The Abdus Salam
International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

International Atomic Energy Agency

SMR.1670 - 2

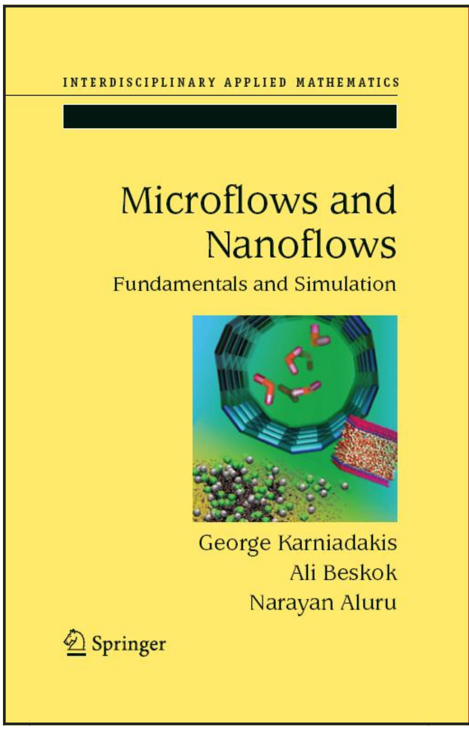
INTRODUCTION TO MICROFLUIDICS

8 - 26 August 2005

Gas Micro Flows

Shear Driven Flows

A. Beskok
Texas A&M University. U.S.A.



Ali Beşkök

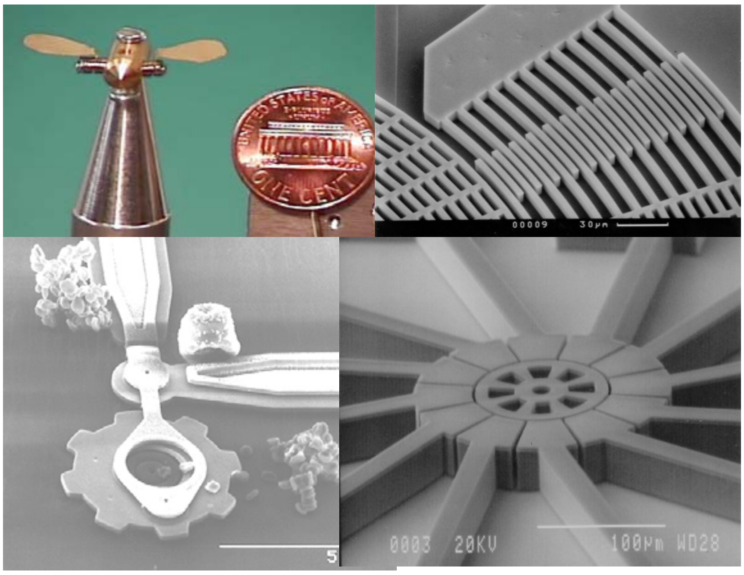
Texas A&M University
Mechanical Engineering Department
College Station, TX 77843
abeskok@tamu.edu

Introduction to Microfluidics

8-26 August, 2005

The Abdus Salam
International Centre for
Theoretical Physics

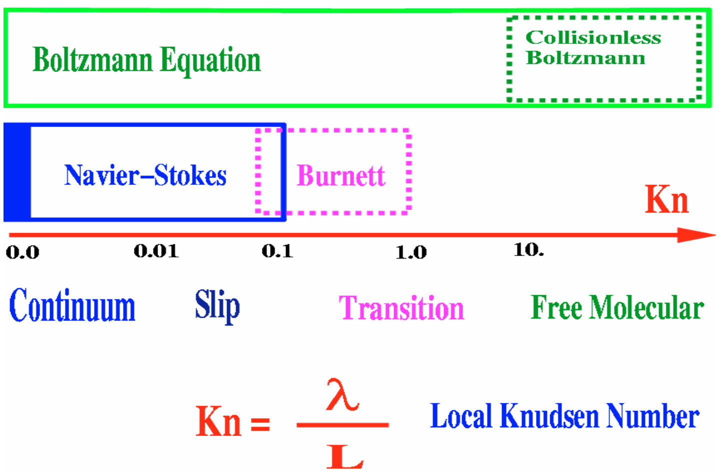
Gas Micro Flows: Examples



Mean free path
λ
an ***intrinsic***
length scale

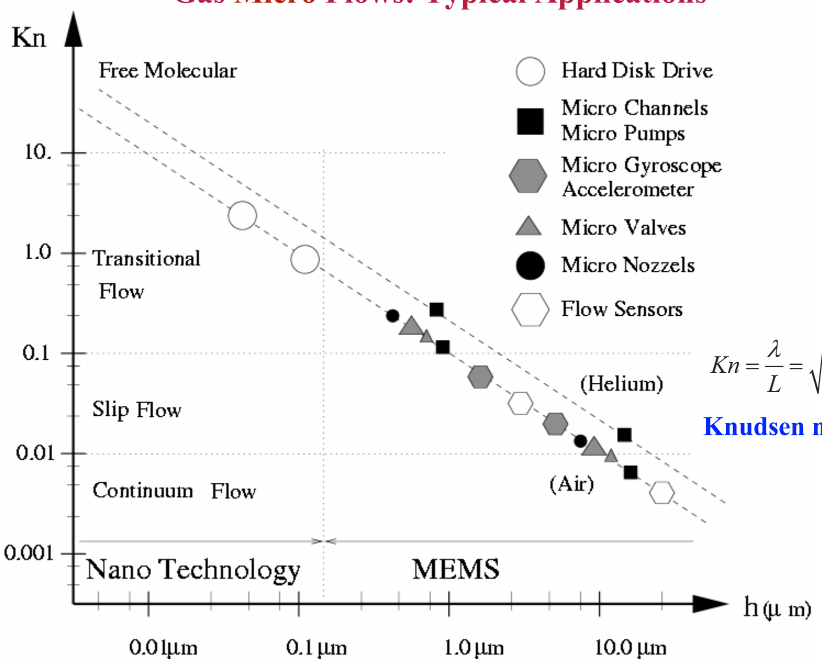
$l \approx 1\mu m$
$\lambda \approx 0.065\mu m$
$$Kn = \frac{\lambda}{l}$$

FLOW REGIMES



•*Chapman-Enskog expansion:* $f = f_0(1 + aKn + bKn^2 + \ldots)$

Gas Micro Flows: Typical Applications

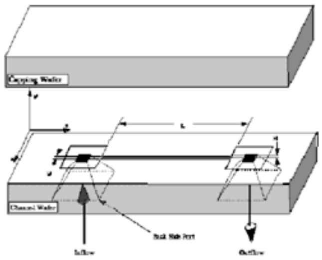


$$Kn = \frac{\lambda}{L} = \sqrt{\frac{\gamma\pi}{2}}\frac{M}{\mathrm{Re}}$$

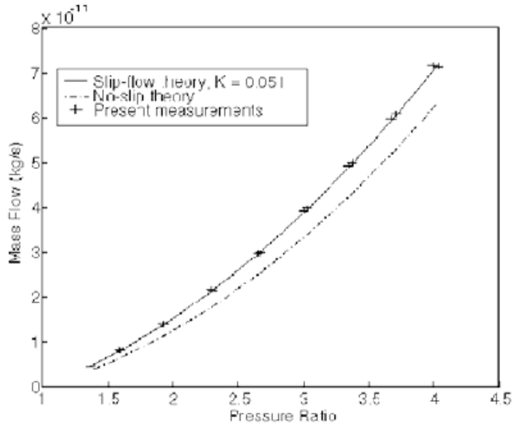
Knudsen number

Experimental Results

Micro Channel Measurements

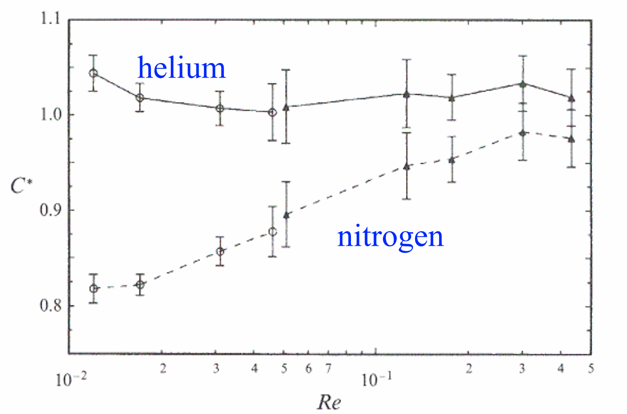


Courtesy of K. Breuer



$$\frac{\dot{M}_{slip}}{\dot{M}_{no-slip}} = 1 + 12\left(\frac{2-\sigma}{\sigma}\right)\frac{Kn_{out}}{\Pi + 1}, \qquad \Pi = \frac{P_{in}}{P_{out}}$$

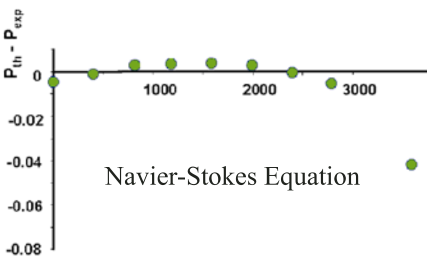
Deviations from Continuum

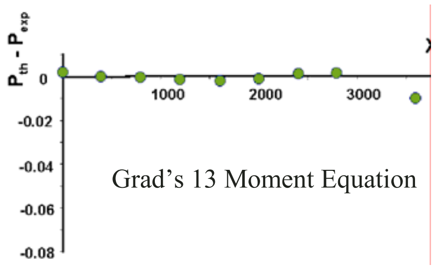


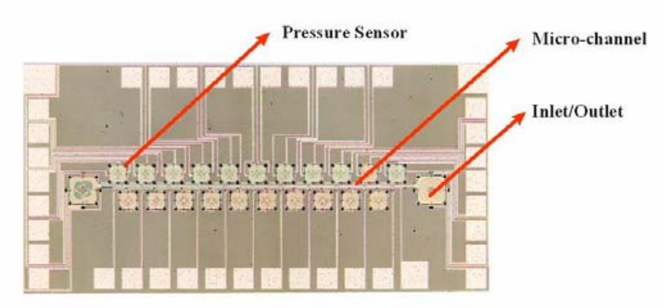
•***Microchannel***: 0.51 microns (*Bau et al., U Penn, 1988*)

- $C^* = Po_{ex}/Po_{th}$ *where* $Po = C_f Re$
- *Po=64 (pipe)*
- *Po=96 (2D channel)*

Pressure Measurements in Early Transition Regime







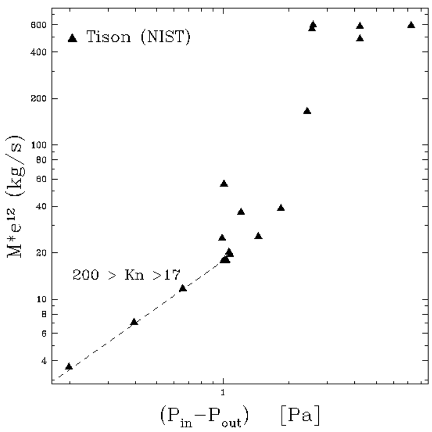
Kn=0.15

Courtesy of C.M. Ho

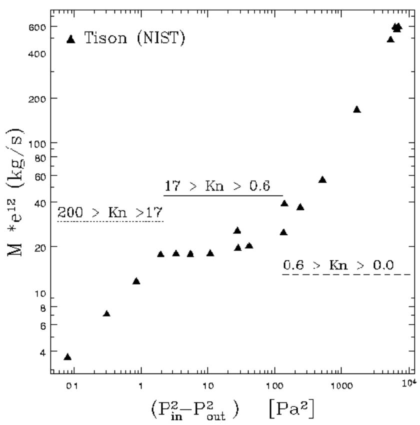
Mass Flow Rate versus Pressure Drop

(Smooth Tubes)

- Pipe Flow (2mm x 200 mm; gas at low pressure)



- Linear Scaling

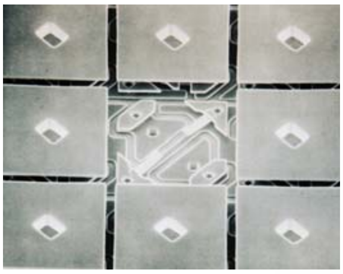


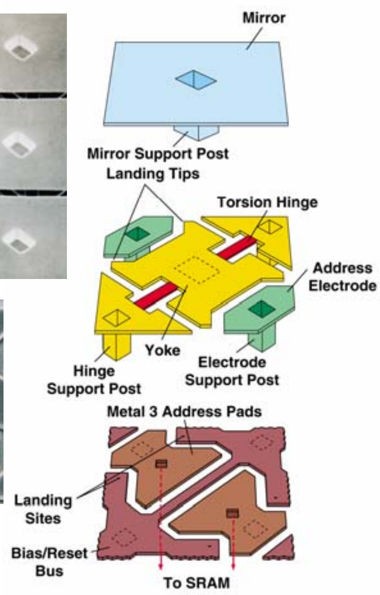
- Quadratic Scaling

A Realistic Geometry: Digital Micro-Mirror Device™

Digital Light Processing™

- 848 x 600 pixels
- 1280 x 1024 pixels
- 16μm x 16μm w/ 1 μm separation

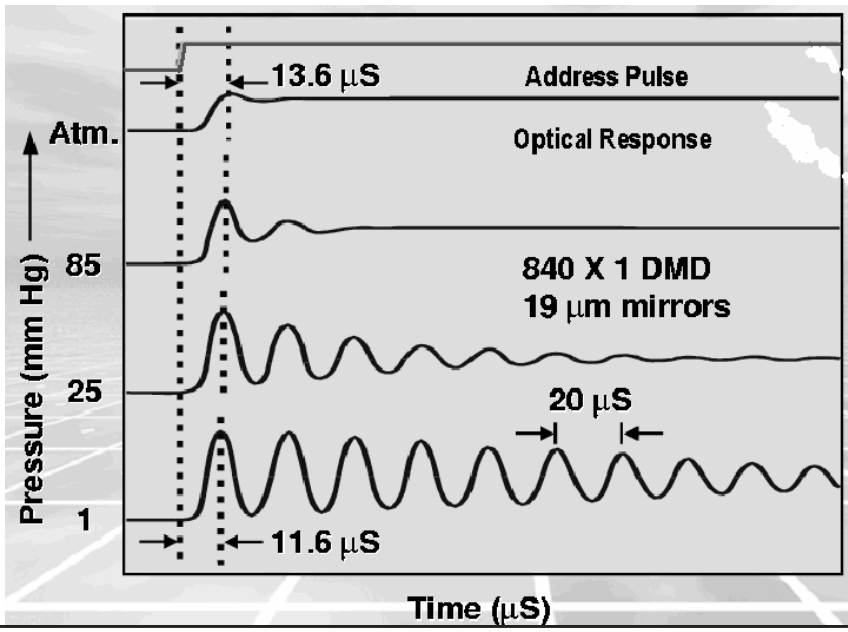




Courtesy of Texas Instruments

DMD™ Air Damping Effects & Transient Response

Courtesy of Texas Instruments



Challenges

- Fundamental understanding of transport in slip, transition and free molecular flow regimes (including the compressibility, rarefaction, viscous heating & thermal creep)
- Engineering models for prototype flows
- Simulation methods for gas micro flows & model verification.

