verified by many experiments (Harley et al. 1995; Liu et al. 1995; Shih et al. 1996). However, for $K_n > 0.1$, in the transition flow regime, the analytical result derived from the first-order boundary condition have shown considerable discrepancy and approved by many experimental studies (Maurer et al. 2003; Colin et al. 2004; Sreekanth 1969) and numerical studies (Barber et al. 2004) based on the DSMC.

To extend the validity of Maxwell's slip model to the high Knudsen number flow regime ($K_n > 0.1$), many researchers have proposed different slip models, which can be simply classified into two fields: the modified first-order slip model and the second-order slip model.

2.1.1 The Modified First Order Slip Model

Xue and Fan (2000) proposed a hyperbolic tangent function of Knudsen number K_n in the power series of slip boundary. The proposed $C(K_n)$ function should satisfy two conditions:

1. It should be at the same order of K_n when it is small.
2. The function should approach unity as $K_n \rightarrow \infty$.

The proposed $C(K_n)$ function was expressed as:

$$\tanh(K_n) = \frac{e^{K_n} - e^{-K_n}}{e^{K_n} + e^{-K_n}} \quad (2-3)$$

The slip velocity is written as:

$$u_s - u_w = \frac{2 - \sigma}{\sigma} (\tanh(K_n)) \left(\frac{\partial u}{\partial y} \right)_w \quad (2-4)$$

The objective of this new model is to extend the validity of application of Maxwell's slip model from the slip flow regime to the transition flow regime. Although the author validated some accuracy of this new slip model in transition flow regime by comparing with the DSMC results, more validation is still required. Another drawback of this slip model is that the expression of the $C(K_n)$ function lacks physical meaning.

In 1999, Pan et al. (1999) first used the qualitative analysis to determine the slip coefficient as a function of two dimensionless parameters. The DSMC method was used for simulation in Couette flows. Based on the Bird's conclusion (1994) and the discussion made by Beskok and Karniadakis (1994), the slip velocity on the boundary was expressed as:

$$u_s - u_w = S_v \left(\frac{\partial u}{\partial y} \right)_w \quad (2-5)$$

where S_v is the velocity-slip coefficient, which is related to the macro-scale parameters (such as wall temperature, velocity) and micro-scale parameters (such as mass, diameters and number density of gas molecules). By using the qualitative analysis, the authors reduce six dimensional parameters related to the slip coefficient S_v , to the two dimensionless parameters. Finally, the slip coefficient S_v can be written as:

$$S_v = S_v(\lambda_{gw}, L_c) \quad (2-6)$$

where λ_{gw} is a statistical average parameter of gas molecules impacting on the wall,

and it is a function of temperature-viscosity, diameter of gas molecules and wall temperature. L_c is a characteristic length of the whole flow system.

The advantage of this slip model is that two dimensionless parameters are adopted to substitute some parameters that have been used before in other models, such as accommodation constant σ and the high order slip coefficient b , which need to be either assumed or determined by experiments. The slip coefficient S_v obviates any experimental parameters and is just related to two dimensionless parameters. This slip model also includes the micro-scale parameters, such as diameters of gas molecules, which are neglected in other slip models. The drawback of Pan's slip model is that it uses the DSMC method for simulation, so the calculation process will be more complex as compared with other slip models and therefore it will not be suitable in engineering field. The qualitative analysis is still needed to be testified in the transition flow regime.

Many researchers also proposed several empirical models. Beskok and Karniadakis (1999) proposed an empirical model, which is designed to give accurate velocity profiles normalized by the average velocity over a wide range of Knudsen numbers for Poiseuille flow:

$$u_s = \frac{K_n}{K_n + 1} \cdot L_c \cdot \frac{2 - \sigma_v}{\sigma_v} \frac{\partial u}{\partial y} \Big|_w \quad (2-7)$$

Another empirical model is based on the DSMC results, where a correction factor was added to best match the slip model results to the DSMC results:

$$u_s = 1.253 \cdot K_n \cdot L_c \cdot \frac{2 - \sigma_v}{\sigma_v} \frac{\partial u}{\partial y} \Big|_w \quad (2-8)$$

These empirical slip models are very simple in mathematical form to be easily used with the continuum equations (such as Navier-Stokes equation). Studies show that these empirical models predicted well for the velocity profile and mass flow rate in the slip flow regime. In the transition flow regime, the slip model yields reasonable results, which is within 10% of the DSMC solution for Couette flow and the normalized flow. Although these empirical models can get reasonable results for large Knudsen number, their applicability is usually limited to very specific cases.

2.1.2 High Order Slip Model

In transition flow regime, several experimental studies and numerical studies showed that the first-order slip model is not accurate any more. Several researchers have proposed the second-order slip model. The objective of the second-order slip model is to extend the validity of the slip flow regime to higher Knudsen numbers.

In 1964, Deissler proposed a second-order slip boundary condition:

$$u_s = \pm \frac{(2-\sigma)}{\sigma} \lambda \frac{\partial u}{\partial y} \Big|_w - \frac{9}{16} \lambda^2 \left(2 \frac{\partial^2 u}{\partial y^2} \Big|_w + \frac{\partial^2 u}{\partial x^2} \Big|_w + \frac{\partial^2 u}{\partial z^2} \Big|_w \right) \quad (2-9)$$

Karniadakis and Beskok (2002) defined the second-order slip boundary condition by using a Taylor series expansion as:

$$u_s = \pm \frac{(2-\sigma)}{\sigma} \left(\lambda \frac{\partial u}{\partial y} \Big|_w \mp \frac{\lambda^2}{2!} \frac{\partial^2 u}{\partial y^2} \Big|_w \right) \quad (2-10)$$

It is obvious that the second term in the right side of Eq. (2-10) will induce greater difficulty in the solving process, especially in complex geometry. To overcome this difficulty, later, a general non-dimensional velocity slip boundary was proposed by the

same authors as follows:

$$u_s = \pm \frac{(2-\sigma)}{\sigma} \frac{K_n}{1-bK_n} \frac{\partial u}{\partial y} \Big|_w \quad (2-11)$$

where b is an empirical slip coefficient determined from Direct Simulation Monte Carlo (DSMC) data or from experimental results. This slip boundary is just expressed as the first-order slip model form, but has accuracy up to the second order.

Lockerby et al. (2004) recently proposed a second-order slip boundary condition by substituting the Burnett stress tensor and heat flux vector into the Maxwell's first-order slip model and restricting the analysis to linear higher-order terms only. The proposed model is as follows:

$$\begin{aligned} u_s = \pm \frac{(2-\sigma)}{\sigma} \left(\lambda \frac{\partial u}{\partial y} \Big|_w + \lambda \frac{\partial v}{\partial x} \Big|_w \right) + \frac{3}{4} \frac{\mu}{\rho T} \frac{\partial T}{\partial x} \Big|_w + \frac{(2-\sigma)}{\sigma} \lambda \left(2 \frac{\mu}{\rho^2} \frac{\partial^2 \rho}{\partial x \partial y} - \frac{\mu}{\rho T} \frac{\partial^2 T}{\partial x \partial y} \right) \\ + \frac{3}{16\pi} \frac{(\gamma-1)}{\gamma} P_r \lambda^2 \left[(45\gamma-61) \frac{\partial^2 u}{\partial x^2} + (45\gamma-49) \frac{\partial^2 v}{\partial x \partial y} - 12 \frac{\partial^2 u}{\partial y^2} \right] \end{aligned} \quad (2-12)$$

A new simple model for ultra-thin film gas bearing was presented by Cheng et al. (1999) to overcome the complicated and time-consuming difficulty of solving the linearized Boltzmann equation. A similar manner was used as the high-order slip flow models for this modified equation. Three adjustable coefficients a, b and c were used to increase the accuracy of this model for a wide range of Knudsen number, according to the linearized Boltzmann equation. The simulation result agreed well with the solution obtained by the linearized Boltzmann equation. It is assumed that the velocity component v is negligible compared with velocity component u . As a result, the velocity boundary conditions are as follows:

$$\begin{aligned} u_z|_{y=0} &= u_0 + a \cdot \lambda \frac{\partial u}{\partial y} \Big|_{y=0} - \frac{1}{2} \cdot b \cdot D^c \cdot h^2 \frac{\partial^2 u}{\partial y^2} \Big|_{y=0} + \dots \\ u_z|_{y=h} &= -a \cdot \lambda \frac{\partial u}{\partial y} \Big|_{y=h} - \frac{1}{2} \cdot b \cdot D^c \cdot h^2 \frac{\partial^2 u}{\partial y^2} \Big|_{y=h} + \dots \end{aligned} \tag{2-13}$$

where $D = \sqrt{\pi} h / 2 \lambda = \sqrt{\pi} / 2 K_n$ is the inverse K_n .

Mitsuya (1993) proposed a 1.5-order modified Reynolds equation for solving the ultra-thin film gas lubrication problem to improve the prediction accuracy of the load-carrying capacity. The so-called 1.5-order slip model provides predictions between those from first-order slip and second-order slip models. The mean free path λ is replaced by $\frac{2}{3} \lambda$ and an accommodation coefficient is involved in the slip model.

The second-order slip model in the general form can be written as:

$$u_s = \pm A_1 \lambda \frac{\partial u}{\partial y} \Big|_w + A_2 \lambda^2 \left(\frac{\partial^2 u}{\partial y^2} \Big|_w \right) \tag{2-14}$$

The theoretical coefficients for main models for second-order boundary conditions are illustrated in Table 2-1.

Table 2-1: Theoretical coefficients for main models for second-order conditions.

Source	A ₁	A ₂
Schamberg (1947)	1	-5 π /12
Chapman and Cowling (1952)	$\approx$ 1	$\approx$ 0.5
Cercignani and Daneri (1963)	1.1466	-0.9756
Deissler (1964)	1	-9/8
Hsia and Domoto (1983)	1	-0.5
Mitsuya (1993)	1	-2/9
Karniadakis and Beskok (2002)	1	0.5
Lockerby (2004)	1	0.15-0.19

2.1.3 Other Approach Proposed to Improve the Slip Model.

Some researchers found that the slip velocity is not only influenced by the shear rate, but also by other terms. Jie et al. (2000) substituted the second term $\left. \frac{\partial^2 u}{\partial y^2} \right|_w$ by pressure gradient term in the second-order slip model to avoid the calculation difficulty. The slip boundary condition is expressed as:

$$u_s = \pm \frac{(2 - \sigma)}{\sigma} \left(K_n \left. \frac{\partial u}{\partial y} \right|_w + \frac{K_n}{2} \text{Re} \left. \frac{\partial p}{\partial x} \right|_w \right) \quad (2.15)$$

where x, y are the stream-wise and normal coordinates respectively, normalized to the channel height and Re is the local Reynolds number.

Ng et al. (2002) studies showed that the slip velocity is affected not only by shear stress, but also by fluid density. The slip boundary condition can be rewritten as:

$$u_s = \frac{(2 - \sigma)}{\sigma} \frac{1}{\sqrt{(2RT/\pi)}} \frac{\tau_w}{\rho} \quad (2.16)$$

They stated this model is particularly suitable in the transition flow regime.

Shen et al. (2007) extended the first-order slip model based on the kinetic theory. The slip boundary condition is deduced by using the solution of the Krook equation. The pressure gradient was introduced as an additional term influencing the slip velocity. The slip model is described as:

$$u_s = \frac{(2 - \sigma)}{\sigma} \tau \left(\frac{\pi k T}{2m} \right)^{1/2} \left. \frac{\partial u}{\partial y} \right|_{y=0} - \frac{\pi d t}{\sigma m n \left[2 \tau \left(\frac{\pi k T}{2m} \right)^{1/2} + \sqrt{3} d \right]} \frac{dP}{dx} \quad (2.17)$$

where t is relaxation time. m is the mass of molecule, n is number density.

Compared with other first-order and second-order slip models, their work showed that the Poiseuille flow rate predicted by this slip model agrees well with the results calculated by the linearized Boltzmann equation.

Sun et al. (2002) proposed a new slip model by using VHS and VSS molecular effects. The molecular dynamics was used to study the impact of molecular collision with the wall. The mean free path was redefined. Her results showed that the second-order slip model overestimates the flow rate while the first-order slip model underestimates the flow rate. The 1.5-order slip model proposed by Mitsuya (1993) sounds a better alternative method.

Although several second-order slip models have been proposed as summarized in Table 2-1, in general, none of them can provide satisfactory application in high Knudsen number flow regime. Schamberg's second-order slip model was found to be accurate just for $K_n < 0.2$ (Zhong 1993). Zhong simulated a hypersonic flow past a circular blunt leading edge in the transition flow regime by using the Burnett equations with Schamberg's second-order slip boundary. His results showed that Schamberg's second-order slip model could not be used for $K_n > 0.2$. Cercignani's second-order slip model has been overlooked for many years because Sreekanth's paper claims that this model cannot fit his experimental data. He modified the second empirical coefficient c_2 to 0.14, which was significantly different from the value proposed in Cercignani's slip model. He compared his experimental results with the prediction of the modified slip model and found the model could be applied up to $K_n = 1.5$. However, recently, Hadjiconstantinou (2003) pointed out Sreekanth misinterpreted the Cercignani's slip

model. With appropriate modification, Cercignani's slip model can be in good agreement with solutions of the Boltzmann equation in a wide range of K_n number. Karniadakis and Beskok's (2002) second-order slip model was based on a simple Taylor series expansion of Maxwell's slip boundary condition. It predicted a decrease in slip velocity as compared with Maxwell's slip model. However, experimental study by Colin (2003) showed that the Maxwell's slip model underestimates the slip velocity on the wall, and the second-order slip model should lead to an increase in the slip velocity at the wall, which indicates that Karniadakis and Beskok's second-order slip model is not correct. It was found that the first-order slip model underestimates the slip velocity while the second-order slip model overestimates the slip velocity. The 1.5-order slip model seems to be better than the first-order and second-order slip model. Actually, the only difference between the 1.5-order and second-order slip model is that the second coefficient is different.

As summarized above, the lack of validation of slip coefficient and exact slip model remain as a major obstacle we encounter in developing a reliable model to predict the flow behavior in the regime with higher Knudsen number. The first-order slip model was proven to underestimate the slip velocity on the boundary by experimental data and Direct Simulation Monte Carlo (DSMC) method, while the confusion between the first and second slip coefficient of second-order slip model led to considerable uncertainty when trying to apply the second-order slip model to high Knudsen number flow regime. It seems that without empirical modification on the first and second slip coefficient, the second-order slip model cannot be applied in the flow regime with high Knudsen number, which is almost as the same as the first-order slip condition.

2.2 Experimental Study on Gas Flow at Micro-Scale and Nano-Scale

Fluid flows have been investigated for a long period at macro-scale. Keenan and Neumann (1946) found that at a distance greater than 50 diameters from the inlet, the friction coefficient for compressible flow is approximately equal to that for incompressible flow with same Reynolds numbers at Mach numbers near 1. The friction factors were measured by Sreekanth (1968) for 2 inch diameter brass tubes under high pressure gradients. The flow regime at the entrance is from the slip flow regime to the transition flow regime, and the Knudsen number varied from 0.007 to 0.24. The experimental result agreed well with theoretical predictions based on the assumption of isothermal and locally fully developed flow. These experiments cannot be directly applied to the micro-scale flow regime because the scale length is very large as compared with micro-scale.

2.2.1 Friction Factor

The first work to measure the friction coefficient through silicon micro-channels is attributed to Wu and Little (1983). They measured friction factors experimentally for both laminar and turbulent gas (N_2 , H_2 , Ar) flows in trapezoidal channels. The channels were etched on glass and silicon was bonded to flat cover glasses. The width of the channels was 130-200 μm and depth was 30-60 μm . The measured values of the friction factor were larger (10%-30%) than those predicted by the conventional theory. A transition to turbulent flow occurred at Reynolds number as low as 400. The authors explained the disparity by considering the effect of surface roughness and the uncertainty in the measurement of the dimensions of the channels.

However, an opposite trend is found in by Choi et al. in 1991. Their experiments were performed for nitrogen flow through micro-tubes. The diameters of the tubes were 3-81 μm and the length to diameter ratios were 640-8100. The relative roughness ranged from 0.00017 to 0.0116. The measured value of $f^*\text{Re}$ for micro-tubes with a diameter less than 10 μm was 53, while the conventional value is 64 for fully developed laminar flow in tubes. Yu et al. (1995) extended the work of Choi by conducting experimental and theoretical studies of flow and heat transfer in micro-tubes. Nitrogen and water were used as the test fluids in micro-tubes ranging in diameter from 12 to 102 μm . They observed friction factor to be lower than that predicted by conventional theory at macro-scale. The role of the relative roughness was analyzed.

Pfahler et al. (1991) performed a series of experiments for measuring the friction factor and viscosity of fluids (gas and liquids respectively) in micro-channels. The test rectangular channels have a diameter range from 1.6 to 3.4 μm . The trapezoidal micro-channels were used, nominally 100 μm wide and 0.5-50 μm deep. The gases used in the study were helium and nitrogen. The measured friction factor was lower than the theoretical results. The researcher also found that the friction factor will be influenced by the polar nature of the fluids.

Gases flow in two-dimensional (2-D) micro-channels for various Knudsen numbers was studied by Harley et al. (1995). They performed experimental and theoretical investigation of subsonic, compressible flow of nitrogen, helium and argon gases in long micro-channels. The channels were typically 10 mm long, 100 μm wide and ranged in depth from 0.5 to 20 μm . The negligible wall-normal pressure gradients were assumed, and the stream-wise momentum equation of the Navier-Stokes equations was applied in

this rarefied flow field, with the nonlinear terms being neglected. The solution for the boundary condition consisted of the first-order wall boundary conditions, validated the slip velocity is nonzero in slightly rarefied flow. From the experimental and theoretical studies, the reduction in Poiseuille number $C^* = (P_o)_{\text{exp}} / (P_o)_{\text{theo}}$ was attributed to the slip effect. It was observed that slip effect was more pronounced at low Reynolds numbers. The experimental result also indicated that the Navier-Stokes equations with no-slip boundary conditions over-predict the pressure drop, especially at low values of Reynolds number. The contribution of the nonzero slip to the mass flow rate and pressure drop relationship was also validated.

