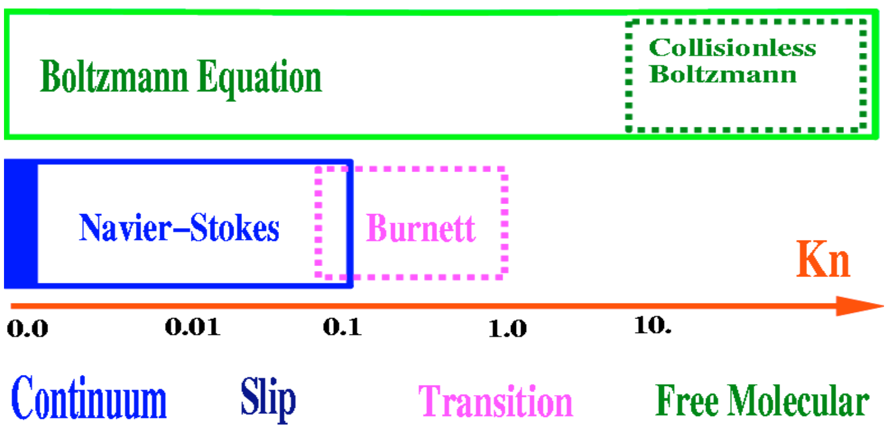
Micro-Scale Gas Transport Modeling

FLOW REGIMES



$$Kn = \frac{\lambda}{L}$$ Local Knudsen Number

•Continuum & Slip Flow Regimes:
- Navier-Stokes Equations
- Slip Boundary Conditions

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

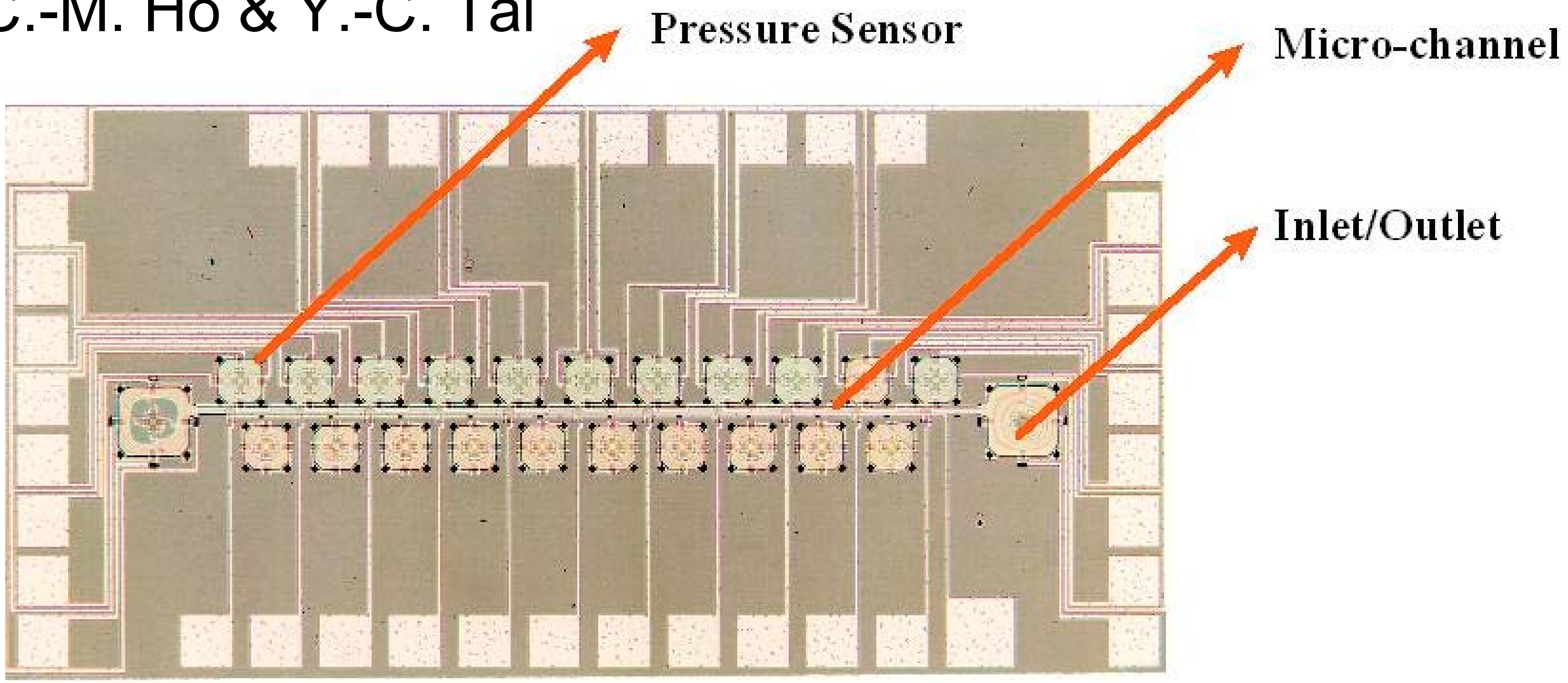
•Slip, Transitional & Free Molecular:
- Direct Simulation Monte Carlo - **DSMC**

$$f = f_0(1 + aKn + bKn^2 + \ldots)$$

•*Chapman-Enskog expansion*

Gas flow through micro channel

C.-M. Ho & Y.-C. Tai



- *Pressure distribution is very insensitive to accommodation constant*
  - *remove the uncertainty of the matching constant*
- *Applying Grad's 13-moment equation (1949)*
  - *establishing constant temperature along the channel*
  - *wall slip at Kn = 0.15*

Compressible Navier-Stokes Equations

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

- •Valid for continuum and rarefied
- •Newtonian fluid
- •Thermal stresses (derived from Boltzmann) not included

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

- •Also the following term is not included in the energy equation:

$$\frac{\partial^2 u_i}{\partial x_j^2}$$

Compressible Microflows: First-Order Models

Stress Tensor:

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

Boundary Conditions:

$$U_s - U_w = \frac{2-\sigma_v}{\sigma_v} Kn \frac{\partial U_s}{\partial n} + \frac{3}{2\pi}\frac{\gamma - 1}{\gamma}\frac{Kn^2 \,\mathrm{Re}}{Ec}\frac{\partial T}{\partial s}$$

$$T_s - T_w = \frac{2-\sigma_T}{\sigma_T}\frac{2\gamma}{\gamma+1}\frac{Kn}{\mathrm{Pr}}\frac{\partial T}{\partial n}$$

Non-dimensional Numbers:

$$M = \frac{u}{\sqrt{\gamma R T_0}}$$ *Mach number*

$$\mathrm{Re} = \frac{\rho u h}{\mu}$$ *Reynolds*

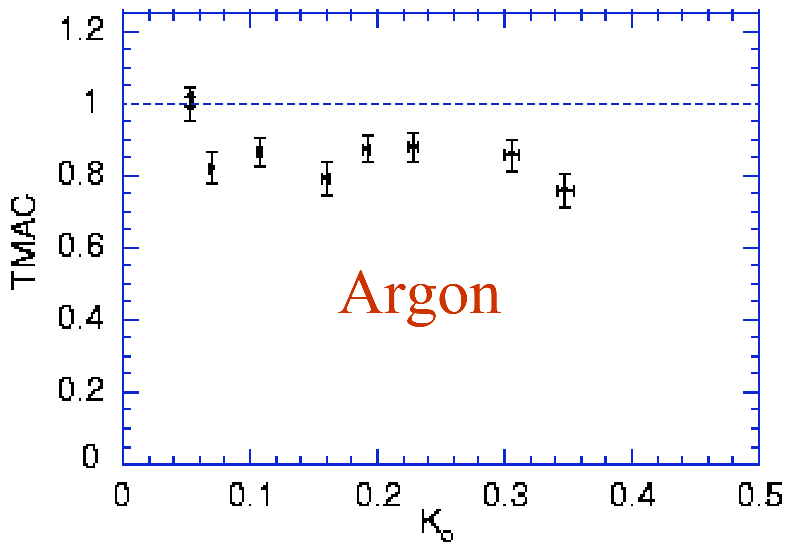
$$Ec = \frac{u^2}{C_p \Delta T} = (\gamma - 1)\frac{T_0}{\Delta T}M^2$$ *Eckert*

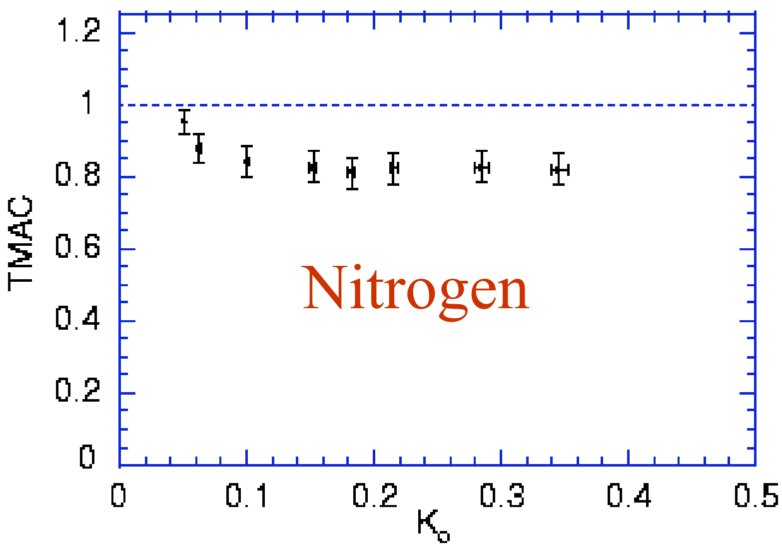
$$Kn = \frac{\lambda}{h} = \sqrt{\frac{\pi\gamma}{2}}\frac{M}{\mathrm{Re}}$$ *Knudsen*

- Independent parameters: **Re, Pr and Kn**

Accommodation Coefficients

•*(Breuer et al.)*





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

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

<u>References:</u> *Seidl & Steible* (1974); *Lord* (1976)

Compressible Microflows: High-Order Models

Stress Tensor:

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

Burnett Stress

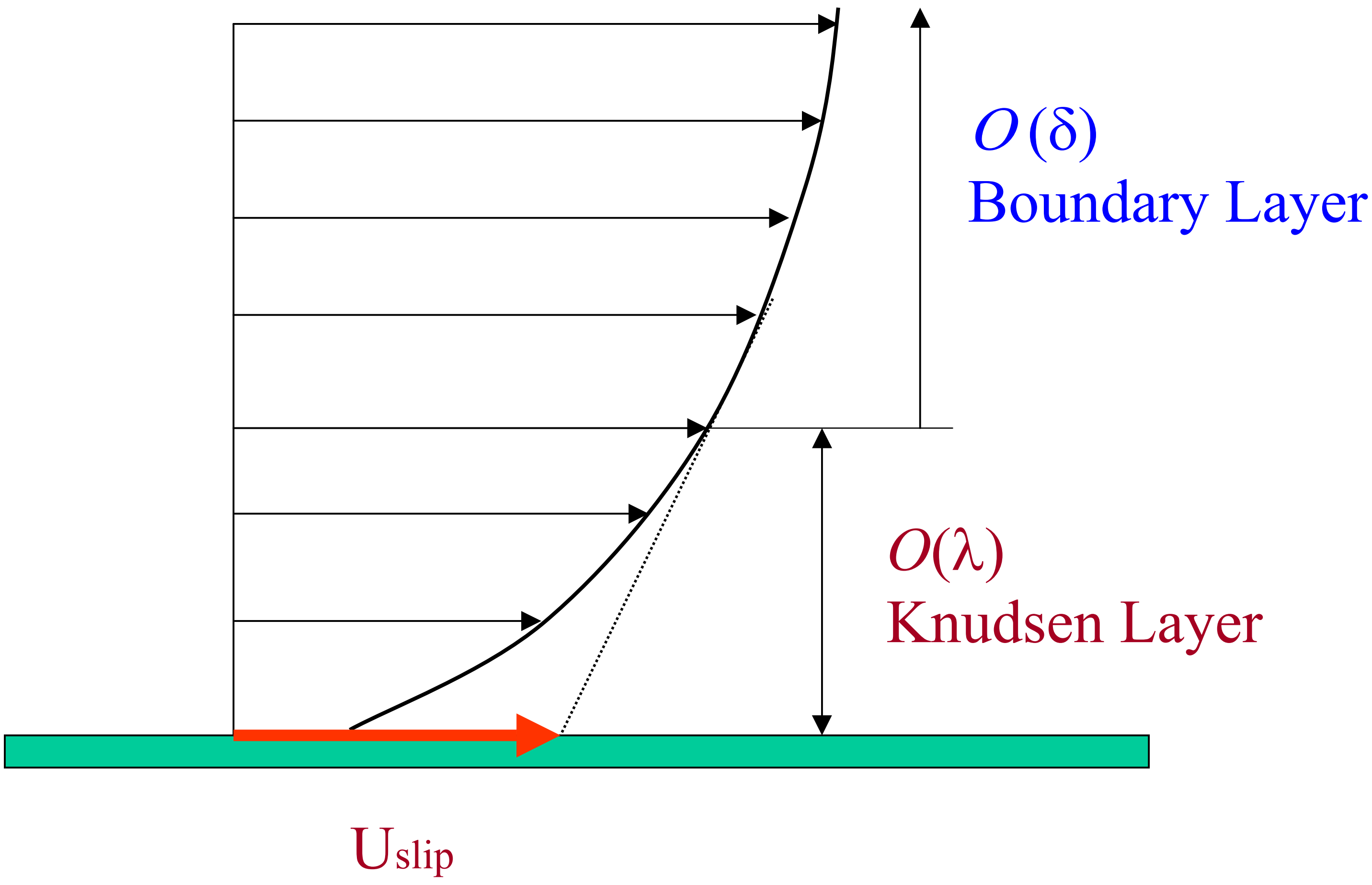
$$+\frac{\mu^2}{p}\left[\omega_4 \frac{1}{\rho T}\frac{\partial p}{\partial x_i}\frac{\partial T}{\partial x_j} + \omega_5 \frac{R}{T}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_j} + \omega_6 \frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j}\right]$$

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 a second-order Chapman-Enskog expansion for Kn and they require second-order slip conditions. (sections 2.3, 4.4 and 5.1 in K & B (2002).*

Why Slip ?