Review of Molecular Magnitudes for Gas Flows

Consider Air at 0°C, and 1 atm

$P = nk_bT$, (Perfect Gas Law)

$n \approx 2.69 \times 10^{25}$ molecules/m^{-3} (Number Density)

$\delta = n^{-3} \approx 3.3 \times 10^{-9}$ m (Mean Molecular Spacing)

$d \approx 3.7 \times 10^{-10}$ m (Molecular Diameter)

} $\delta/d >> 1$ Dilute Gas

$\lambda = 1/\sqrt{2}\pi nd^2 \approx 6.5 \times 10^{-8}$ m (Mean Free Path)

$\bar{c} = \sqrt{3RT} \approx 486$ m/s (Mean Square Molecular Speed)

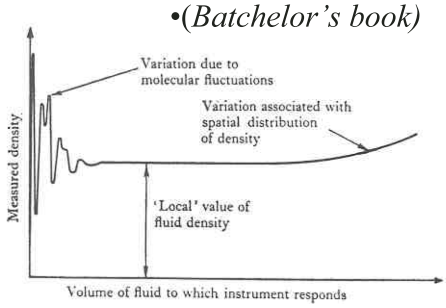
$t_c \approx 10^{-10}$ s (Mean Collision time)

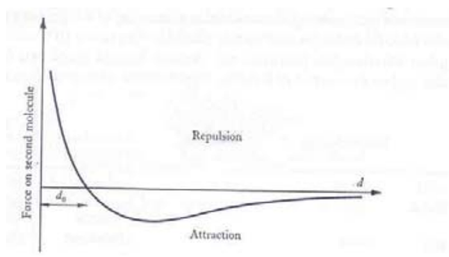
The Continuum Hypothesis

- How small should a volume of fluid be so that we can assign it *mean* properties?
- At what scales will the statistical fluctuations be significant?
- Are the low-pressure rarefied gas flows *dynamically similar* to the gas micro-flows?

The Continuum Hypothesis

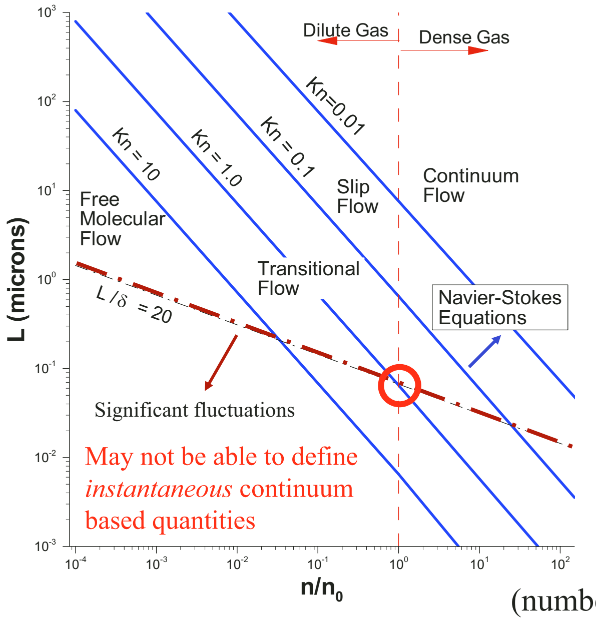
•(*Batchelor's book)*





Type	Force (molec)	Motion (d_0)	Structure (molec)	statistics
Solid	Strong	<<1	ordered	quantum
Liquid	Medium	O(1)	Semi-order	quantum+ classical
gas	weak	>>1	disordered	classical

The Continuum Hypothesis



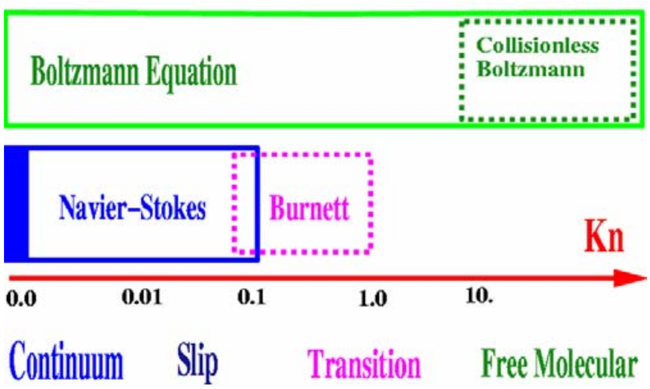
(number density)

1% Statistical Fluctuations for sample volume that contains 10,000 molecules

At standard conditions, a sample volume of 3.7×10^{-10} m^3 results in 1% statistical fluctuations. This corresponds to a cubic volume with side 65nm.

Continuum & Slip Flow Regimes

Kn<0.1



Conservation Laws

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u_1\\ \rho u_2\\ E\end{pmatrix} + \frac{\partial}{\partial x_1}\begin{pmatrix}\rho u_1\\ \rho u_1^2 + p + \sigma_{11}\\ \rho u_1 u_2 + \sigma_{12}\\ (E + p + \sigma_{11})\cdot u_1 + \sigma_{12}\cdot u_2 + q_1\end{pmatrix} + \frac{\partial}{\partial x_2}\begin{pmatrix}\rho u_2\\ \rho u_1 u_2 + \sigma_{21}\\ \rho u_2^2 + p + \sigma_{22}\\ (E + p + \sigma_{22})\cdot u_2 + \sigma_{21}\cdot u_1 + q_2\end{pmatrix} = 0$$

Constitutive Equations:
(Navier-Stokes level stress tensor)

$$\sigma_{ij}^{N-S} = -\mu\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) + \mu\frac{2}{3}\frac{\partial u_m}{\partial x_m}\delta_{ij} - \zeta\frac{\partial u_m}{\partial x_m}\delta_{ij},$$

Compressible Navier Stokes Equations

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ E\end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix}\rho u\\ \rho u^2 + p\\ \rho uv\\ (E+p).u\end{pmatrix} + \frac{\partial}{\partial y}\begin{pmatrix}\rho v\\ \rho vu\\ \rho v^2 + p\\ (E+p).v\end{pmatrix} = \frac{1}{\mathrm{Re}}\frac{\partial}{\partial x}\begin{pmatrix}0\\ \frac{2}{3}\mu(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y})\\ \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})\\ \frac{2}{3}\mu(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}).v + \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}).u + \frac{\kappa\gamma}{\mathrm{Pr}}\cdot\frac{\partial T}{\partial y}\end{pmatrix} +$$

$$\frac{1}{\mathrm{Re}}\frac{\partial}{\partial y}\begin{pmatrix}0\\ \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})\\ \frac{2}{3}\mu(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y})\\ \frac{2}{3}\mu(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}).v + \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}).u + \frac{\kappa\gamma}{\mathrm{Pr}}\cdot\frac{\partial T}{\partial y}\end{pmatrix}$$

$p = (\gamma - 1)\,\rho T$ **Ideal gas equation of state**

$E = \rho\,(T + \frac{1}{2}(u^2 + v^2)),$

$T_o = U_o^2/C_v$

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2}\frac{T_0 + S_1}{T + S_1}$$

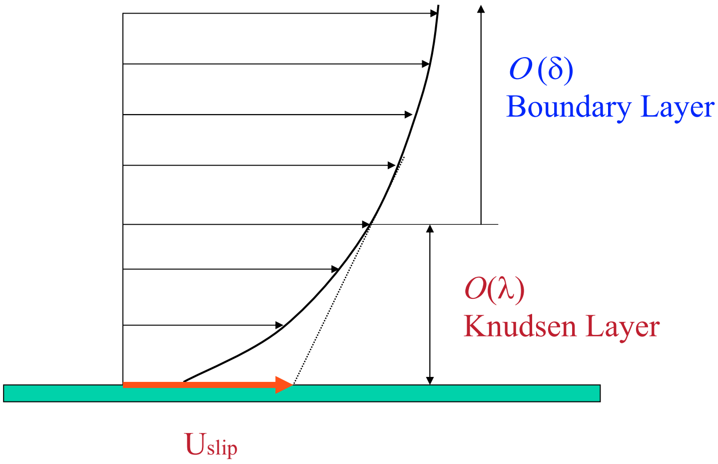
GOVERNING EQUATIONS
Compressible Navier-Stokes Equations

- Valid for continuum and slip flow regimes (Kn<0.1)
- Newtonian fluid
- Thermal stresses (derived from Boltzmann) not included

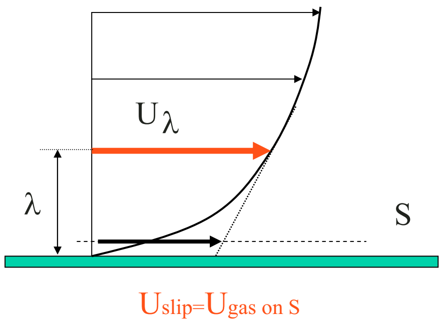
$$\frac{\partial^2 T}{\partial x_i \partial x_j} - \frac{1}{3}\frac{\partial^2 T}{\partial x_k^2}\delta_{ij}$$

How About the Boundary Conditions?

Why Slip ?



Tangential velocity of gas near an isothermal surface



$$U_s = \frac{1}{2}\left[U_\lambda + (1-\sigma)\,U_\lambda + \sigma\,U_w\right]$$

Can be used as a generalized slip model

Tang velocity of impinging molecules

Tang velocity of reflected molecules

Taylor series expand U_λ

$$u_s = \frac{1}{2}\left[u_s + \lambda\left(\frac{\partial u}{\partial n}\right)_s + \frac{\lambda^2}{2}\left(\frac{\partial^2 u}{\partial n^2}\right)_s + \cdots\right] + \frac{1}{2}\left\{(1-\sigma_v)\left[u_s + \lambda\left(\frac{\partial u}{\partial n}\right)_s + \frac{\lambda^2}{2}\left(\frac{\partial^2 u}{\partial n^2}\right)_s + \cdots\right] + \sigma_v \cdot u_w\right\},$$

Rearrange

$$u_s - u_w = \frac{2-\sigma_v}{\sigma_v}\left[\lambda\left(\frac{\partial u}{\partial n}\right)_s + \frac{\lambda^2}{2}\left(\frac{\partial^2 u}{\partial n^2}\right)_s + \cdots\right].$$

$$U_s = \frac{1}{2}\left[U_\lambda + (1-\sigma)\,U_\lambda + \sigma\,U_w\right]$$

Nondimensionalize

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v}\left[Kn\left(\frac{\partial U}{\partial n}\right)_s\right]$$ Truncate

First Order Slip Boundary Conditions

$$u_s - u_w = \frac{2-\sigma_v}{\sigma_v}\,\frac{1}{\rho(2RT_w/\pi)^{1/2}}\tau_s + \frac{3}{4}\frac{Pr(\gamma-1)}{\gamma\rho RT_w}(-q_s)$$

Thermal Creep

$$T_s - T_w = \frac{2-\sigma_T}{\sigma_T}\left[\frac{2(\gamma-1)}{\gamma+1}\right]\frac{1}{R\rho(2RT_w/\pi)^{1/2}}(-q_n),$$

Tangential Momentum Accommodation Coefficient

$$\sigma_v = \frac{\tau_i - \tau_r}{\tau_i - \tau_w}$$

$\sigma_v = 0$ is called **specular reflection**,

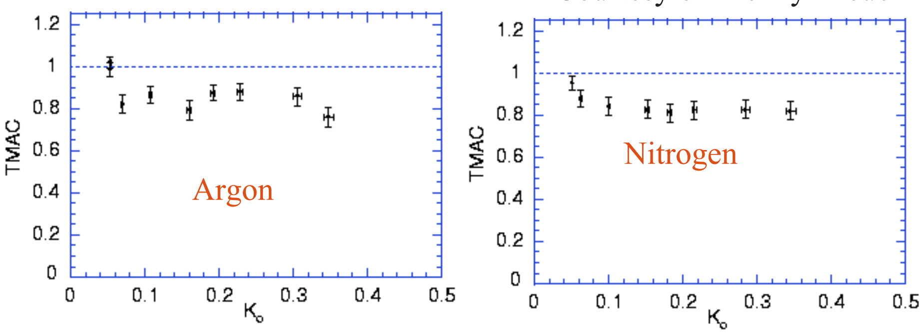
$$\frac{\partial u_s}{\partial n} \to 0 \quad \text{as} \quad \sigma_v \to 0,$$

$\sigma_v = 1$ is called **diffuse reflection**.

$$\sigma_T = \frac{dE_i - dE_r}{dE_i - dE_w},$$ Energy Accommodation Coef.

Accommodation Coefficients

• Courtesy of Kenny Breuer

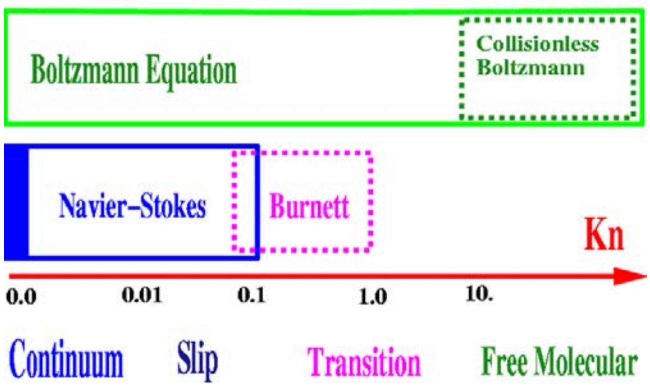


★ σ_v=0 corresponds to *specular reflection*
★ σ_v=1 corresponds to *diffuse reflection*

$$\sigma_v = \frac{\tau_i - \tau_r}{\tau_i - \tau_w}$$

References: *Seidl & Steible* (1974); *Lord* (1976)

Transition Regime Flows



Conservation Laws

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho \\ \rho u_1 \\ \rho u_2 \\ E\end{pmatrix} + \frac{\partial}{\partial x_1}\begin{pmatrix}\rho u_1 \\ \rho u_1^2 + p + \sigma_{11} \\ \rho u_1 u_2 + \sigma_{12} \\ (E + p + \sigma_{11}) \cdot u_1 + \sigma_{12} \cdot u_2 + q_1\end{pmatrix} + \frac{\partial}{\partial x_2}\begin{pmatrix}\rho u_2 \\ \rho u_1 u_2 + \sigma_{21} \\ \rho u_2^2 + p + \sigma_{22} \\ (E + p + \sigma_{22}) \cdot u_2 + \sigma_{21} \cdot u_1 + q_2\end{pmatrix} = 0$$

Governing Equations: Burnett Equations

Stress Tensor:

$$\sigma_{ij} = -2\mu \frac{\overline{\partial u_i}}{\partial x_j} + \frac{\mu^2}{p}\left[\omega_1 \frac{\partial u_k}{\partial x_k}\frac{\overline{\partial u_i}}{\partial x_j} + \omega_2\left(\frac{D}{Dt}\frac{\overline{\partial u_i}}{\partial x_j} - 2\frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j}\right) + \omega_3 R \frac{\partial^2 T}{\partial x_i \partial x_j}\right]$$
$$+ \frac{\mu^2}{p}\left[\omega_4 \frac{1}{\rho T}\frac{\partial p}{\partial x_i}\frac{\partial T}{\partial x_j} + \omega_5 \frac{R}{T}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_j} + \omega_6 \frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j}\right]$$

Where bar defines a non-divergent symmetric tensor:

$$\overline{f_{ij}} = (f_{ij} + f_{ji})/2 - \delta_{ij} f_{mm}/3$$

Boundary Conditions: *The Burnett equations are derived via a second-order Chapman-Enskog expansion in Kn, and they require second-order slip conditions. See Schamberg's second-order slip models.*

A Regularized Slip Condition

Perturbation expansion of the velocity field

$$U = U_0 + KnU_1 + Kn^2U_2 + Kn^3U_3 + \mathcal{O}(Kn^4).$$

Plug in to the generalized slip model

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

$$\mathcal{O}(1): \quad U_0|_s = U_w$$

$$\mathcal{O}(Kn): \quad U_1|_s = \frac{2-\sigma}{\sigma}(U_0')|_s$$

$$\mathcal{O}(Kn^2): \quad U_2|_s = \frac{2-\sigma}{\sigma}\left(\frac{1}{2}U_0'' + U_1'\right)|_s$$

$$\mathcal{O}(Kn^3): \quad U_3|_s = \frac{2-\sigma}{\sigma}\left(U_2' + \frac{1}{2}U_1'' + \frac{1}{6}U_0'''\right)|_s,$$