There are still many experiments on the friction factors for micro-channels in recent years. Araki et al. (2002) investigated frictional characteristics of nitrogen and helium flows through three different trapezoidal micro-channels. These channels have a hydraulic diameter ranging from $3 \mu\text{m}$ to $10 \mu\text{m}$. The experimental result showed that the friction factor was smaller than the prediction of the conventional theory. The rarefaction effects were used to account for the decrease of friction factor. Li et al. (2000) measured the friction factor through five micro-tubes with diameters ranging from 80 to $166.6 \mu\text{m}$. The test fluid was nitrogen. The experimental results indicated that the pressure drop along the tube became nonlinear at the Mach number higher than 0.3 . The friction factor was found to be higher than that predicted by the conventional theory. Turner et al. (2004) carried out an experimental investigation on compressible gas flow through rough and smooth micro-channels with diameters ranging from 4 to $100 \mu\text{m}$. Nitrogen, helium and air were used as the test fluids. The friction factor for both smooth and rough micro-channels was indicated to agree well with the prediction of the conventional theory.

2.2.2 Mass Flow Rate and Pressure Distribution

Pong et al. (1994) was the first to explore the experimental measurements of pressure distribution along micro-channels, by using an array of surface pressure sensors. The previous studies focused only on measurement of mass flow rate and pressure measurements at inlet and outlet. Nitrogen and helium were tested and the pressure distributions at different Knudsen number were measured. The channels were $1.2\text{ }\mu\text{m}$ deep, $3000\text{ }\mu\text{m}$ long and ranged in width from 5 to $40\text{ }\mu\text{m}$. In their experiments they showed that the pressure distribution was lower than that predicted by the continuum flow theory and that it was not linear in the flow direction. The compressible and rarefaction effects play the opposite role to influence the final pressure distribution, and cause a nonlinear pressure distribution. However, no mass flow rate data was reported in this experiment. More experimental data were obtained by Liu et al. (1995), with experiments conducted using the same flow system as described by Pong et al. They found that the pressure distribution was nonlinear and the pressure drop was smaller than that expected. From the analysis, Liu concluded that a slip boundary condition with an accommodation factor that equals to unity could accurately model the flow behavior. However, the model could not explain the small pressure gradient measured near the inlet and the outlet.

Shih et al. (1996) completed the measurements of Liu et al. by using nitrogen and helium as test fluids. The test channel was $40\text{ }\mu\text{m}$ wide, $1.2\text{ }\mu\text{m}$ deep and $4000\text{ }\mu\text{m}$ long. Mass flow rate and pressure distribution were measured along the channels. Their results were in agreement with the prediction, based on the first-order correction of the Navier-Stokes equations for helium gas. However there were deviations between

theoretical and experimental result for nitrogen gas. The theoretical model cannot indicate a non-linear dependence of the mass flow rate on the pressure drop as observed in experimental data.

Arkilic et al. (1997) investigated gases flow with slight rarefaction through long micro-channels both experimentally and analytically. The channel was $52.25\ \mu\text{m}$ wide, $1.33\ \mu\text{m}$ deep and $7500\ \mu\text{m}$ long. A two-dimensional analysis of the Navier-Stokes equations incorporating with a first-order slip velocity boundary condition was adopted to the existence of the compressibility and rarefied effect in long micro-channels. The results showed that the pressure drop through the channel was less than the continuum flow results. They also found that the zero-order analytic solution for the stream-wise mass flow agrees well with the experimental results. The effect of slip upon the pressure distribution is also verified. The experimental results were cited by many researchers because of the well-controlled surface structure and accurate measuring technique.

Maurer et al. (2003) performed gas flow experiments in a shallow micro-channel, $200\ \mu\text{m}$ wide, $1.14 \pm 0.02\ \mu\text{m}$ deep. This is the first investigation to extend a range of averaged Knudsen numbers, roughly, from 0.05 to 0.8 in experiments. The researchers incorporated second-order term in the boundary conditions and concluded that second-order effects do play an important role with increasing Knudsen number. Later, Colin et al. (2004) performed similar experiments with rectangular micro-channels, from 4.4 to $0.5\ \mu\text{m}$ in depth and with aspect ratios from 1-9%. Nitrogen and helium were used as the test fluids. The experimental data showed that the proposed second-order model is accurate for Knudsen number up to about 0.25, whereas the first-order model is no longer valid for Knudsen number higher than 0.05. These two experiments confirmed that the additional term in the second-order boundary conditions could be useful in

transition flow regime that with high Knudsen number.

In a recent study, Roy et al. (2004) performed the experiments to measure the mass flow rate and pressure distribution through anodized alumina with 200 nm diameter pores. The Knudsen number for the experiments ranged from slip ($K_n=0.058$) flow regime to transition ($K_n=7.36$) flow regime. The theoretical approach was a hydrodynamics model based on finite element method, which incorporated Navier-Stokes equations with a first-order slip boundary condition. The experimental results were consistent with the theoretical prediction and a tangential momentum accommodation coefficient (TMAC) $\sigma = 1$ was confirmed. Later, experiments were performed to determine the slip coefficient for tubular carbon structures that were produced on a porous alumina substrate with nominal pore diameters of almost 200 nm (Cooper et al. 2003). The experimental results were nearly identical to the results obtained in the previous experimental work. The estimation of TMAC $\sigma = 0.52$ was different from the previous conclusion due to the effect of small relative roughness of the surface and a shift in pore diameter. The researchers concluded that the hydrodynamics Navier-Stokes method with first-order slip condition was valid even in the high Knudsen number flow regime. It was indicated that the hydrodynamic models for micro- and nano-scale flows should be investigated thoroughly before discarding them.

The experimental results are summarized in Table 2-2.

Authors	Fluid	Description of the work	Conclusion
Measurements of friction factors in micro-channels			
Wu and Little (1983)	N_2, H_2, Ar	EDP etching for Si channels, abrasive etching for glass channels. Width:130-200 μm , Depth:30-60 μm , Hydraulic diameter:55-83 μm , Length: 7.5-40 μm , Relative roughness: 0.2-0.3	$f \cdot Re$ higher than the conventional theory, due to the very large relative roughness and uncertainty in measurements.
Choi et al. (1991); Yu et al. (1995)	N_2	Silica circular tube, Diameter:3-81 μm , Relative roughness: 0.00017-0.011; (Choi) Silica circular tube, Diameter: 12-10 μm , Relative roughness:0.0003 for 52 μm tube. (Yu)	$f \cdot Re$ lower than the conventional theory, can not be explained by slip effect.
Pfahler et al. (1991); Harley et al. (1995)	N_2, H_e, Ar	Trapezoid microchannel, Width:75-2 μm , Depth: 0.5-50 μm , Length:10 μm . Hydraulic diameter: 1.6-3.4 μm , Roughness:5 nm for 0.5 μm deep channel	C^* decreases as channel depth decreases. f decreases as Re decreases for the smallest channel size. Slip effect was more pronounced at low Reynolds numbers.
Araki et al. (2002) Li et al. (2000) Turner et al. (2004)	H_e , N_2 , Ar	Hydraulic diameter: 3-10 μm . Microtube diameter: 80-167 μm Microtube diameter: 4-100 μm	Friction factor small than the conventional theory due to the rarefaction effect (Araki et al.) ; Friction factor was found higher than that predicted by the conventional theory (Li et al.); Friction factor for both smooth and rough micro-channels same as the prediction of the conventional theory. (Turner et al.).

Pressure distribution and Mass flow rate			
Pong et al. (1994) Liu et al.(1995)	$H_e,$ N_2	Micro-channels, Width: 5-40 μ m, Depth: 1.2 μ m, Length: 3000 μ m, surface micromachined polysilicon piezoresistors and sacrificial layer etching	Nonlinear pressure distribution, the pressure drop smaller than the conventional theory; A slip boundary condition with an accommodation factor equal to 1 could accurately model the flow.
Shih et al. (1996)	$H_e,$ N_2	Micro-channels, Width: 40 μ m, Depth: 1.2 μ m, Length: 4000 μ m, well controlled surface roughness	First-order slip model justified, deviations between theoretical model and experimental result for nitrogen gas, non-linear dependence of the mass flow rate on the pressure drop
Arkilic et al. (1997)	$H_e, N_2, Ar,$ CO_2	Micro-channel with 1.33 μ m height, 52.25 μ m width, and 7500 μ m length, oxidation up to the depth of channels and silicon direct bounding	Pressure drop through the channel less than the continuum flow results. The effect of slip upon the pressure distribution validated. Well-controlled surface structure and accurate measuring technique
Maurer et al. (2003)	H_e, N_2	Micro-channel: 200 μ m wide, 1.14 $\pm$ 0.02 μ m deep Knudsen number range: 0.05-0.8	The slip coefficient S as a function of mean Knudsen was plotted. The polynomial of second order was compared with first order slip model and experimental results. The second order effect should be taken into account in studying micro flow
Colin et al. (2004)	H_e, N_2	Rectangular micro-channels, from 4.4 to 0.5 μ m in depth and with aspect ratios from 1-9%	The second-order model with coefficient $\sigma = 0.93$ was used to fit the experimental data and compared with first order slip model. The trend is agreed for Knudsen number up to about 0.25, the first-order model is no longer valid for Knudsen number higher than 0.05.
Roy et al. (2004)	N_2, Ar, O_2	Anodized alumina with 200 nm diameter pore Knudsen number range: 0.58-7.36	Tangential momentum accommodation coefficient $\sigma_v = 1$ confirmed, Navier-Stokes equations with a first-order slip boundary condition validated
Cooper et al. (2003)	Ar	Porous alumina substrate with nominal pore diameters from 169 to 235 nm; Relative small surface roughness	Tangential momentum accommodation coefficient $\sigma_v = 0.52$ confirmed, Navier-Stokes equations with first-order slip condition valid even in the high Knudsen number flow regime.

Table 2-2: Previous studies of gas flow experiments in micro-channels.

2.2.3 Experimental Techniques to Measure Slip Velocity at Micro-Scale and Nano-Scale

The previous experiments that measured the pressure distribution and mass flow rate, friction factors can be considered as indirect methods in obtaining the slip boundary condition for gases flow at micro-scale and nano-scale. However, the slip velocity was not probed directly, but instead was estimated by some other parameters measured in macroscopic. Tretheway et al. (2002) used micro-resolution particle velocimetry (μ -PIV) to measure the velocity profile of water flowing through $30 \times 300 \mu\text{m}$ micro-channels. μ -PIV uses tracing particles as substitute materials for fluid motion and can be treated as a direct method to investigate the fluid/solid boundary at small length scales. The experimental results indicated that the slip velocity on the solid boundary was approximately 10% of the stream-wise velocity and the slip length was near $1 \mu\text{m}$. The researchers concluded that the slip boundary conditions must be taken into account at the micro- and nano-scales. For gases flow at micro-scale, the particle tracers do not collide with the wall in the same way as the gas molecules do, especially when non-continuum effects are evident in the region near wall, so the particle-based velocity-measurement technique, such as μ -PIV, is not an option for gas flow. There are several new diagnostic techniques developed to measure the velocity for gases flow at micro-scale, including fluorescent Doppler anemometry (FDA), emission detection of Doppler-shifted absorption (EDDA) and Raman excitation plus laser-induced electronic fluorescence (RELIEF). (see Reese, J.M. et al. 2003 for more details).

FDA: Optics is located upstream and downstream of the measure location, the flow-field velocity is determined by heterodyning the Doppler-shifted fluorescence signal gathered from collection. The advantage of FDA technique is that it increases measurement

sensitivity and loose constraints on the spectral linewidth of the laser illumination. However, the experimental set-up is more complex and sensitive to alignment.

EDDA: NO and I_2 fluorescence is used in this technique. It has been successfully implemented in supersonic and subsonic macro-flows. The experimental set-up is relatively simple compared with that for FDA technique. The disadvantage is that the spectral linewidth of the exciting laser beam must be very small to provide enough sensitivity.

RELIEF: Molecular tagging technique is used in this method. Compared with particle-based techniques, the velocity profile can be seen immediately, with no data reduction or data analysis. The optical set-up is more straightforward compared with that for the FDA technique. However, the quantum efficiency of the process is very low, and the application is limited due to the focus of the Raman-excitation beams and diffusion of gas particles.

The difficulties in measuring the slip velocity at micro-scale and nano-scale indicate that the amount of reliable experimental data is very small, and the above-mentioned techniques (FDA, EDDA, RELIEF) are still far from fully developed. However, the direct experimental method, without any artificial parameters, is still the potential method to measure the slip velocity at micro-scale and nano-scale flows.

2.3 Modeling for Gas Flow

2.3.1 Boltzmann Equation

Boltzmann equation is the fundamental kinetic equation, which describes gas flow in all regimes. The later introduced method, DSMC and extended hydrodynamics can be considered as different ways of solving Boltzmann equation for transition-continuum flow. By clarifying the irreversibility implicated by the second law of thermodynamics and the reversibility of the microscopic equation of small particles motion, Boltzmann developed a statistical theory and the Boltzmann equation can be written as (Bird 1994):

$$c \cdot \frac{\partial(nf)}{\partial r} dcd r + F \cdot \frac{\partial(nf)}{\partial c} dcd r + \frac{\partial(nf)}{\partial t} dcd r = \int_{-\infty}^{\infty} \int_0^{4\pi} n^2 (f^* f_1^* - ff_1) c \cdot \sigma_c d\Omega dc_1 dcd r \quad (2.18)$$

where $f(r, c, t)$ is the velocity distribution in space and time, r denotes the position vector and c is the molecular velocity vector. The rate of change of number of molecules in an element is $\frac{\partial(nf)}{\partial t} dcd r$, n is the number density, dr represents the physical space and dc represents the velocity space.

Three processes contribute to the change in the number of molecules within $dcd r$:

$-c \cdot \frac{\partial(nf)}{\partial r} dcd r$: expresses the convection of molecules across the face of dr by molecular velocity c .

$-F \cdot \frac{\partial(nf)}{\partial c} dcd r$: represents the convection of net inflow molecules across the surface of dc as a result of the external force per unit mass F .

$\int_{-\infty}^{\infty} \int_0^{4\pi} n^2 (f^* f_1^* - ff_1) c_r \sigma_c d\Omega dc_1 dcd r$: represents the scattering of molecules into and out of $dcd r$ as a result of intermolecular collisions.

The right side of Eq.(2.18) is the collision function, which induces the main source of difficulty. Because of this obstacle, an analytical solution for gas flow in complex geometries is intractable, and a formidable problem is encountered in solving the Boltzmann equation in three dimensions by using a numerical approach. To overcome these difficulties, two practical and competing approaches simulating gas flows are proposed: (i) the DSMC, simulating the movement and collisions of gas molecules directly; and (ii) extending the continuum equations, using an approximation based on K_n .

2.3.2 The DSMC Method

In the late 1950's, a new numerical method, called molecular dynamics simulation (MD) was introduced by Alder and Wainwright (1957). This molecular model considered the fluid as a collection of discrete particles at specific positions with specific velocities. Since MD is based on the most fundamental equation of motion, it can be applied in the whole range of Knudsen number. However, as pointed by Gad-el-Hak (1999), the major disadvantage of MD simulation is how to select a proper and convenient potential for a particular fluid and solid interface. The MD simulation is commonly used in dense gases and liquids because the above-mentioned difficulty limits its application in dilute gases (Risso et al 1997). In general, the MD simulation method cannot be used in complex flow patterns and tends to be computationally expensive.

To overcome the difficulty in applying the MD simulation in flow regimes, an alternative method called DSMC (Direct Simulation Monte Carlo), was proposed by Bird in 1963 (Bird 1994). Bird calculated the molecular collisions using a stochastic approach, rather than a deterministic procedure. One advantage of this method is that the computational efficiency improves greatly because the tracks molecular velocities and positions are based on representative collisions and boundary interaction. Another advantage is that the DSMC is a useful tool to test the validation of theoretical models, especially in high Knudsen number flow regime. However, the DSMC becomes computationally expensive in subsonic flows and statistical errors are unavoidable, which makes it unlikely to be used as a design tool in both the industry and research.

2.3.3 Extended Hydrodynamics

With increasing Knudsen number, the relation that stress that assumed to be linearly proportional to the gradients of velocity breaks down. Extended hydrodynamics uses standard fluid equations of mass, momentum and energy, but the stress tensor and heat flux vector are constructed to be more applicable to the flow regime with high Knudsen number. Many competing sets of higher-order constitutive relations are derived from the Boltzmann equation by using different ways. The commonly used solution to the Boltzmann equation can be obtained by using Chapman-Enskog method. The distribution function is expanded as an infinite series in terms of the Knudsen number:

$$f = f^0 + K_n \cdot f^1 + \dots + K_n^{Z+1} \cdot f^Z \quad (2-19)$$

where f^0 is the equilibrium Maxwellian distribution function.

The constitutive relation for the governing equation can be written as (Zhong, 1993):

$$\begin{aligned}\sigma_{ij} &= \sigma_{ij}^0 + \sigma_{ij}^1 + \dots + \sigma_{ij}^\chi + \dots \\ q_i &= q_i^0 + q_i^1 + \dots + q_i^\chi + \dots\end{aligned}\tag{2-20}$$

where σ_{ij} is the stress tensor, q_i is the heat flux vector.