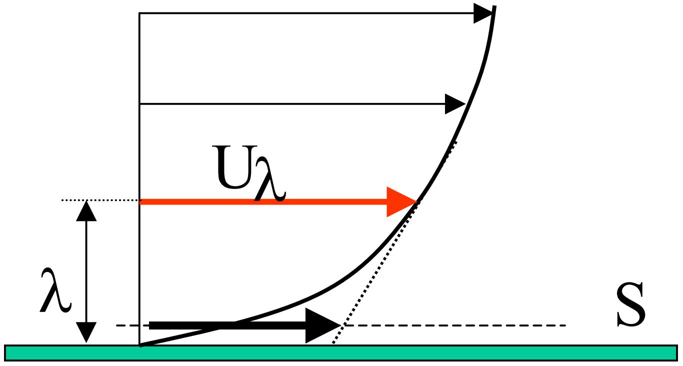


Slip Boundary Conditions

$$U_g - U_w = \frac{(2-\sigma)}{\sigma} Kn \frac{\partial U}{\partial n} + \frac{3(\gamma - 1)}{2\pi} Kn^2 \operatorname{Re} \frac{\partial T}{\partial s}$$

Maxwell 1879

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



U_{slip}=U_{gas} on S

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

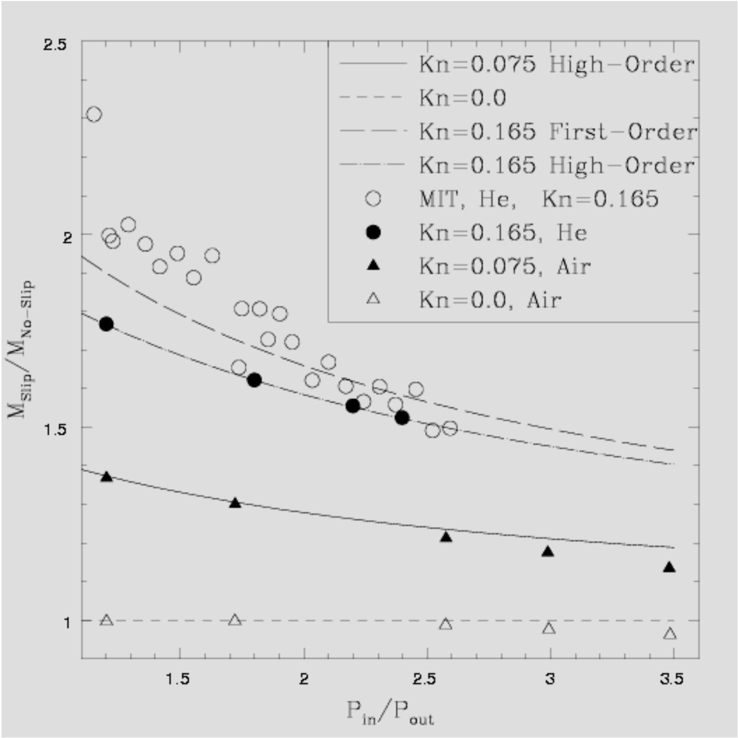
$$U_g - U_w = \frac{(2-\sigma)}{\sigma}\left(\frac{Kn}{1 - b\, Kn}\right)\frac{\partial U}{\partial n}$$

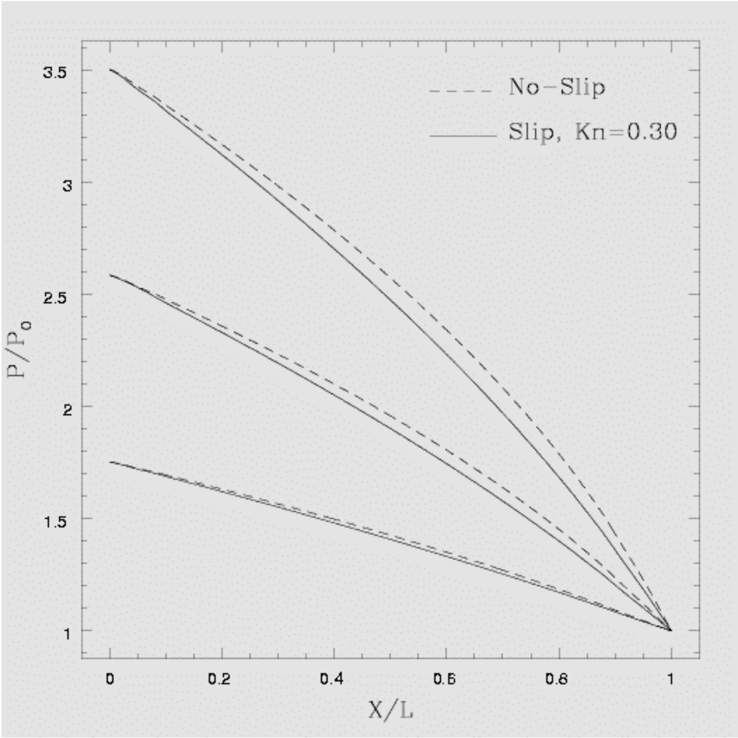
$$b = \left.\frac{U_o''}{2U_o'}\right|_s$$

Slip Flow Regime ($Kn<0.1$)

- **Compressibility**
- **Rarefaction**
- **Viscous Heating**
- **Thermal Creep**

Compressibility versus Rarefaction



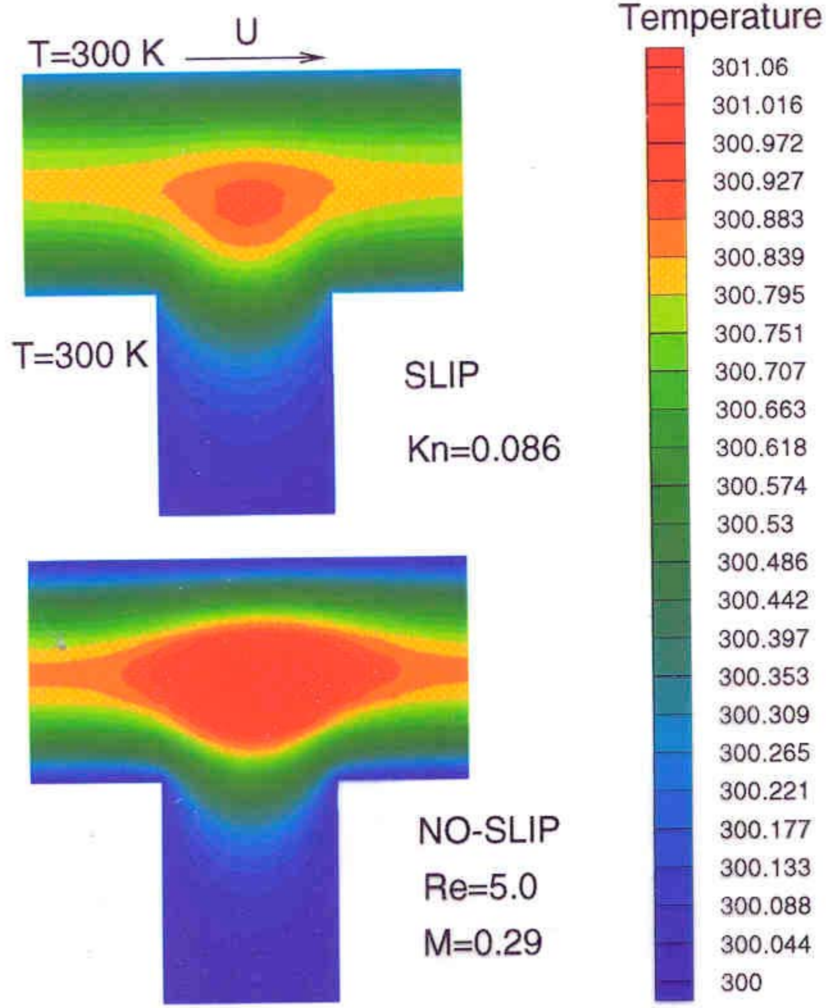


Increase in the mass flowrate compared to the No-Slip Flow

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

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

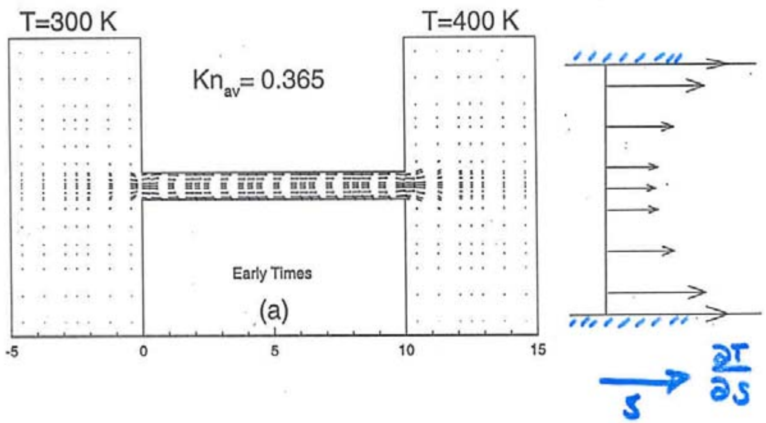
Viscous Heating

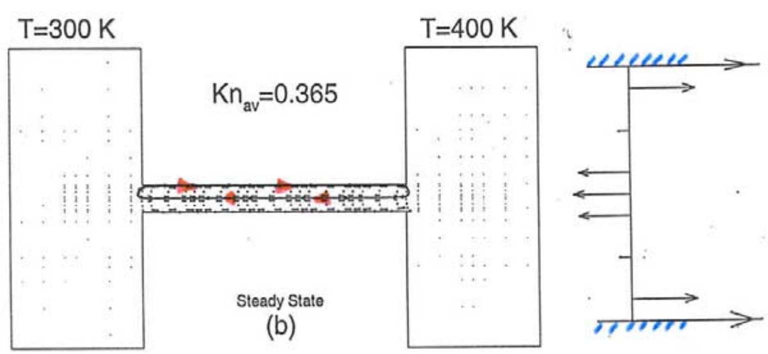


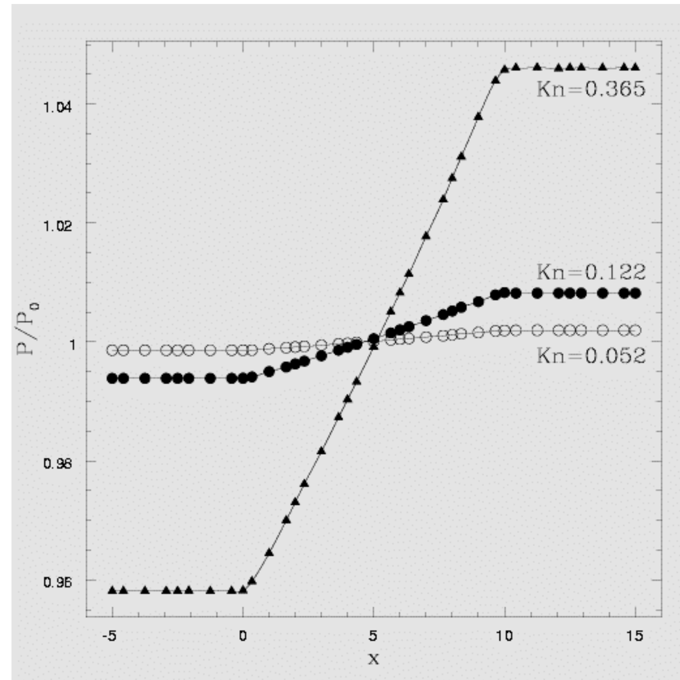
$$\Delta T = 1\ K$$

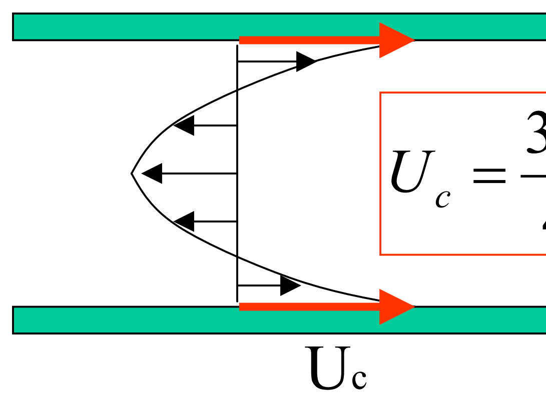
$$\frac{\partial T}{\partial n} \approx 10^6\ (K/m)$$

Thermally Induced Flows:
Thermal Creep







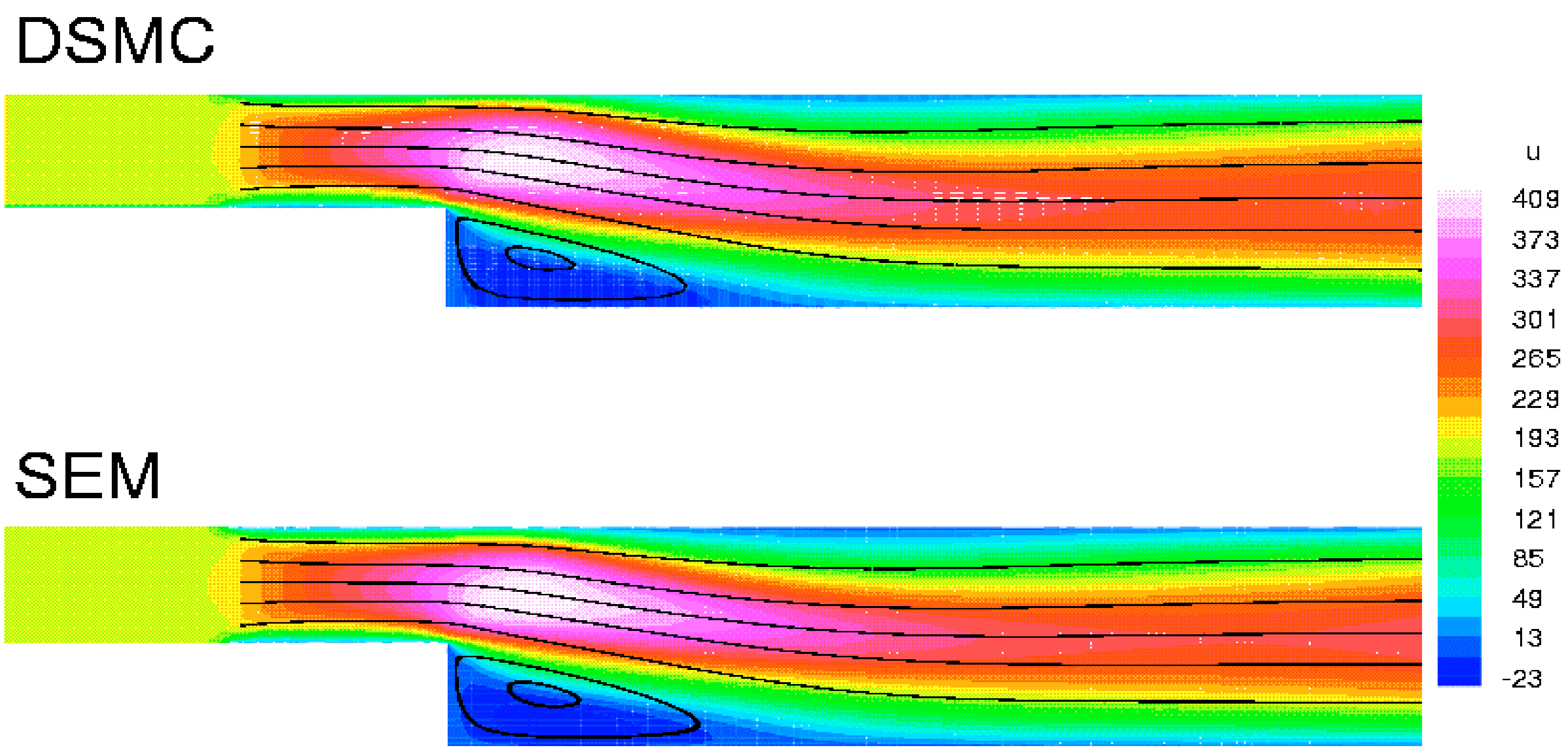


$$U_c = \frac{3\mu R}{4P}\frac{\partial T}{\partial s}$$

Comparisons of Molecular versus Continuum Solutions

(Velocity Contours)