Postulate a regularized slip condition

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v}\frac{Kn}{1 - B(Kn)\,Kn}\left(\frac{\partial U}{\partial n}\right), \quad (1)$$

$$B(Kn) = B|_0 + \frac{dB}{dKn}|_0\; Kn + \cdots = b + Kn\; c + \cdots$$

For *BKn <<1* Use Geometric Series Expansion

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v}Kn\frac{\partial U}{\partial n}[1 + bKn + (b^2 + c)Kn^2 + \cdots]. \quad (2)$$

Perturbation expansion of the velocity field

$$U = U_0 + KnU_1 + Kn^2U_2 + Kn^3U_3 + \mathcal{O}(Kn^4).$$

Using (2) We get

$$\mathcal{O}(1): \quad U_0|_s = U_w$$

$$\mathcal{O}(Kn): \quad U_1|_s = \frac{2-\sigma_v}{\sigma_v}(U_0')|_s$$

$$\mathcal{O}(Kn^2): \quad U_2|_s = \frac{2-\sigma_v}{\sigma_v}(bU_0' + U_1')|_s$$

$$\mathcal{O}(Kn^3): \quad U_3|_s = \frac{2-\sigma_v}{\sigma_v}(U_2' + bU_1' + (b^2+c)U_0')|_s.$$

$$\mathcal{O}(1): \quad U_0|_s = U_w$$

$$\mathcal{O}(Kn): \quad U_1|_s = \frac{2-\sigma}{\sigma}(U_0')|_s$$

$$\mathcal{O}(Kn^2): \quad U_2|_s = \frac{2-\sigma}{\sigma}\left(\frac{1}{2}U_0'' + U_1'\right)|_s$$

$$\mathcal{O}(Kn^3): \quad U_3|_s = \frac{2-\sigma}{\sigma}\left(U_2' + \frac{1}{2}U_1'' + \frac{1}{6}U_0'''\right)|_s,$$

Choose to match the second order terms

$$b = \left.\frac{U_o''}{2U_o'}\right|_s = \frac{1}{2}\frac{\left(\frac{\partial \omega}{\partial n}\right)_0}{\omega_0}$$

- *The parameter b in equation (2.39) is the ratio of the vorticity flux to the wall vorticity, obtained in no-slip flow conditions. The value of b for simple flows can be found analytically.*

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v}\frac{Kn}{1-BKn}\frac{\partial U}{\partial n} = \frac{2-\sigma_v}{\sigma_v}\frac{Kn}{1-bKn}\frac{\partial U}{\partial n} + \mathcal{O}(Kn^3),$$

$$U_s - U_w = \frac{(2-\sigma)}{\sigma}\left(\frac{Kn}{1-b\,Kn}\right)\frac{\partial U}{\partial n}$$

This is a second-order slip BC in Kn.
Regularized for large Kn

Summary of Slip Boundary Conditions

$$U_g - U_w = \frac{(2-\sigma)}{\sigma} Kn \frac{\partial U}{\partial n}$$ Maxwell 1879

$$U_g = \frac{1}{2}\left[U_\lambda + (1-\sigma)\, U_\lambda + \sigma\, U_w\right]$$ Generalized model

$$U_g - U_w = \frac{(2-\sigma)}{\sigma}\left\{ Kn \frac{\partial U}{\partial n} + \frac{Kn^2}{2} \frac{\partial^2 U}{\partial n^2} \right\}$$ Second-order Model

$$U_g - U_w = \frac{(2-\sigma)}{\sigma}\left(\frac{Kn}{1 - b\, Kn}\right) \frac{\partial U}{\partial n}$$

Regularized model
Second-order if $b = \left.\frac{U_o''}{2U_o'}\right|_s$

Notes

- In the small Reynolds number limit, i.e., $Re \ll Kn \ll 1$, asymptotic analysis of the Boltzmann equation shows that a consistent set of governing equations and boundary conditions up to $\mathcal{O}(Kn^2)$ is the Stokes system with second-order slip boundary conditions, see section 15.4.2 and for details (Sone, 2002; Aoki, 2001).
- Rarefaction effects both in the aforementioned limit as well as in the limit of $Re \sim \mathcal{O}(1) \rightarrow M \sim \mathcal{O}(Kn)$ come in only through the boundary condition. This has been proven rigorously using the Boltzmann equation in (Sone, 2002).
- The high-order boundary conditions proposed include Maxwell's first-order slip conditions (2.18, 2.19), as the leading order term. Hence, these results are correct up to $\mathcal{O}(Kn)$ in the slip flow regime, irrespective of the formal order of the utilized slip conditions.
- The general boundary condition for slip (equation (2.43)) converges to a finite value for large Kn unlike the first-order Maxwell's boundary condition.

For non isothermal surfaces include thermal creep effects

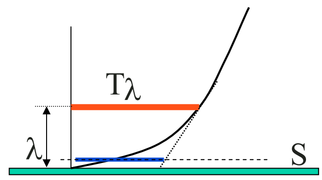
$$u_s = \frac{1}{2}[u_\lambda + (1-\sigma_v)u_\lambda + \sigma_v u_w] + \frac{3}{4}\frac{Pr(\gamma-1)}{\gamma\rho R T_w}(-q_s).$$

Temperature Jump:-

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

von Smoluchowski

$$T_g = \frac{\frac{(2-\sigma_T)}{\Pr}\frac{2\gamma}{(\gamma+1)}T_\lambda + \sigma_T T_w}{\sigma_T + \frac{(2-\sigma_T)}{\Pr}\frac{2\gamma}{(\gamma+1)}}$$



$T_{slip} = T_{gas\ on\ S}$

Pressure Driven Flows

Slip Flow Regime

Kn < 0.1

1-D Analysis of Pressure Driven Gas Microflows

$\rho_i u_i = \rho_o u_o,$ Continuity

$(P_i - P_o)h - 2L\tau = \dot{M}(u_o - u_i).$ Momentum (per unit width)

$$\frac{(P_i - P_o)}{P_o} = \frac{\Delta P}{P_o} = 2\frac{L}{h}\frac{\tau}{P_o} + \frac{\dot{M}(u_o - u_i)}{hP_o},$$

where $\frac{\Delta P}{P_o}$ represents the non-dimensional pressure drop. Concentrating on the term $\frac{\dot{M}}{hP_o} = (\rho_o u_o)/P_o$ and using the continuity equation ($u_o = u_i \rho_i/\rho_o$) and the equation of state for an ideal gas ($\rho_i/\rho_o = P_i/P_o$, assuming isothermal conditions) we obtain

$$\frac{\Delta P}{P_o} = 2\frac{L}{h}\frac{\tau}{P_o} + \frac{\rho_o u_o u_i}{P_o}\left(\frac{P_i}{P_o} - 1\right).$$

Since $P_o = \rho_o RT$, and $c_s^2 = \gamma RT$, where c_s is the speed of sound, the above equation can be simplified as

$$\frac{\Delta P}{P_o} = 2\frac{L}{h}\frac{\tau}{P_o} + \gamma M_o M_i \frac{\Delta P}{P_o}, \tag{4.2}$$

where M denotes the Mach number at respective locations. Rearranging, we obtain

$$\boxed{\frac{\Delta P}{P_o}(1 - \gamma M_o M_i) = 2\frac{L}{h}\frac{\tau}{P_o}.}$$

Without further simplification we see that the inertial terms in the momentum equation (right-hand-side of equation (4.1)) can be neglected if $\gamma M_o M_i \ll 1$. To this end, we note that:

$$\frac{\Delta P}{P_o}(1 - \gamma M_o M_i) = 2\frac{L}{h}\frac{\tau}{P_o}.$$

1. In microchannels with $\frac{L}{h} \simeq 10^3 \sim 10^4$ relatively large pressure drops can be sustained for small Mach number flows.
2. Since the Mach number in microflows is usually small, the inertial effects are small. Therefore, we expect semi-analytic formulas based on balancing the pressure drop with drag on the channel walls to work reasonably well. (This is not true for micronozzles; see section 6.6.)
3. If the diffusion term is simplified by approximating the wall shear stress as $\tau \sim \mu u/h$ and recognizing $\mu/P_o \sim \lambda/c_s$, we obtain

$$\frac{\Delta P}{P_o}(1 - \gamma M_o M_i) \simeq 2\frac{L}{h} M_o Kn_o. \quad (4.3)$$

The above relation indicates the relative importance of compressibility effects in the slip flow regime.

In order to identify the relative importance of inertial terms in the momentum equation compared to the diffusion terms we compare their respective magnitudes

$$\frac{\rho u \frac{\partial u}{\partial x}}{\mu \frac{\partial^2 u}{\partial y^2}} \sim \frac{\rho u^2/L}{\mu u/h^2} = \frac{\rho u h}{\mu}\left(\frac{h}{L}\right) = Re\left(\frac{h}{L}\right).$$

A similar estimate can be obtained by taking the ratio of inertial terms to diffusion terms in equation (4.3) as

$$\frac{\frac{\Delta P}{P_o}(\gamma M_o M_i)}{\frac{L}{h} M_o Kn_o} \simeq \frac{M_i}{Kn_o}\frac{h}{L}\frac{\Delta P}{P_o} \simeq \frac{M_i}{Kn_i}\frac{h}{L}\frac{\Delta P}{P_i} \simeq \frac{h}{L} Re \frac{\Delta P}{P_i},$$

where we have used

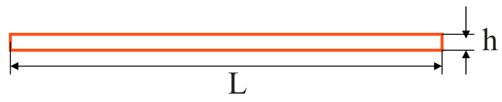
$$Kn_o = \frac{P_i}{P_o} Kn_i, \quad \text{and} \quad Kn \sim \frac{M}{Re},$$

in order to arrive at the third and the fourth equations, respectively. Therefore, the above two estimates are similar, with an exception of the term

$$\frac{\Delta P}{P_i} = \frac{P_i - P_o}{P_i},$$

which is always smaller than unity. This analysis verifies that for relatively low Re flows ($Re \le \mathcal{O}(1)$) in large aspect ratio channels ($L/h \gg 1$) the inertial effects in the momentum equation can be neglected. Under such conditions the momentum equation in the streamwise direction is reduced to the familiar form

$$\frac{dP}{dx} = \mu \frac{\partial^2 u}{\partial y^2}.$$



at y=0 & y=h $\quad U_g - U_w = \frac{(2-\sigma)}{\sigma} Kn \frac{\partial U}{\partial n}$

Can you solve for the velocity profile?

Using the second-order effects, we get

$$U(y) = \frac{h^2}{2\mu}\frac{dP}{dx}\left[\frac{y^2}{h^2} - \frac{y}{h} + \frac{2-\sigma_v}{\sigma_v}(Kn^2 - Kn)\right],$$

Mass flowrate

$$\dot{M} = \rho \int_0^h U(y)dy,$$

Equivalent
$\mathcal{O}$(Kn) Result

$$\dot{M} = \frac{h^3 P_o^2}{24\mu RTL}[(\Pi^2 - 1) + 12\frac{2-\sigma_v}{\sigma_v}(Kn_o(\Pi - 1) - Kn_o^2 \log_e \Pi)],$$

Π is P_{in}/P_{out} $\quad$ Also note that $p/\mu \propto \lambda$ & $pKn = p_o Kn_o$

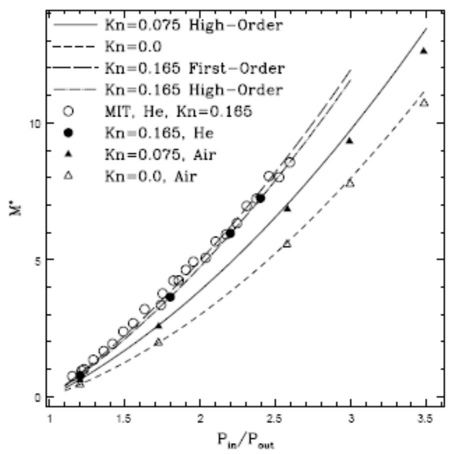
$$\dot{M}_{ns} = \frac{h^3 P_o^2}{24\mu RTL}(\Pi^2 - 1).$$

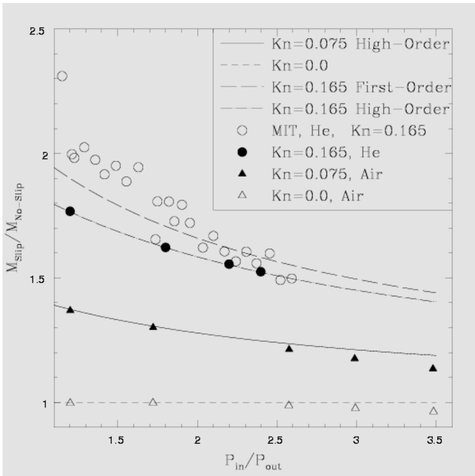
$$\frac{\dot{M}}{\dot{M}_{ns}} = 1 + 12\frac{2-\sigma_v}{\sigma_v}\frac{Kn_o}{\Pi + 1} - 12\frac{2-\sigma_v}{\sigma_v}Kn_o^2\frac{\log_e \Pi}{\Pi^2 - 1}. \qquad \mathcal{O}(Kn^2)$$

$$\frac{\dot{M}_{slip}}{\dot{M}_{no-slip}} = 1 + 12\left(\frac{2-\sigma}{\sigma}\right)\frac{Kn_{out}}{\Pi + 1}, \qquad \Pi = \frac{P_{in}}{P_{out}} \qquad \mathcal{O}(Kn)$$

Which one is a better fit to the experimental data?

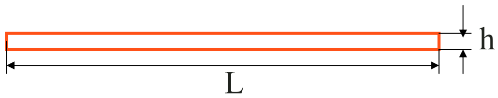
Increase in the mass flowrate compared to the No-Slip Flow





We see that the effect of the second order term is to *reduce* the increase in mass flowrate due to the first-order slip. This is in *disagreement* with the experimental data, since the flowrate increases faster than the predictions of the first order slip theory in the transition flow regime.

Pressure distribution in a micro channel



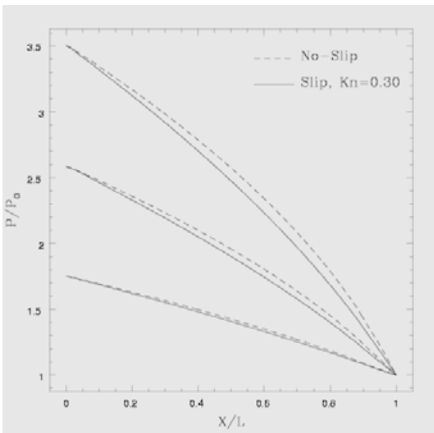
$$\dot{M} = \frac{h^3 P_o^2}{24\mu RTL}[(\Pi^2 - 1) + 12\frac{2-\sigma_v}{\sigma_v}(Kn_o(\Pi - 1) - Kn_o^2 \log_e \Pi)],$$

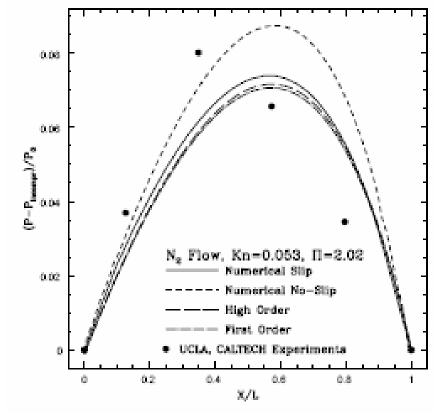
Π is P_{in}/P_{out} Also note that $p/\mu \propto \lambda$ & $pKn=p_oKn_o$

$$1 - \tilde{P}^2 + 12\frac{1-\sigma_v}{\sigma_v}Kn_o(1-\tilde{P}) + 12\frac{2-\sigma_v}{\sigma_v}Kn_o^2 \log_e(\tilde{P}) = B(L-x),$$

where B is a constant such that $\tilde{P}(0) = \Pi$. Here we have defined $\tilde{P} = P/P_0$, i.e., the pressure at a station x normalized with the outlet pressure. The above equation provides an implicit relation for $\tilde{P}$; the pressure distribution for a first-order boundary condition is obtained explicitly by neglecting the second-order terms $(\mathcal{O}(Kn^2))$ in equation (4.9).