The stress tensor and heat flux vector for various formulations are given by:

• $\chi = 0$	Euler equations	• $\chi = 1$	Navier-Stokes equations
• $\chi = 2$	Burnett equations	• $\chi = 3$	Super-Burnett equations

Burnett Equations

Burnett (1935) derived the Burnett equation from Boltzmann equation by considering the first three terms of Chapman-Enskog expansion. Fisko and Chapman (1988) and Zhong (1991) have employed the Burnett equation into continuum-transition flow regime by incorporating the additional linear and nonlinear stress and heat flux terms. From their study, it was validated that the Burnett equations do indeed describe the normal shock structure better than Navier-Stokes equations at high Mach numbers. Agarwal and Balakrishnan (2001) have recently proposed a new set of Burnett equations called as “BGK-Burnett” equations, to avoid the instability at high Knudsen numbers and violation of second law of thermodynamics for the Burnett equations.

The main advantage of the Burnett equation is that the solving process is not more complicated than solving the standard Navier-Stokes equations. Second, the Burnett equations are demonstrated to be more useful in solving the rarefied hypersonic flows as compared with the Navier-Stokes equations. However, there are still three major hurdles that need to be overcome in the development of the Burnett equations. The first problem is that although some ways are used try to eliminate the instability (Fisko and Chapman 1988; Zhong 1991; Agarwal 2001), no approach seems to give us a satisfactory solution in stabilizing the equation sets. The second problem is that Burnett equations is difficult to

be applied in the commercial fields because of the lack of efficient fluid dynamics codes and numerical techniques. The last problem is that the selection of appropriate boundary conditions, which is also a major problem. The high-order equation sets need the high-order boundary conditions, which means the high-order gradient should be included in the boundary conditions, and will cause the computational difficulty. The underlying physics also cannot be clearly figured out.

The comparison between simulation tools and experimental works are illustrated in Table 2-3.

Tools in simulating gas flow at micro and nano-scale		
Tools	Description of the simulation results compared with the experimental works	Advantage/Disadvantage
Lattice Boltzmann Equation	<ul style="list-style-type: none">Nie et al. (2001) compared mass flow rate as a function of pressure drop between LBM simulation and experimental work (Arkilic et al. 1997), show a better agreement with experimental data than Beskok et al. (1996) second order slip model. A quadratic dependence of slip velocity on Knudsen number was assumed in this simulation	<i>Application field:</i> Low speed rarefied gas flow in MEMS (slip flow regime). <i>Advantage:</i> Ease in handling in complex geometry; Simplicity in implementation and high efficiency.
	<ul style="list-style-type: none">Lim Shu et al. (2002) compared nonlinearity pressure distribution with LBM simulation and experimental results (Pong et al. 1994). It was found the simulation result was closer to experimental work than Arkilic's analytical work.	<i>Disadvantage:</i> Only suitable to simulate gas flow for very small Knudsen number. An apparent deviation from DSMC result was found when Kn reach to 0.2.
	<ul style="list-style-type: none">Sbragaglia et al. (2005) calculated the slip coefficient as a function Knudsen number using LBM solution. The result agrees well with the experimental work (Maurer et al. 2003).	
DSMC	<ul style="list-style-type: none">Ewart et al. (2009) compared DSMC simulation with the experimental results (Ewart et al. 2007). The mass flow rate was compared from the slip flow to transition flow regime ($0.086 < Kn < 8.86$). A qualitative agreement was found except in the range $0.17 < Kn < 0.5$. Maxwell's slip model with TMAC value 0.91 was adopted.	<i>Application field:</i> Rarefied atmospheric gas flow; Material design and processing; Microfluidics.
	<ul style="list-style-type: none">Piekos et al. (1996) use DSMC to obtain the pressure distribution in slip flow regime ($Kn=0.05$). An agreement was found by comparing with Arkilic analytical solution. A trend of increasing pressure curve linearity with increasing rarefaction is obtained in transition flow regime, which is contrast with experimental results of Pong et al. (1994)	<i>Advantage:</i> Can be applied in whole flow regime and complex geometry. <i>Disadvantage:</i> Computationally expensive in rarefied low-speed flows.

Tools in simulating gas flow at micro and nano-scale		
Tools	Description of the simulation results compared with the experimental works	Advantage/Disadvantage
Linearized Boltzmann Equation	<ul style="list-style-type: none">Ohwada et al. (1989) calculated the mass flow rate as a function of Knudsen number by using linearized Boltzmann equation. The calculation showed an agreement with Dong et al. (1956) experiments in a wide range Knudsen number from 0.1 to 20.The linearized Boltzmann equation was used to study Poiseuille flow for high Knudsen number gas films by Fukui and Kaneko (1989). The mass flow rate database for rapid calculation was provided. The simulation results were compared with Cercignani et al. (1963) and Loyalka (1971).	<p><i>Application field:</i> Low speed rarefied gas flow in whole flow regime</p> <p><i>Advantage:</i> Its solution may be served as criteria of testing other models.</p> <p><i>Disadvantage:</i> Solution only limited to simple geometry</p>
	<ul style="list-style-type: none">Bao et al. (2008) computed pressure distributions of nitrogen flow along the microchannel and compared with experimental data of Pong et al. (1994). The results agree well with the experimental data as well as Navier-Stokes equation with slip boundary.	<p><i>Application field:</i> rarefied gas flow in MEMS (slip flow regime)</p>
	<ul style="list-style-type: none">BGK-Burnett solution was used to study the microchannel flow in slip regime by Xu et al. (2004). The pressure distribution along the channel and mass flow rate were compared between simulation results and experiments of Pong et al. (1994), Zohar et al. (2002). The simulation results agree well with the experiments compared to BGK-NS solver. Maxwell first order slip model with full accommodation coefficient was adopted in the simulation.A Maxwell-Burnett second order slip model was incorporated with the first order constitutive equation (Weng et al. 2008). The mass flow rate was compared with experiment of Ewart et al. (2007).	<p><i>Advantage:</i> Solving process is simple; More useful in hypersonic flow than Navier-Stokes method.</p> <p><i>Disadvantage:</i> The convergent solution of micro Poiseuille flow could only be obtained when Knudsen number is less than 0.2.</p>

Table 2-3: Comparison between simulation tools and experimental works.

2.4 Summary

In this chapter, several slip models are reviewed, which can be mainly classified as first-order and second-order slip models. Compared with molecular-based models, slip models are more useful because analytical results can be obtained using continuum description. It is noted that the relative accurate results can be obtained in the slip regime with the incorporation of appropriate first-order slip models. In order to extend the validity of the slip regime to high Knudsen numbers, second-order slip models have been proposed. The efforts were mainly focused on finding the correct slip coefficients, but none of them has been proven to yield satisfactory results in the transition flow regime in general. Another argument is that second-order slip models are based on mathematics and lack physical interpretation.

From the experiments conducted in micro-channels, it was found that friction factors are still controversial. Some of them showed friction factors smaller or larger than that predicted by macro-scale fluid theory, which cannot be understood clearly. The slip models also cannot be validated by the experiments. First-order slip models are validated by some experiments, while second-order slip models are certified by others.

The models to describe gas flow are reviewed in the Section 2.3 in this chapter. However, the computational complexity associated with the linearized Boltzmann equation or the DSMC method is prohibitive and often inappropriate in the engineering field. Burnett equation and lattice Boltzmann equation also cannot be applied with acceptable accuracy in high Knudsen number flow regime. It is therefore desirable to develop an appropriate slip model incorporating with the constitutive equation, which can accurately describe micro and nano fluid flow.

Chapter 2 Literature Review

In conclusion, the literature survey shows in spite of the great efforts in studying micro-flows, a generally accepted slip model is still a valuable research topic and an important step towards resolving discrepancies.

Chapter 3 Scattering Model

3.1 The Weakness of Maxwell's Scattering Model

As discussed in literature review, in Maxwell's landmark paper (1879), kinetic theory was used to study the slip length associated with fluid flow close to a solid surface. A linear combination of two kinds behavior was postulated when a molecule was incident on the boundary. (it is either specularly reflected or it penetrated so deeply and undergoes many collisions with the wall molecules, then it forgets the direction in which it had approached and emerges with a velocity characteristic of the wall temperature). Later, although the model was proven to be appropriate only if the Knudsen number is sufficiently small, it continues to be the widely used as the fundamental assumption about molecules scattering behavior on a weakly adsorbing surface.

When we study the slip boundary condition and take the Maxwell's model for granted, the following general questions naturally arise:

1. Although the Maxwell's model is easily applied, it does not take into account the interaction between different components in the impinging particles' velocities, which determines the particles' reflections. Therefore, it seems necessary to consider the dependence of the accommodation coefficient on the molecular properties of interface.
2. The use of a constant accommodation coefficient in the Maxwell's model does not seem suitable to be applied to a wide range of incident velocity. There should be a relationship between the accommodation coefficient and the incident

molecules' properties, such as velocities of molecules, impinging direction, internal state, etc.

3. The internal-translational energy conversion may play an important role in determining the re-emitted particle velocity. The rotational-tangential energy conversion should be taken into account for rough surfaces.
4. On the weakly adsorbing boundary, the stick-slip can occur for a molecule on the boundary before it re-emits. Obviously, Maxwell's model does not take this into consideration.

It is found that the Maxwell's scattering model does not accommodate all the features of the interaction at the interface. More research is necessary to obtain useful information about the molecules scattering properties and to improve the Maxwell's scattering model.

3.2 New Scattering Model for Molecules

Before we study the scattering properties of the incident molecules on the surface, the surface roughness effect should be discussed in detail. In the previous study, the accommodation coefficient is generally treated as one unit. This means the boundary is so rough that the incident molecules penetrate deeply and collide with the wall molecules many times, losing their memory after being re-emitted. In the previous experiments, the characteristic length is of the order $100\text{ }\mu\text{m}$, although the relative roughness is small, the surface roughness ($\sim 10^1\text{ nm}$) is quite large comparable to the molecules diameter ($\sim 10^{-1}\text{ nm}$), so it is reasonable to consider the reflected molecules as having lost their memory after being re-emitted and treat the accommodation coefficient

as one unit.

However, with the size reduction of transport carrier and improvements with fabrication techniques, the surface roughness becomes smaller and comparable to the order of the diameter of incident molecules. Experiments conducted by Arkilic et al. (1997) were performed using micro-channels with height $1.33\ \mu\text{m}$. The micro-channels were very smooth and roughness was less than $0.65\ \text{nm}$, which is nearly three molecular diameters of helium. Tretheway and Meinhart (2002) used micro particle image velocimetry to measure velocities for the flow of fluids in rectangular glass micro-channels. When the wall was treated by a coating of OTS with nanometer thickness, surface roughness was about $0.2\ \text{nm}$. Cheng and Giordano (2002) reported flow rate versus pressure drop measurements for the flow in rectangular glass channels of width of about $10\ \mu\text{m}$, with various heights on the scale of tens to hundreds of nanometers, surface roughness of about $0.5\ \text{nm}$.

The combined experimental and hydrodynamics modeling also successfully revealed the significant deviation from totally diffused scattering for various gas transport in nano-pores and nano-tubes. Argon transport in amorphous nano-tubes with diameter $170\ \text{nm}$ (Cooper et al. 2003) was successfully modeled by describing the gas-wall interaction with a value of TMAC $\sigma = 0.52 \pm 0.1 (K_n = 7)$. That means more molecules were specularly reflected and retained more tangential momentum based on Maxwell's assumption. Because of the small characteristic length ($170\ \text{nm}$), the surface roughness can be assumed smaller compared to that for large tubes. The disparity of the scattering behavior in the nano-tube and large tube is due to the fact that the surface roughness plays an important role and changes the scattering character of molecules.

The diameter for several gas molecules and surface roughness in some experiments are

illustrated in Table 3-1.

Table 3-1 Comparison between diameter of gas molecules and surface roughness in some experiments.

Gas	Diameter (nm)	Surface Roughness (nm)	Source
Argon	0.36	≤ 0.65	Arkilic et al. (1997)
N ₂	0.37	0.2	Tretheway et al. (2002)
CO ₂	0.46	0.5	Cheng et al. (2002)
Helium	0.21	~ 2	Turner et al. (2002)

From Table 3-1, we can conclude that Maxwell’s scattering model simply divides the reflected molecules as specular or diffuse reflection, and is not enough to describe the real interaction between the molecules and the wall. A new model should be proposed based on the assumption that a fraction of molecules collide with the rough, frictional wall only once and then re-emit. The reflected molecular velocity should be related to the incident velocity, direction of incidence, the surface roughness and molecular properties of the interface.

The evident influence of the surface roughness prompts us to introduce a new simple scattering model to consider the surface roughness effect. In this model, a fraction of molecules f is reflected diffusely on the surface, and a complementary fraction of molecules $(1 - f)$ is reflected after colliding with the flat, frictional boundary. The reflected velocities, both tangential and normal to the surface, denoted by $u_{t,r}$ and $u_{n,r}$ respectively, depend on the incident molecular velocities, surface frictional coefficient, and the type of molecules at the interface.

The mean tangential reflected velocities of molecules can be written as:

$$u_{t,r} = (1 - f)u_{t,r1} + fu_{t,w} \quad (3-1)$$

where f is a parameter determined by the surface roughness and diameter of molecules. $u_{t,r}$ is the average reflected stream-wise velocity for all molecules and $u_{t,w}$ is the stream-wise velocity of the surface. $u_{t,r1}$ is the mean reflected stream-wise velocity for molecules, that are involved in colliding with the flat friction wall once and then re-emitted.

3.2.1 Collision for Molecule and Flat, Frictional Surface

The collision between molecules and flat wall is frictional, which indicates the linear and angular momentum can convert. Frictional force generated by rough surface is important since it allows for an exchange of translational and rotational energy and influences the reflected molecules velocities. Coulomb's law of friction is adopted to describe the frictional interaction of the molecules and wall. In this work, we propose a more realistic frictional law involving the Coulomb frictional force, which depends on the impact angle, i.e., the angle between the contact normal and the relative velocity of the contact points.

During a collision, energy is stored due to the deformations, which is related with both the normal and tangential direction of the contact point relative to the center of the molecules. Release of this energy will influence the rebounded molecules velocity significantly, so we introduce coefficients of restitution associated with both the normal and tangential components of the velocity at the point of contact.

Following Jenkins J.T. (1992), we distinguish between two kinds of binary collisions.

The first is called a sliding collision, a friction coefficient μ and a normal restitution coefficient e are introduced to describe the interaction between molecules and wall. The other is called a sticking collision, a tangential restitution coefficient β_0 and the same coefficient e are employed.

Binary Collision

In general case, a collision between two inelastic, frictional spherical particles 1 and 2 is considered, with diameter σ_1 and σ_2 and mass m_1 and m_2 with center located at r_1 and r_2 (see Figure 3-1). During the collision, particle 2 exerts an impulse J onto particle 1. Prior to the collision, the particles have translational velocities u_1 and u_2 , angular velocities ω_1 and ω_2 . The corresponding post-collision velocities are denoted by primes.

Figure 3-1 A binary collision between sphere 1 and sphere 2

Based on linear momentum conservation, it gives:

$$\begin{aligned} m_1(u'_1 - u_1) &= J \quad \text{and} \\ -m_2(u'_2 - u_2) &= J \end{aligned} \quad (3-2)$$

Similarly, the balance of angular momentum provides the relationship between the

angular velocities ω_1 and ω_2 as:

$$\begin{aligned}\omega_1' &= \omega_1 + \frac{\sigma_1}{2I_1} k \times J \quad \text{and} \\ \omega_2' &= \omega_2 + \frac{\sigma_2}{2I_2} k \times J\end{aligned}\quad (3-3)$$

where $I = m\sigma^2/10$ is the moment of inertia about the center of a homogeneous particle. The unit normal vector k is defined as the direction from center of particle 1 to the center of particle 2 and expressed as:

$$k = \frac{r_2 - r_1}{|r_1 - r_2|} \quad (3-4)$$

The relative velocity of centers of the particles is given as:

$$g = u_1 - u_2 \quad (3-5)$$

The relative velocities in the normal direction before and after collision are related through:

$$g' \cdot k = -e(g \cdot k) \quad (3-6)$$

where e is the coefficient of restitution in the normal direction.

The mean angular velocity can be written as:

$$S = \frac{1}{2}(\sigma_1 \omega_1 + \sigma_2 \omega_2) \quad (3-7)$$

The relative velocity G of the contact point before collision can be defined as:

$$G = g + S \times k \quad (3-8)$$

Using Eq. (3-2) and (3-3), the contact velocities before and after the collision are related by:

$$G' - G = \frac{7}{2m^*} J - \frac{5}{2m^*} (J \cdot k) \vec{k} \quad (3-9)$$

where $m^* = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass.

The impulse can be decomposed into its normal and tangential components:

$$J = m^* (A_1 k + A_2 j) \quad (3-10)$$

where the unit tangent vector is defined as:

$$j = \frac{(G \times k) \times k}{|G \times k|} \quad (3-11)$$

The coefficient A_1 is found by combining Eq. (3-2) and (3-11) and expressed as:

$$A_1 = -(1 + e) g \cdot k \quad (3-12)$$

Sliding Versus Sticking Collision

In sliding collision, using Coulomb friction model, the tangential component A_2 of J , is proportional to the normal component.

$$|k \times J| = \mu(k \cdot J) \quad (3-13)$$

where μ is the friction coefficient, $\mu \geq 0$. During a sliding collision, the tangential relative velocity of the particles contact point should be reduced by the friction force. The tangential relative velocity of the contact point can not reverse its direction and at most decreases to zero.

Combining the Eq. (3-12), (3-13), for sliding collision,

$$A_2 = \mu(1 + e) g \cdot k \quad (3-14)$$

If the tangential impulse is less than the product of the normal impulse and friction coefficient, i.e., $|k \times J| \leq \mu(k \cdot J)$, sticking collision occurs. A tangential coefficient of restitution of β_0 is introduced to model this case:

$$G' \cdot j = -\beta_0 (G \cdot j) \quad (3-15)$$

where β_0 is a positive number no greater than unity. The tangential component β_0 of J is not proportional in sticking collision.