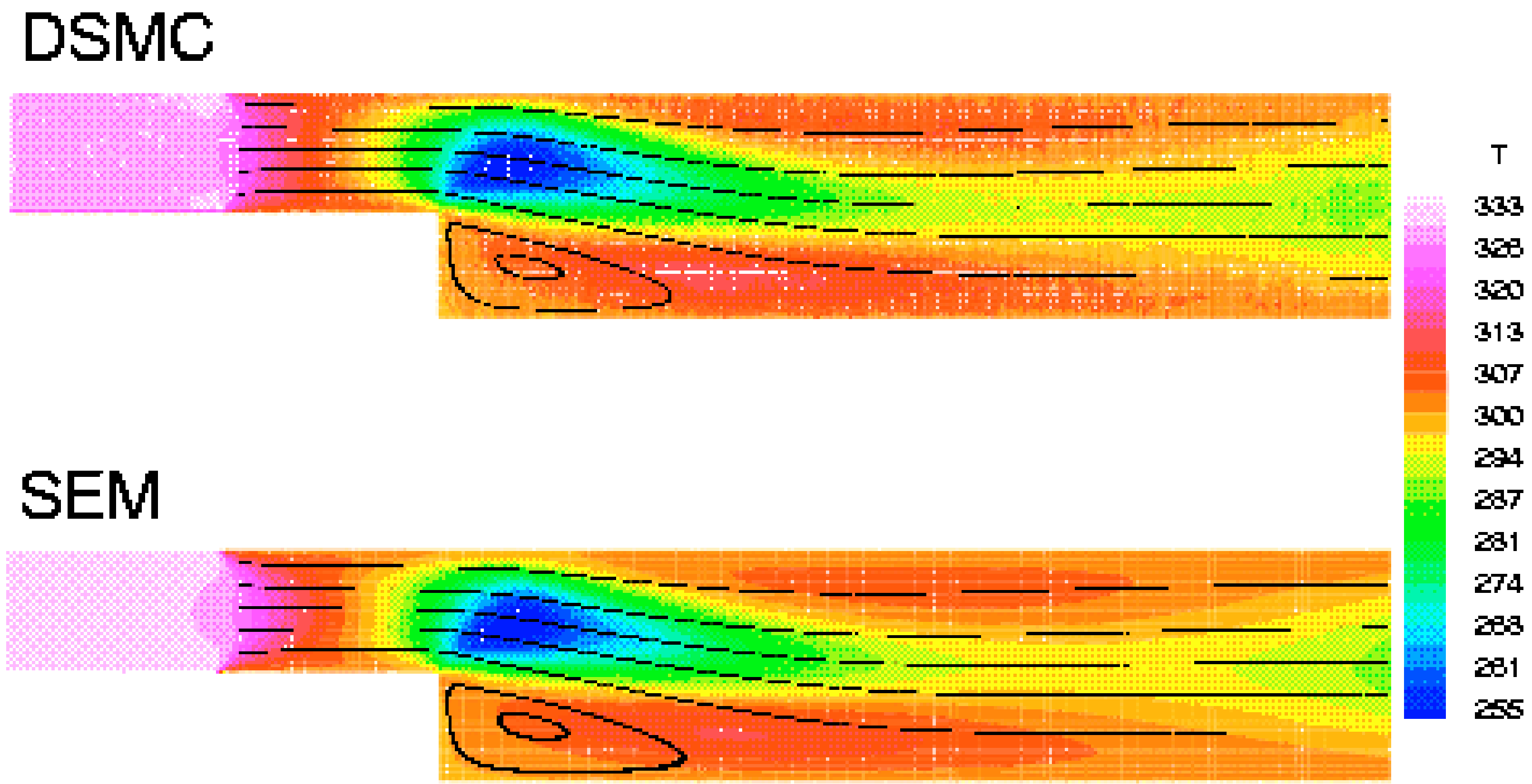
$Re=80, \quad Kn_o=0.05, \quad M_i=0.55, \quad Pr=0.7$



Comparisons of Molecular versus Continuum Solutions

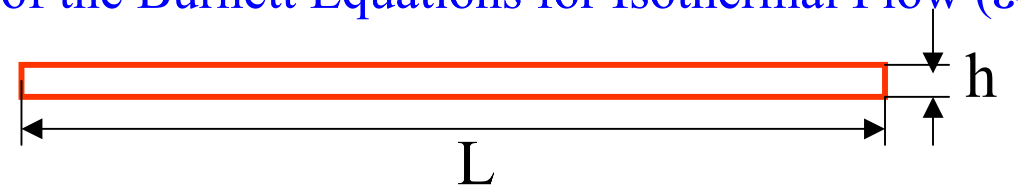
Temperature Contours

$Re=80, \quad Kn_o=0.05, \quad M_I=0.55, \quad Pr=0.7$



Transitional & Freemolecular Flow Regimes (Kn>0.1)

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



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

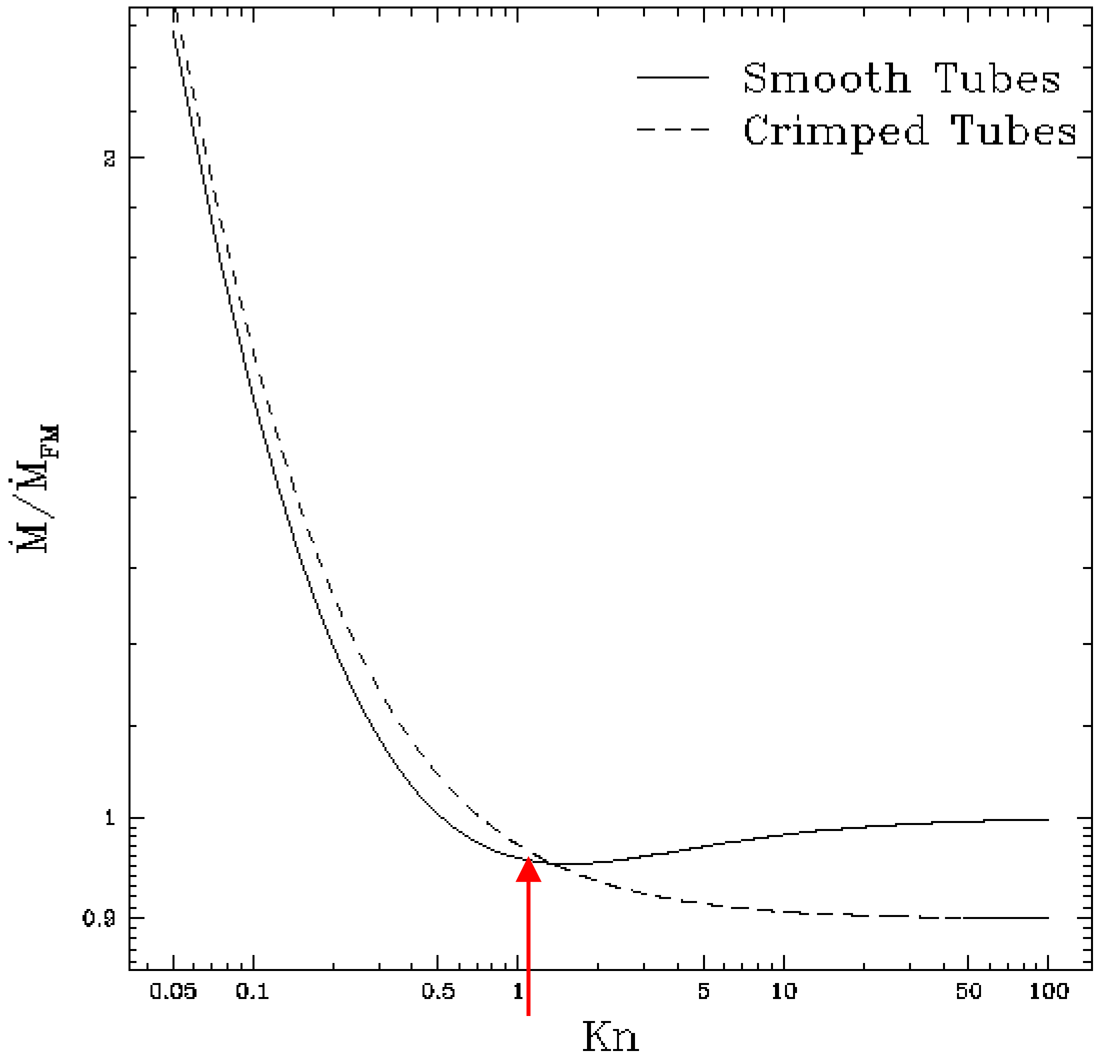
$$P_y\left[1-\frac{\pi\gamma}{3}Kn_{out}^2\ M_{out}^2\left(\frac{P_{out}}{P}\right)^2 U_y^2\right]= \frac{4\sqrt{\pi\gamma/2}}{3}Kn_{out}\ M_{out}\left(\frac{P_{out}}{P}\right)U_yU_{yy}+O(\varepsilon)$$

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

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

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

Transition and Free Molecular Flow Regimes and Knudsen's Minimum



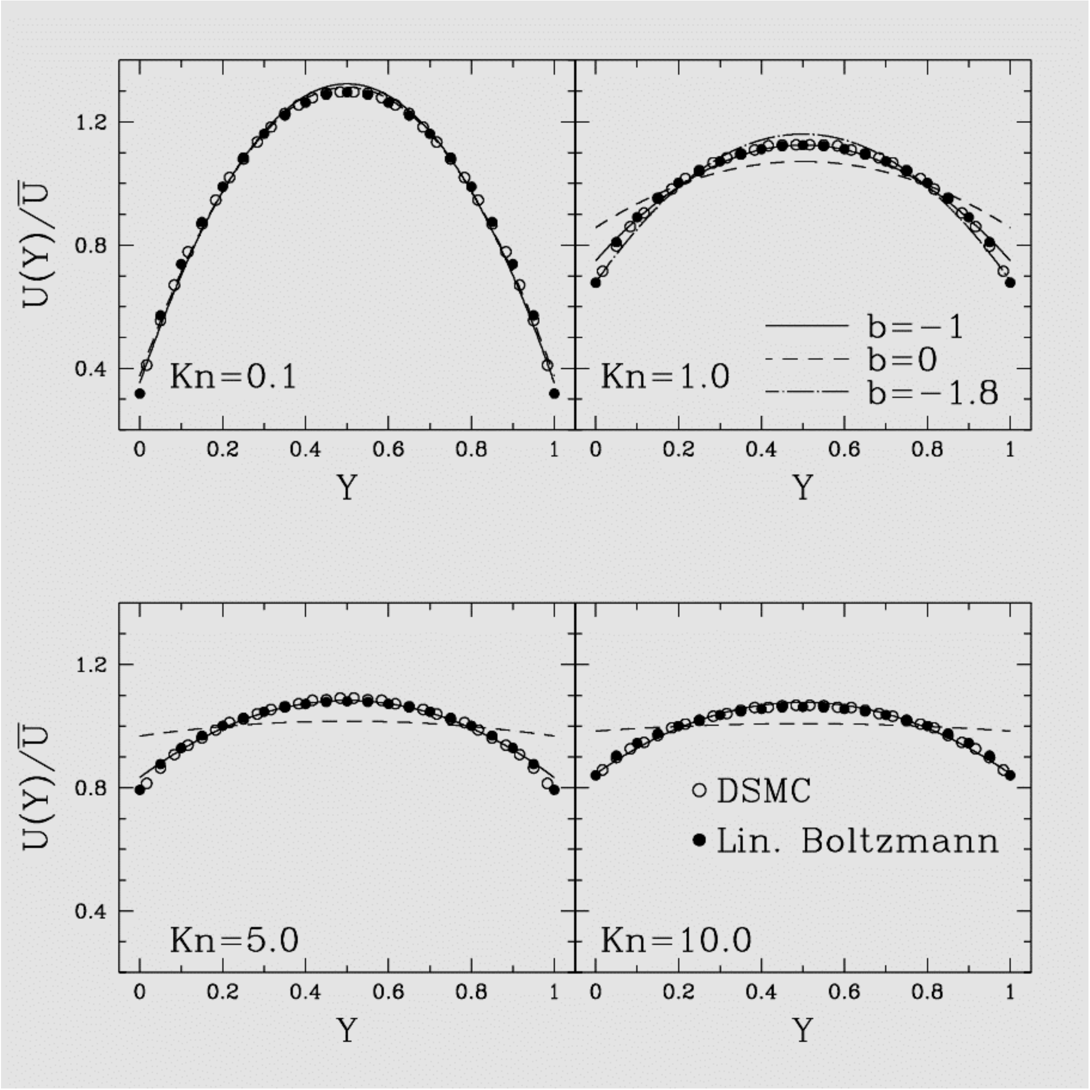
Knudsen's Minimum

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

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

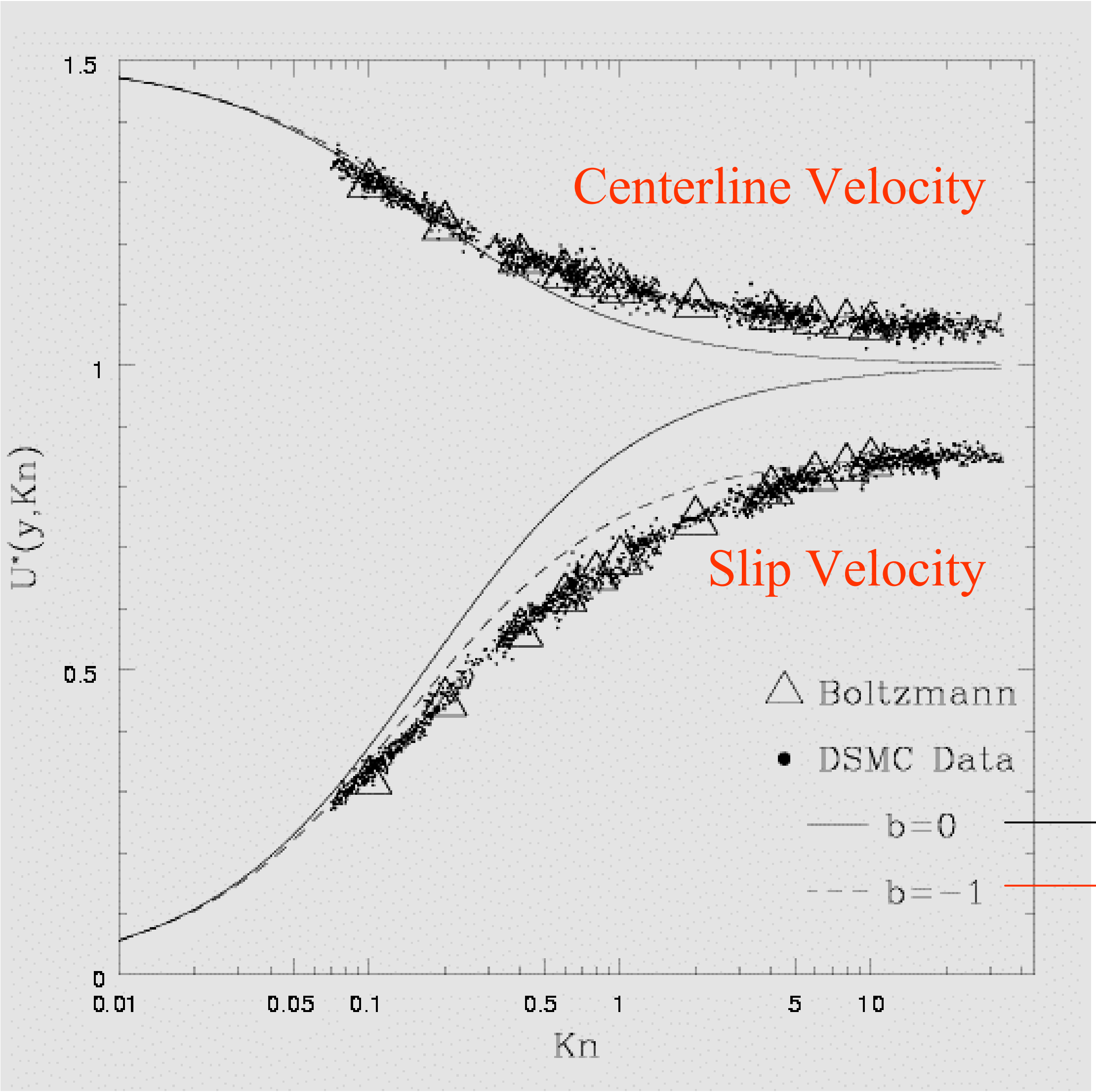
is plotted against the average pressure!