Compressibility vs Rarefaction





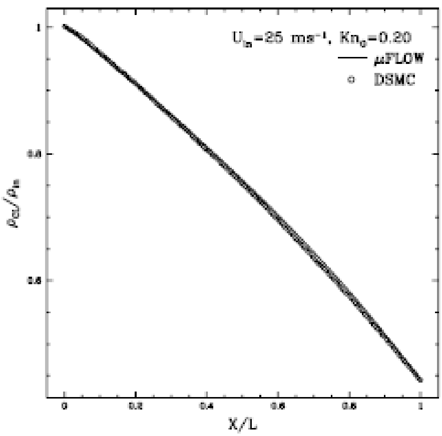
Decrease in the pressure gradient compared to the No-Slip flow

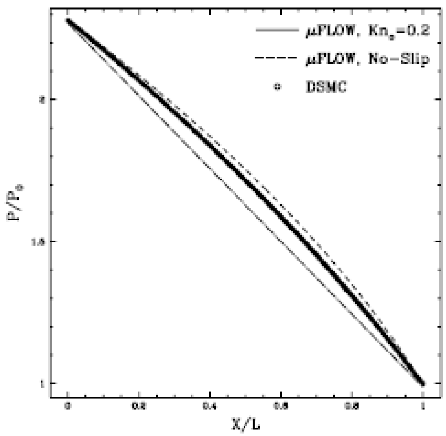
Yet it is still difficult to make comparisons with the experiments

Model Verification Using the DSMC & LB

- Tried to validate various slip models using experimental data, but experimental data have large noise…
- Perhaps we can verify these models by comparisons with atomistic simulations (DSMC) & solutions of the linearized Boltzmann equation.
- Need to see what happens to the
  - Velocity profile?
  - Mass flow rate?
  - Pressure distribution?
- Compare DSMC/LB & continuum based models.

DSMC Simulations in Slip Flow Regime

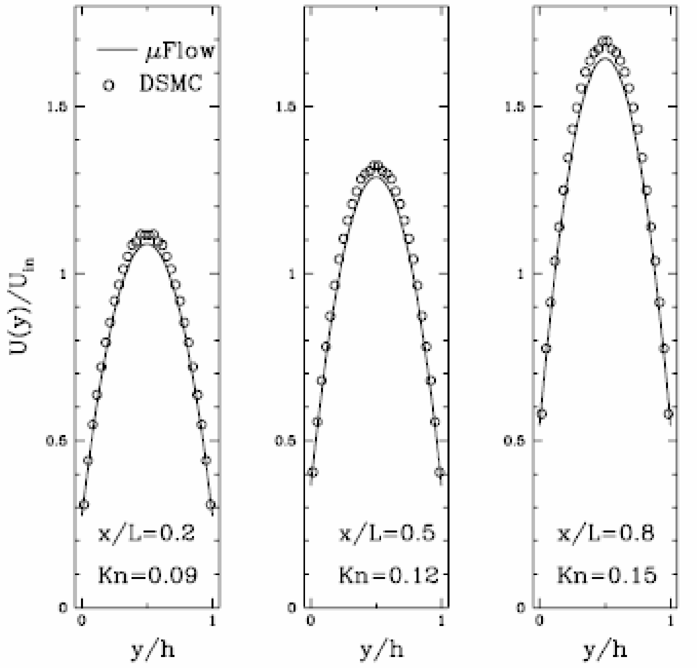




Using

$$U_g = \frac{1}{2}\left[U_\lambda + (1-\sigma)\,U_\lambda + \sigma\,U_w\right]$$

There is a decrease in the pressure gradient compared to the noslip flow



Velocity profiles are normalized by U_{in}.

The channel inlet is at y/h=0

Comparison of various slip models for pressure driven gas flow

$$U_s - U_w = C_1 Kn \left(\frac{\partial U}{\partial n}\right)_s - C_2 Kn^2 \left(\frac{\partial^2 U}{\partial n^2}\right)_s,$$

Author	C_1	C_2
Cercignani (Cercignani and Daneri, 1963)	1.1466	0.9756
Cercignani (Hadjiconstantinou, 2003a)	1.1466	0.647
Deissler (Deissler, 1964)	1.0	9/8
Schamberg (Schamberg, 1947)	1.0	$5\pi/12$
Hsia and Domoto (Hsia and Domoto, 1983)	1.0	0.5
Maxwell (Kennard, 1938)	1.0	0.0
Equation (2.29)	1.0	−0.5

$$U(x,y) = -\frac{dP}{dx}\frac{h^2}{2\mu}\left[-\left(\frac{y}{h}\right)^2 + \left(\frac{y}{h}\right) + C_1 Kn + 2C_2 Kn^2\right]$$

$$\dot{Q}(x) = -\frac{dP}{dx}\frac{h^3}{2\mu}\left(\frac{1}{6} + C_1 Kn + 2C_2 Kn^2\right)$$

$$U^*(y, Kn) \equiv \frac{U(x,y)}{\bar{U}(x)} = \frac{\left(-(\frac{y}{h})^2 + \frac{y}{h} + C_1 Kn + 2C_2 Kn^2\right)}{\frac{1}{6} + C_1 Kn + 2C_2 Kn^2},$$

Shows the shape of the velocity profile

$$U^*(y, Kn) \equiv \frac{U(x,y)}{\bar{U}(x)} = \frac{\left(-(\frac{y}{h})^2 + \frac{y}{h} + C_1 Kn + 2C_2 Kn^2\right)}{\frac{1}{6} + C_1 Kn + 2C_2 Kn^2},$$

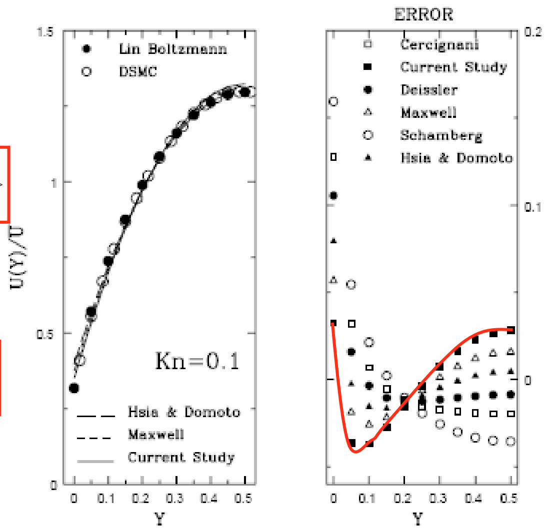
$$E = U_{Model} - U_{LB},$$

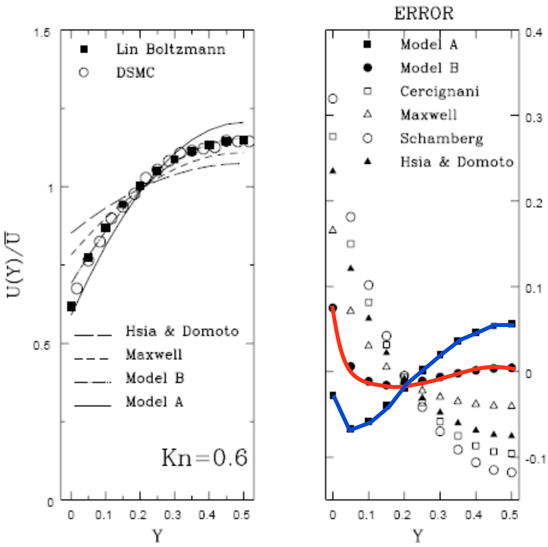
$$U_g - U_w = \frac{(2-\sigma)}{\sigma}\left\{Kn\frac{\partial U}{\partial n} + \frac{Kn^2}{2}\frac{\partial^2 U}{\partial n^2}\right\}$$

↕

$$U_s = \frac{1}{2}\left[U_\lambda + (1-\sigma)\,U_\lambda + \sigma\,U_w\right]$$

Since the velocity profile is parabolic





$$U_g - U_w = \frac{(2-\sigma)}{\sigma}\left\{Kn\frac{\partial U}{\partial n} + \frac{Kn^2}{2}\frac{\partial^2 U}{\partial n^2}\right\}$$

$$U_s - U_w = \frac{(2-\sigma)}{\sigma}\left(\frac{Kn}{1-b\,Kn}\right)\frac{\partial U}{\partial n}$$

Observations

- *In the model of equation (2.29) the second-order slip contribution leads to a reduction in the volumetric flowrate compared to the first-order model.*
- *Other models with second-order slip conditions can predict flowrate accurately but only at the expense of accuracy in the velocity profile.*

$$U_g - U_w = \frac{(2-\sigma)}{\sigma}\left\{ Kn\frac{\partial U}{\partial n} + \frac{Kn^2}{2}\frac{\partial^2 U}{\partial n^2} \right\}$$

This inconsistency becomes more dominant for large Kn flows, and cannot be resolved by simply using a slip correction!

Transition & Free Molecular Flow Regimes

Kn>0.1

Governing Equations: Burnett Equations

Stress Tensor: $$\sigma_{ij} = -2\mu\frac{\overline{\partial u_i}}{\partial x_j} + \frac{\mu^2}{p}\left[\omega_1\frac{\partial u_k}{\partial x_k}\frac{\overline{\partial u_i}}{\partial x_j} + \omega_2\left(\frac{D}{Dt}\frac{\overline{\partial u_i}}{\partial x_j} - 2\frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j}\right) + \omega_3 R\frac{\partial^2 T}{\partial x_i \partial x_j}\right]$$

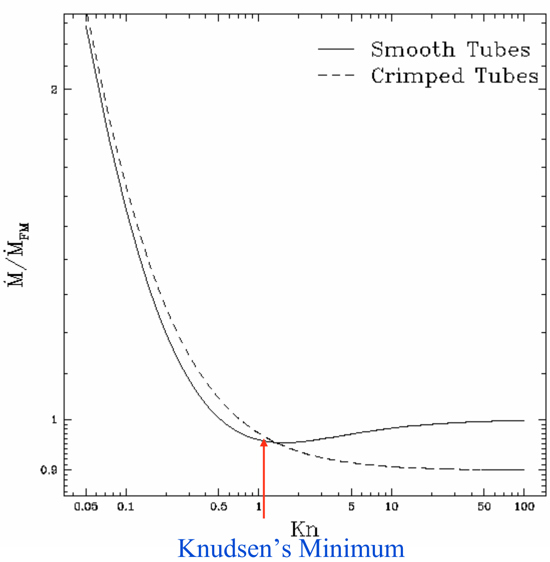
$$+\frac{\mu^2}{p}\left[\omega_4\frac{1}{\rho T}\frac{\partial p}{\partial x_i}\frac{\partial T}{\partial x_j} + \omega_5\frac{R}{T}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_j} + \omega_6\frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j}\right]$$

Where bar defines a non-divergent symmetric tensor:

$$\overline{f}_{ij} = (f_{ij} + f_{ji})/2 - \delta_{ij} f_{mm}/3$$

Boundary Conditions: *The Burnett equations are derived via a second-order Chapman-Enskog expansion in Kn, and they require second-order slip conditions. (sections 2.3, 4.4 and 5.1 in K & B (2002).*

Transition and Free Molecular Flow Regimes and Knudsen's Minimum



In 1909, Knudsen discovered that there is a minimum, when

$$\frac{\dot{Q}}{P_i - P_o}$$

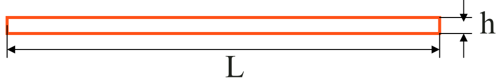
is plotted against the average pressure!

$$\dot{M}_{FM} = \frac{4}{3}a^3\frac{\Delta P}{L}\sqrt{\frac{2\pi}{RT}}.$$

Pipe Flows

Channel Flow Analysis for Kn>0.1 Flows

Analysis of the Burnett Equations for Isothermal Flow (ε=h/L<<1)



$$P_x\left[1-\frac{2\pi\gamma}{3}Kn_{out}^2\, M_{out}^2\left(\frac{P_{out}}{P}\right)^2 U_y^2\right] = U_{yy} + O(\varepsilon)$$

$$P_y\left[1-\frac{\pi\gamma}{3}Kn_{out}^2\, M_{out}^2\left(\frac{P_{out}}{P}\right)^2 U_y^2\right] = \frac{4\sqrt{\pi\gamma/2}}{3}Kn_{out}\, M_{out}\left(\frac{P_{out}}{P}\right)U_y U_{yy} + O(\varepsilon)$$

If $Kn_{out} \leq 1$ & $M_{out} << 1$

$P_x = U_{yy}$ → ***Parabolic Velocity Profile?***

$$P_y = \frac{4\sqrt{\pi\gamma/2}}{3}Kn_{out}\, M_{out}\left(\frac{P_{out}}{P}\right)U_y U_{yy}$$

A Unified Flow Model for Pressure Driven Gas Micro Flows

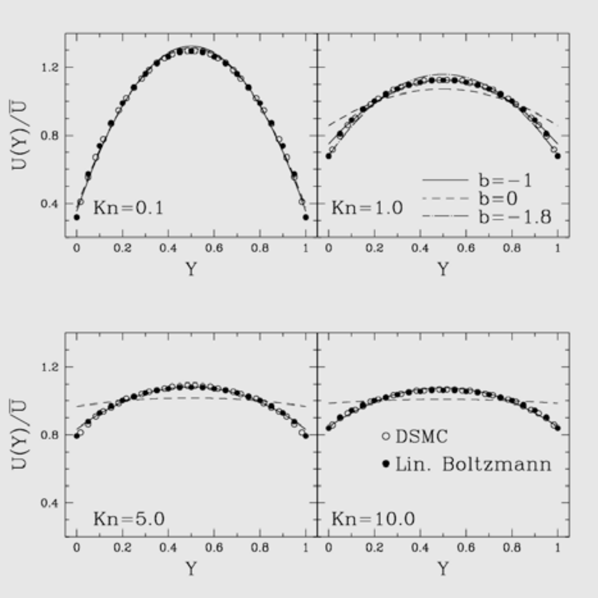
$$U(x,y) = \mathcal{F}\left(\frac{dP}{dx},\mu_o,h,\lambda\right)\left[-(\frac{y}{h})^2 + (\frac{y}{h}) + U_s\right],$$ Parabolic profile w/ U_s

$$U(x,y) = \mathcal{F}\left(\frac{dP}{dx},\mu_o,h,\lambda\right)\left[-(\frac{y}{h})^2 + (\frac{y}{h}) + \left(\frac{2-\sigma_v}{\sigma_v}\right)\frac{Kn}{1-bKn}\right].$$ Regularized model

$$\bar{U}(x) = \mathcal{F}\left(\frac{dP}{dx},\mu_o,h,\lambda\right)\left[\frac{1}{6} + \left(\frac{2-\sigma_v}{\sigma_v}\right)\frac{Kn}{1-bKn}\right]$$ Averaged velocity

$$U^*(y,Kn) \equiv U(x,y)/\bar{U}(x) = \left[\frac{-\left(\frac{y}{h}\right)^2 + \frac{y}{h} + \frac{Kn}{1-bKn}}{\frac{1}{6} + \frac{Kn}{1-bKn}}\right]$$ Normalized velocity