Combining Eq. (3-9), (3-13) and (3-15), we get:

$$A_2 = -\frac{2}{7}(1 + \beta_0)(G \cdot j) \quad (3-16)$$

It should be noted that during the sticking collision, the relative velocity at the contact point can reverse its direction due to the release the deformation. Whether a collision is sliding or sticking depends on the angle γ between G and k . When this angle is less than the critical angle γ^* , the collision is sticking. When the angle is greater or equal to the critical angle, a sliding collision occurs. When $\gamma = \gamma^*$, the above expression for A_2 should agree at critical angle γ^* . From this, we can obtain tangential coefficient of restitution β_0 as:

$$\beta_0 = -1 + \frac{7}{2}(1 + e)\mu \cot \gamma^* \quad (3-17)$$

The critical angle γ^* is determined by:

$$\gamma^* = \arctan \left[\frac{7}{2}(1 + e)\mu / (1 + \beta_0) \right] \quad (3-18)$$

From Eq. (3-12) and (3-14), in sliding collision,

$$J^{(1)} = -m^*(1 + e)(G \cdot k)\vec{k} + m^*\mu(1 + e)(G \cdot k)\vec{j} \quad (3-19)$$

From Eq.(3-12) and (3-16), in sticking collision,

$$J^{(2)} = -m^*(1 + e)(G \cdot k)\vec{k} - \frac{2}{7}m^*(1 + \beta_0)(G \cdot j)\vec{j} \quad (3-20)$$

Reflected Velocity after Colliding with Wall

The objective of this section is to analyze the tangential velocity relationship of a molecule before and after the collision. A roughness coefficient β is introduced to express the ratio of tangential component of relative velocity before and after collision. In general case, the value of the coefficient β is assumed to be between -1 and $+1$. When β equals to -1 , the molecules and wall are considered as frictionless and the tangential component of the relative velocities after collision is same as that before collision. When β equals to $+1$, the tangential component of the relative velocity reverses completely after collision. The interface is treated as perfectly rough. Whether the collision is sliding or sticking, roughly said, near head-on collision generates sticking collisions, while grazing collision causes sliding collision.

Considering a molecule with the tangential and normal velocity u_{1t} , u_{1n} respectively collide with the wall. For simplicity, the internal freedom of the incident molecule is not considered, so the rotational velocity $\omega_1 = 0$. The wall is treated as stationary, and the tangential and normal velocity $u_{2t} = 0$, $u_{2n} = 0$. By applying the Eq.(3-2) (3-19), in sliding collision,

$$m_1(u_1' - u_1) = -m^*(1+e)(G \cdot k)\vec{k} + m^*\mu(1+e)(G \cdot k)\vec{j} \quad (3-21)$$

in stick collision:

$$m_1(u_1' - u_1) = -m^*(1+e)(G \cdot k)\vec{k} - \frac{2}{7}m^*(1+\beta_0)(G \cdot j)\vec{j} \quad (3-22)$$

The wall can be considered as a particle with infinite mass m_2 , so $m^* = m_1$, where m_1 is the gas molecule mass.

From the Eq. (3-21) and Eq. (3-22), the tangential velocity of a molecule colliding with

the wall can be expressed as:

$$u_{t,rs} - u_{t,is} = -\frac{2}{7}(1 + \beta(\gamma))u_{t,is} \text{ and}$$

$$\beta(\gamma) = \min\left[-1 + \frac{7}{2}\mu(1 + e)\cot\gamma, \beta_0\right] \quad (3-23)$$

where $u_{t,rs}$ and $u_{t,is}$ express the tangential reflected and incident velocity for a molecule. The value of tangential restitution coefficient β varying with impact angle and frictional coefficient are illustrated in Figure 3-2.

Figure 3-2 Tangential restitution as a function of the impact angle γ for different values of coefficient of friction μ ($\beta_0 = 0.5$).

3.2.2 Mean Tangential Restitution

From Figure (3-2), it is obvious that the coefficient of the tangential restitution is not a constant. The average coefficient of tangential restitution over all impact angles was used to simplify the many molecules-wall collision rules, thereby reducing the problem to one with a constant coefficient of tangential restitution. To obtain an average coefficient, the first step is to know the probability distribution of impact angles.

Here we assume the probability of molecules hitting the wall is proportional to the normal velocity of molecules, so the distribution of $\sin \gamma$ is constant: $P'(\sin \gamma) \equiv 1$. A uniform probability P' implies for the distribution of the angle $P(\gamma) = \cos \gamma$, so that grazing contacts sound less probable than central collisions within a fixed interval $d\gamma$, which is consistent with the CLL scattering model. (Cercignani, C. et al. 1997)

Mean Tangential Restitution $\beta = \langle \beta(\gamma) \rangle$

From Eq. (3-23), if we assume the incident angle is from 0 to $\frac{\pi}{2}$, the average coefficient of tangential restitution over all impact angle range is:

$$\beta = \langle \beta(\gamma) \rangle = \int_0^{\frac{\pi}{2}} P(\gamma) \beta(\gamma) d\gamma = \int_0^{\gamma^*} P(\gamma) \beta_0 d\gamma + \int_{\gamma^*}^{\frac{\pi}{2}} P(\gamma) \beta(\gamma) d\gamma \quad (3-24)$$

The integral over from 0 to $\frac{\pi}{2}$, is composed of two parts. One corresponding to the range $0 \leq \gamma \leq \gamma^*$, for which sticking collision occurs with a constant restitution $\beta = \beta_0$, the other part corresponding to the range $\gamma^* < \gamma < \frac{\pi}{2}$, for which a sliding collision takes place with the tangential restitution $\beta(\gamma) = -1 + \frac{7}{2} \mu(1+e) \cot \gamma$

Recall the Eq. (3-18) and obtain the critical angle:

$$\cot \gamma^* = \frac{2(\beta_0 + 1)}{7(1+e)\mu} \quad (3-25)$$

Combining the Eq. (3-24) and (3-25), we obtain the mean tangential restitution:

$$\beta = \langle \beta(\gamma) \rangle = -1 + \frac{7}{2}(1+e)\mu \cdot \ln(\cot \gamma^* + \sqrt{1 + \cot^2 \gamma^*}) \quad (3-26)$$

The values of mean tangential restitution coefficient varying with frictional coefficient are illustrated in Figure 3-3.

Figure 3-3 Mean tangential restitution versus the friction coefficient and normal restitution coefficient.

3.2.3 Tangential Momentum Accommodation Coefficient in the Scattering Model

In Maxwell's scattering model, it was postulated that when molecules incident on a

surface, some fraction of them rebound from the surface without transferring any of their stream-wise momentum, others transfer all of their momentum. To express the ratio that relates the amount of stream-wise momentum which is transferred to the wall upon collision, the TMAC was defined as:

$$\sigma = \frac{u_{t,r} - u_{t,i}}{u_{t,w} - u_{t,i}} \quad (3-27)$$

where $u_{t,i}$ is the average incident stream-wise velocity.

To describe the TMAC in the new scattering model, we combine the Eq. (3-1) and (3-23), the tangential velocity of the reflected molecules can be expressed as:

$$u_{t,r} = (1 - f)\varepsilon u_{t,i} + f u_{t,w} \quad (3-28)$$

where ε is the parameter which expresses the mean ratio of tangential velocity after collision to the value before collision for molecules, that are involved in colliding with the flat frictional wall once and then re-emit.

If the impact angle varies from 0 to $\frac{\pi}{2}$, ε can be calculated as:

$$\begin{aligned} \varepsilon &= \langle \varepsilon(\gamma) \rangle = \int_0^{\frac{\pi}{2}} P(\gamma) \left(1 - \frac{2}{7} (1 + \beta(\gamma)) \right) d\gamma \\ &= \int_0^{\gamma^*} P(\gamma) \left(1 - \frac{2}{7} (1 + \beta_0) \right) d\gamma + \int_{\gamma^*}^{\frac{\pi}{2}} P(\gamma) (1 - ((1 + e) \cdot u \cdot \cot \gamma)) d\gamma \end{aligned} \quad (3-29)$$

Comparing with the definition of the tangential momentum accommodation coefficient in Maxwell's scattering model and further assume the tangential momentum of the wall $u_{t,w} = 0$, the value of TMAC in our scattering model can be defined as:

$$\sigma = 1 - (1 - f)\varepsilon \quad (3-30)$$

3.3 Temperature Dependence of TMAC for Gas Flow

In the previous work, the tangential momentum accommodation coefficient (TMAC) was usually treated as unity in most engineering application. However, it was found that the TMAC is very sensitive to gas and wall conditions. The values of TMAC have been demonstrated to be influenced by many factors, such as material properties, surface roughness. These investigations alert us to be very cautious when choosing value of TMAC, because it depends strongly on the conditions parameters. Another important parameter, temperature, was rarely mentioned in the existing literatures because the values of TMAC were obtained mostly at a limited room temperature. Using MD simulations, Cao, B.Y. et al (2005) and Collins et al. (1994) pointed out the temperature is another important factor which has effects on the TMAC as well. Cao reported a decrease in TMAC for argon on platinum plates, from 0.28 at 119.8 K to 0.18 at 349.5 K. Further, he described this decrease by an exponential function which shows TMAC decrease more sensitive to low temperature than higher one. Unfortunately, no detailed physical interpretation was offered to the temperature dependence of the TMAC except these simulation results. In the present study, our purpose is to using the new scattering model and explaining the temperature dependence of TMAC for gases flow.

The normal restitution coefficient e was found as a function of impact velocity by many researchers. According to Lun and Savage (1986), restitution coefficient e is dependent on impact velocity of the particle in the normal direction. At very low impact velocity, the particle deformation is nearly elastic and the energy dissipation is small, thus particle keeps more momentum in the normal direction after reflected and e is closed to unity. At high impact velocity, the effects of plastic deformation and energy dissipation are significant, e approaches zero, which means the colliding particles do not rebound

after the collision.

Lun et al. (1985) proposed that the restitution coefficient e is decayed exponentially with respect to the impact velocity (see Figure 3-4):

$$e = \exp\left(-\delta\left(\frac{\rho}{E}\right)^{1/2} u_{i,n}\right) \quad (3-31)$$

where ρ and E are referred to particles density and modulus of elasticity respectively, δ is a dimensionless coefficient, the term $u_{i,n}$ is referred to incident velocity of molecule in the normal direction.

McNamara et al. (2008) proposed another model to describe this dependence. The restitution coefficient e was expressed as:

$$e = \begin{cases} 1 - (1 - e_0) \left(\frac{u_{i,n}}{u_0}\right)^{1/5} & , u_{i,n} \leq u_0 \\ e_0 \left(\frac{u_{i,n}}{u_0}\right)^{-1/4} & , u_{i,n} \geq u_0 \end{cases} \quad (3-32)$$

where e_0 , u_0 express the critical restitution coefficient and critical velocity.

Figure 3-4 Variation of coefficient of restitution e with impact velocity. (Lun et al. 1985)

Based on these investigations, we can conclude that the normal restitution coefficient decreases with increasing impact velocity in the normal direction. At the same impact-angle probability distribution, the mean velocity normal to the surface is determined only by the gases temperature (for the same molecules), that is, the mean velocity normal to the surface will increase with higher temperature. According to Eq. (3-29), the parameter ε will increase due to the lower value of e , which indicates the reflected molecules will keep more tangential momentum if the temperature is higher. This predication is consistent with the simulation results by Cao and Collins. Our scattering model can provide qualitative explanation to the temperature dependence of TMAC.

3.4 Incident Angle Dependence of TMAC for Gas Flow

Understanding the microscopic properties of momentum and energy transfer between gas and surface is of fundamental and practical importance to the study of micro-channel flows. One method to measure the tangential momentum accommodation coefficient (TMAC) is to use the beam technique. Omelik (1977) measured the forces acting on a flat plate to determine the normal and tangential momentum accommodation coefficients. Supersonic beams of gases were directed at the surface at different angles of incidence. It was validated that the nature of reflected molecules approaches specular reflection as the angle of incidence, i.e, from the normal to the surface, increases. The variation of TMAC with incident angle of gas, as reported by Omelik, is in qualitative agreement with the results of Knechtel et al. (1969) and Seidel et al. (1974) who used a similar measurement technique.

Another approach to derive the TMAC is through the molecular dynamics (MD) technique. MD is used to study the impact of individual gas molecule upon solid surfaces, in order to understand how inter-molecular forces, surface geometry and the incident angle of molecules influence their scattering behavior. Finger et al. (2007) used Lennard-Jones potential to describe the impact model, using angles of incidence that varied from 10 to 70 degrees from the normal of the surface. The simulation results agreed within 3% of experimental values and correctly validated that TMAC changes with different incident angle. The estimated TMAC values were from a high of 1.2 to a low of 0.25, generally with lower values at larger incident angles.

The value of TMAC as a function of incident angle in the collision model and experimental/simulation data is illustrated in Figure 3-5.

Figure 3-5: TMAC value as a function of incident angle.

From Figure 3-5, the prediction from the collision model we adopted agrees well with the experimental and simulation results. It is found that the prediction agrees well especially at larger incident angle, but deviates at smaller incident angle, which is not a surprised result. At the small angle, the stick-slip collision occurs and the TMAC value is a constant. The deviation for the small incident angle does not illuminate the collision model is invalid. The parameter f should increase when the incident angle decrease. In Figure 3-5, if the value of f is allowed to be larger at small incident angle, a desired result can be obtained.

Overall, the experimental and MD simulation results do follow the same trends that molecules scatter from the surface more specularly with increasing incident angle.

One interesting experiment performed by Cook (1997) is to measure TMAC between the space shuttle reaction control jet plume gases and solar panel array materials. Measurements were made with H_2 , N_2 , CO and CO_2 gases incident upon the solar array material, Kapton, SiO_2 -coated Kapton and Z93-coated Al. It was found that TMAC also decreases with increasing incident angles for most surface materials except the Z93-coated Al. The experiment shows that gas molecules scattering from Z93-coated Al are nearly diffused for all angles of incidence, which is most likely attributed to the extremely rough surface of Z93-coated aluminum.

From the experimental and MD simulation results, two conclusions are drawn:

1. In general, molecules scatter from the surface more specularly as the incident angle increases.
2. Diffused scattering happens mostly for rough surfaces regardless of the incident angle.

Considering the interaction model of molecules and surface that we introduced in section 3.2, it is easily deduced that with the same impact velocity, when the incident angle of the particles γ increases, frictional force decreases and the reflected molecules retain more tangential momentum after collision with the wall. This indicates that our impact model is consistent with the results obtained in the molecular beam experiment and the MD simulation. For a rough surface, the parameter f , as defined, can be assumed as one unit, and the scattering molecules are totally diffusely reflected, which indicates that our scattering model can also describe the phenomenon happened in Cook's experiments.

Based on the above, it is reasonable to draw the conclusion that our scattering model is in qualitative agreement with the experimental and MD simulation results and suitable for studying the microscopic behavior of momentum transfer at the fluid/solid interface.

3.5 Impact Tangential Velocity Dependence of TMAC for Gas Flow

It is expected that the TMAC strongly depends on the angle at which the gas molecules impact on the wall. At zero impact tangential velocity, the mean angle at which the molecules collide with respect to the surface normal is zero (see Figure 3-6). With a finite impact tangential velocity, the mean angle is non-zero and increases with the magnitude of the tangential velocity. From the experimental and theoretical studies, the impact tangential velocity approximately one mean free path from the walls is found to be between 20-30% of the maximum stream velocity for helium gas and 5-36% of the maximum velocity for steady state flow of various gases (Wleklinski, J.J 2001). Therefore, it validates that the mean angle is non-zero and varies with the magnitude of the tangential velocity for the most flows. However, in Maxwell's slip model, the TMAC

is generally defined using all incident molecules to the wall irrespective of their magnitude of tangential velocity, which should be an important parameter that influences the value of TMAC in our scattering model. In this section, our main purpose is to derive the value of TMAC that is dependent on the impact tangential velocity.

Let us assume an isothermal flow, with the incident molecules obeying the Maxwell's distribution. The x, y velocity components are then random and the impact angle is assumed evenly distributed. Considering the case of the mean tangential velocity $u_{t,i} = 0$, the velocity distribution of molecules colliding on the wall can be represented by the vectorial diagram in Figure 3-6. The average Maxwell distribution of speeds is given by u_m as follows:

$$u_m = \int_0^{\infty} \sqrt{\frac{m}{KT}} u e^{-(m/2KT)u^2} du = \sqrt{\frac{2KT}{\pi m}} \quad (3-33)$$

At a finite “drift” velocity, the impact angle distribution is not even. Subjected to a Galilean transformation, the velocity angular distribution in the wall frame can be represented by the diagram in Figure 3-7.

The graphical method is used to calculate the mean change in tangential velocity for all molecules hitting the wall and then the TMAC value can be derived. We should note that u is now a function of θ and that the probability of molecule incidence at a given angle θ is now a function of θ' .

From the Figure 3-7,

$$u_m^2 = u_{t,i}^2 + u^2(\theta) - 2u_{t,i}u(\theta)\cos(\theta) \quad (3-34)$$

where $u_{t,i}$ is the mean tangential velocity of incident molecules.