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



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

Universal Velocity Scaling

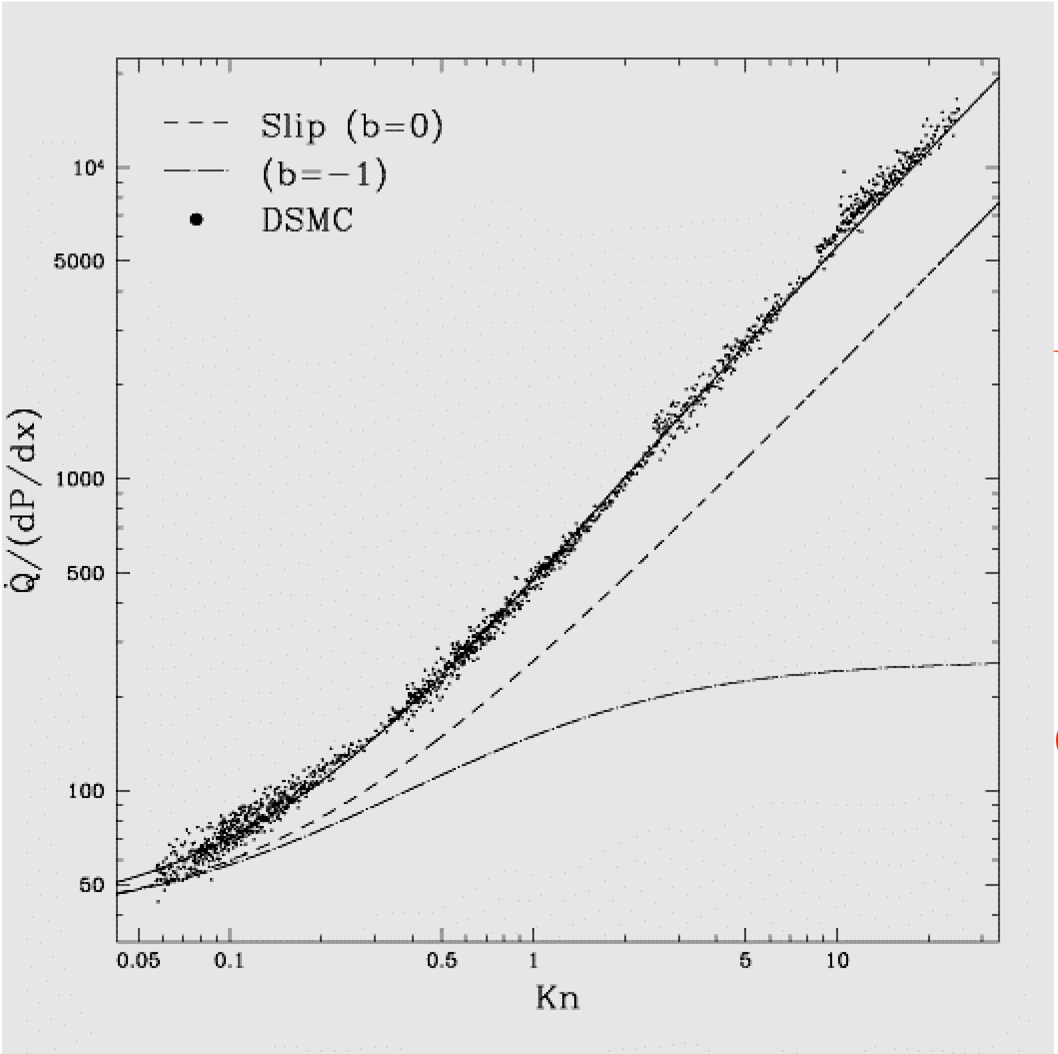


$$U(Y,Kn) = \left[\frac{-\left(\frac{y}{h}\right)^2 + \left(\frac{y}{h}\right) + \frac{Kn}{1-b\,Kn}}{\frac{1}{6} + \frac{Kn}{1-b\,Kn}} \right]$$

Maxwell's

New Model

Modeling Flowrate



Volumetric Flowrate

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

Using Navier-Stokes w/ Slip

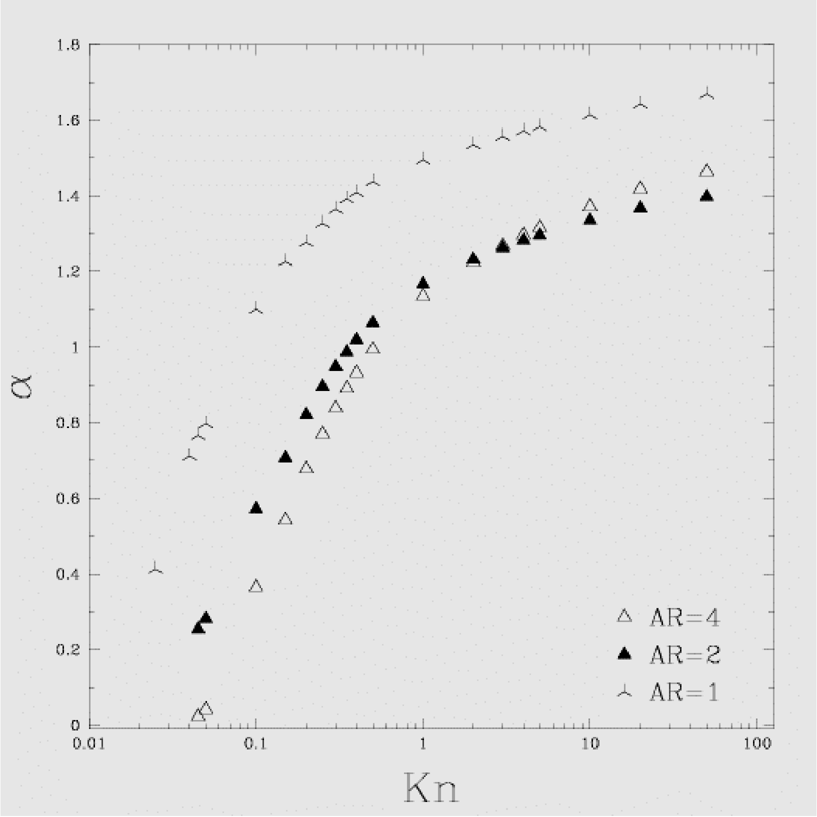
$$\frac{\dot{Q}}{W} = -\frac{h^3}{12\mu}\frac{dP}{dx}\left[1 + \frac{6Kn}{1 - bKn}\right]$$

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



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

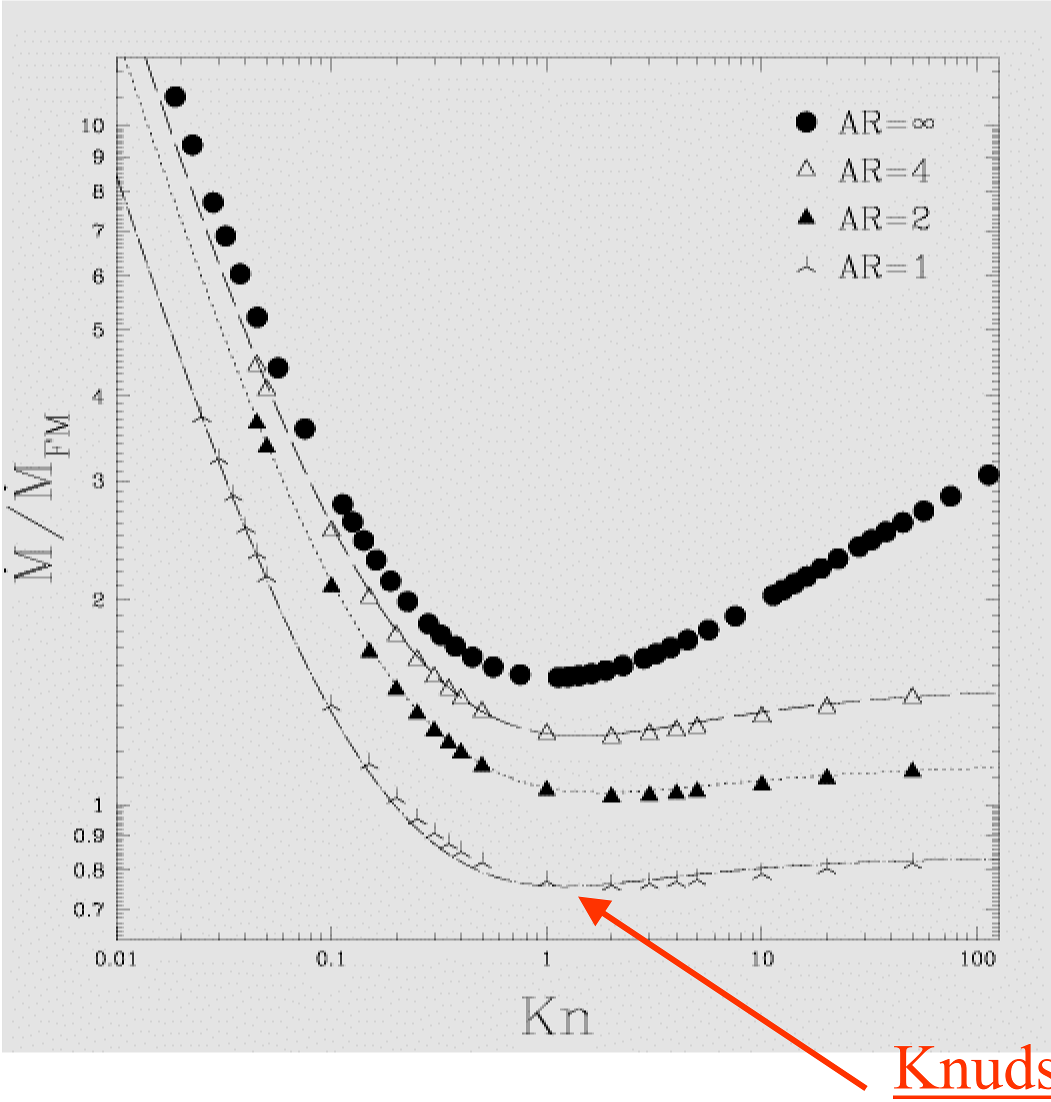
$$\alpha \Rightarrow 0 \quad as \quad Kn \Rightarrow 0$$

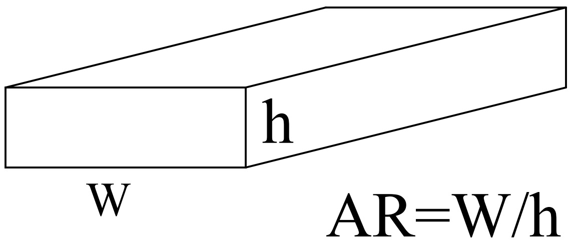
$$\alpha \Rightarrow \alpha_o \ \ as \ \ Kn \Rightarrow \infty$$

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

α_1 & β are empirical parameters

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

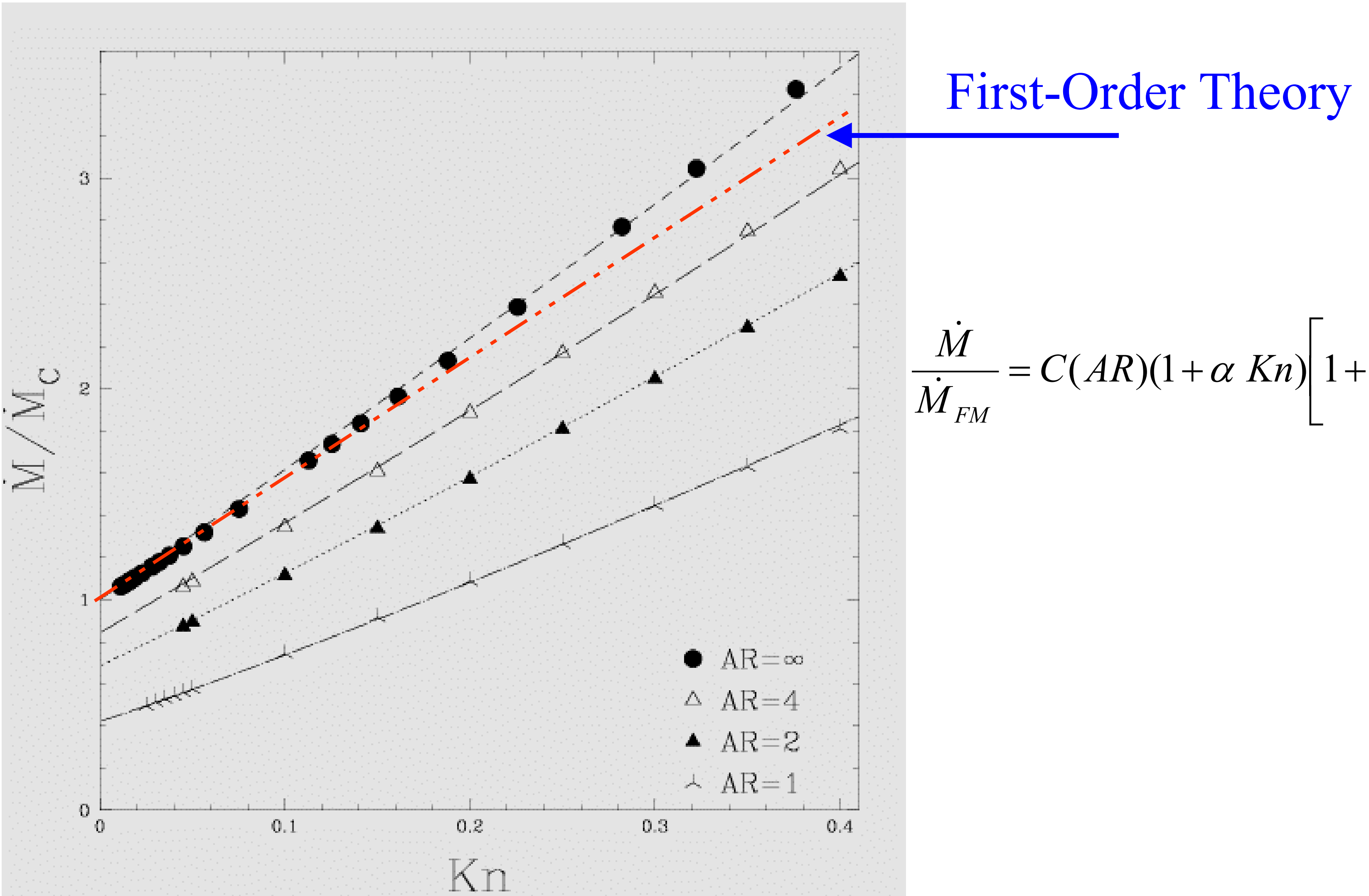




$$\frac{\dot{M}}{\dot{M}_{FM}} = \frac{C(AR)}{6\,Kn}(1+\alpha Kn)\left[1+\frac{6Kn}{1-b\,Kn}\right]$$