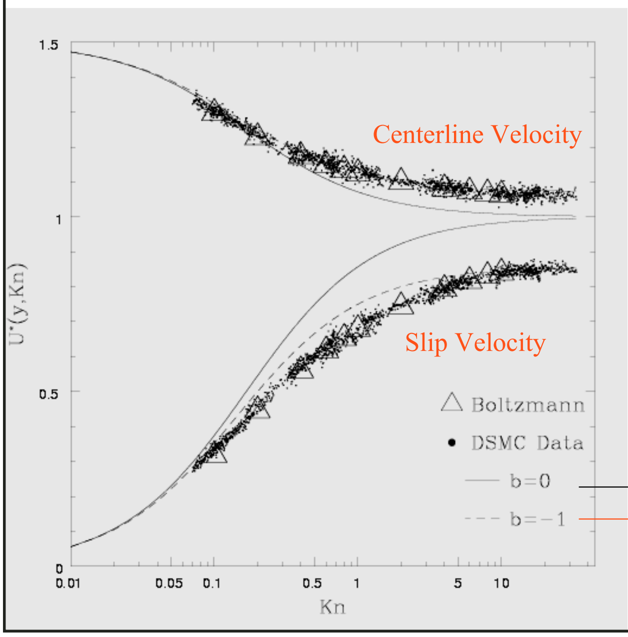
Transitional & Freemolecular Flow Regimes via Direct Simulation Monte Carlo (DSMC)



Velocity Distributions

$$U(Y,Kn)=\left[\frac{-\left(\frac{y}{h}\right)^2+\left(\frac{y}{h}\right)+\frac{Kn}{1-b\,Kn}}{\frac{1}{6}+\frac{Kn}{1-b\,Kn}}\right]$$

Universal Velocity Scaling

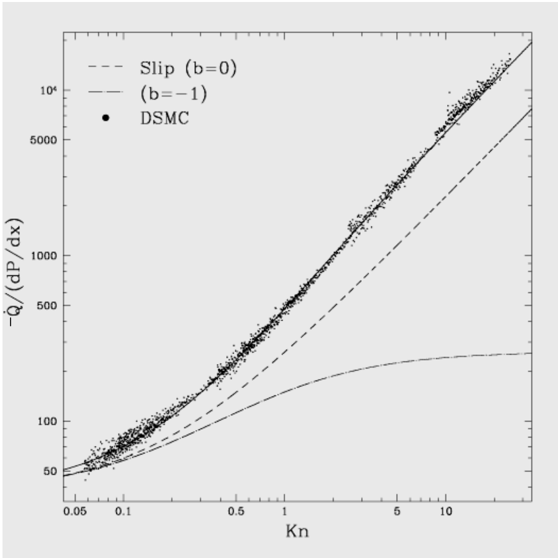


$$U(Y,Kn)=\left[\frac{-\left(\frac{y}{h}\right)^2+\left(\frac{y}{h}\right)+\frac{Kn}{1-b\,Kn}}{\frac{1}{6}+\frac{Kn}{1-b\,Kn}}\right]$$

Maxwell's

New Model

Modeling Flowrate



Volumetric Flowrate

$$\dot{Q} = G\left(\frac{dP}{dx}, \mu, h, \lambda\right)$$

Using Navier-Stokes w/ Slip

$$\frac{\dot{Q}}{W} = -\frac{h^3}{12\mu}\frac{dP}{dx}\left[1 + \frac{6Kn}{1 - bKn}\right]$$

Correct for Rarefaction

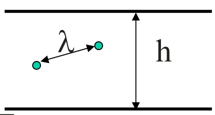
$$\frac{\dot{Q}}{W} = -\frac{h^3}{12\mu}\frac{dP}{dx}\left[1 + \frac{6Kn}{1 - bKn}\right]C_r(Kn)$$

Rarefaction Coefficient

Rarefaction Coefficient (Cont.)

Physical Meaning *1*: Switch over of characteristic length in definition of apparent diffusion coefficient

Absolute Viscosity: $\mu_o \approx \rho\lambda\bar{v}$



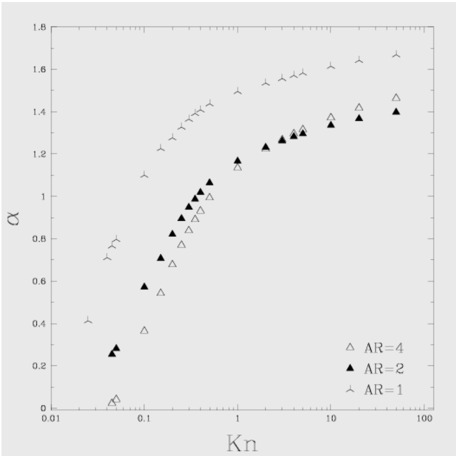
Free Molecular Flow Diffusion Coef: $\mu \approx \rho h \bar{v}$

A Hybrid Model: $$\mu = \rho\bar{v}\frac{1}{1/h + 1/\lambda} = \frac{\rho\bar{v}\lambda}{1 + Kn} = \frac{\mu_0}{1 + Kn}$$

$$C_r(K) = 1 + \alpha Kn, \quad \alpha = \alpha(Kn)$$

A similar model can be developed by considering the intermolecular and molecule/wall collision frequencies. See Karniadakis & Beskok, sec. 5.3.2

Rarefaction Coefficient



$$C_r(Kn) = 1 + \alpha\ Kn$$

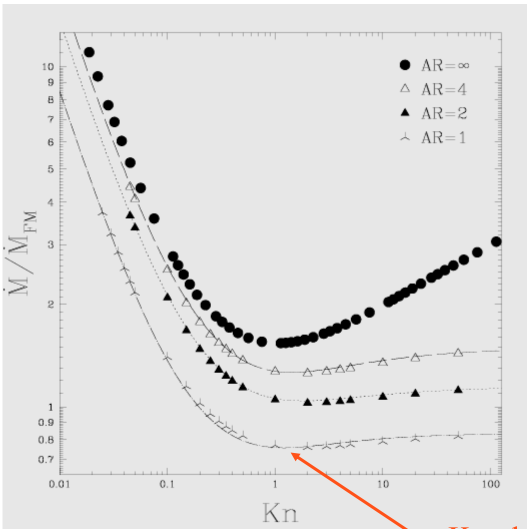
$$\alpha \Rightarrow 0 \quad as \quad Kn \Rightarrow 0$$

$$\alpha \Rightarrow \alpha_o \quad as \quad Kn \Rightarrow \infty$$

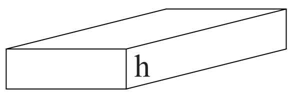
$$\alpha = \alpha_o \frac{2}{\pi} \tan^{-1}(\alpha_1 Kn^{\beta})$$

α_1 & β are empirical parameters

Flowrate Scaling in Arbitrary Aspect-Ratio Rectangular Ducts (Based on the Free Molecular Limit)



Knudsen's Minimum

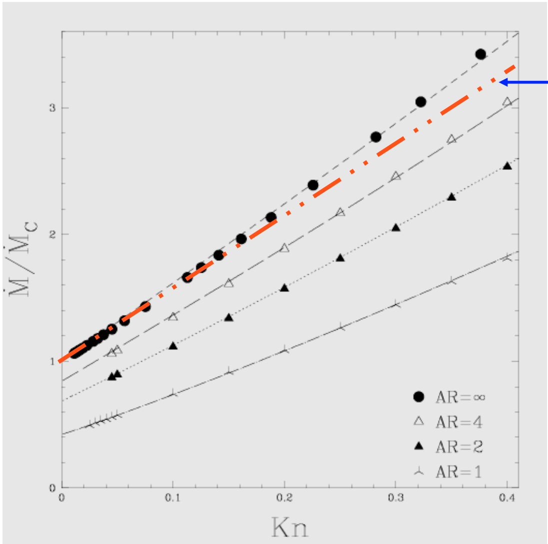


$$\frac{\dot{M}}{\dot{M}_{FM}} = \frac{C(AR)}{6\,Kn}(1+\alpha Kn)\left[1+\frac{6Kn}{1-b\,Kn}\right]$$

$$\dot{M}_{FM} = \frac{h^2 W}{\sqrt{2RT_o}} \frac{\Delta P}{L}$$

$$C(AR) = \left[1 - \frac{192(AR)}{\pi^5} \sum_{i=1,3,5,\ldots}^{\infty} \frac{\tanh(i\pi/2(AR))}{i^5}\right]$$

Flowrate Scaling in Arbitrary Aspect-Ratio Rectangular Ducts (Based on the Continuum Limit)

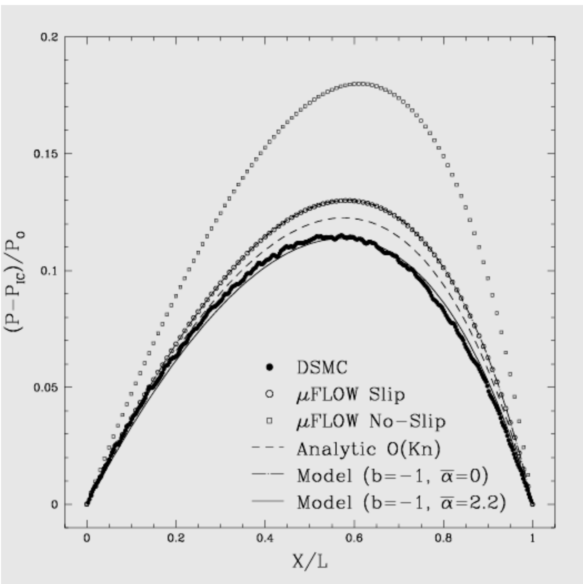


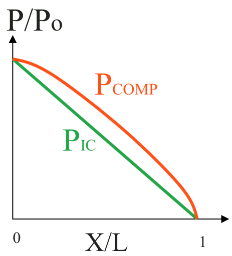
First-Order Theory

$$\frac{\dot{M}}{\dot{M}_{FM}} = C(AR)(1+\alpha\, Kn)\left[1+\frac{6Kn}{1-b\, Kn}\right]$$

$$C(AR) = \left[1 - \frac{192(AR)}{\pi^5}\sum_{i=1,3,5,\ldots}^{\infty}\frac{\tanh(i\pi/2(AR))}{i^5}\right]$$

Channel Flow, Nonlinear Pressure Distribution





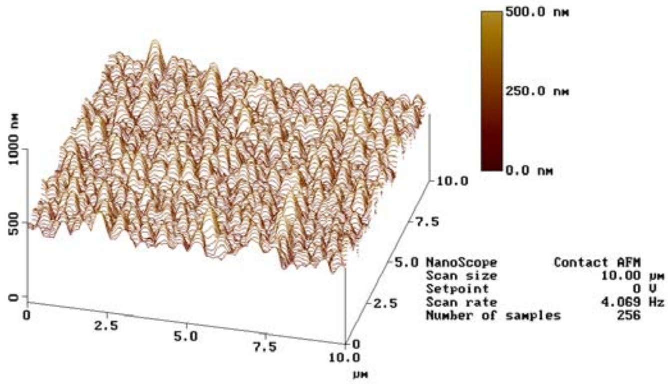
Regarding the new model

- Model accurately predicts the volumetric flowrate, velocity and pressure distribution for rectangular ducts (and circular pipes) in the entire Knudsen regime, including the Knudsen's minimum.
- The new model is based on the hypothesis that the velocity distribution remains parabolic in the transition regime, which is supported by the asymptotic analysis of Burnett equations.

- The general slip boundary condition (equation (2.43)) gives the correct non-dimensional velocity profile, where the normalization is obtained using *the local channel averaged velocity*. This eliminates the flowrate dependence in modeling the velocity profile. For channel flows, using equation (2.39), we obtain $b = -1$ in the slip flow regime. Evidence based on comparisons of the model with the DSMC and Boltzmann solutions shows that $b = -1$ in the *entire* Knudsen regime.
- In order to model the flowrate variations with respect to the Knudsen number, Kn, we introduced the rarefaction correction factor as $C_r = 1 + \alpha Kn$. This form of the correction factor was justified using two independent arguments: First, the apparent diffusion coefficient; and second, the ratio of intermolecular collisions to the total molecular collisions. We must note that α cannot be a constant. Physical considerations to match the slip flowrate require $\alpha \to 0$ for $Kn \lesssim 0.1$, while $\alpha \to \alpha_o$ in the free molecular flow regime. The variation of α between zero and a known α_0 value is approximated using equation (4.34) that introduced two empirical parameters α_1 and β to the new model.

Therefore, the unified model employs two empirical parameters (α_1 and β) and two known parameters $b = -1$ and α_0. Although this empiricism is not desired, the α value in C_r varies from zero in the slip flow regime to an *order one* value of α_0 as $Kn \to \infty$. Finally, the model is adopted to the finite aspect ratio rectangular ducts using a standard aspect ratio correction given in equation (4.35).

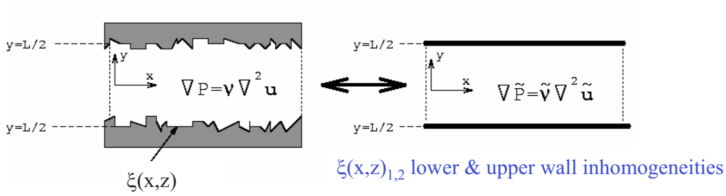
Modeling Roughness in Micro-Geometries



- **Regularized roughness**
- **Equivalent effect**
- **Random walls**

Modeling Roughness Effects

- Model the extra chaotic motion due to the rough boundary using correlation function of surface inhomogeneities



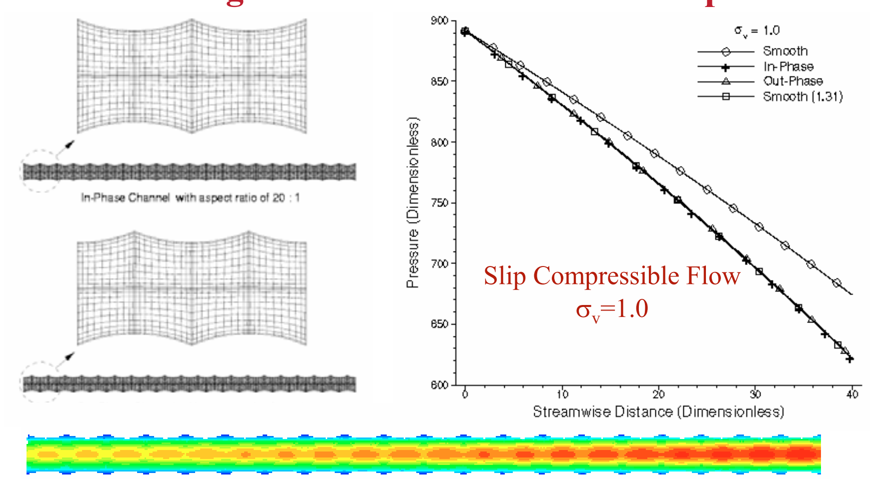
- Use Migdal transformation from nuclear physics

$$Y = \frac{L[y - 1/2[\xi_2(x,z) - \xi_1(x,z)]]}{L - [\xi_1(x,z) + \xi_2(x,z)]}$$

- Renormalize the viscosity to account for extra diffusion

- Solve new equation in simple domain

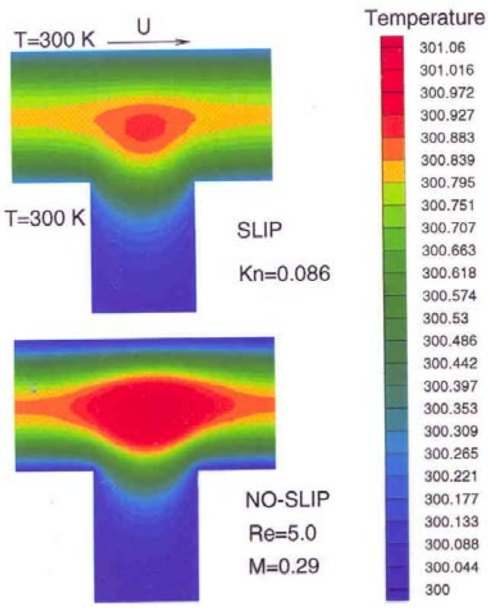
Roughness Effect on Pressure Drop



- Re = 0.36; with enhanced viscosity Re = 0.276
- Enhanced viscosity factor: 1.31