$u(\theta)$ can be obtained as the function of θ and impact tangential velocity $u_{t,i}$.

$$u(\theta) = u_{t,i} \cos(\theta) + \sqrt{u_m^2 - u_{t,i}^2 \sin^2(\theta)} \quad (3-35)$$

$$u_m \cos(\theta') + u_{t,i} = u(\theta) \cos(\theta) \quad (3-36)$$

$$\theta' = \arccos[(u(\theta) \cos(\theta) - u_{t,i}) / u_m] \quad (3-37)$$

In the original Maxwell's distribution, the impact angle distribution is even and described as:

$$\int_0^\pi P(\theta') d\theta' = 1; \quad P(\theta') = \frac{1}{\pi} \quad (3-38)$$

$$P(\theta') d\theta' = P(\theta) d\theta = \frac{d\theta'}{\pi} \quad (3-39)$$

From the Figure 3-8, we derived:

$$\cos(\theta' - \theta) = \frac{u(\theta) d\theta}{u_m d\theta'} \quad (3-40)$$

The angular distribution with the drift velocity $u_{t,i}$ is (see Figure 3-7):

$$P(\theta) = \frac{d\theta'}{\pi d\theta} = \frac{u(\theta)}{u_m \cos(\theta' - \theta) \pi} \quad (3-41)$$

Based on our impact model, the reflected tangential velocity for one molecule after hitting the wall can be rewritten as:

$$u_{t,rs} - u_{t,is} = -\frac{2}{7} (1 + \beta(\theta)) u_{t,is}$$

$$\beta(\theta) = \min \left[-1 + \frac{7}{2} \mu(1+e) |\tan(\theta)|, \beta_0 \right] \quad (3-42)$$

The mean tangential velocity of reflected molecules, that is not diffusely reflected, is then given by:

$$u_{t,r1} = \varepsilon \cdot u_{t,i} = \left(\int_0^\infty \int_0^\pi \psi \frac{u(\theta)}{u_m \cos(\theta - \theta') \pi} \left[\left(1 - \frac{2}{7} (1 + \beta(\theta)) \right) \right] d\theta du \right) \cdot u_{t,i} \quad (3-43)$$

where ψ is the Maxwell distribution of speeds probability defined in Eq. (3-33). u_m is replaced by u in $u(\theta)$

Figure 3-6. Profile of molecular velocity incident on a surface

Figure 3-7. Galilean transformation of molecular velocities (exaggerated).

Figure 3-8. Sector transformation from reference frames.

Impact angle distribution

Figure 3-9 Incident angle probability dependent on incident tangential velocity at $u_{t,i} = 0.02u_m$

Figure 3-10 Incident angle probability dependent on incident tangential velocity at $u_{t,i} = 0.1u_m$

Figure 3-11 Incident angle probability dependent on incident tangential velocity at $u_{t,i} = 0.2u_m$

Figure 3-12 Incident angle probability dependent on incident tangential velocity at $u_{t,i} = 0.4u_m$

Figures (3-9) to Figure (3-12) show the impact angle probability distribution versus incident tangential velocity of gas molecules. The value of ε , i.e., the mean ratio of reflected tangential velocity to the incident tangential velocity as calculated in Eq. (3-43), is illustrated in Figure (3-13).

Figure 3-13 ε versus incident tangential velocity with various value of friction coefficient. ($e = 0.95$; $\beta_0 = 0.95$)

From Figure (3-13), it can be concluded that the value of ε is not a constant, and increases near linearly with increasing incident tangential velocity, thus ε can be expressed as:

$$\varepsilon = \frac{u_{t,r1}}{u_{t,i}} = (\varepsilon_0 + \varepsilon_1 u_{t,i}) \quad (3-44)$$

where ε_0 expresses the mean ratio of reflected tangential velocity to the incident

tangential velocity when the incident tangential velocity is small, i.e., at low shear rate.

ε_1 is the parameter to describe the influence of incident tangential velocity on momentum transferring to the wall.

3.6 Summary

In this chapter, our main objective is to propose a new scattering model for molecules. It is demonstrated that one parameter σ is not enough to describe the interaction of molecules and wall as used in Maxwell's scattering model. In Arkilic et al. (1997) experiments, operating with the same channel and at same flow conditions, the accommodation coefficients for argon and nitrogen are different (for argon, $\sigma_{ar} = 0.8 \pm 0.1$; for nitrogen, $\sigma_{N_2} = 0.88 \pm 0.06$). The Maxwell scattering model can not explain this deviation. In our scattering model, the parameter f describes the effect of surface roughness, which is defined to express the percentage of single collision and multiple-collision. The friction and restitution coefficient are introduced to account for the different type of molecules interaction with the wall. The translational-rotational energy conversion will be generated by the frictional force, so the molecules with the same velocity but different incident direction will produce the different frictional force and different translational-rotational energy conversion. Our scattering model can also provide a physical interpretation to the temperature dependence of TMAC, which is in agreement with the simulation results. The value of TMAC is also found to be influenced by the incident angle and mean tangential velocity of molecules. In general, our scattering model can provide a more realistic description to the interaction model of molecules and wall.

Chapter 4 Wall Boundary Conditions for Gas Flow

4.1 New Slip Model

Maxwell's most famous slip model proposed in 1879 was based on the kinetic theory. For isothermal flow, a similar boundary with the approximate analysis of the motion of gas was derived by Beskok (2002). For the convenience of illustrating the new slip model, the similar method as Beskok's is adopted but the influence of the incident tangential velocity is also considered. At a surface 's' near the wall, half of the molecules pass through the surface are coming from a distance of one mean free path λ away from this surface. These molecules can be considered as the incident molecules. Other half of the molecules pass through the surface 's' can be considered as the reflected molecules. For the reflected molecules, f is defined as the fraction of diffused reflection, where the reflected molecules lost the 'memory' on their velocity after the collision with the boundary and are reflected randomly in all directions, the average velocity of the molecules for the diffused reflection corresponds to that of the wall (see Figure 4-1). The remaining fraction of molecules, $1-f$, which is not specularly reflected as Maxwell's slip model, collides with the flat rough wall once and are then re-emitted (see Figure 4-2). The reflected velocities depend on the incident angle distribution, normal restitution coefficient and frictional coefficient.

Figure 4-1 Diffuse reflection of a molecule colliding with a wall

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Figure 4-2 The reflection of a molecule on a flat rough wall

The total tangential momentum flux is written as:

$$\frac{1}{4} n_s m \bar{u} u_s = \frac{1}{4} n_{t,i} m \bar{u}_g u_{t,i} + \frac{1}{4} n_w m \bar{u}_w u_{t,r} \quad (4-1)$$

Assuming that there is no condensation of gas on the surface, the number density of the reflected molecules can also be related as:

$$n_{t,i} = n_w = \frac{1}{2} n_s \quad (4-2)$$

With the assumption that the temperature of the gas and the wall are same, the mean thermal speeds are identical: $\bar{u} = \bar{u}_g = \bar{u}_w$

Combining the Eq. (3-28) and Eq. (3-44), the reflected velocity at the surface 's' $u_{t,r}$, is:

$$u_{t,r} = (1-f)(\varepsilon_0 + \varepsilon_1 u_{t,i}) u_{t,i} + f u_{t,w} \quad (4-3)$$

From Eq.(4-1),Eq.(4-2) and Eq.(4-3), we get

$$u_s = \frac{1}{2} u_{t,i} + \frac{1}{2} (1-f)(\varepsilon_0 + \varepsilon_1 u_{t,i}) u_{t,i} + \frac{1}{2} f u_w \quad (4-4)$$

Assuming the velocity of the wall is zero and use Taylor series expansion, the above equation becomes

$$u_s = \frac{1}{2} (u_s + \lambda \frac{\partial u}{\partial y}) + \frac{1}{2} (1-f) \left(\varepsilon_0 + \varepsilon_1 (u_s + \lambda \frac{\partial u}{\partial y}) \right) (u_s + \lambda \frac{\partial u}{\partial y}) \quad (4-5)$$

For simplicity, Eq. (4-5) changes to

$$u_s = A(u_s + \lambda \frac{\partial u}{\partial y}) + B(u_s + \lambda \frac{\partial u}{\partial y})^2 \quad (4-6)$$

where $A = \frac{1}{2} + \frac{1}{2}(1-f) \cdot \varepsilon_0$, $B = \frac{1}{2}(1-f) \cdot \varepsilon_1$

Eq. (4-6) is the new slip model we derived.

For the ease of comparison to other slip models, we rewrite the Eq. (4-6) as:

$$u_s = \frac{2 - \sigma_{s-d}}{2} (u_s + \lambda \frac{\partial u}{\partial y}) + B(u_s + \lambda \frac{\partial u}{\partial y})^2 \quad (4-7)$$

where $\sigma_{s-d} = 1 - (1-f) \cdot \varepsilon_0$, the subscript $s-d$ indicates the shear-dependent.

Physical Meaning of Parameters σ_{s-d} , B in Our Slip Model

As defined, the parameter σ_{s-d} is:

$$\sigma_{s-d} = 1 - (1-f) \cdot \varepsilon_0 \quad (4-8)$$

where ε_0 is the parameter defined in Eq. (3-44). Comparing with the TMAC value defined in Eq. (3-30) in the last chapter, σ_{s-d} is nearly the TMAC value in our slip model, i.e., it expresses the ratio that relates the amount of stream-wise momentum which is transferred to the wall upon collision at low shear rate. In Maxwell's slip model, the value of TMAC is defined as the fraction of gas molecules reflected diffusively from a solid surface, while σ is the parameter that mainly indicates the surface roughness. In our slip model, parameter σ_{s-d} is a function of f, μ and e . f, μ are the parameters to describe the surface roughness effects influencing the collision between gas molecules and wall. Parameter e describes the interaction properties of gas molecules and wall, which can explain the different values for slip coefficient for different kinds of gas molecules under the same experimental conditions. Parameter B is a coefficient

that describes the influence of shear rate. When the reflected molecules are totally diffuse-reflected, the value of σ_{s-d} in our slip model equals to unity and the coefficient B equals to zero. Our slip model then reduces to the Maxwell’s slip model.

From Eq. (4-6), a nonlinear relationship between shear rate and slip velocity is indicated in our slip model, which is never mentioned in other slip models. To verify our slip model, we present the comparison between experimental work conducted by Arkilic (1997T) (the detailed experimental condition and detailed derivation are presented in section 4-3) and prediction of our slip model. The predictions of the first-order slip models and second-order slip models are also included. Figure (4-3) shows the comparison between our slip model to experimental work and first-order slip models.

Figure 4-3 Comparison between predictions of first-order slip models and experimental work (Arkilic, E.B. 1997T)

Figure (4-4) shows the comparison between our slip model to experimental work and second-order slip models.

Figure 4-4 Comparison between predictions of second-order slip models and experimental work (Arkilic, E.B. 1997T)

For the ease of comparison, we rewrite the first-order slip models and second-order slip models as the form in Eq.(4-7), the TMAC value σ_{s-d} and B for this experiment are illustrated in Table (4-1).

Table 4-1: Coefficients σ_{s-d} and B in slip models

Slip Models	σ_{s-d}	B
Our slip model	0.804	0.004
Xue and Fan (2002)	0.8	0
Beskok and Karniadakis (1999)	0.8	0
Schamberg (1947)	0.38	0
Cercignani and Daneri (1963)	0.44	0
Deissler (1964)	0.42	0
Hsia and Domoto (1983)	0.6	0
Mitsuya (1993)	0.79	0

It is obvious that either the first-order slip modes or the second-order slip models cannot explain the phenomena observed in this experiment, in which a nonlinear relationship between slip velocity and shear rate is apparent. The main differences between the first-order and second-order slip models are that the slip coefficients in these slip models are varying to account the rarefaction effect, however, the linear relationship between shear rate and slip velocity is always hold for these slip models. On the contrary, this concept is no longer valid in our slip model. The nonlinear relationship is not only testified by the experiments in gas flow, but also observed by many experimentalists in liquid flow. In the following part of this chapter and next chapter, more work will be presented to validate our slip model.

4.2 Compare the Shear-Dependent Slip Model to Boltzmann Equation Solution and Other Slip Models in Poiseuille Flow

Now, we apply the Navier-Stokes equations to a micro-channel flow as shown in Figure 4-5. For simplicity, all derivations are based on the following assumptions:

1. The flow in the micro-channel is steady.
2. The flow is assumed to be isothermal, compressible, time independent and one-dimensional.
3. The fluid pressure is assumed to be only a function of stream-wise direction.
4. The pressure drop related to the contraction and expansion at the inlet and outlet are neglected.

Figure 4-5 Poiseuille flow in micro-channel

The continuity equation is given by:

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \quad (4-9)$$

For simplicity, the order-of-magnitude relations, which are in m-kg-sec units for most micro-channel flows, are considered in the momentum equation.

Length $L \sim 10^{-3} m$, height $d \sim 10^{-6} m$, stream velocity $u \sim 10^1 m/s$, the velocity in the

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y, z direction is zero, kinematic viscosity $\nu = \mu / \rho \sim 10^{-5}$, density $\rho \sim 10^0 \text{ kg/m}^3$.

With these properties, the momentum equation in the stream-wise direction, incorporating the order of magnitude of terms, can be expressed as:

$$\text{x-momentum} \quad \frac{\partial u}{\partial t} + \underbrace{u \frac{\partial u}{\partial x}}_{10^5} + \frac{1}{\rho} \frac{\partial p}{\partial x} = \frac{1}{\rho} \underbrace{\frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right)}_{10^8} \quad (4-10)$$

Based on the above assumptions, the time-derivative terms can be neglected. The momentum equation in most micro-channel flows in the stream-wise direction can be written as:

$$\frac{\partial p}{\partial x} = \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) \quad (4-11)$$

From the above equation, the stream-wise velocity profile can be obtained with a analytical solution as follows:

$$u = \frac{1}{2\mu} \frac{\partial p}{\partial x} y^2 + c_1 y + c_2 \quad (4-12)$$

By using the new slip model we proposed in Eq. (4-7), the slip velocities for Poiseuille flow at the boundary are written as:

$$\begin{aligned} y = -\frac{d}{2}, u_s &= \frac{\sigma_{s-d} - 4B\lambda \frac{\partial u}{\partial y} - \sqrt{\sigma_{s-d}^2 - 16B\lambda \frac{\partial u}{\partial y}}}{4B} \\ y = \frac{d}{2}, u_s &= \frac{\sigma_{s-d} + 4B\lambda \frac{\partial u}{\partial y} - \sqrt{\sigma_{s-d}^2 + 16B\lambda \frac{\partial u}{\partial y}}}{4B} \end{aligned} \quad (4-13)$$

Constant c_1, c_2 in Eq. (4-12) can be derived from the above boundary conditions.

4.2.1 Velocity Profile for Poiseuille Flow

The velocity profile can be strongly influenced by the slip boundary conditions. To validate our slip model, the velocity distribution for Poiseuille flow is presented. Comparisons between our slip model, other slip models and the linearized Boltzmann equation's results are made using a wide range of Knudsen numbers.

The bulk velocity at the central line with non-slip boundary in micro-channel can be written as:

$$u_0 = -\frac{d^2}{8\mu} \frac{\partial p}{\partial x} \quad (4-14)$$

Based on Eq. (4-12), Eq. (4-13), the velocity profile for Poiseuille flow in micro-channel is:

$$u = -\frac{d^2}{2\mu} \frac{\partial p}{\partial x} \left(\frac{1}{4} - \left(\frac{y}{d} \right)^2 + \left(\frac{\sigma_{s-d} - \sqrt{\sigma_{s-d}^2 - 64Bu_0K_n}}{16BK_nu_0} - 1 \right) K_n \right) \quad (4-15)$$

Generally, the velocity formula of the Poiseuille flow through a micro-channel with a constant height d can be expressed as:

$$u = -\frac{d^2}{2\mu} \frac{\partial p}{\partial x} \left(\frac{1}{4} - \left(\frac{y}{d} \right)^2 + C_1 K_n^2 + C_2 K_n \right) \quad (4-16)$$

The values of C_1, C_2 for different slip models are described in Table (4-2).

Table 4-2 The value of C_1, C_2 in Poiseuille flow for different slip models

Model	C_1	C_2
Continuum	0	0
Maxwell Slip Model	0	$(2 - \sigma) / \sigma$
Schamberg Slip model	$-5\pi / 6$	1
Hsia slip Model	1	1
Mitsuya Slip model	4/9	1
The VHS Slip Model	0.3872	0.62228
The VSS Slip Model	0.408	0.63875
Our Slip Model	$\frac{64Bu_0}{\sigma_{s-d}}$	$\frac{2 - \sigma_{s-d}}{\sigma_{s-d}}$

In our model, if all the reflections are diffused, $C_1 = 0, C_2 = 1$ and our slip model simplifies to the first-order slip model.

For convenience, we introduce a non-dimensional parameter, the inverse Knudsen number D , which is defined as $D = \frac{\sqrt{\pi}}{2K_n}$. Figures (4.6-4.8) are the non-dimensional velocity profile for Poiseuille flow at different inverse K_n numbers, D . The velocity

u has been non-dimensionalized by a factor B_1 where $B_1 = \sqrt{\frac{RT}{2}} \frac{d}{p} \frac{dp}{dx}$.

Figure 4-6 Non-dimension velocity profile at $Kn=0.088623$ ($D=10$)

Figure 4-7 Non-dimension velocity profile at $Kn=0.88623$ ($D=1$)

Figure 4-8 Non-dimension velocity profile at Kn=11.3 (D=0.0724)

From the figures, comparing the predictions of slip models and the solution of linearized Boltzmann equation, it is apparent the accuracy of prediction is worse as Knudsen number increases. For small Knudsen numbers, say, $K_n = 0.088623(D = 10)$, the first-order and second-order slip models provide good predictions of slip velocities at the wall, but the mean flow velocities are underestimated compared with the solution of linearized Boltzmann equation. The modified VHS slip model underestimates the slip velocities at the wall and the mean flow velocities at this small Knudsen number. On the other hand, our slip model agrees well with the velocities given by the linearized Boltzmann equation.