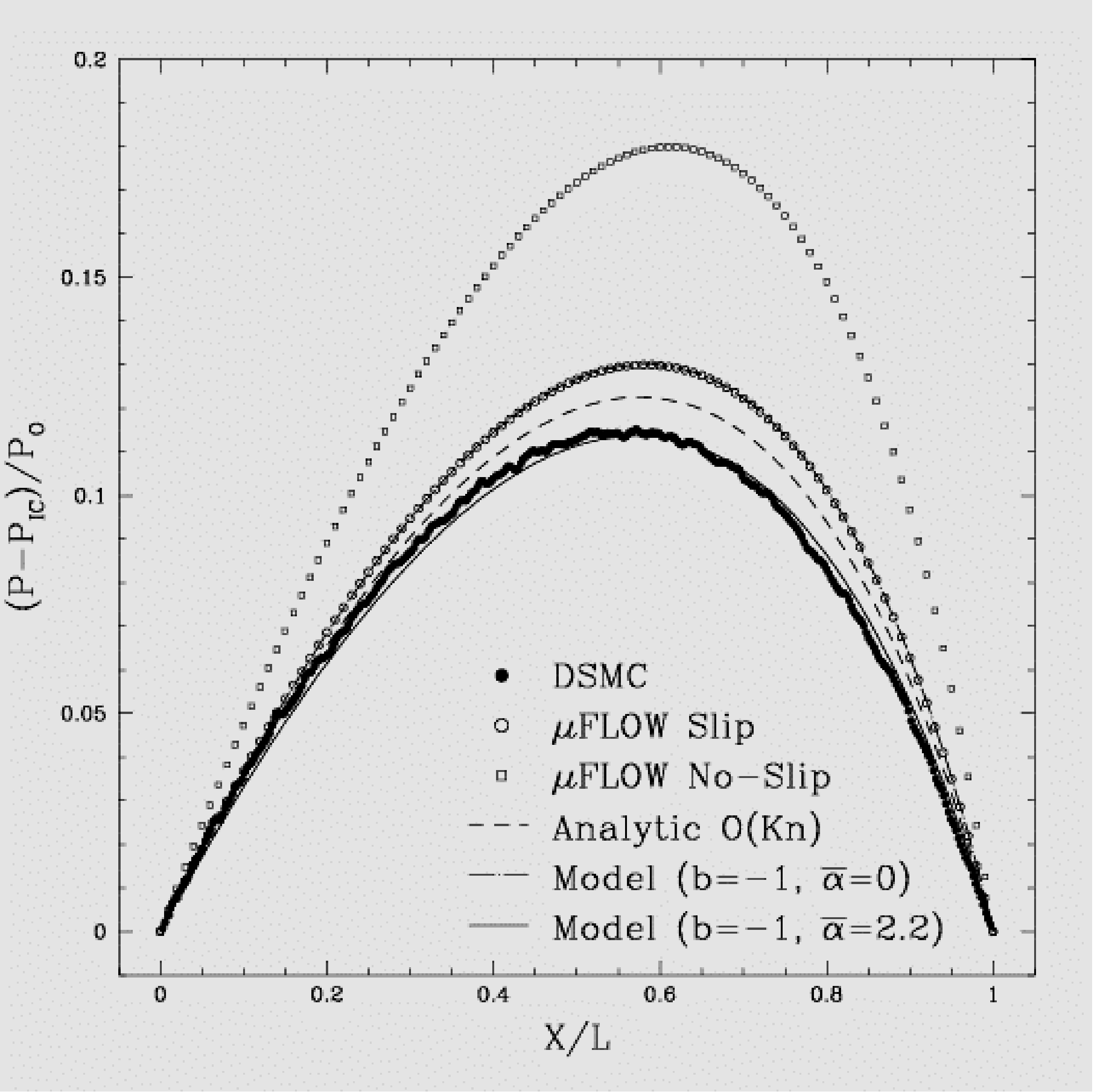
$$\dot{M}_{FM} = \frac{h^2 W}{\sqrt{2RT_o}}\frac{\Delta P}{L}$$

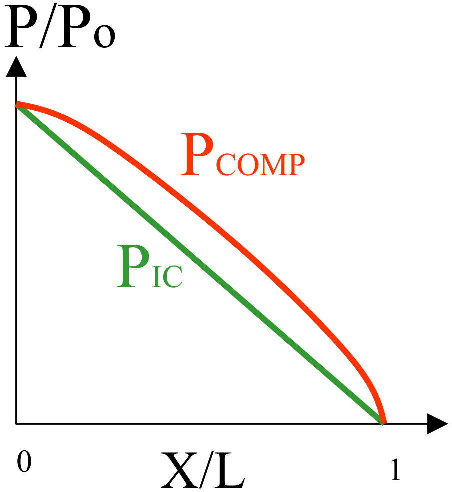
Flowrate Scaling in Arbitrary Aspect-Ratio Rectangular Ducts (Based on the Continuum Limit)



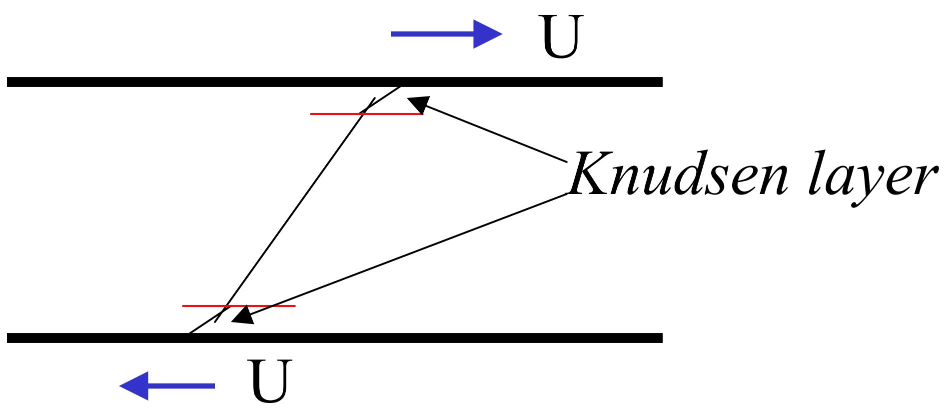
$$\frac{\dot{M}}{\dot{M}_{FM}} = C(AR)(1+\alpha\ Kn)\left[1+\frac{6Kn}{1-b\ Kn}\right]$$

Channel Flow, Nonlinear Pressure Distribution





A Unified Model for Plane Couette Flows



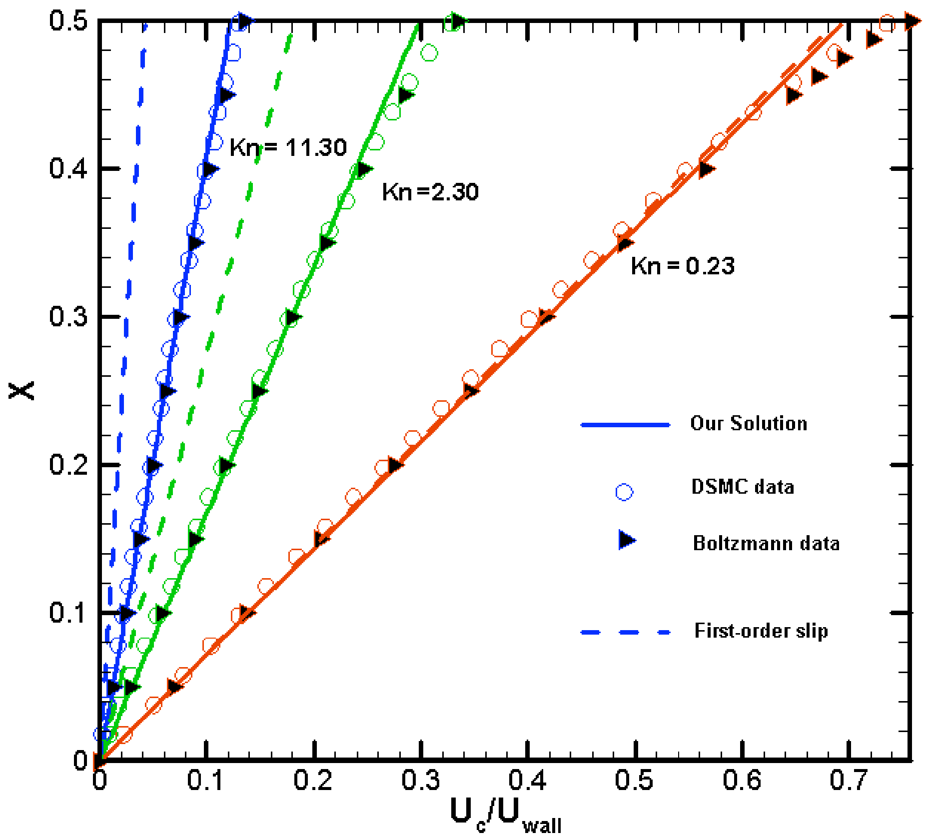
$$U_c(y) = \frac{2U}{1+2\alpha Kn}\frac{y}{D} \qquad \alpha = a + b\tanh(cKn^d)$$

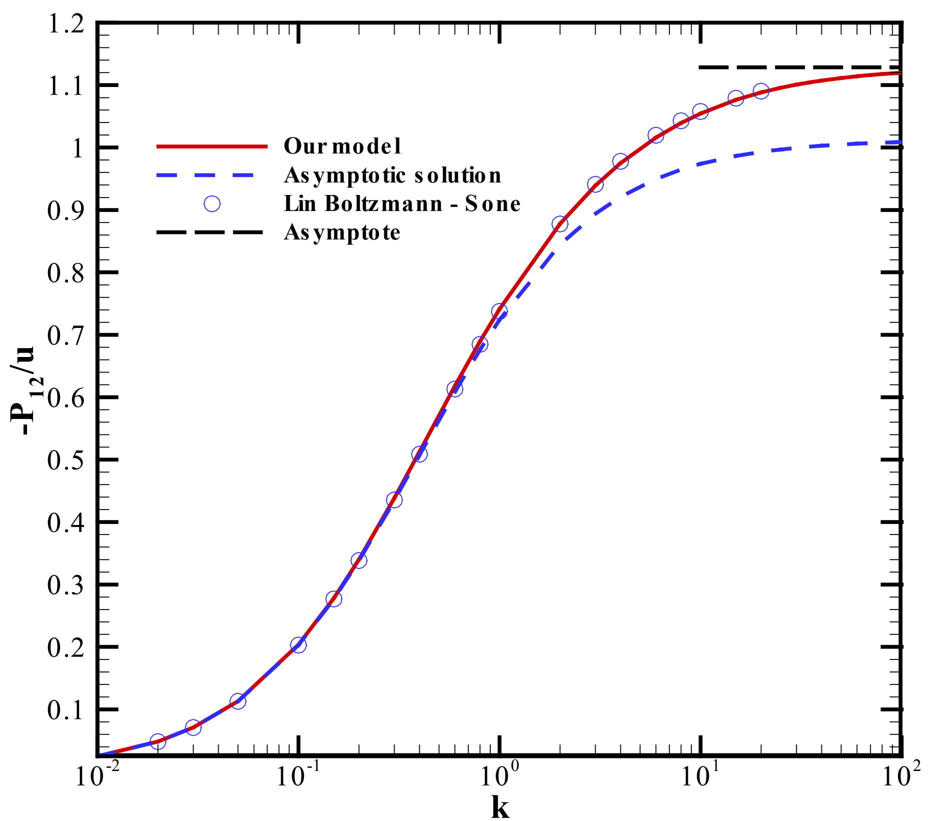
Macromodel

$$P_{12} = -\frac{g\theta k+1}{\theta k+1}\left\{\frac{2\beta kU}{1+2\gamma k}\right\} \qquad k = \frac{\sqrt{\pi}}{2}Kn$$

•Validation against: DSMC (argon, hard spheres) and *linearied* Boltzmann solutions

A Unified Model for Plane Couette Flows

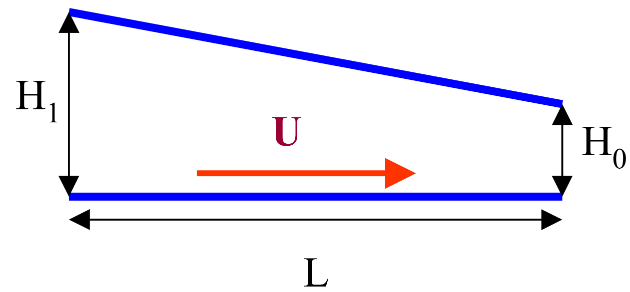




Analytical models of velocity profile & shear stress for $0 < Kn < \infty$

P. Bahukudumbi, TAMU, MSME, August 2002

Gas Damping/Lubrication: Reynolds Equation



General equation:

$$\nabla \bullet \left[\left(\frac{\rho h^3}{\mu} \right) \nabla p \right] = 12 \frac{\partial(\rho h)}{\partial t} + 6 \nabla \bullet (\rho h U)$$

Inertial-free flow if: $\mathrm{Re} \times \left(\frac{H_0}{L} \right)^2 << 1$

Then, leading-order solution: $\frac{dp}{dx} = \mu \frac{\partial^2 u}{\partial x^2}$ *where p=p(x)*

•Constant flowrate:

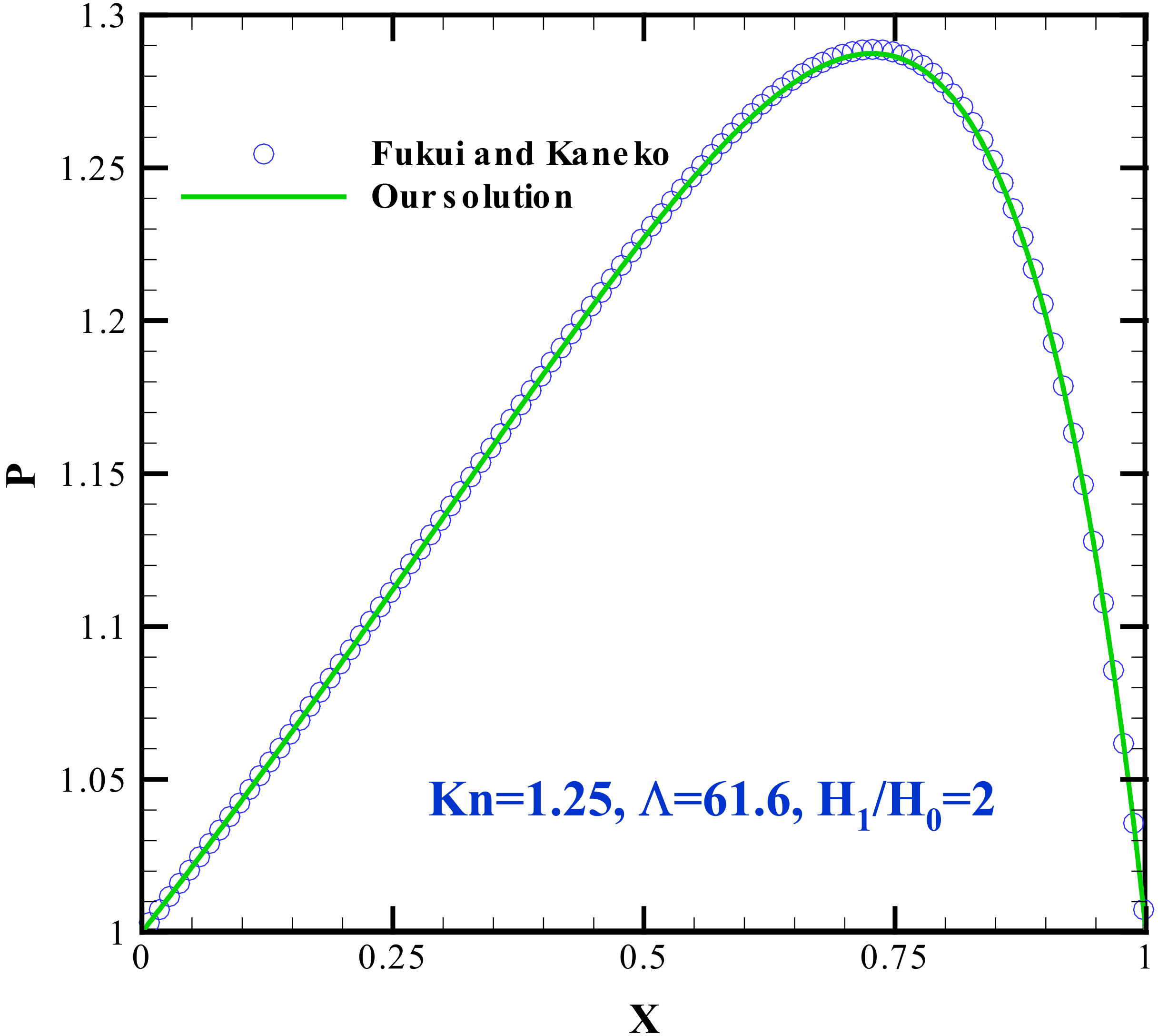
$$\frac{\partial}{\partial X} \left(H^3 P \frac{dP}{dX} \right) = \Lambda \frac{\partial}{\partial X} (PH) \qquad \Lambda = \frac{6 \mu U L}{p_0 H_0^2}$$