Courtesy of Karniadakis

Viscous Heating

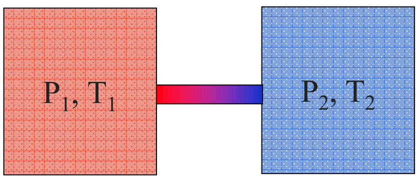


$$\Delta T = 1\ \mathrm{K}$$

$$\frac{\partial T}{\partial n} \approx 10^6\ (\mathrm{K/m})$$

$$\int_{CS} (n_j \tau_{ji}).\mathrm{v}_i dS$$

Thermally Induced Flows:
Thermal Creep/Transpiration
(O. Reynolds & Maxwell)



$P_1 = P_2 \qquad T_1 > T_2$

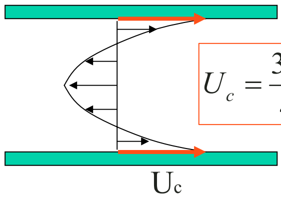
$\rho \propto n, \qquad T \propto \bar{c}^2$

Mass Flux from hot & cold ends are: $\quad m n_1 \bar{c}_1$ and $m n_2 \bar{c}_2$

Using $\quad P = \rho R T$ and $\dfrac{P_1}{P_2} = 1.$

$$\frac{m n_1 \bar{c}_1}{m n_2 \bar{c}_2} \simeq \frac{\rho_1}{\rho_2}\left(\frac{T_1}{T_2}\right)^{0.5} = \frac{P_1}{P_2}\left(\frac{T_2}{T_1}\right)^{0.5} = \left(\frac{T_2}{T_1}\right)^{0.5} \leq 1,$$

Hence, there is creeping flow from cold to hot



$$U_c = \frac{3\mu R}{4P}\frac{\partial T}{\partial s}$$

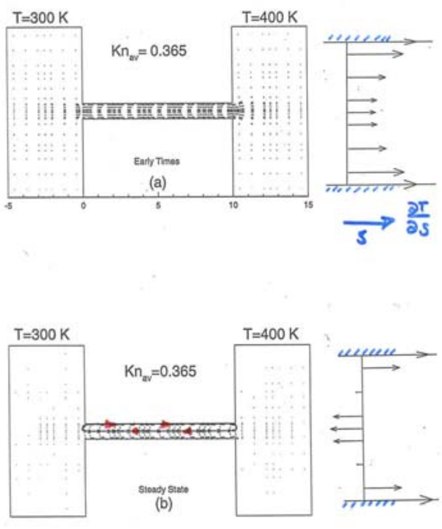
$$U_s = \frac{1}{2}[(2-\sigma)U_\lambda + \sigma U_w] + U_c.$$

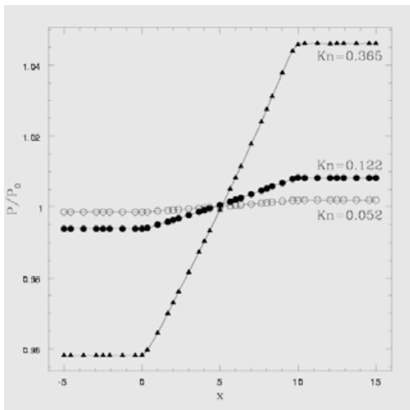
$$\dot{M} = -\frac{h^3 P}{12\mu RT}\frac{dP}{dx}\left[1 + 6\frac{2-\sigma_v}{\sigma_v}(Kn - Kn^2)\right] + \frac{3}{4}\frac{\mu h}{T}\frac{dT}{dx}.$$

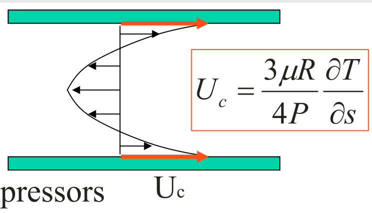
We conclude that thermal creep can change the mass flowrate in a channel. If the pressure gradient and the temperature gradient along the channel walls act along the same direction the flowrate is decreased; otherwise the flowrate is increased.

- *Therefore, it is possible to have non-zero flowrate in a microchannel even in the case of zero pressure gradient.*
- Also there can be no net flow under a pressure difference

Thermally Induced Flows: Thermal Creep







$$U_c = \frac{3\mu R}{4P}\frac{\partial T}{\partial s}$$

Similar ideas are used in Knudsen compressors

A Unified Slip Model for Shear Driven Flows

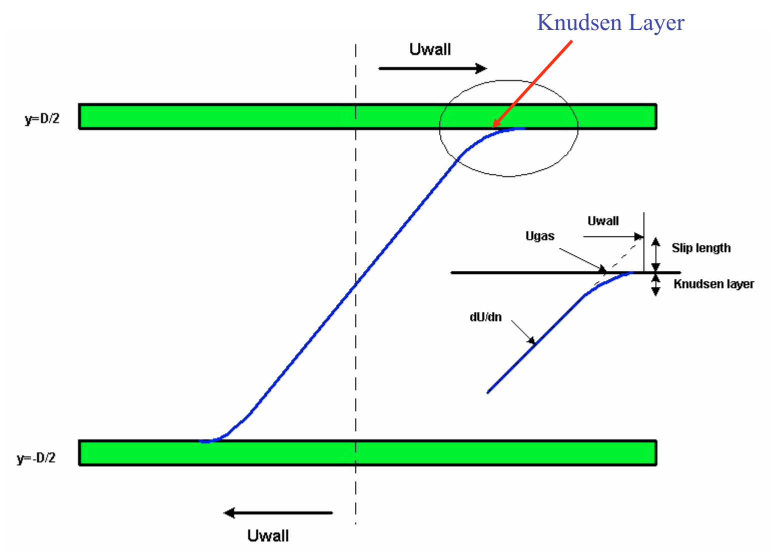
Ali Beskok

Texas A&M University
Mechanical Engineering Department

College Station, TX 77845
abeskok@tamu.edu

in collaboration with
Pradipkumar Bahukudumbi & Jae Hyun Park

Shear Driven Flows: Linear Couette Flow



Shear Driven *Steady* Flows:

Linear Couette Flow

Governing equation : $$\frac{\partial^2 u(y)}{\partial y^2} = 0$$ ← Based on Navier-Stokes

Boundary conditions :

$$u - u_w = \frac{2-\sigma_v}{\sigma_v} \alpha \lambda \frac{\partial u}{\partial y}$$

where, α is the slip coefficient and λ is the mean-free path.

α = 1 **[Maxwell's classical velocity slip formulation]**

α = 1.111 **[Obtained by Ohwada et.al. for hard-sphere molecules using the linearized Boltzmann equation]**

Analytical expression for the velocity profile (u_c)

$$u_c = \frac{2U_o}{1 + 2\frac{2-\sigma_v}{\sigma_v}\alpha Kn} \frac{y}{D}$$

where, we have defined Kn=λ/D.

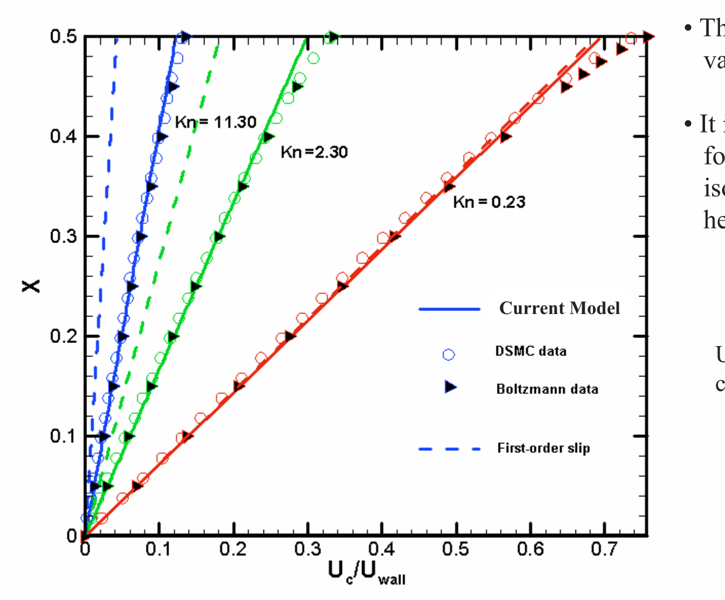
Generalized Slip coefficient

$$\alpha_m = \beta_0 + \beta_1 \tan^{-1}(\beta_2 Kn^{\beta_3})$$

$$\beta_0 = 1.2977; \beta_1 = 0.71851; \beta_2 = -1.17488; \beta_3 = 0.58642$$

- **Extends the validity of first-order slip condition.**
- **Converges to the first order slip condition for Kn<0.1.**

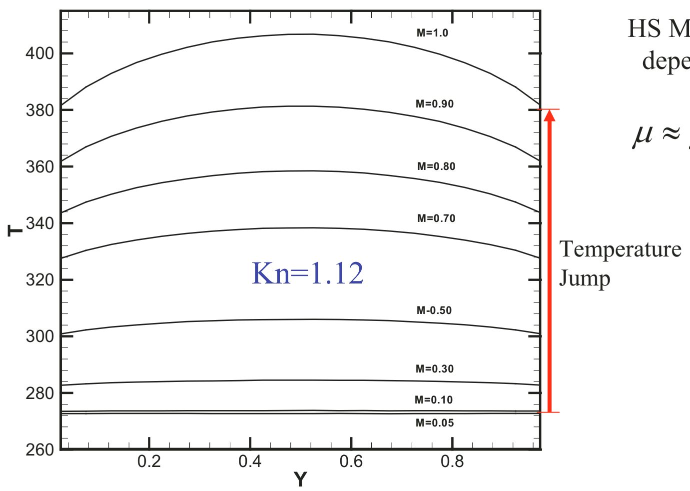
Velocity Distribution of Plane Couette Flows



- The Model is valid for Kn<12.
- It is appropriate for (nearly) isothermal flows, hence M<0.3

Upper half of the channel is shown

Viscous Heating: Plane Couette Flow Temperature Distribution

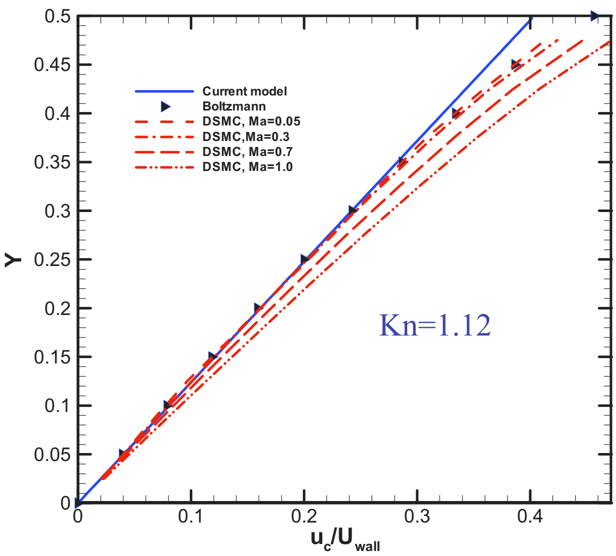


HS Model viscosity dependence on T

$$\mu \approx \mu_o \left(T / T_o \right)^{1/2}$$

A significant increase in mean temperature with Mach number is observed, indicating dominant viscous heating effects

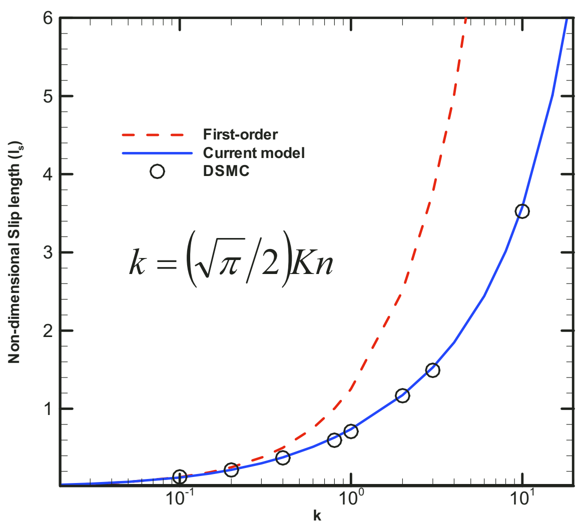
Viscous Heating Induced Compressibility Effects



New Velocity model is valid for Ma<0.3.

Upper half of the channel is shown

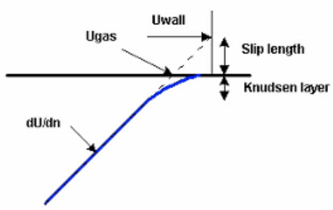
Variation of Normalized Slip-Length with Knudsen Number



$$l_s = \frac{u(y = D/2) - U}{D\dfrac{\partial u(y)}{\partial y}}$$

$$l_s = \alpha Kn$$

Distance from the wall, where the extrapolated bulk flow velocity is equal to the wall velocity.



Shear-Stress Model :

- Least-square fit to linearized Boltzmann solution of Sone *et al* (1990).
- Uniformly converges to correct asymptotic limits as Kn→ 0 and Kn→ ∞.
- Accurate prediction of shear stress for Kn<∞ and for Ma<0.3.

Free-molecular shear stress : $\tau_{xy,\infty} = -\rho_o U \sqrt{\dfrac{2RT_w}{\pi}}$

Continuum shear stress : $\tau_{xy,cont} = -2\mu \dfrac{U}{D}$

where, the dynamic viscosity $\mu = \sqrt{\dfrac{2RT_w}{\pi}} \rho_o \lambda$ is independent of pressure.