In Figure (4-7) when $K_n = 0.88623 (D = 1)$, the second-order slip models give a better prediction than the first-order slip model if the TMAC is assumed equal to unity, but

substantial deviations still exist when compared with the results given by the linearized Boltzmann equation. In Figure (4-8) when $K_n = 11.7 (D = 0.0724)$ which corresponds to the free molecular flow regime, it is evident that the first-order and second-order slip models are no longer accurate to describe the velocity profile in this range of Knudsen number, either the velocity at the wall or for the mean flow is not accurate. Compared with the first-order and second-order slip model, our proposed slip model demonstrates that it agrees reasonably well with the linearized Boltzmann equation, and is more accurate than the other slip models. When the Knudsen number is small, the curvature of the velocity profile predicted by our slip model agrees well with that of the linearized Boltzmann equation. As the Knudsen number increases, our proposed slip model can still predict the velocities at the wall well, although there are some differences in the mean flow given by the linearized Boltzmann equation. In the effective viscosity model used by Beskok et al. (2002) and Sun et al. (2002), the viscosity is not a constant and modified to account for the increased rarefaction effects in the transition and free molecular regimes. The curvature based on their slip model is not as flat as the result of the first and second-order slip models and provides a better agreement with the linearized Boltzmann equation even in the free molecular regime. In our slip model, the influence of the rarefaction effects on the viscosity is not considered, thus a relatively large error is observed in the curvature of velocities profile with increasing Knudsen number. Although the prediction of the mean flow still needs to be improved, our proposed slip model can still provide a better prediction compared with other slip models.

4.2.2 Flow Rate Profile for Poiseuille Flow

The mass flow rate depends on pressure gradient, velocity and temperature. In our study, adiabatic conditions are assumed and heat caused by viscous effect can be neglected.

The mass flow rate per unit width is $Q = \int_{-\frac{d}{2}}^{\frac{d}{2}} \rho u dy$, and the flow rate based on the velocity

profile Eq. (4-16) is:

$$Q = -\frac{d^3 \rho}{2\mu} \frac{\partial p}{\partial x} \left(\frac{1}{6} + K_n \left(\frac{\sigma_{s-d} - \sqrt{\sigma_{s-d}^2 - 64Bu_0K_n}}{16BK_nu_0} - 1 \right) \right) \quad (4-17)$$

The non-dimensional flow rate is defined as:

$$Q_p = \frac{Q}{-\frac{d^3 \rho}{2\mu D} \frac{\partial p}{\partial x}} = \left(\frac{D}{6} + \frac{\sqrt{\pi}}{2} \left(\frac{\sigma_{s-d}D - \sqrt{\sigma_{s-d}^2 D^2 - 32Bu_0D\sqrt{\pi}}}{8Bu_0\sqrt{\pi}} - 1 \right) \right) \quad (4-18)$$

The Poiseuille flow rate Q_p for the existing slip models are also non-dimensionalized by

the factor $\left(-\frac{d^3 \rho}{2\mu D} \frac{\partial p}{\partial x} \right)$ and given in the Table (4-3).

Table 4-3 The value of non-dimensionalized flow rate in Poiseuille flow for different slip models

	Q_p
Continuum	$\frac{D}{6}$
Maxwell Slip Model	$\frac{D}{6} + \frac{(2-\sigma)\sqrt{\pi}}{4}$
Hsia Slip Model	$\frac{D}{6} + \frac{\sqrt{\pi}}{2} + \frac{\pi}{4D}$
Mitsuya slip Model	$\frac{D}{6} + \frac{\sqrt{\pi}}{2} + \frac{\pi}{9D}$
The VHS Slip Model	$\frac{D}{6} + 0.62228\frac{\sqrt{\pi}}{2} + 0.3872\frac{\pi}{4D}$
The VSS Slip Model	$\frac{D}{6} + 0.63875\frac{\sqrt{\pi}}{2} + 0.408\frac{\pi}{4D}$
Our Slip Model	$\left(\frac{D}{6} + \frac{\sqrt{\pi}}{2} \left(\frac{\sigma_{s-d}D - \sqrt{\sigma_{s-d}^2 D^2 - 32Bu_0 D\sqrt{\pi}}}{8Bu_0\sqrt{\pi}} - 1 \right) \right)$

The results for flow rate as a function of inverse Knudsen number D are shown in Figure (4-9).

Comparing with the continuum result with non-slip boundary condition, as seen in Figure (4-9), it is observed that the flow rate will increase due to the slip effect. When the Knudsen number is small (D is around 100), the differences for all the slip models can hardly be discerned. All slip models agree well with the result of the linearized Boltzmann equation. As the Knudsen number increases to a range of $K_n = 0.1 \sim 10$, which corresponds to the transition regime, the flow rate is underestimated by the first-order slip model, while overestimated by the second-order slip models. This

concurr with the velocity prediction by these slip models. Compared with the other slip models, our proposed slip model agrees reasonably well with the linearized Boltzmann equation, which makes it possible to be applied in engineering field. What more important is that our slip model provides physical interpretations because it indicates that the slip length is a nonlinear function of the shear rate, which is never indicated in other slip models. This non-linear relationship will be validated in the next section by studying some experimental results.

Figure 4-9 Non-dimension flow rate versus inverse Knudsen number.

4.3 Compare the Shear-Dependent Slip Model to Experimental Works

As reviewed in the chapter two, there are several techniques that can be used to examine the boundary condition at surface-fluid interfaces. These techniques are broadly classified into either direct or indirect methods. Fluorescent Doppler anemometry (FDA), emission detection of Doppler-shifted absorption (EDDA) and Raman excitation plus laser-induced electronic fluorescence (RELIEF) are considered as the direct way to measure the slip velocity of gas molecules at the boundary. However, these direct methods, without any artificial parameters, are still far from fully developed. Because we lack the reliable experimental data, comparisons between the results from our slip model and these direct methods are not included in our work. The indirect model is valid for a particular geometry. A slip length is inferred by a correction to the model used to fit macroscopic observations. Pressure driven flow is a popular indirect method to study the slip velocity of gas molecules at the boundary. The advent of micro-fabrication has allowed for construction of channels with dimensions on the order of micrometers and nanometers. In our work, we carefully choose four experiments conducted by Arkilic et al. (1997,1997T), Colin et al. (2003). These experiments had been conducted using well-controlled surface structure and accurate measuring technique. The experimental results are cited by numerous researchers (citation times: Arkilic et al:251; Colin:43). The Knudsen number at the channel outlet is from 0.05~2.5, which cover a wide range of flows, from the continuum slip regime to the translational regime. Our main purpose is to test whether our slip model can describe the slip phenomenon observed in these experiments and verify whether the slip coefficient is dependent on the shear rate or not.

Before we validate our slip model, let us first look at the derivation of extracting slip

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length based on the experimental parameters.

We consider the flow of a Newtonian fluid through a micro-channel of height d , as represented in Figure (4-10).

Figure 4-10 Velocity distribution of the flow in micro-channel

The boundary condition can be written as:

$$u\Big|_{y=\frac{d}{2}} = u\Big|_{y=-\frac{d}{2}} = u_{slip} \quad (4-19)$$

where u_{slip} is the fluid velocity at the wall. Integrating Eq.(4-12) for u and combining Eq. (4-19), the boundary conditions, so the velocity in the micro-channel is:

$$u = -\frac{1}{2\mu} \frac{dp}{dx} \left(\frac{d^2}{4} - y^2 \right) + u_{slip} \quad (4-20)$$

If we assume the micro-channel has a high aspect ratio $d \ll w$. Integrating Eq. (4-20) and flow rate Q can be expressed as:

$$Q = \rho w \int_{-\frac{d}{2}}^{\frac{d}{2}} u \cdot dy = -\frac{\rho w d^3}{12\mu} \frac{dp}{dx} + \rho d w \cdot u_{slip} \quad (4-21)$$

where the first term on the right hand side is consistent with the theoretical prediction for Poiseuille flow with a non-slip boundary condition, while the second term is added to account for the extra flow rate due to the slip velocity at the wall.

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Assuming the flow is incompressible and with a constant density, the pressure gradient is also constant and is conveniently expressed as:

$$\frac{dp}{dx} = -\frac{\Delta P}{L} \quad (4-22)$$

The flow rate consists of two components, $Q_{Poiseuille}$ and Q_{slip} , which can be expressed separately as:

$$Q_{Poiseuille} = \frac{1}{12} \frac{\rho w d^3}{L} \frac{\Delta P}{\mu} \quad (4-23)$$

and

$$Q_{slip} = \rho w d \cdot u_{slip} \quad (4-24)$$

then the slip velocity can be derived from experimental parameters alone as:

$$u_{slip} = \frac{Q}{\rho w d} - \frac{1}{12} \frac{d^2}{L} \frac{\Delta P}{\mu} \quad (4-25)$$

If the slip velocity is proportional to the shear stress τ at the surface, as contemplated by the Navier hypothesis, the slip velocity can be expressed as a function of the slip length b :

$$u_{slip} = a \cdot \tau_w = a \cdot \mu \cdot \left(\frac{du}{dy} \right)_w = b \cdot \dot{\gamma}_w \quad (4-26)$$

where $\dot{\gamma}_w$ is the strain rate at the wall. τ_w , $\dot{\gamma}_w$ and b can also be determined based on the experimental parameters alone:

$$\dot{\gamma}_w = \frac{d}{2L} \cdot \frac{\Delta P}{\mu} \quad (4-27)$$

$$\tau_w = \frac{d}{2L} \cdot \Delta P \quad (4-28)$$

$$b = \frac{u_{slip}}{\dot{\gamma}_w} = 2\mu \cdot \frac{L}{\rho w d^2} \frac{Q}{\Delta P} - \frac{d}{6} \quad (4-29)$$

The ratio between the flow rate due to the slip condition and the prediction using

continuum theory with non-slip boundary, is:

$$\frac{Q_{slip}}{Q_{Poiseuille}} = 6 \cdot \frac{b}{d} \quad (4-30)$$

Eq.(4-30) gives us evidence that the slip effect can be detectable only when the characteristic length is comparable to the slip length, thus also explain why slip is not observed in some previous experiments.

By using this method to investigate the boundary condition, the accuracy of height in micro-channel should be well controlled, which is an important parameter influencing experimental results.

Consider the compressible effect and the density is not a constant, the strain rate at the wall $\dot{\gamma}_w$ can be expressed as:

$$\dot{\gamma}_w = -\frac{d}{2\mu} \cdot \frac{dP}{dx} \quad (4-31)$$

Substitute Eq. (4-31) into Eq. (4-29) and integrate, the slip length is:

$$b = \frac{u_{slip}}{\dot{\gamma}_w} = 4\mu \cdot \frac{RTL}{wd^2} \frac{Q}{P_0^2 (\Pi^2 - 1)} - \frac{d}{6} \quad (4-32)$$

where Π indicates an inlet over outlet pressure ratio.

To clarify the experimental conditions, Table (4-4) illustrates the micro-channel characterization in Colin et al. (2003), Arkilic, et al. (1997,1997T) experiments. For convenience, we mark these four experiments as #1, #2, #3 #4. Experiments #1, 2, 4 used helium as the working fluid and argon was used as test fluid in experiment #3.

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Table 4-4 Micro-channel characterization

Experiment #1 Colin et al. (2003)

Parameter	Nominal value (μm)	Variation (μm)	Parameter	Range of Mean Value
Length(L)	5000	± 5	Outlet Pressure (P_0)	190KPa
Width(w)	21.2	± 0.15	Pressure Ratio (Π)	1.3-1.9
Height(d)	1.88	NA	Temperature (T)	294.2K
Surface roughness	NA	NA	Outlet K_n Number	0.053

Experiment #2 (Arkilic, et al. 1997)

Parameter	Nominal value (μm)	Variation (μm)	Parameter	Range of Mean Value
Length(L)	7500	± 10	Outlet Pressure (P_0)	100KPa
Width(w)	52.25	± 0.25	Pressure Ratio (Π)	1.6-4.2
Height(d)	1.33	± 0.01	Temperature (T)	314K
Surface roughness	$\leq 0.65 \times 10^{-3}$	NA	Outlet K_n Number	0.155

Experiment #3, 4 (Arkilic 1997T) used the same micro-channel as experiment #2. The experimental differences are shown below:

#3: Outlet pressure P_0 : 13 KPa; Pressure ratio Π : 10~32.5; Outlet K_n number: 0.41.

#4: Outlet pressure P_0 : 6.5 KPa; Pressure ratio Π : 20.5~60.5; Outlet K_n number: 2.5.

Figures (4.11-4.14) illustrate the mass flow rate at different pressure ratio for these experiments. The original data for experiment #3, #4 is based on a normalized mass flow rate as a function of mean pressure. For the ease of comparison, we express mass flow rate as a function of pressure ratio as shown in Figure (4-13), Figure (4-14).

Figure 4-11 Mass flow versus pressure ratio for 1.88 um channel ($K_{n_{out}}=0.053$)

Figure 4-12 Mass flow versus pressure ratio for 1.33 um channel ($K_{n_{out}}=0.155$)

Figure 4-13 Mass flow versus pressure ratio for 1.33 um channel ($K_{nout}=0.41$)

Figure 4-14 Mass flow versus pressure ratio for 1.33 um channel ($K_{nout}=2.5$)

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For Figure (4-11) to Figure (4-14), the fit lines are plotted using the Maxwell's slip model, with the TMAC value σ shown in each figure.

It is apparent that the full diffused slip model ($\sigma = 1$) does not yield satisfactory results between the theoretical model and the experimental mass flow rate values. This implies that the momentum exchange between the impinging gas and the wall is not complete and the rebounding gas leaves the wall while keeping its stream-wise momentum to the surface, so we cannot take for granted and use the assumption of totally diffused reflection. This conclusion is consistent with Arkilic's work, which proved that the value of TMAC is less than unity and appears to be around 0.8.

Another finding we can conclude from Figure (4-13), Figure (4-14) is that with the higher pressure ratio, i.e., with higher shear rate, considerable discrepancies are observed between the experimental data and the predictions by the first-order slip model. The mass flow rates in these experiments are higher than that predicted by the first-order slip model with increasing pressure ratio. The second-order slip model also cannot explain these deviations. The additional term in the second-order slip model is to account for the rarefaction effect. When the Knudsen number increases, the second term plays an important role and the mass flow rate increases more significantly as compared with the first-order slip model. In Figure (4-13)-(4-14), with increasing pressure ratio, the average Knudsen number for the micro-channel flow is smaller. That means the disparity should become smaller with increasing pressure ratio if the second-order slip model is valid. However, the predictions from the second-order slip model contradict the experimental results. Obviously, the first-order and second-order slip models cannot explain the phenomenon observed in these experiments with increasing pressure ratio.

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Other mechanisms should account for these disparities. Our proposed slip model, which indicates that slip velocity is a non-linear function of shear rate, is able to model the experimental results more closely.

Slip coefficient

To verify this nonlinear relationship, let us examine the slip coefficient for these experiments. In Maxwell's slip model, the slip velocity at the boundary is:

$$u_s = b \left(\frac{\partial u}{\partial y} \right)_w = \left(\frac{2-\sigma}{\sigma} \right) \lambda \left(\frac{\partial u}{\partial y} \right)_w \quad (4-33)$$

where b is the slip length as defined in Eq. (4-32).

For our proposed slip model, the slip velocity at the boundary also can also be expressed

as:

$$u_s = b_g \lambda_m \left(\frac{\partial u}{\partial y} \right)_w \quad (4-34)$$

where $b_g = \frac{b}{\lambda_m}$ is the slip coefficient, λ_m is the average mean free path in the flow.

In Maxwell's slip model, the slip coefficient b_g equals to $\frac{2-\sigma}{\sigma}$ and can be treated as a constant within specific flow conditions. By using Eq. (4-32), we can get the slip length from the experimental parameters, and then the slip coefficient is easily derived. If the slip coefficient is a constant, it validates that the slip velocity is a linear function of the shear rate. Otherwise, if the slip coefficient varies with an increasing shear rate, the nonlinear relationship proposed in our slip model is then verified.

Figure (4-15)-(4-18) represent the slip coefficients extracted from the experiments.

Figure 4-15 Slip coefficients as a function of the shear rate ($K_{nout}=0.053$).

Figure 4-16 Slip coefficients as a function of the shear rate ($K_{nout}=0.155$).

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Figure 4-17 Slip coefficients as a function of the shear rate ($K_{nout}=0.41$).

Figure 4-18 Slip coefficients as a function of the shear rate ($K_{nout}=2.5$).

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From the figures above, when the Knudsen number is small ($K_{\text{nout}}=0.053$), the slip coefficient varies from 1.18~1.23 as shear rate increases from $7.2 \times 10^5 \text{ s}^{-1}$, which indicates the first-order slip model is appropriate. When the Knudsen number is moderate ($K_{\text{nout}}=0.155$), the slip coefficient varies from 1.32~1.51 as shear rate increases from $2.5 \times 10^5 \text{ s}^{-1}$. When the Knudsen number is large ($K_{\text{nout}}=2.5$), the slip coefficient varies substantially from 1.6~2.05 with a shear rate range of $(5.9 \sim 17.7) \times 10^5 \text{ s}^{-1}$ and increases abruptly as shear rate increases further. This demonstrates that slip coefficient is not a constant and increases with shear rate. This figure also validates a nonlinear relationship between slip velocity and shear rate, which can be conjectured that a larger fraction of gas molecules grazes the surface during the collision when the shear rate increases, leading to reduced frictional force and momentum exchange between the gas and the wall. Therefore, the reflected molecules retain more tangential momentum and the value of slip coefficient increases.

Slip velocity versus shear rate

Figures (4-19) to (4-22) show the slip velocity as a function of shear rate extracted from these experiments. The experimental results are theoretically compared with slip model in Eq. (4-7).

Figure 4-19 Slip velocity versus shear rate for 1.88 um channel (K_{nout}=0.053)

Figure 4-20 Slip velocity versus shear rate for 1.33 um channel (K_{nout}=0.155).