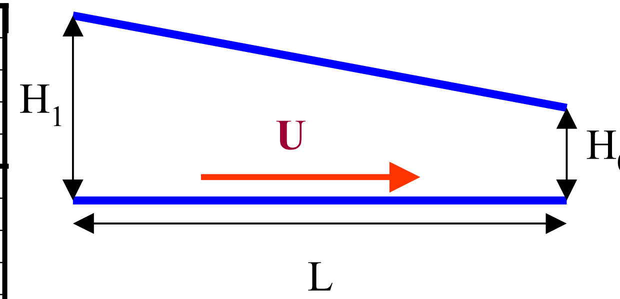
Bearing number

•Slip-Flow:

$$\frac{\partial}{\partial X} \left([1 + 6 \frac{2 - \sigma_v}{\sigma_v} Kn] H^3 P \frac{dP}{dX} \right) = \Lambda \frac{\partial}{\partial X} (PH)$$

Slider Bearing Pressure Distribution





$$\Lambda = \frac{6\mu UL}{p_o H_o^2}$$

$$P = \frac{p}{p_o}, \quad X = \frac{x}{L}$$

Accurate Predictions of Pressure, Velocity, Shear Stress & Flowrate

An Analytical model for generalized Reynolds equation

$0 < Kn < \infty$

Numerical Simulation for Gas Micro-Flows

DSMC Method:

- **Slow Convergence:**

$$\varepsilon \propto \frac{1}{\sqrt{n}}$$

- **Large Statistical Error:**

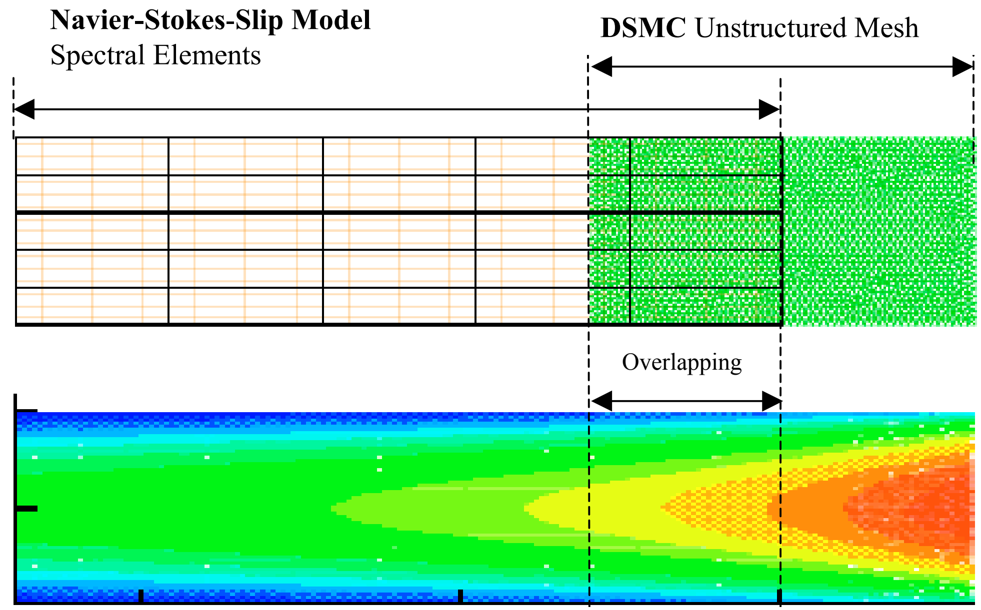
  (10^8 samples)

- **Extensive Number of Particles:**

  3 cells per λ
  and 20 particles per cell

Multi-Domain Simulation:

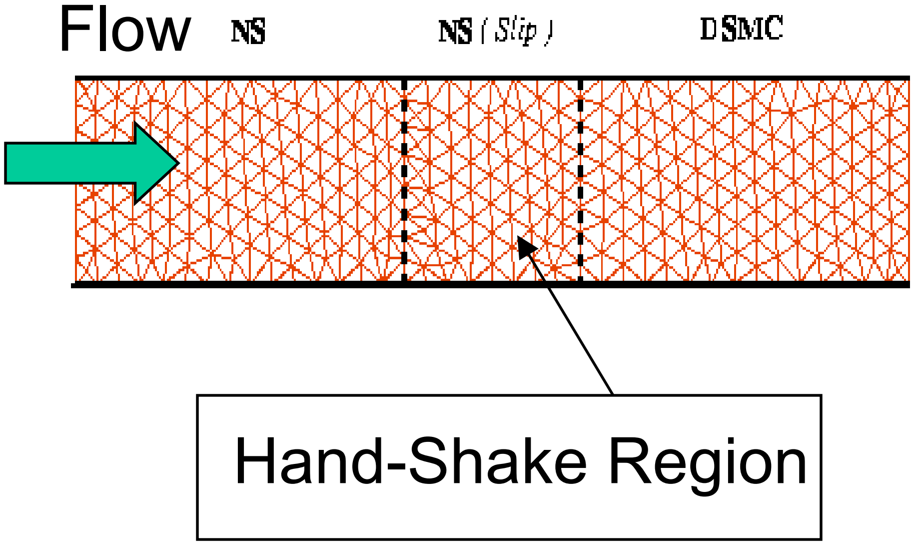
DSMC/Continuum Coupling

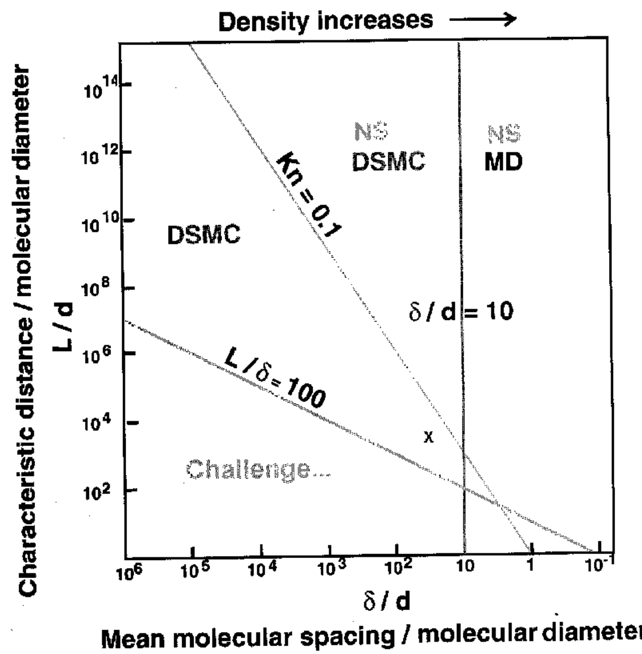


I. Boyd, AIAA 2001-0876 (14:30)

Micro-Macro Interface

- Hash & Hassan (1995)
- Garcia et al. (1999)
- Hadjiconstantinou (1999)
- Liu (1999)
- Aluru (2001)



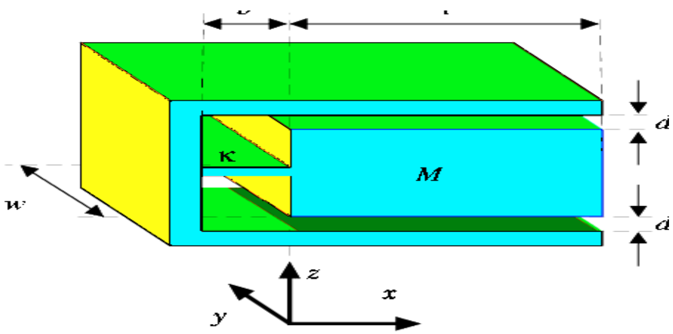


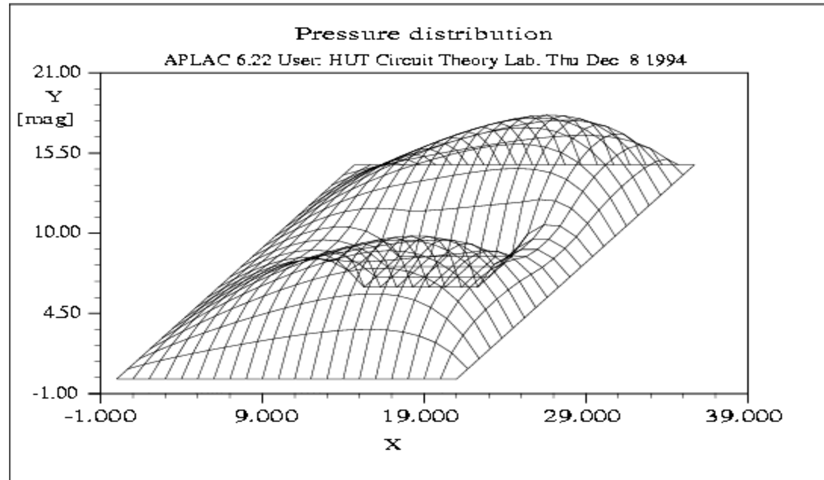
- Oran et al. (1998)

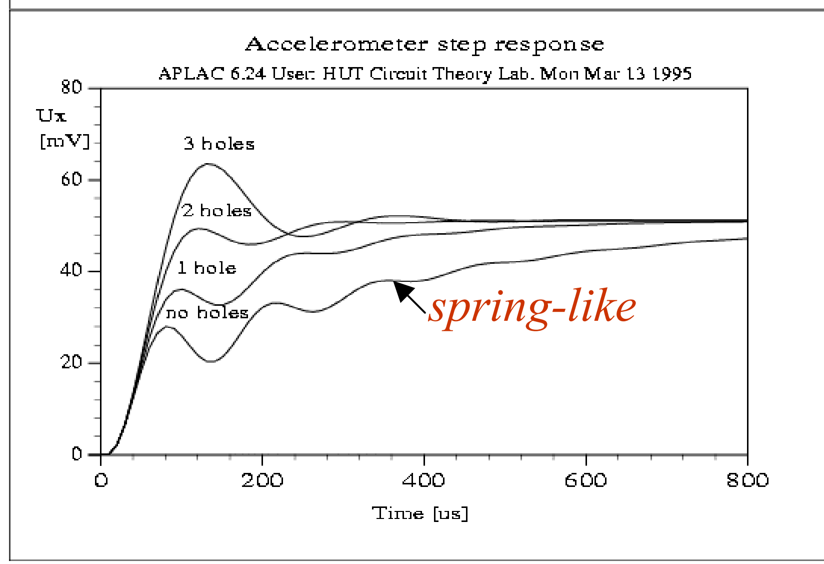
- Zanolli iterative patching

Coupled Domain Simulations

- Titling rectangular accelerometer
- Gap of 2 microns



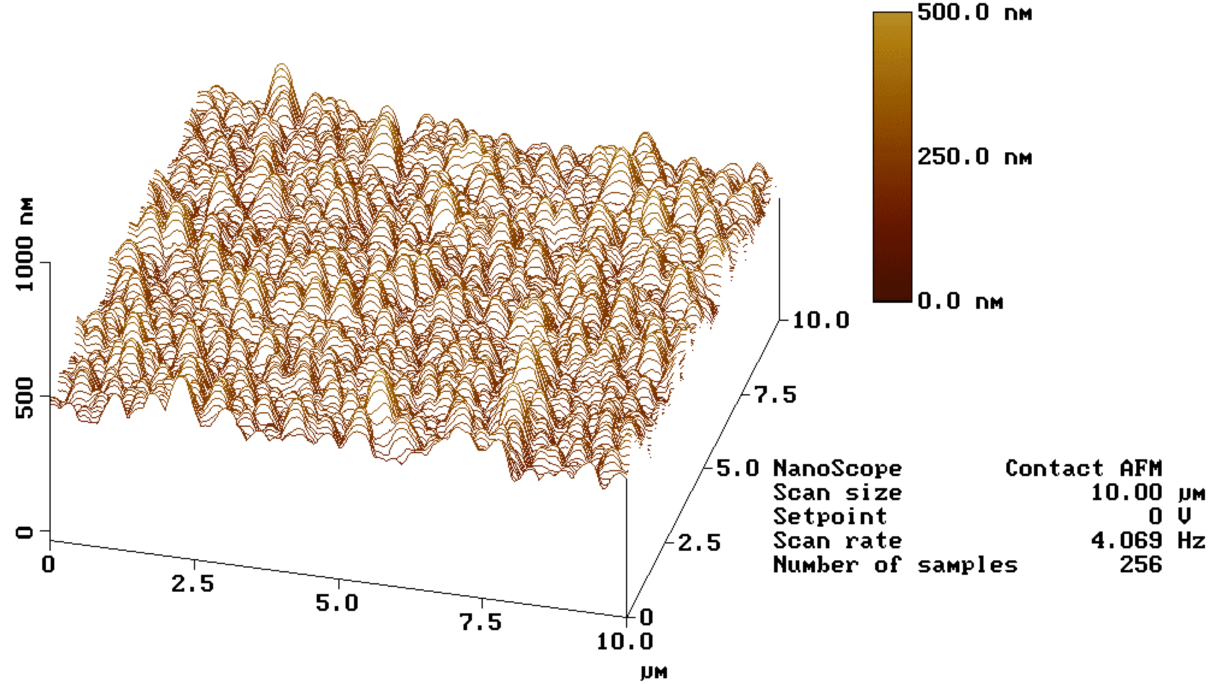




•Generalized Reynolds equation with electrostatic actuation.
•Dynamic response of a micro accelerometer with holes.

Courtesy of T. Veijola

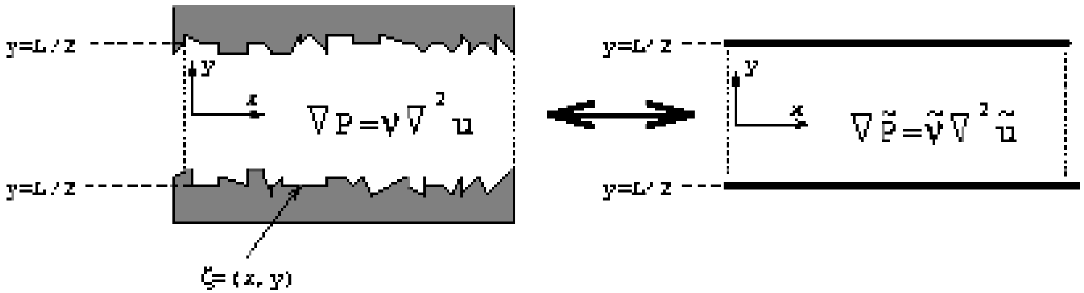
Modeling Roughness in Micro-Geometries



- Regularized roughness
- Equivalent effect
- Random walls

Apparent Diffusion: Roughness

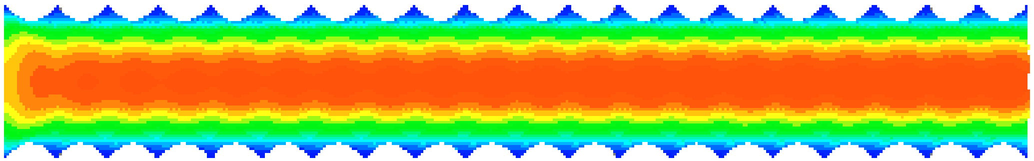
- Model the extra chaotic motion (extra diffusion) due to the rough boundary using correlation function of surface inhomogeneities



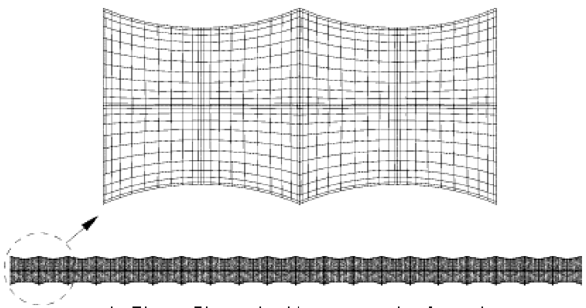
- Use Migdal tranformation from nuclear physics