Shear-stress Model (contd..):

$$\frac{\tau_{xy}}{\tau_{xy,\infty}} = \pi_{xy} = \frac{aKn^2 + 2bKn}{aKn^2 + cKn + b}$$

$$\frac{\tau_{xy}}{\tau_{xy,cont}} = \Pi_{xy} = \frac{1}{2}\frac{aKn + 2b}{aKn^2 + cKn + b}$$

$$a = 0.529690; b = 0.602985; c = 1.627666$$

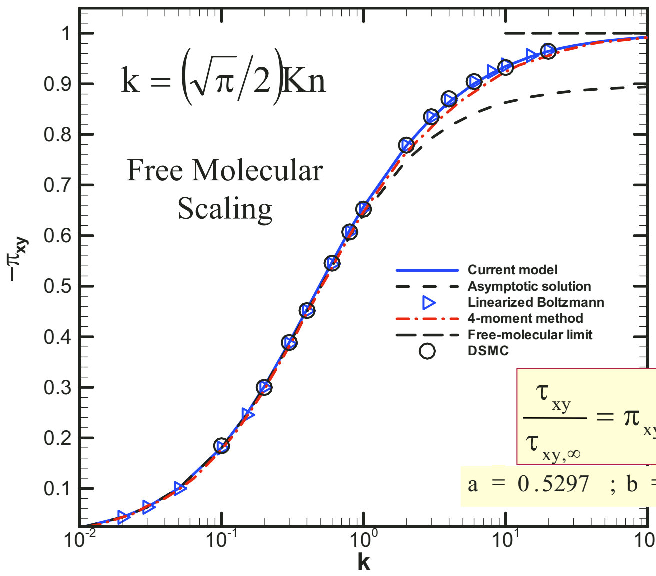
Asymptotic expansions for Kn→∞ and Kn→0

$$\pi_{xy} = 1 + \frac{2b-c}{a}\frac{1}{Kn} + \frac{-b - \left(\frac{-2b-c}{a}\right)c}{a}\frac{1}{Kn^2} + O(Kn^{-3}) \quad \text{as } \mathbf{Kn \to \infty}$$

$$\Pi_{xy} = 1 + \frac{a-2c}{2b}Kn + \frac{\left(\frac{2c-a}{b}\right)c - 2a}{2b}Kn^2 + O\left(Kn^3\right) \quad \text{as } \mathbf{Kn \to 0}$$

$$\frac{a-2c}{2b} = -2.2601 \approx -2\alpha$$

Normalized Shear-Stress Variation with Kn



Free-molecular:

$$\tau_{xy,\infty} = -\rho_o U_o \sqrt{\frac{2RT_w}{\pi}}$$

Continuum:

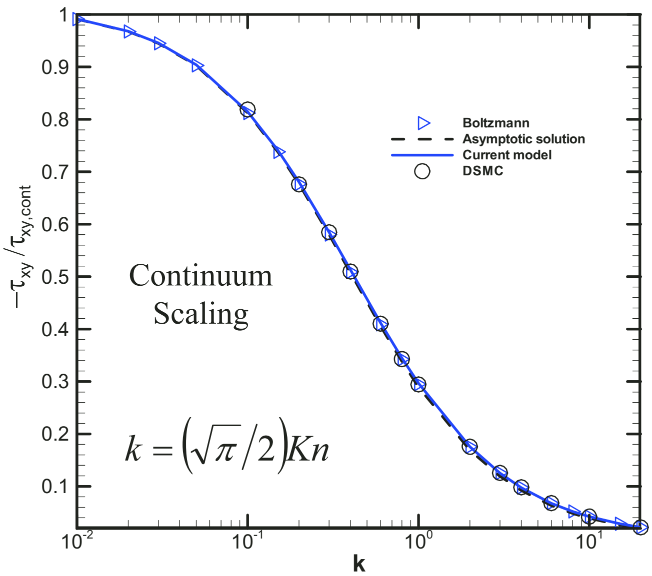
$$\tau_{xy,cont} = -2\mu \frac{U_o}{D}$$

Model:

$$\frac{\tau_{xy}}{\tau_{xy,\infty}} = \pi_{xy} = \frac{aKn^2 + 2bKn}{aKn^2 + cKn + b}$$

a = 0.5297 ; b = 0.6030 ; c = 1.6277

Normalized Shear-Stress Variation with Kn



Shear Stress & Velocity Model Correlation

Define an effective viscosity:

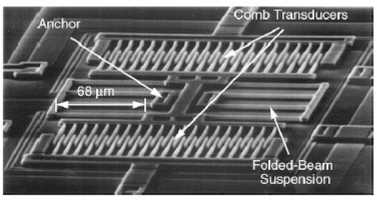
$$\mu_{eff} = \frac{\tau_{model}}{\left(\frac{du}{dy}\right)_{model}} = \frac{\mu_0 U_0}{2}\frac{aKn + 2b}{aKn^2 + cKn + b}\left(1 + 2\alpha_m Kn\right)$$

$\left(\frac{du}{dy}\right)^{-1}$ of steady flow

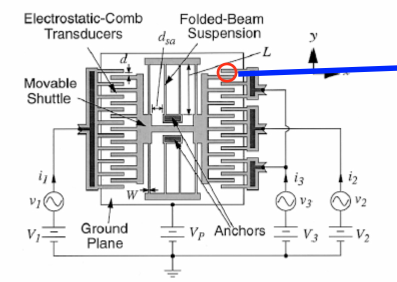
Shear stress of steady flow

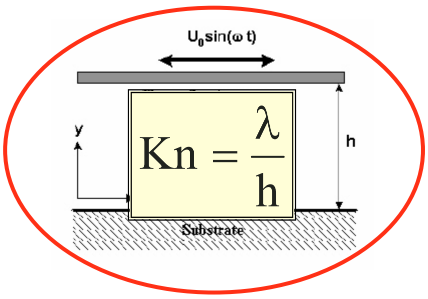
Laterally Oscillating MEMS Structures

Nguyen and Howe (1999): Comb-micro-resonator



SEM of a 100-KHz folded-beam, comb-micro-resonator





Oscillatory Couette Flow

Motivations

❑ Recent experiments in ultra high vacuum chambers ($P < 10^{-8}$ mbar) to achieve high quality factor Q (Yang, et al., 2000).

→ Expect significant rarefaction effects.

❑ Recent micro-resonators at 10-100 MHz (Mattila, et al., 2002; Wang et al., 2000). Comparable to gas *collision frequency* (~1 GHz).

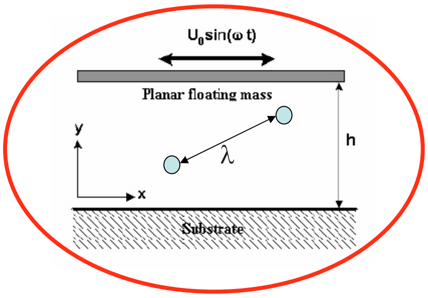
→ Expect strong nonequilibrium effects.

⇨ Accurate analysis of oscillatory Couette flow in the *entire Knudsen regime* and *wide frequency range* is essential for improved design.

Organization

- Develop empirical models for velocity slip & shear stress for steady Couette flows, using hard-sphere direct simulation Monte Carlo (HS-DSMC),
- Extend the empirical model to quasi-steady oscillatory Couette flows and validate using the HS-DSMC,
- Using HS-DSMC, study high-frequency oscillatory Couette flows, and validate the DSMC results for $Kn \to \infty$, using the analytical solutions of the *unsteady collisionless Boltzmann equation*.

Schematic of Oscillatory Couette Flow



Oscillatory Couette Flow

Nondimensional parameters

$$Kn = \frac{\lambda}{h} \quad \text{: Knudsen \#}$$

$$\beta = \sqrt{\frac{h^2\omega}{\nu}} \quad \text{: Stokes \#}$$

Physical Parameters:
ν, ω, λ, h

Continuum-Based Approach

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2}$$

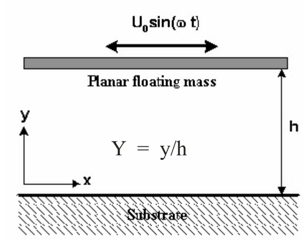
$$u - u_w = \frac{2-\sigma_v}{\sigma_v}\alpha\lambda\frac{\partial u}{\partial y} \quad ; \quad y = 0, h$$

Velocity Response:

$$u(y,t) = \mathrm{Im}\{V(y)\exp(j\omega t)\}$$

$$\beta = \sqrt{\frac{\omega h^2}{\nu}}$$ **Stokes number**

$$u(Y) = C_1\sinh(\sqrt{j}\beta Y) + C_2\cosh(\sqrt{j}\beta Y)$$



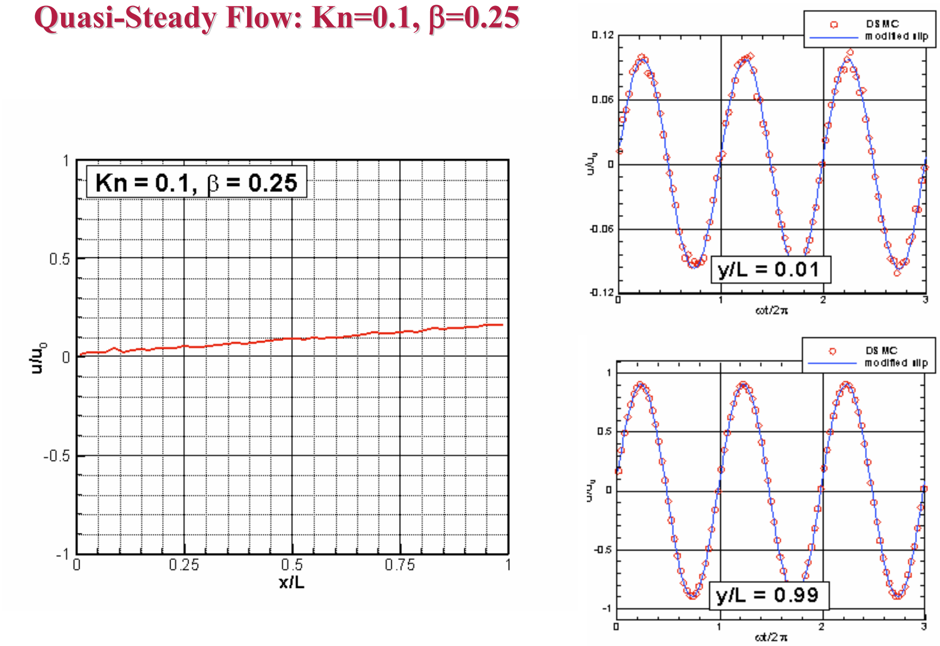
Solution with the generalized slip boundary condition:

$$u(Y) = \mathrm{Im}\left\{U_0 \frac{\sinh(\sqrt{j\beta}Y) + \sqrt{j\beta}\alpha_m Kn\cosh(\sqrt{j\beta}Y)}{(1 + j\beta^2\alpha_m^2 Kn^2)\sinh(\sqrt{j\beta}) + 2\sqrt{j\beta}\alpha_m Kn\cosh(\sqrt{j\beta})}\exp(j\omega t)\right\}$$

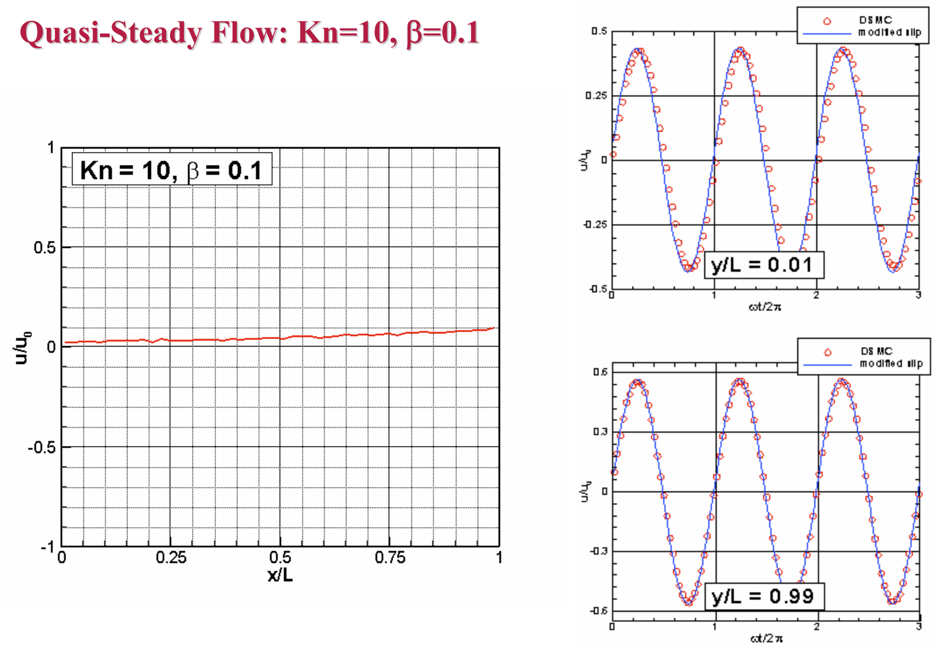
α_m :Generalized slip coefficient

U_o : Amplitude of lateral oscillations.

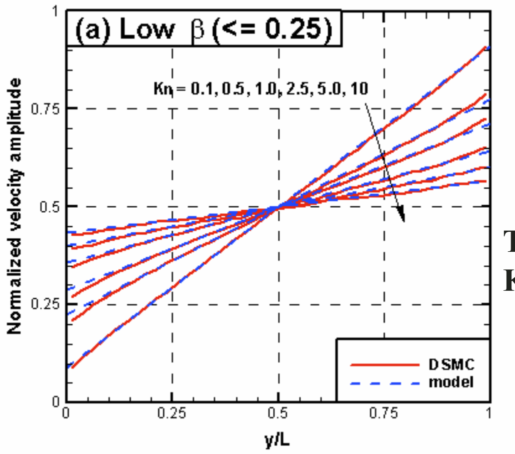
Quasi-Steady Flow: Kn=0.1, β=0.25



Quasi-Steady Flow: Kn=10, β=0.1



Model Summary for Quasi-Steady Flows

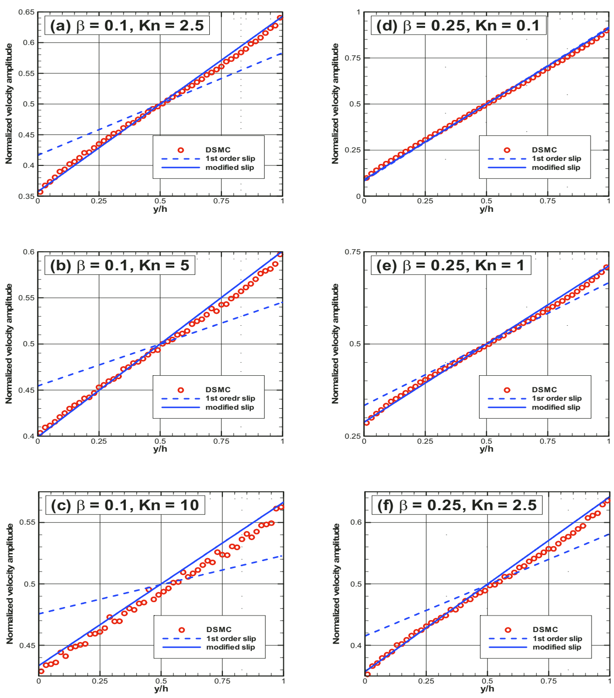


$\beta < 0.25 \Rightarrow$ **Quasi-steady**

Slip on the top and bottom walls are equal, and the velocity profile passes through (V,Y)=(0.5,0.5)

The velocity model is valid for Kn<12, for β<0.25.

Bahukudumbi, Park, Beskok, *Microscale Thermophysical Engineering*, Vol 7(4). 2003.

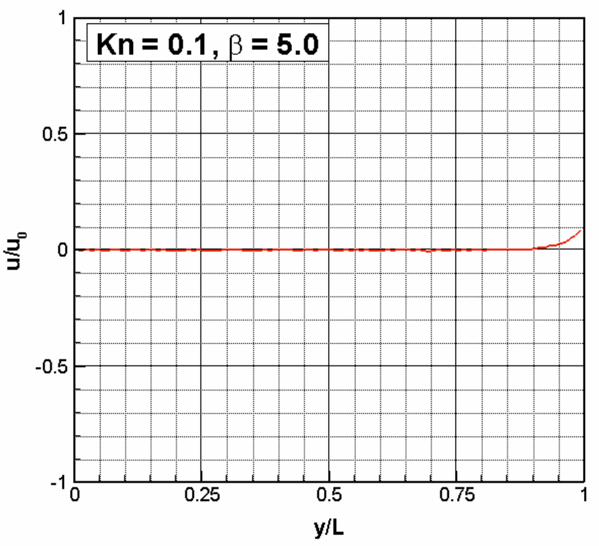


High Frequency Oscillations

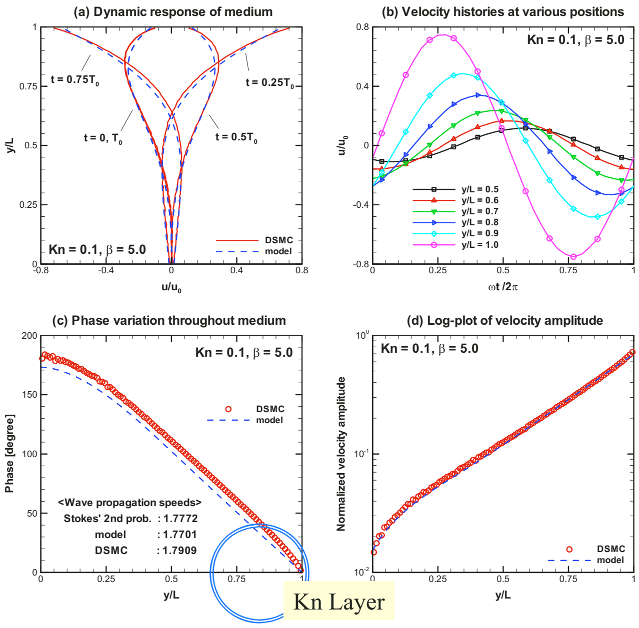
in

Slip Flow Regime

High Frequency Slip Flows (Kn ≤ 0.1 & β ≥ 0.25)



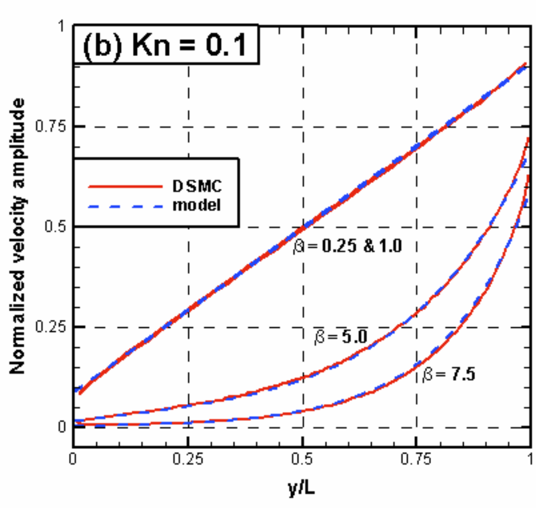
Details of Dynamic Response (Kn = 0.1 & β = 5.0)



Slip Flow Regime

- Exponential decay of velocity amplitude
- Constant wave speed and linearly varying phase angle in most of the domain.
- Interactions between two surfaces result in variations of the wave speed deeper in the domain
- All predicted by the analytical model.