Figure 4-21 Slip velocity versus shear rate for 1.33um channel (K_{nout}=0.41)

Figure 4-22 Slip velocity versus shear rate for 1.33um channel (K_{nout}=2.5)

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In Figure (4-19), when Knudsen number is small, say $K_{nout}=0.053$, the slip velocity appear to be a linear function of shear rate. When Knudsen number K_{nout} reaches to 0.155 (Figure 4-20), $K_{nout}=0.41$ (Figure 4-21) and $K_{nout}=2.5$ (Figure 4-22) separately, the linear fitting is not appropriate whereas the quadratic one is in good agreement. The slip velocity in Figure (4-22) exhibits a strong nonlinear function of the shear rate. We can conclude that with the increasing Knudsen number, the nonlinear effect appear more significant. It is also observed that TMAC value σ_{s-d} in theoretical model decreases with increasing Knudsen number, which means the reflected gas molecules keep more tangential momentum with increasing Knudsen number. This is consistent with the findings by many researchers.

4.4 Summary

In this chapter, using the similar method as Beskok's (2002), a shear-dependent slip boundary condition is proposed based on our scattering model. Compared with other slip models and the solution of linearized Boltzmann equation, our shear-dependent slip model can provide a better prediction of slip velocity and flow rate for Poiseuille flow. By studying the experimental results for gas flow, it is demonstrated that the slip coefficient is not a constant and varies with increasing shear rate, which indicates a nonlinear function of slip velocity and shear rate. The shear-dependent slip model can also theoretically predict the results of these experiments, the value of the parameter is consistent with the physical meaning in our slip model.

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In last chapter, we proposed the new slip model and testified it is applicable to describe the boundary conditions at solid/gases interface. The objective of this chapter is to validate that the slip model is also suitable in liquid flow.

5.1 History of the Non-Slip Boundary Condition

The boundary condition is a controversial topic, which has been studied by many researchers. The origination of non-slip boundary condition is not based on physical principles, but instead deduced on experimental observation. At macroscopic length scales, the non-slip boundary was usually employed to describe the fluid behavior in a continuum field and verified by many experiments. However, a non-zero slip length is observed and plays an important role in micro-scale and nano-scale flow. Now, researchers can investigate at smaller and smaller scales with advent of new technology, so the boundary condition attracted more attention in recent decades in microscopic flow.

A mathematical expression for the non-slip boundary condition is:

$$u_x|_{wall} = U_x \quad (5.1)$$

where u_x is the component of velocity of fluid in the x direction, and U_x is the x component of velocity of the surface. Although the non-slip boundary has been dominated for a long period in fluid dynamics, the rationality of this boundary condition is still puzzling. The non-slip boundary conditions were stated by Fox and McDonald (1998) as ‘an experimental fact based upon numerous observation of fluid behavior.’, and Schlichting (1987) stated, ‘In real fluids, the existence of intermolecular attraction

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causes the fluid to adhere to a solid wall...’. However, the slip velocity observed in many experiments cannot be explained by the latter statement when the interface interaction is hydrophobic. Another assumption is proposed by Panton (1996) to verify the non-slip boundary conditions. He assumes that a diffused reflection should happen after fluid molecules collide with the wall, thus the reflected molecules have the same tangential momentum as the wall, with zero tangential momentum.

The diffused assumption was testified later by Schlichting (1987) and Panton (1996). Schlichting put forth that fluid molecules are attached to the surface due to intermolecular forces between fluids and surface. For non-wetting liquids, the intermolecular forces within the liquid are known to be greater than that of the interface, so this theory cannot provide us a reasonable explanation. Panton assume the surface are rough on microscopic length scale, fluid molecules should be stationary due to viscous dissipation at the interface. The strength of the intermolecular force between the liquid and the surface is not an important factor to influence the boundary conditions. However, the following question naturally arise ‘how much surface roughness is needed for the fluid molecules to rest?’.

Since there are no rational interpretations about the non-slip boundary condition, other boundary condition have been explored. The first mathematical slip model was proposed by Navier in 1823 (Lamb, H. 1932). The main concept of this slip model is that the tangential component of fluid velocity on the wall, should be proportional to the shear rate.

$$u_s = b \left. \frac{\partial u}{\partial y} \right|_w \quad (5.2)$$

where u is the velocity of the fluid tangential to the surface in the bulk , y is the

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direction perpendicular to the surface, and b is the slip length. If the slip length is small compared to the length scales of the flow, then the non-slip condition is recovered for those flows.

Since the lack of physical interpretation to the boundary conditions, the experimental techniques are treated as useful tool to probe the slip velocity at the interface. These techniques enable us explore the nature of fluid at small scales.

5.2 Examining the Boundary Condition for Liquids in Micro-Fluidic Devices

Several novel techniques were developed to investigate the boundary condition at solid/liquid interfaces in recent years. Like the techniques to probe the solid/gases boundary condition, these techniques are also broadly classified into two categories: indirect or direct methods. As for indirect way, a slip length is deduced by other flow quantities. These indirect methods mainly include: the Surface Force Apparatus (SFA), measuring drainage force acting on a sphere by using Atomic Force Microscopy (AFM); Total Internal Reflectivity-Fluorescence Recovery After Photobleaching (TIR-FRAPB); Pressure driving flow, measuring pressure drop and mass flow rate in micro-channels. In contrast, direct methods have resulted in direct measurements of near surface liquid velocities using tracer particles, such as μ -PIV (Particle Image Velocimetry) method. The details of these techniques are discussed below.

5.2.1 Indirect Method

Surface Force Apparatus

The surface force apparatus (SFA) is a device measuring intermolecular forces. Typically, two solid crossed cylinders of radius R at a spacing of D are laid up for the test (see Figure 5-1). Liquid is filled between the gaps. A force F_H can be measured directly when the two cylinder approach or retreat from one another. The force F_H is

$$F_H = \frac{f^* 6\pi R^2 \mu}{D} \left(\frac{dD}{dt} \right) \quad (5.3)$$

where μ is the viscosity of the liquid and f^* is a correction factor account for slip effect. For $f^* < 1$, indicates the measured hydrodynamics force is smaller than the prediction with non-slip condition. The correction factor f^* is:

$$f^* = 2 \cdot \frac{D}{6b} \left[\left(1 + \frac{D}{6b} \right) \ln \left(1 + \frac{6b}{D} \right) - 1 \right] \quad (5.4)$$

If the cylinders are oscillated at a frequency ω with the vibration amplitude d , the peak velocity is $v_{peak} = d\omega$. A wide range of velocities can be provided because of the independence of the amplitude and frequency of the driving oscillation. Shear rate, $\dot{\gamma}_{max}$, is proportional to the flow rate by a geometry factor κ (Vinogradova, O. I. 1995):

$$\dot{\gamma}_{max} = \kappa \sqrt{R/D} (v_{peak}/D), \text{ where } \kappa = \sqrt{28/127} \quad (5.5)$$

By using Eq. (5.4) and (5.5), we can deduce the relationship between shear rates and slip velocity based on the experimental results.

Figure 5-1 Schematic of Surface Force Apparatus. (Neto, C. et al. 2005)

Two crossed cylinders of radius R ($\sim 1\text{cm}$) are oscillated with respect to one another by amplitude d ($\sim 1\text{nm}$). A drop of liquid is squeezed out of the gap of size D ($\sim 100\text{nm}$) between the cylinders. The force resisting the motion of the cylinders, $F_{H,Peak}$ ($\sim 100\text{ }\mu\text{N}$) is measured.

Drainage Forces

Another method similar to the SFA is that the drainage force is measured by using Atomic Force Microscope (AFM). A cantilever is mounted in Atomic Force Microscope and a single sphere is attached to this cantilever. A hydrodynamics force is generated when the sphere approaches a flat surface. When the spring constant of the cantilever is known, the hydrodynamics force can be derived by using theoretical model. The hydrodynamic force, which takes the slip condition into account, is:

$$F_H = \frac{6\pi R^2 \mu v}{h} f^* \quad (5.6)$$

where h is the distance from the surface to the center of the sphere. R is the radius of the sphere, and v is the approach velocity to the surface (see Figure 5-2). f^* , the same meaning as that for the SFA, is a correction parameter that accounts for the slip effect. Vinogradova (1995) pointed out that the correction factor in Eq. (5.6) can be expressed

as:

$$f^* = \frac{h}{3b} \left[\left(1 + \frac{h}{6b} \right) \ln \left(1 + \frac{h}{6b} \right) - 1 \right] \quad (5.7)$$

where b is the slip length.

The spring constant of the cantilever is an important parameter determining the accuracy in the measurement. In addition, an effective radius R^* of the cantilever/sphere system is usually adopted in Eq. (5.6) (Bonaccorso et al. 2002).

The maximum shear rate at a separation distance h can be calculated as (Horn, R.G., et al. 2000):

$$\dot{\gamma}_{\max} = 9\nu \sqrt{\frac{2R}{3h^3}} \cdot \frac{\sqrt{g^* - 1 - 3b/h}}{(2 - 3b/h + g^*)(2 + 15b/h + g^*)} \quad (5.8)$$

where

$$g^* = \sqrt{4 + 24b/h + 9(b/h)^2} \quad (5.9)$$

b is the slip length and ν is the approaching velocity.

Figure 5-2 Schematic of AFM to measuring the drainage force. (Neto, C. et al. 2005)

A sphere attached to a cantilever is immersed in a liquid. The radius of the sphere is r . The sphere approaches to the solid wall with a velocity ν . The closet approach distance $h \ll r$. An opposite drainage force F_H arise when the sphere approach to the wall.

Pressure driven flow in micro-channels

Another commonly used method to investigate slip is measurement of flow quantities of liquid flow through micro-channels. As discussed in last chapter, for incompressible liquid flow, the relative change of flow rate due to the slip effect is:

$$\frac{Q_{slip}}{Q_{Poiseuille}} = 6 \cdot \frac{b}{d} \quad (5.10)$$

and the slip length can be expressed as: $b = \frac{u_{slip}}{\dot{\gamma}_w} = 2\mu \cdot \frac{L}{\rho w d^2} \frac{Q}{\Delta P} - \frac{d}{6}$ (5.11)

Using these expressions, we are able to provide a comparison between an existing slip model and experiments performed. The relationship between shear rate and slip velocity also can be deduced from experimental parameters.

TIR-FRAP

Total Internal Reflection-Fluorescence Recovery after Photobleaching (TIR-FRAP) is another indirect method applied in the measurement. A liquid is filled between two discs. One is fixed and another is rotating (see Figure 5-3). The light from a laser excites the fluorescent probes, which are part components in the liquid. Remain part of laser beam is totally reflected inside the disc, excites the probes at the distance less than 100 nm from the liquid surface. The detailed process measuring the slip velocity at the interface can be found in Pit's experiments (1999, 2000).

Figure 5-3 A schematic of a TIR-FRAP system (Pit, R. et al 1999)

Molecular Dynamics Simulations

Molecular dynamics (MD) simulations is a useful tool examining the boundary conditions. A generalized boundary condition has been proposed by Thompson and Troian (1997), which is based on the results of molecular dynamical simulations. The model they proposed indicates that the slip length is a nonlinear function of the shear rate, given by:

$$L_s = L_s^0 \left(1 - \frac{\dot{\gamma}}{\dot{\gamma}_c} \right)^{-\frac{1}{2}} \quad (5.12)$$

where L_s^0 is a constant slip length, $\dot{\gamma}_c$ is the critical shear rate.

The drawback of their work is that the magnitude of pressure and shear rate in their

simulations, in order to conserve mass, exceed those possible in the laboratory. For this reason, MD simulations' results are not included in our work for comparison.

5.2.2 Direct Method

Particle Image Velocimetry

The Direct methods of measuring the slip velocity are not based on the derivation from the macroscopic parameters measured in the experiments. μ -PIV is a commonly used technique measuring the slip velocity at the solid/liquid interface. Slip velocity is obtained by tracking images of the particles in the flow field. The location of zero velocity will be provided by a theoretical fit in the boundary layer. When the velocity vectors become random, the location of the wall of the micro-channels is obtained. The difference of location of zero velocity and wall is the slip length.

5.3 Generating Mechanisms for Slip

Even though the magnitude of slip at a surface is still controversial, slip does exist without any doubt, which has been proven by many experimental works. Only after we figure out the mechanism behind the slip, the discrepancy observed in the previous work may be resolved

Now, there are two schools about the mechanism for slip. The first explanation assumes a lowered viscosity region or an air gap exist near the solid/liquid interface. However, the process which could generate such a gas layer is elusive, and as pointed by de Gennes (2002), Lauga and Stone (2003), the layer would be energetically unstable,

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especially on hydrophilic surface. The observed slippage on a hydrophilic wall cannot be explained by the existence of air gap. Some experiments claim that slippage is due to depletion at the solid/liquid interface, which could produce a local reduced viscosity. However, slippage has also been observed in some experiments (Zhu and Granick 2002PRL, Bonaccorso et al. 2002, Vinogradova et al. 2003), by using polydimethylsiloxane (PDMS), aqueous electrolytes and organic solvents as testing liquids, where no viscosity reduction can be invoked. The assumptions that slip caused by an air gap or the lower viscosity in the region near the surface cannot be validated, we therefore believe that slippage occurs by a different mechanism.

The second explanation using microscopic view, individual molecules of liquid are assumed move past the surface. The key point of the molecular slip argument is that the previous thoughts that liquid molecules should bind to the wall is discarded. Liquid molecules have random motion near the surface, so we cannot take the assumption that liquid molecules have the same tangential momentum as the surface for granted. This assumption was firstly quantified by Tolstoi in 1953. By considering the relationship between molecular mobility and surface energy, he calculated the energy required for a molecule to make space for movement for itself near the interface. A different molecular mobility was found near the interface than in a bulk liquid. For complete wetting surface, the no-slip boundary condition is recovered due to strong intermolecular attraction of liquid and wall. For partial wetting surface, molecules have greater mobility due to weak attraction of molecules of liquid and wall, in which non-zero slip velocity can occur.

5.4 Factors Effecting Slip

5.4.1 Shear Rate

The boundary condition first proposed by Navier (1823) is linear and the slip length is a parameter determined by property of the liquid/solid interface. Independence of the slip length upon the shear rate was testified by many experiments, providing evidence of a linear boundary condition (Pit et al. 1999, Pit et al 2000, Baudry et al. 2001, Cottin-Bizonne et al. 2002, Bonaccorso et al. 2002, Cheng and Giordano 2002, Hervet and Leger 2003, and Cottin-Bizonne et al. 2005). Other experimental studies of simple liquids have proven that the slip length increases nonlinearly with the shear rate (Churaev et al. 1984, Zhu and Granick 2001, Craig et al. 2001, Zhu and Granick 2002PRL, Zhu and Granick 2002L, Bonaccorso et al. 2003, Neto et al 2003, Choi et al. 2003, Henry et al. 2003, Huang et al. 2006, Ulmanella et al. 2008), and the shear-independence slip condition is valid only in the limit of low shear rates. Compared with the studies of roughness effect on the slip boundary conditions, the dynamic behavior of the slip length with increasing shear rate has received much less attention. Only a few mathematical models have been put forward to theoretically explain the observed phenomena of shear-dependence, and more efforts are required to provide a general mechanism explaining the new results.

For gas flow, the distance for each molecule is far apart and the interactions are therefore simple compared with that in liquids. As discussed in the last chapter, if the interaction force between gas molecules and wall is just due to collision, the surface slip of gas flow is a function of surface roughness, properties of gas/solid interface, Knudsen number and shear rates. Although the structure of a liquid molecule is more complicated than the smaller gas molecules, and the interactions model are different, we can still validate if

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our shear-dependence slip model is suitable to characterize the slip behavior for liquids based on the previous experimental works.

As in chapter 4, for liquids, we rewrite the slip boundary condition as:

$$u_s = \frac{2 - \sigma_{s-d}}{\sigma_{s-d}} \cdot \left(u_s + b \frac{\partial u}{\partial y} \Big|_w \right) + B \cdot \left(u_s + b \frac{\partial u}{\partial y} \Big|_w \right)^2 \quad (5.13)$$

The experimental results are summarized in Table 5-1 and the comparison between experimental results and theoretical model are illustrated from Figure 5-4 to 5-15. The values of coefficients σ_{s-d} and B are indicated in each experimental work while b is the slip length when slip can be detected. The values of the coefficient σ_{s-d} and B in Eq. (5.13) are tabulated in Table 5-2.