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

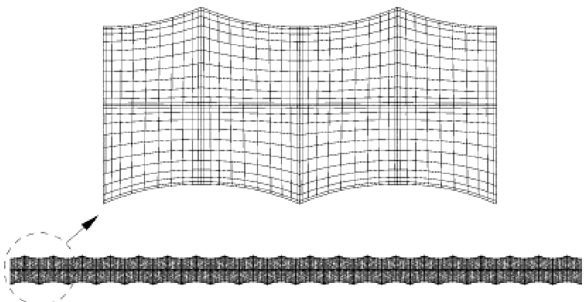
- Renormalize the viscosity to account for extra diffusion
- Solve new equation in simple domain
- Start with regular roughness



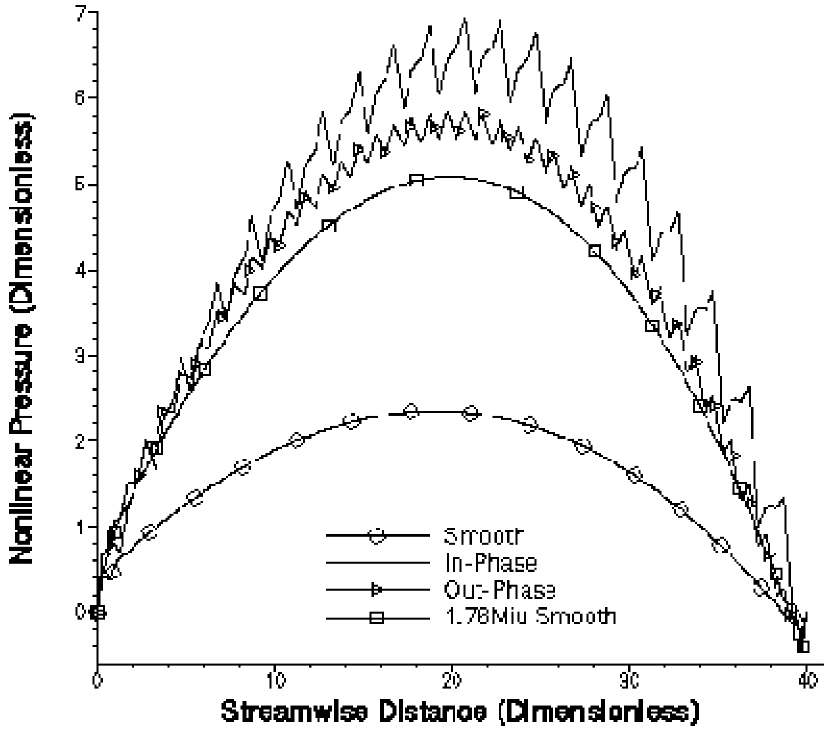
Roughness Effect on Pressure Drop

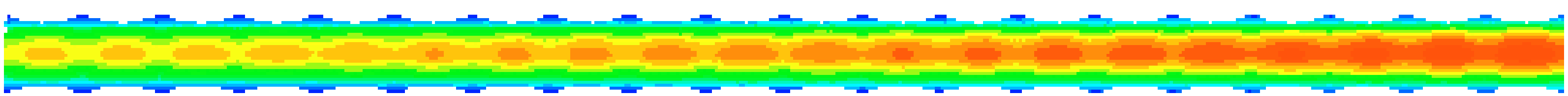


In-Phase Channel with aspect ratio of 20 : 1

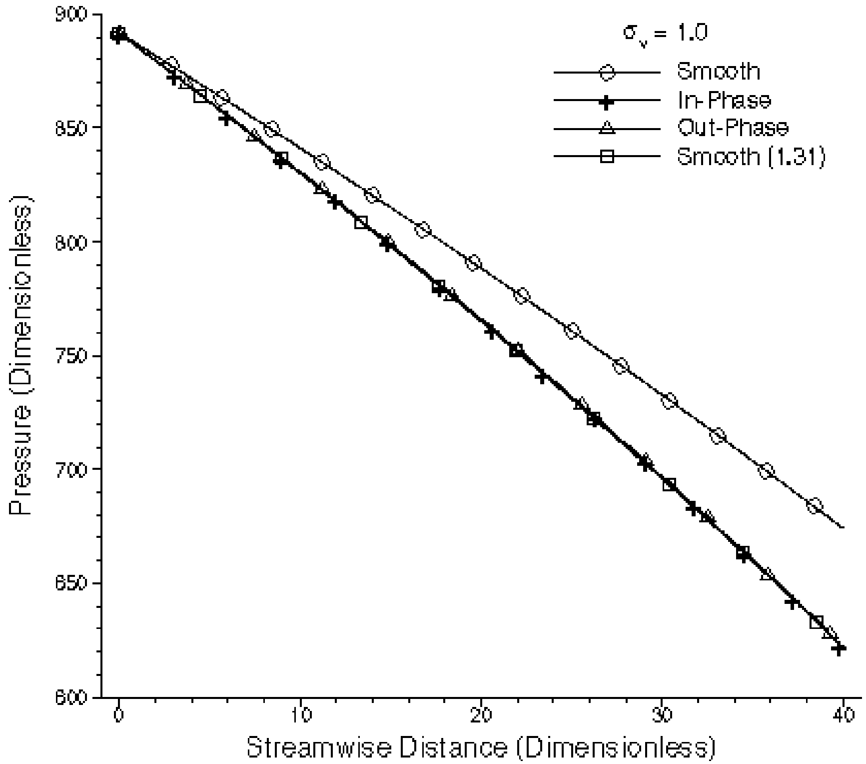


Out-Phase Channel with aspect ratio of 20 : 1





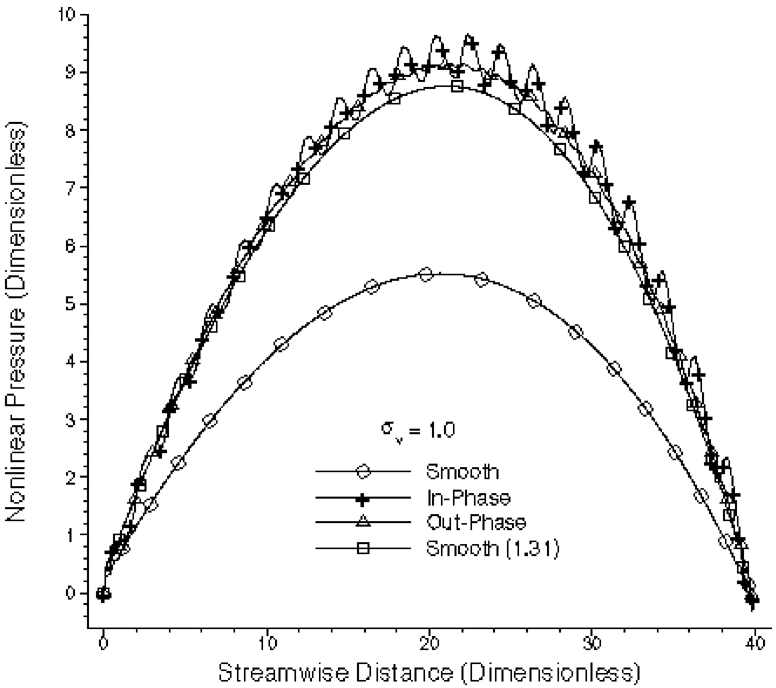
Slip Compressible Flow σ_v=1.0

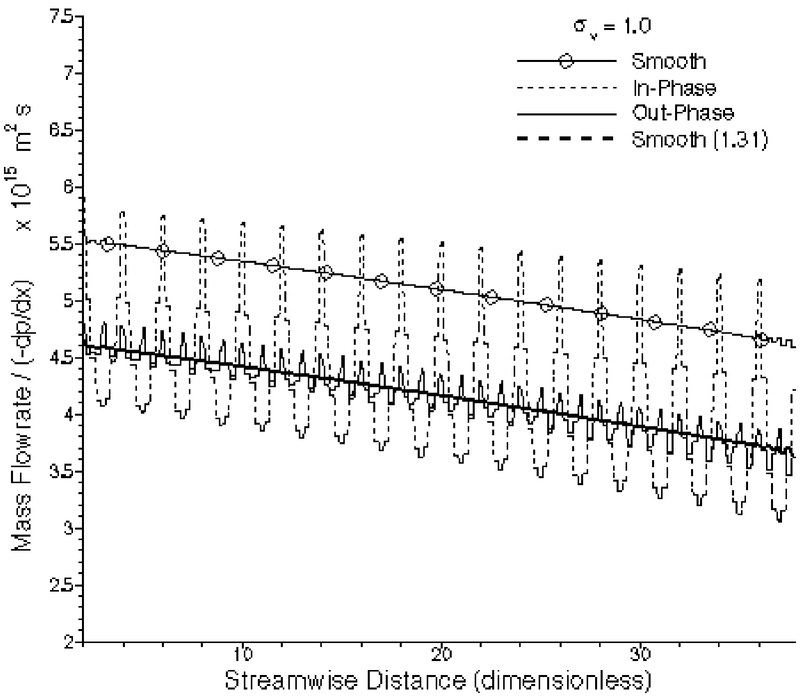


- Re = 0.36; with enhanced viscosity Re = 0.276
- Simulation - 0.640×10^{-5} kg/s, formula - 0.641×10^{-5} kg/s

  Simulation - 0.640×10^{-5} kg/s, formula - 0.643×10^{-5} kg/s(enhanced)
- Enhanced viscosity factor: 1.31

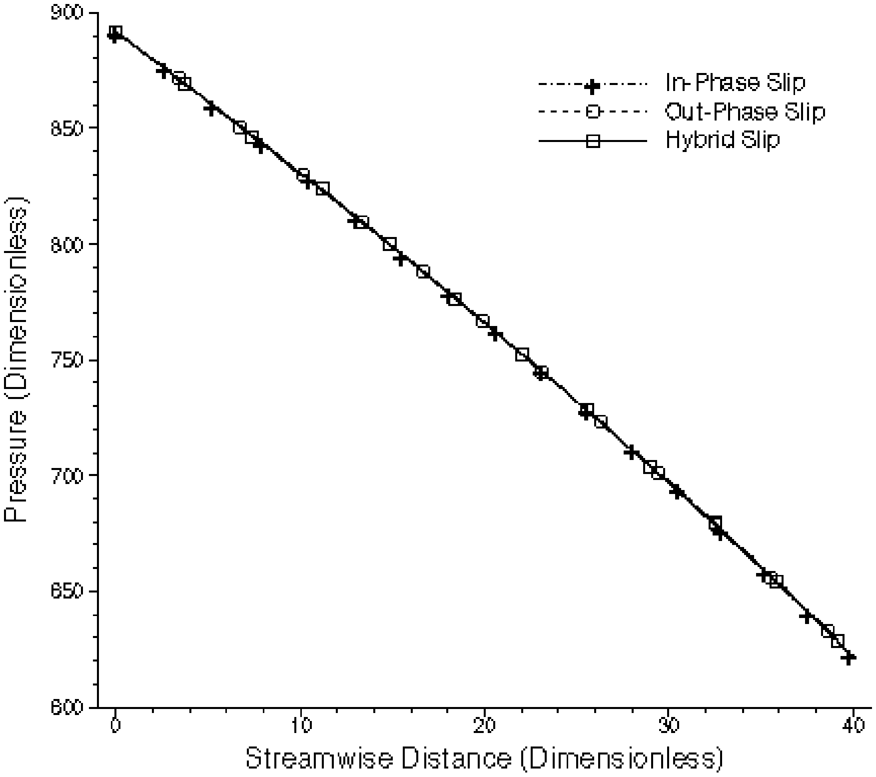
Slip Compressible Flow σ_v=1.0 (continued)





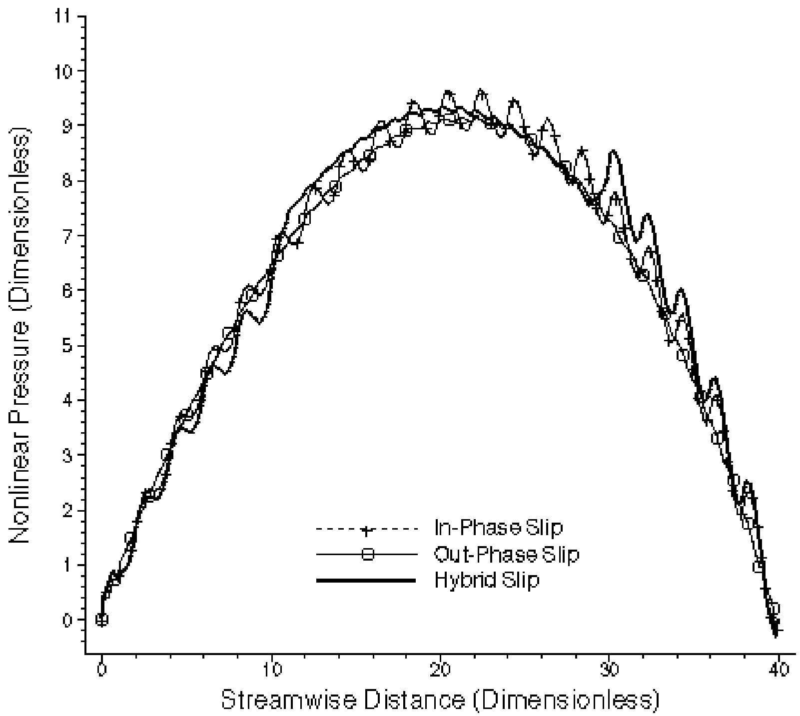
- Slip walls make the flow less compressible than noslip walls
- Slip flow needs more extra viscosity than noslip flow

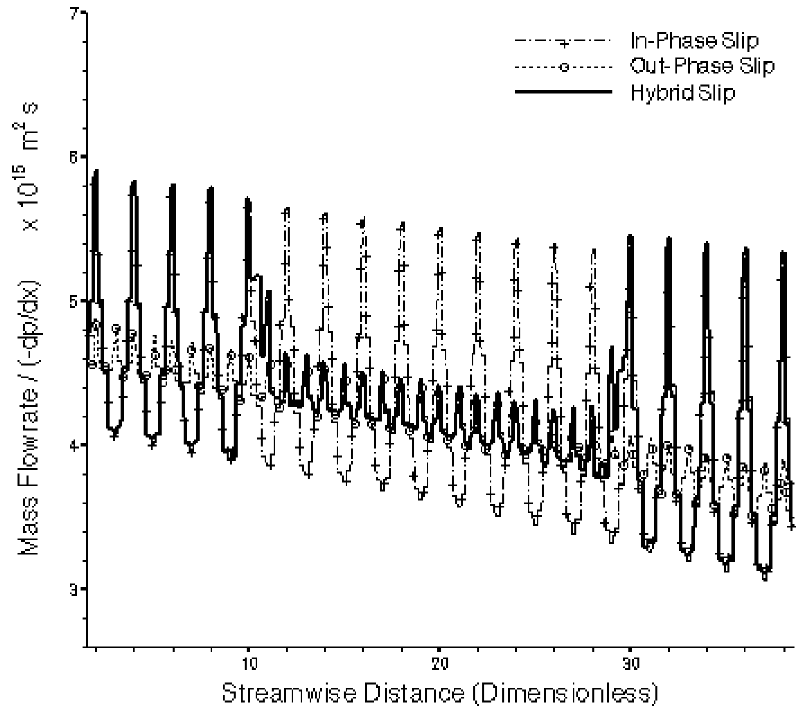
In-Phase, Out-of-Phase & Hybrid Channels