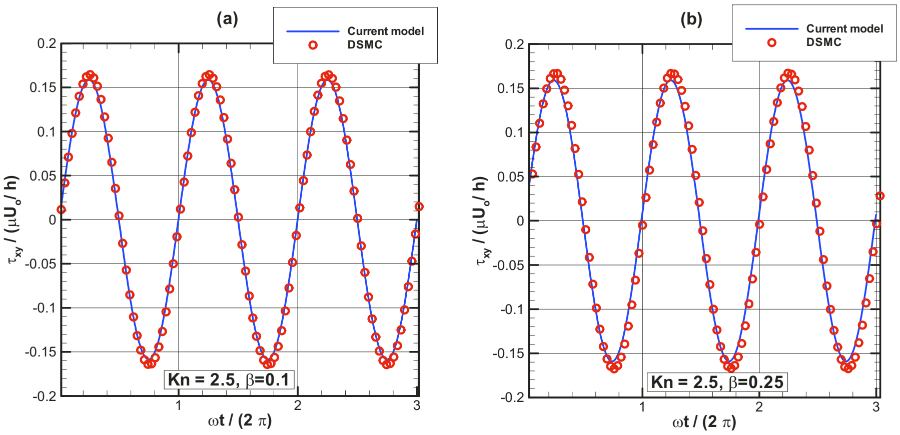
Model Summary for High Frequency Slip Flows ($Kn \leq 0.1$ & $\beta \geq 0.25$)



The velocity model is also valid for $Kn < 0.1$, for $\beta > 0.25$
→ High frequency slip flow.

For $\beta > 5.0$, we observe bounded Stokes layers in the slip flow regime.

Time history of shear stress at the oscillating wall



Shear stress on the oscillating plate:

$$\tau_{xy} = \mu_{eff}\left(\frac{du_{oscillating}}{dy}\right)_{y=h}$$

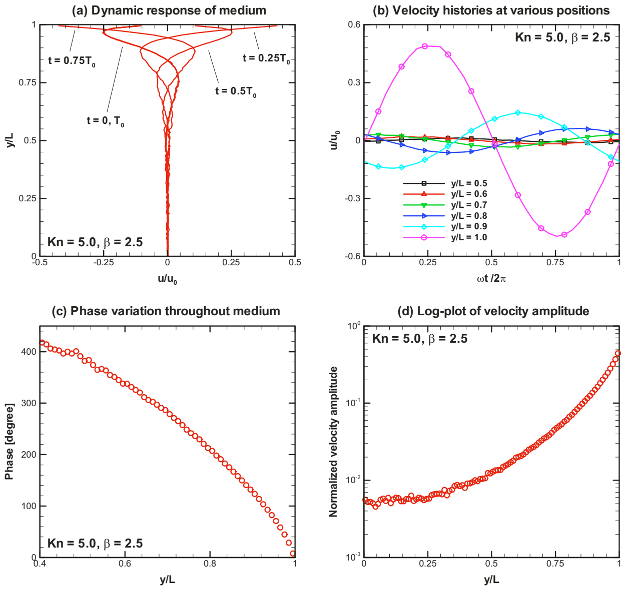
The shear stress model is valid for:

a) Kn < 0.1 & β > 0.25 → High frequency slip flow

b) Kn < 12 & β < 0.25 → quasi-steady flow

High Frequency flows in the *transition* and *free molecular* flow regimes

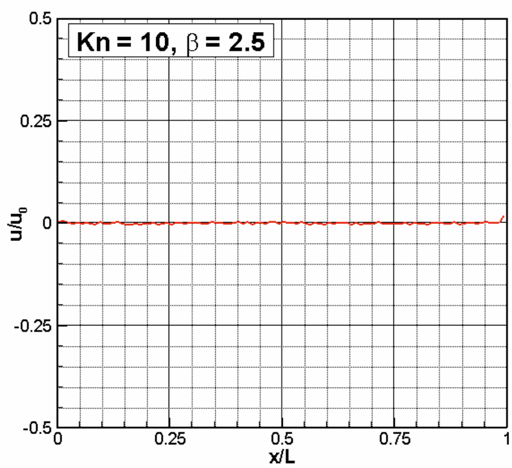
Details of Dynamic Response (Kn = 5.0 & β = 2.5)



Transition Flow Regime

- **Bounded Stokes layer type behavior**
- **Non-exponential decay of the velocity magnitude**
- **Variable wave speed**

Dynamic Response of Free Molecular Flow

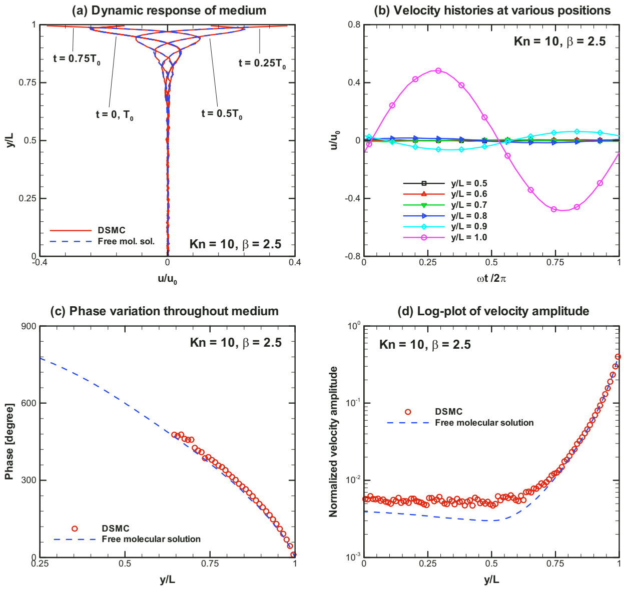


Transitional/Free Molecular Characteristics

- **Bounded layers** (β & Kn)
- **Non-exponential decay of the velocity magnitude**
- **Variable wave speed**
- **Slip Velocity increases with** (β & Kn)
- **As Kn→ ∞, slip velocity and shear stress for *oscillatory flows* reach to the *steady free molecular solution***

Park et al, *Physics of Fluids*, 2004

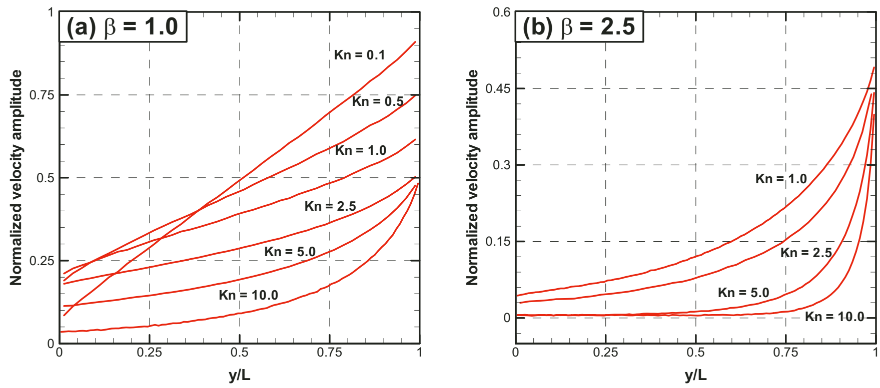
Details of Dynamic Response (Kn = 10, β = 2.5)



Transitional/Free Molecular Flow Regimes

- Bounded Stokes layer type behavior
- Non-exponential decay of the velocity magnitude
- Variable wave speed

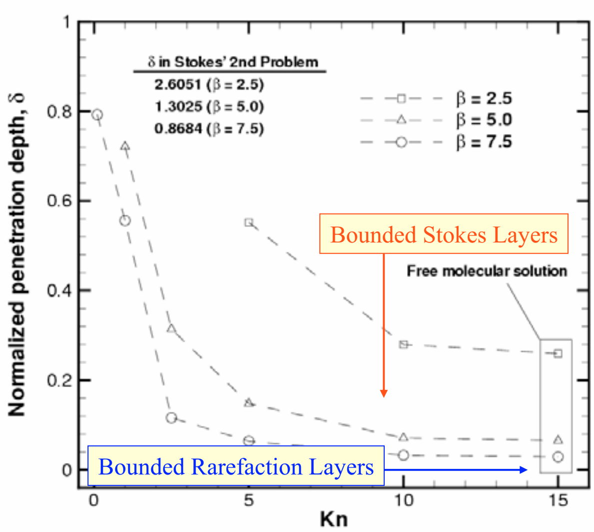
Effects of Kn for fixed β



Increasing Kn for fixed β results in *bounded rarefaction layers!*

Park, Bahukudumbi, Beskok, *Physics of Fluids*, Vol 16 No 2, 2004.

Penetration Depth Variation for Bounded Layers



δ is the distance, where

$$\frac{|U|}{U_o} = 0.01.$$

δ values are smaller than that of the continuum flows.

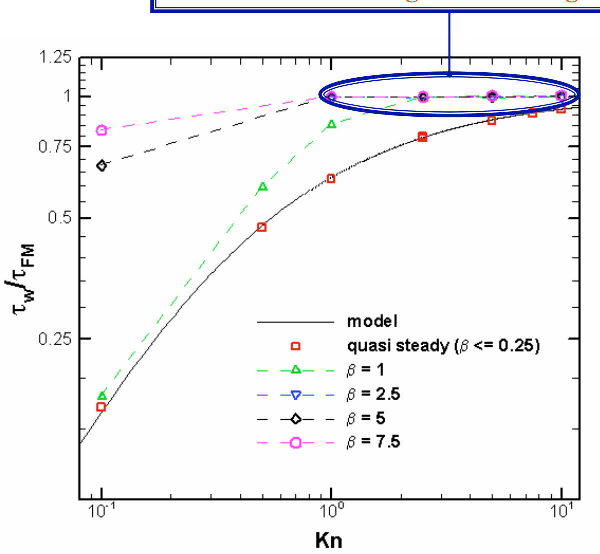
For fixed Kn, δ is reduced by increasing β.

For fixed β, δ is reduced by increasing Kn

Introduction of δ requires length scale change for redefinition of Kn

Effects of Kn & β on Wall Shear Stress

Saturation due to length scale change from h to δ.

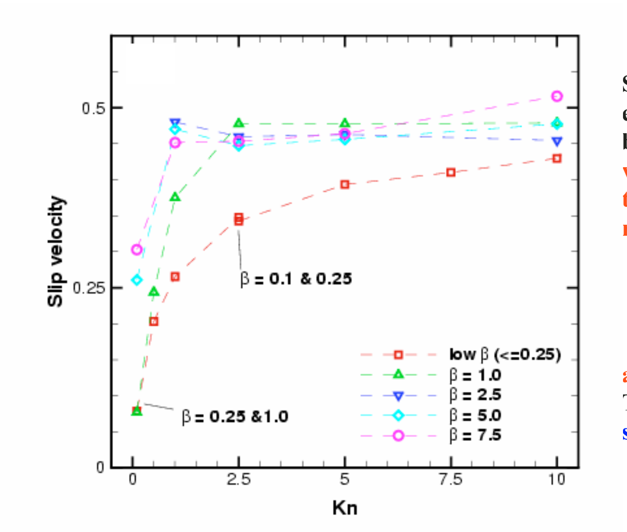


Solution of the Boltzmann equation and the DSMC both predict that the shear stress in oscillatory flows in the free molecular flow regime reaches

$$\tau_{FM} = \frac{1}{2}\rho_0 u_0 \sqrt{\frac{2k_B T_w}{\pi m}}$$

as (Kn → ∞).
This is the value for the steady Couette Flow!

Slip Velocity



Solution of the Boltzmann equation and the DSMC both predict that the slip velocity in oscillatory flows in the free molecular flow regime reaches

$$U_g\big|_w = \frac{1}{2}U_o$$

as ($Kn \rightarrow \infty$).
This is the value for the steady Couette Flow!

Viscous Dissipation

- **Viscous dissipation :** $D = \frac{1}{\omega}\int_0^{2\pi} \tau_w(\omega t) u_w(\omega t) d(\omega t)$
- **Dimensionless Dissipation :** $D^* = \frac{D_{cd}}{D}$

$$D_{cd} = \frac{\pi}{\omega} u_0^2 \left(\frac{\mu_0}{L}\right)$$

μ_0 : absolute viscosity of fluid

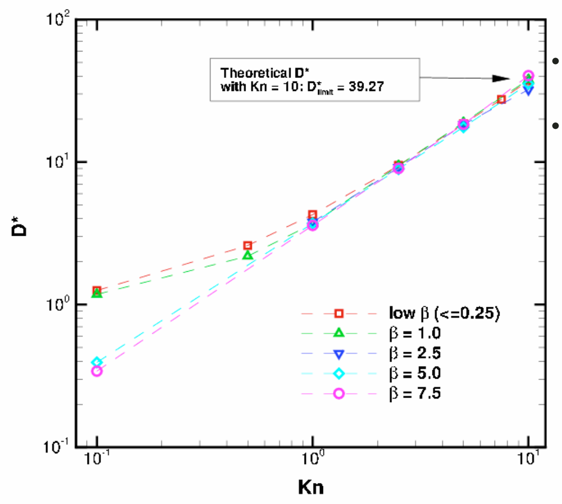
D_{cd} is from steady Couette Flow

In the free molecular flow limit $\tau_{FM} = \frac{1}{2}\rho_0 u_0 \sqrt{\frac{2 k_B T_w}{\pi m}}$

$$U_g\big|_w = \frac{1}{2}U_o$$

This gives: $D^* = \frac{5\pi}{16} Kn$ as $Kn \rightarrow \infty$

Effects of Kn & β on Viscous Dissipation



- D* increases with increased Kn
- D* increases with decreased β

At Kn=10

$$D^* = \frac{5\pi}{16} Kn = 39.27$$

Conclusions

- **We have developed an unsteady DSMC algorithm to study laterally oscillating gas micro flows.**
- **We have developed analytical models for:**
  - **a) Quasi-steady flows (β < 0.25) at *any* Kn**
  - **b) Slip flows (Kn < 0.1) at *any* β**

  These models predict the flow dynamics and dissipation accurately.
- **DSMC results are verified using the *unsteady*, Boltzmann solutions**
  Shear stress and slip velocity for oscillatory Couette flows converge to that of the steady Couette flow for Kn → ∞
- **For β > 0.25 and Kn > 0.1, DSMC data shows rich nonequilibrium physics that can't be predicted by the existing analytical models.**
  First observation of the bounded rarefaction layers