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Table 5-1. Detailed results of slip measured using experimental techniques

Author	Surface	Liquid	Shear Rate (s ⁻¹)	Slip length (nm)	Shear Dependence	Method
Ulmanella, U. et al. (2008)	Silicon	Isopropanol	10-10 ⁵	5-35	D	Pressure-driven flow
Ulmanella, U. et al. (2008)	Silicon	Hexadecane	10-10 ⁵	40-120	D	Pressure-driven flow
Choi CH, et al. (2003)	Silicon+OTS	Water	10 ³ -10 ⁵	5-35	D	Pressure-driven flow
Choi CH, et al. (2003)	Silicon	Water	10 ³ -10 ⁵	0-10	D	Pressure-driven flow
Huang P, et al. (2006)	Glass+OTS	Water	10-10 ³	50-100	D	TIRV
Zhu, Y.X. et al. (2001)	Mica+OTE	Water	10-10 ⁵	0-2500	D	SFA
Zhu, Y.X. et al. (2001)	Mica+OTE	Tetradecane	10-10 ⁵	0-1500	D	SFA
Zhu, Y.X. et al. (2001)	Mica+HDA	Tetradecane	10-10 ⁵	0-1000	D	SFA
Zhu, Y.X. et al. (2002M)	Mica+PVA	Water	10-10 ⁵	0-80	D	SFA
Zhu, Y.X. et al. (2002PRL)	Mica+0.8 PPO	Water	10-10 ⁵	0-5	D	SFA
Zhu, Y.X. et al. (2002PRL)	Mica+0.2 PPO	Water	10-10 ⁵	0-20	D	SFA
Zhu, Y.X. et al. (2002L)	Mica+HDA	Dodecane	10-10 ⁵	0-10	D	SFA

The symbols used in this table are given as: OTS: octadecyltrichlorosilane; OTE: octadecyltriethoxysilane; HDA: 1-hexadecylamine; PVA: polyvinylalcohol; PPO: polystyrene (PS) and polyvinylpyridine (PVP); D: a dependence of slip length on shear rate

Figure 5-4 Slip velocity versus shear rate for silicon/ isopropanol. (Ulmanella, U. et al. 2008)

Figure 5-5 Slip velocity versus shear rate for silicon/ hexadecane. (Ulmanella, U. et al. 2008)

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Figure 5-6 Slip velocity versus shear rate for silicon+OTS/water. (Choi C.H. et al. 2003)

Figure 5-7 Slip velocity versus shear rate for silicon/ water. (Choi C.H. et al. 2003)

Figure 5-8 Slip velocity versus shear rate for glass+OTS/water. (Huang P. et al. 2006)

Figure 5-9 Slip velocity versus shear rate for mica+OTE/ water. (Zhu,Y.X. et al. 2001)

Figure 5-10 Slip velocity versus shear rate for mica+OTE/tetradecane. (Zhu, Y.X. et al. 2001)

Figure 5-11 Slip velocity versus shear rate for mica+HDA/tetradecane. (Zhu, Y.X. et al. 2001)

Figure 5-12 Slip velocity versus shear rate for mica+PVA/water. (Zhu, Y.X. et al. 2002M)

Figure 5-13 Slip velocity versus shear rate for mica+0.8PPO/ water. (Zhu, Y.X. et al. 2002PRL)

Figure 5-14 Slip velocity versus shear rate for mica+0.2PPO/water. (Zhu, Y.X. et al. 2002PRL)

Figure 5-15 Slip velocity versus shear rate for mica+HDA/dodecane. (Zhu, Y.X. et al. 2002L)

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Table 5-2. The values of coefficient σ_{s-d} and B in each experiment.

Author	Surface/ Liquid	σ_{s-d}	B (s/m)	b(nm)	Roughness (nm)
Ulmanella, U. et al. (2008)	Silicon/Isopropanol	0.8	12	8	0.5
Ulmanella, U. et al. (2008)	Silicon/Hexadecane	0.8	3	40	~0.5
Choi CH, et al. (2003)	Silicon+OTS/Water	0.6	40	5	0.3
Choi CH, et al. (2003)	Silicon/Water	0.72	90	2	1.1
Huang P, et al. (2006)	Glass+OTS/Water	0.8	40	40	0.47
Zhu, Y.X. et al. (2001)	Mica+OTE/Water	0.3	100	100	0.1
Zhu, Y.X. et al. (2001)	Mica+OTE/Tetradecane	0.36	80	30	0.1
Zhu, Y.X. et al. (2001)	Mica+HDA/Tetradecane	0.32	30	15	0.1
Zhu, Y.X. et al. (2002M)	Mica+PVA/Water	0.7	40	30	1
Zhu, Y.X. et al. (2002PRL)	Mica+0.8 PPO/Water	1.0	200	2	3.5
Zhu, Y.X. et al. (2002PRL)	Mica+0.2 PPO/Water	1.1	42	5	2
Zhu, Y.X. et al. (2002L)	Mica+HDA/Dodecane	0.6	300	1	-

The results in the Figures (5.4-5.15) extracted from experimental work indicate that a nonlinear slip is apparent with increasing shear rate. A new boundary condition, which includes a shear-rate dependent term, is needed. As Tolstoi (1953) pointed out, liquid molecules have a greater mobility and a weaker intermolecular force at the proximity to the interface than in a bulk liquid, so the similar analysis of molecules/surface collision model for gases flow can be applied to study the liquid slip conditions. In our slip model, we have restricted our study to the boundary condition for the tangential velocity field at the interface. It was found that the frictional force decreases with increasing shear rate and slip velocity is a nonlinear function of the shear rate. From the figures, our shear

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dependence slip model is consistent with the slip behavior discovered in the experiments.

From the figures (5.10-5.11) and (5.14-5.15), we can also conclude that there is a threshold value of the shear rate above which slip is detectable. This can also be interpreted by using our shear dependence slip model. We should note that in our slip model, the value of parameter f , which corresponds to the fraction of molecules scattered diffusely, is varying with shear rate. At lower shear rate, the incident molecules are nearly even distributed, the molecules are totally diffusely reflected, the slip length is zero and a no-slip boundary is applicable. When the shear rate go above the threshold values, a larger fraction of molecules are incident at a larger angle and some molecules are not diffusely reflected while keeping some original tangential momentum, causing slip to occur. The reflected tangential velocities are a nonlinear function of incident velocities. At higher shear rate, the nonlinear effects become more prominent and detectable. Our shear dependence slip model gives us a reasonable explanation as why the evidence for boundary slip have not been observed in earlier experiments and why shear-independence slip condition is valid only in the limit of low shear rates.

5.4.2 Surface Roughness

Roughness was known for a long time to be one of the main parameters influencing boundary slip behavior. For surfaces smooth on a molecular scale, the studies on surface roughness effect on slip condition become more important. If the non-slip boundary condition is caused by frictional interactions between molecules of liquid and the surface, the slip length should decrease with increasing surface roughness. This has been validated by several experiments, in which a decrease in slip length was found with increasing surface roughness (Georges et al. 1993, Pit et al. 1999, Jabbarzadogh et al. 2000, and Zhu and Granick 2002 (PRL)). The analysis of slip condition in a complicated system, which involves several combined effects (i.e., surface roughness, properties and shear rate), is difficult. To avoid the confusion, in our first approach, we investigate the respective role of roughness in the resulting magnitude of slip, with all other parameters that can influence the slip condition being kept constant.

Figures (5.16-5.19) are the detailed results of slip measured with variable roughness by keeping the properties of materials as constant. The values of the coefficient σ_{s-d} and B are tabulated in Table 5-3.

Figure 5-16 Slip velocity versus shear rate at different roughness for silicon/isopropanol (Ulmanella, U. et al. 2008).

Figure 5-17 Slip velocity versus shear rate at different roughness for silicon/ hexadecane (Ulmanella, U. et al. 2008).

Figure 5-18 Slip velocity versus shear rate at different roughness for mica+OTE/water (Zhu, Y.X. et al. 2001; Zhu, Y.X. et al. 2002PRL).

Figure 5-19 Slip velocity versus shear rate at different roughness for mica+OTE/ tetradecane (Zhu, Y.X. et al. 2001; Zhu, Y.X. et al. 2002PRL).

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Table 5-3. The values of coefficients σ_{s-d} and B for same interface with different roughness.

Author	Surface/ Liquid	σ_{s-d}	B (s/m)	b(nm)	Roughness (nm)
Ulmanella, U. et al. (2008)	Silicon/Isopropanol	0.8	12	8	0.5
		-	-	-	8.4
Ulmanella, U. et al. (2008)	Silicon/ Hexadecane	0.8	3	40	~0.5
		-	-	-	8.4
Zhu, Y.X. et al. (2001)	Mica+OTE/Water	0.3	100	100	0.1
Zhu, Y.X. et al. (2002PRL)		0.6	80	3	0.2
Zhu, Y.X. et al. (2001)	Mica+OTE/Tetradecane	0.36	80	30	0.1
Zhu, Y.X. et al. (2002PRL)		0.64	50	2.5	0.2

From the figures and table, we can conclude that the roughness of a surface is a dominative factor in determining the magnitude of wall slip. For rough surface, the slip velocity is observed nearly to zero. Based on these experiments, it is also observed that the threshold values of the shear rate are larger for a rough surface compared with smooth surface when slip can be detected. In our shear-dependent slip model, it is obvious that the critical shear rate, that can guarantee some reflected molecules escape from the surface without trapping by the crevice and losing memory after collision, should be larger for a rough surface. The slip mechanism behind our slip model is consistent with the observation in these experiments.

As discussed in the last chapter, the TMAC value σ_{s-d} expressed the mean ratio of the tangential component of velocity transferring to the wall after a collision for molecules

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at lower shear rate. It is logical that with an increase in surface roughness, the frictional force will increase and the value of TMAC σ_{s-d} will increase. In Zhu's experiments (Table 5-3), for mica+OTE/water interface, the value of TMAC σ_{s-d} varies from 0.30 to 0.60 when surface roughness increases from 0.1nm to 0.2nm. For the mica+OTE/tetradecane interface, the value of TMAC σ_{s-d} is 0.36 at a roughness of 0.1nm, versus 0.64 at roughness of 0.2nm. It also can be derived from Table (5-2) that the value of TMAC σ_{s-d} qualitatively increases when the surface roughness increases. It is concluded that our slip model is able to explain the phenomenon recorded in these experiments

In Ulmanella's (2008) experiments, the relationship between flow rate and pressure drop is linear, which means non-slip boundary conditions is recovered when the roughness reaches to several nanometers. This result agrees well with Cook's (1997) experiment that is mentioned in chapter 3, validates the conclusion that no slip is detectable regardless of the magnitude of shear rate in rough channels.

Through these experiments, roughness has shown as a dominate effect on slip. Our slip model provides an adequate description of the effect of surface roughness on slip, and is a more comprehensive slip model.

5.4.3 Properties of Liquid/Solid Interface

Material property is another important factor influencing the slip condition. For pure liquids, it is reasonable to expect that the boundary condition at a solid surface is affected by properties of liquid/boundary, which is not taken into account in the continuum description. The efforts to decouple the roughness and properties of liquid/solid interface are necessary for researchers in investigations of boundary conditions. Comparing with the method used to study the roughness effect, we take the opposite direction to investigate the influence of properties. Keeping roughness constant, but using several liquids and surfaces, we show that, not only the roughness, involved in influencing the magnitude of slip at the solid interface, but the properties of liquid/surface also play an important role.

Figures (5.20-5.23) are the detailed results of slip measured with variable liquid/solid surface by keeping the roughness as constant. The values of the TMAC σ_{s-d} and B are tabulated in Table 5-4.

Figure 5-20 Slip velocity versus shear rate at same roughness ($Ra \approx 0.5nm$) for different materials. Square indicates the silicon/isopropanol interface; Triangle indicates the silicon/hexadecane interface. (Ulmanella, U. et al. 2008)

Figure 5-21 Slip velocity versus shear rate at same roughness ($Ra=0.1nm$) for different materials. Triangle indicates the mica+OTE/water interface; Square indicates the mica+OTE/tetradecane interface. Diamond indicates mica+HDA/tetradecane interface. (Zhu, Y.X. et al. 2001)

Figure 5-22 Slip velocity versus shear rate at same roughness ($Ra=0.2nm$) for different materials. Square indicates the mica+OTE/water interface; Triangle indicates the mica+OTE/tetradecane interface. (Zhu Y.X. et al. 2002PRL)

Figure 5-23 Slip velocity versus shear rate at same roughness ($Ra \approx 1nm$) for different materials. Square indicates the silicon/water interface (Choi CH. et al. 2003); Triangle indicates the mica+OTE/tetradecane interface (Zhu, Y.X. et al. 2002M).

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Table 5-4. The values of coefficient σ_{s-d} and B for different interfaces with same roughness.

Author	Surface/ Liquid	σ_{s-d}	B (s/m)	b(nm)	Roughness (nm)
Ulmanella, U. et al. (2008)	Silicon/Isopropanol	0.8	12	8	~0.5
	Silicon/Hexadecane	0.8	3	40	
Zhu, Y.X. et al. (2001)	Mica+OTE/Water	0.30	100	100	0.1
	Mica+OTE/Tetradecane	0.36	80	30	
	Mica+HDA/Tetradecane	0.32	30	15	
Zhu, Y.X. et al. (2002PRL)	Mica+OTE/Water	0.6	80	3	0.2
	Mica+OTE/Tetradecane	0.64	50	2.5	
Choi CH. et al. (2003)	Silicon/Water	0.72	90	2	~1
Zhu, Y.X. et al. (2002M)	Mica+OTE/Tetradecane	0.7	40	30	

In these experiments, there exist divergences of slip behavior by using the same boundary roughness. We explain the different extent of slip with the different interaction at the wall.

In Ulmanella’s (2008) experiment, n-hexadecane has shown greater slip velocity than isopropanol, with slip velocity as large as 41 mm/s at a shear rate of $3.5 \cdot 10^5 \text{ s}^{-1}$ for the former, versus 11 mm/s for the latter. This phenomenon can be attributed to the fact the nature of the liquid molecules is different. As we know, hexadecane is a non-polar molecule, while isopropanol is polar molecule. The isopropanol molecule should interact with a stronger interaction with the wall than hexadecane. The different amount of slip velocity on the interface sustains the assumption that if the interaction is smaller with the boundary, the larger the amount of slip occurs.

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From the experiments, it can be qualitatively understood that properties of materials should affect collision behavior, thus affecting the momentum transfer to the wall for liquid molecules.

5.5 Summary

In this chapter, the origins of non-slip boundary conditions are reviewed. It is found the application of non-slip boundary conditions is not from physical principle, but from experimental observation. The mechanism generating the slip velocity is still a hot topic but unsolved. Compared to the methods investigating the slip boundary conditions in gas flow, the techniques measuring the slip at the liquid/solid interface are in many styles. The shear-dependent slip boundary in liquid flow has been an attractive direction in recent years, but the physical interpretation and mathematical modeling are still in initial stage. By studying the experimental results, our shear-dependent slip model can provide a comprehensive description to the phenomenon observed in these experiments. The surface effects and properties of the interface are discussed in this chapter. The values of the parameters in our slip model are essentially coincident with the assumption in our derivation.

Chapter 6 Conclusions and Recommendations

6.1 Conclusions

In this thesis, the main focus is to investigate the slip boundary conditions for fluid flow at micro-scale and nano-scale. A novel shear-dependent slip model was developed to account for fluid molecular effects. An analytical solution can be obtained with this slip model by using continuum description.

In the first part of the study, we analyze the weakness of Maxwell's scattering model and point out that one parameter σ , is not enough to describe the interaction between the gas and wall. The friction and restitution coefficient are introduced to account for the different types of molecules interaction with the wall. The temperature dependence of TMAC can be physically explained based on our scattering model. The validation of our scattering model is shown by MD simulations and beam experiments. It is found that the value of TMAC decreases with increasing incident angle, which is consistent in our scattering model. From our scattering model, it can be shown that the value of TMAC is dependent on the mean tangential incident velocity of gas molecules.

In the second part of the thesis, using the similar analysis as Beskok's (2002), a shear-dependent slip model is developed. The nonlinear function of shear rate and slip velocity is indicated. Unlike the efforts mainly focused on finding the correct slip coefficients by many researchers, the shear-dependent slip model has changed the concept

that slip velocity is linearly proportional to shear rate, which was rarely challenged by researchers. Analytical solutions obtained are then compared with the solutions using linearized Boltzmann equation. The shear-dependent slip model agrees well with the solution and can be applied in a wide range flow regime. By studying experimental results for gas flow in micro-channels, it is demonstrated that slip coefficient is not a constant and increases with shear rate, which is consistent with prediction of the shear-dependent slip model. Either the first order or the second order slip model cannot explained the nonlinear relationship between slip velocity and shear rate observed in the experiments.

In the last part of the thesis, experimental results of liquid flows are extracted and compared with the prediction of shear-dependent slip model. It is validated that the shear-dependent slip model can also be applied in liquid flow. The roughness effects and properties of the interface are also discussed. Our slip model is able to explain the mechanism behind the experimental results.

6.2 Recommendations for Future Work

- Atomic force microscope (AFM) and surface force apparatus (SFA) are the useful method on the measurement of liquid slip on solid surface. However, such apparatuses are not suitable for the study of gas flow. The induced viscous force is very low because of the low value of viscosity for the gas. Recently, Maali et al. (2008) used an AFM in dynamic model to measure the slip length for the confined air flow close to solid surface. Due to the high-quality factor of the cantilever, the additional damping

caused by the hydrodynamic interaction during the confining of the gas can be probed accurately. Although the author mainly focused on measuring the slip length with various Knudsen numbers, it provides us another method to testify the nonlinear relationship between slip velocity and shear rate. Compared with the method measuring the pressure drop and flow rate in micro-channels, this method may give us a direct way to validate the shear-dependent slip boundary conditions for gas flow.

- Although there are many experiments conducted in micro-channels for gas flow, the validation of the first-order or the second-order slip model is the main purpose for the researchers. The shear rate influence on slip length is usually ignored. In the thesis, the parameters σ_{s-d} indicates the intrinsic properties for specific solid/fluid interface. A first and foremost verification on the validity of the new slip model is given by comparing with the experimental results. However, the values of σ_{s-d} are not directly derived from the microscopic parameters in the collision model. The exact value of the microscopic parameters are not clear because of the lack of experimental instruments, which now lends motivation research work to be done on quantifying microscopic parameters in future. Experimental works and simulation tools (e.g. DSMC) should be incorporated to study the microscopic parameters at the boundary
- From the experimental study in liquid flow, the explicit evidence of shear-dependent slip in hydrophobic micro-channels has been proven by many researchers. Owing to the lack of the physical interpretation and mathematical modeling, some researchers just used $u_s = A\left(\frac{\partial u}{\partial y}\right) + B\left(\frac{\partial u}{\partial y}\right)^2$ to represent this nonlinear relationship, but this was

Chapter 6 Conclusions and Recommendations

not from physical derivation. In Chapter 5, we testified the shear-dependent slip model and found that it is suitable to describe the phenomenon observed in these experiments. Due to the complicated molecular structure and interaction, here, we cannot conclude that our slip model is the only mechanisms that generate the nonlinear dependence of slip velocity and shear rate. The simulation tools (e.g. MD) should be utilized in our collision model in the future research.

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