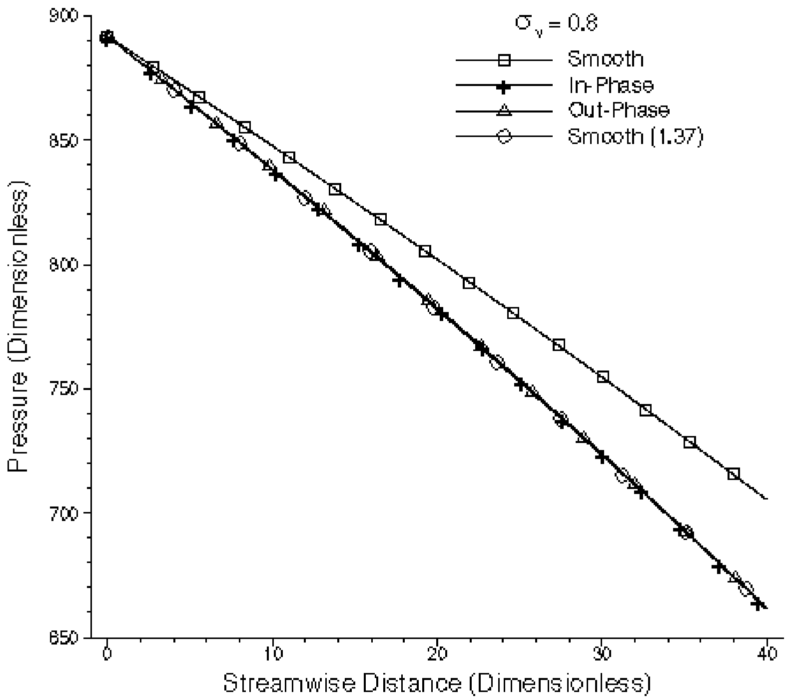
- These channels are hydrodynamically equivalent
- Artificial roughness patterns induce similar apparent diffusion

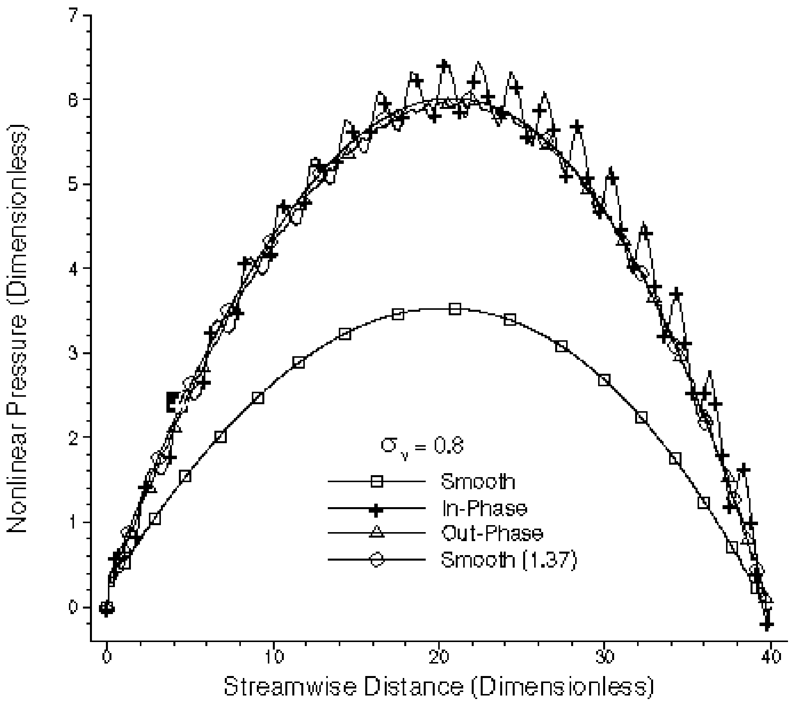
In-Phase, Out-of-Phase & Hybrid Channels (continued)





Slip Compressible Flow σ_v=0.8 and 0.6 (continued)

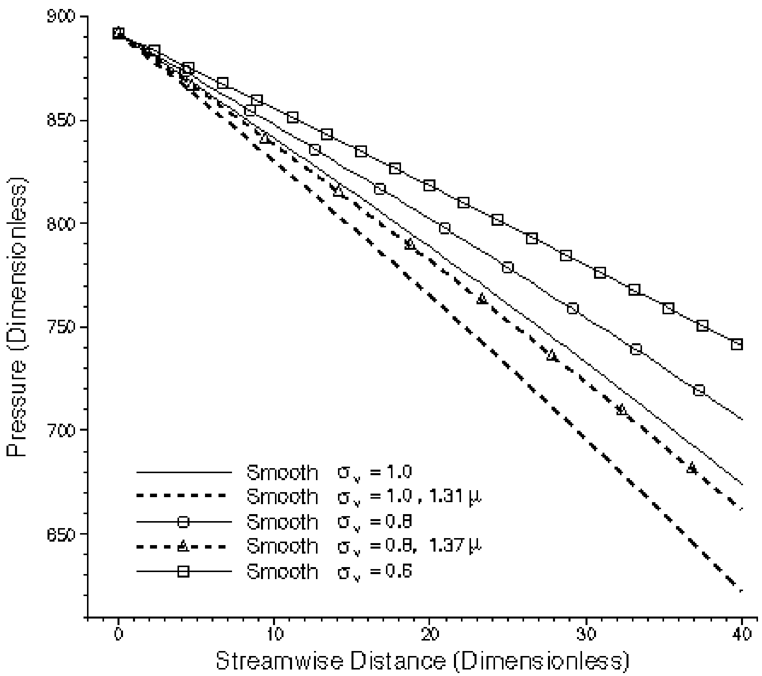


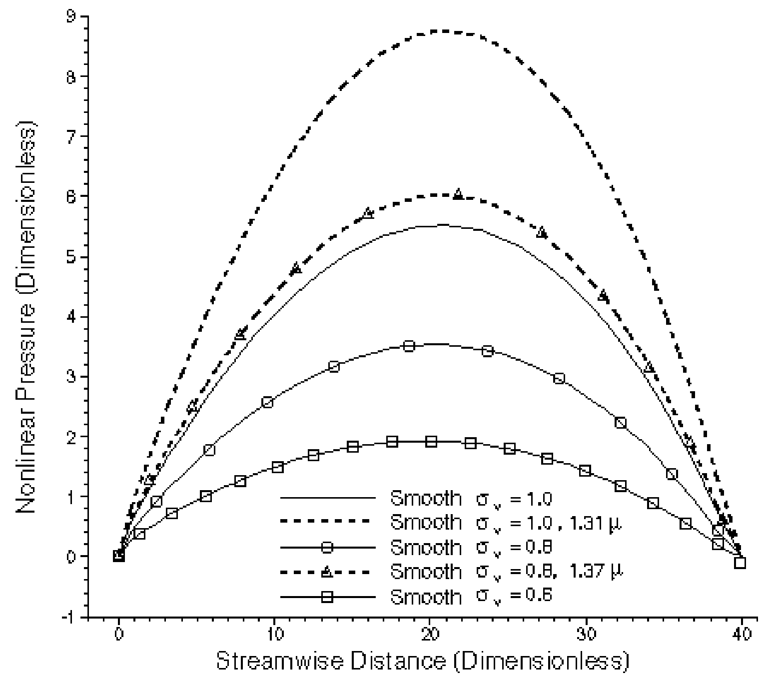


Increased surface smoothness condition

- enlarges the enhanced viscosity factor to 1.37
- lessens the overall pressure drop
- needs more artificial viscosity
- makes the flow less compressible

The Effect of Surface Roughness Condition

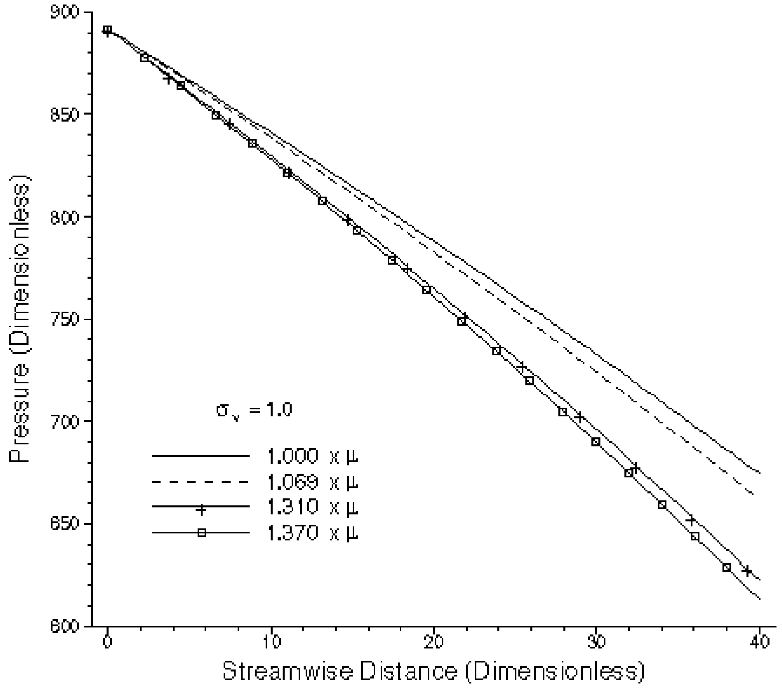


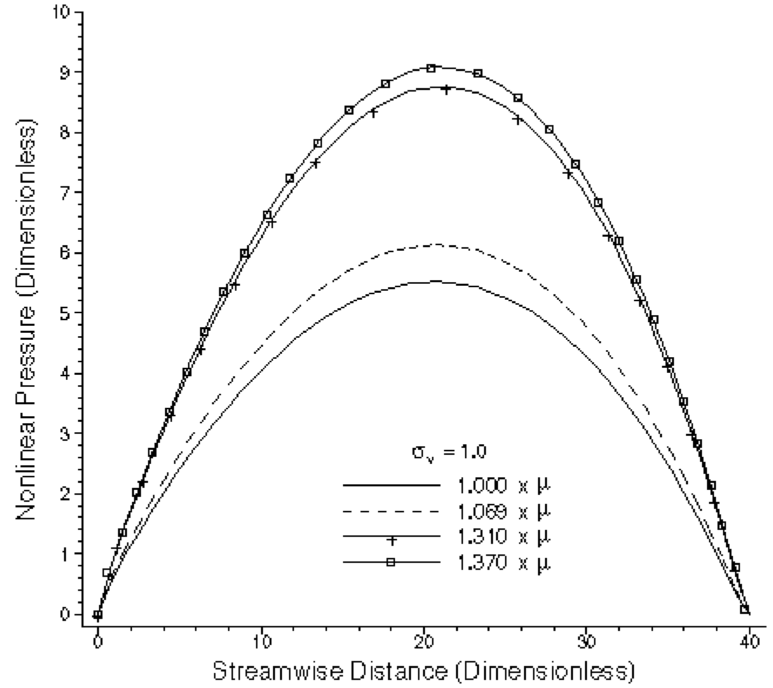


Improved surface roughness condition

- makes the flow less compressible
- decreases the overall pressure drop
- balances more extra artificial viscosity added into the flow

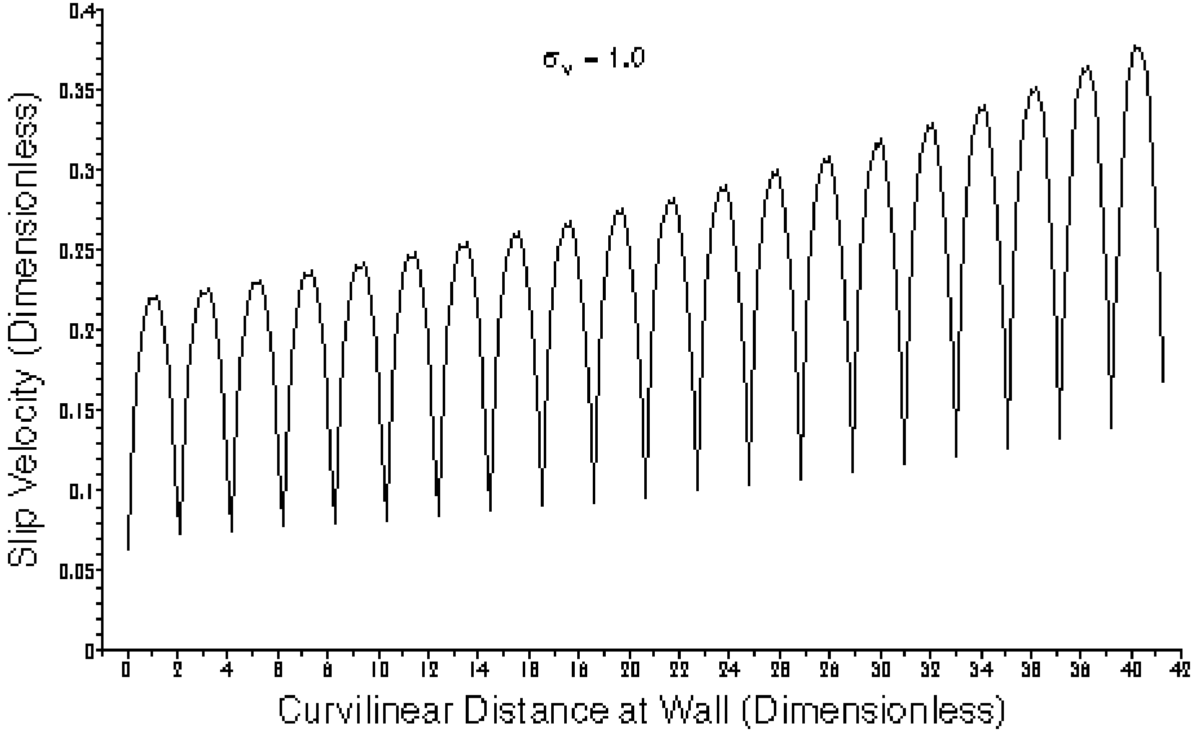
The Effect of Extra Artificial Viscosity





- Enhanced viscosity factor for σ_v= 1.0 was found as 1.069, to match the case σ_v= 0.8, enhanced viscosity factor 1.37
- Enhanced viscosity increases pressure drop and compressibility
- Enhanced viscosity competes improvement of surface condition

Slip Velocity at In-Phase Curvilinear Wall



- Slip velocity fluctuates around artificial roughness
- Slip velocity increases as the main flow develops

Verifications

$$\dot{M} = \frac{h^3 p_i \Delta p}{24\mu_i R T_i L}\left[1+\Pi+2\left(\frac{12-6\sigma_v}{\sigma_v}+\alpha\right)Kn_i + \frac{2-\sigma_v}{\sigma_v}\frac{12(b+\alpha)}{1-\Pi}Kn_i^{\,2}\ln\frac{1-bKn_i}{\Pi-bKn_i}\right]$$

Δp - pressure drop: p_i-p_o

L - total length of microscaled channels

h - channel width

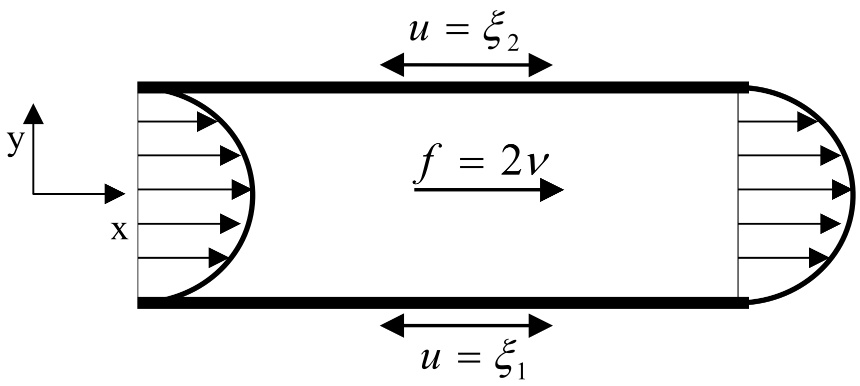
b – slip parameter, b=–1 for fully developed channel flow

Π - pressure ratio: p_o/p_i

α - rarefaction factor, α=0 for Kn<0.5

Case	Π	μ_i (kg/m/s)	Kn_i	σ_v	M_{simu}(kg/s)	$M_{formula}$(kg/s)	Error
1	0.75638	1.7600×10^{-5}	0.07	1.0	6.40×10^{-6}	6.41×10^{-6}	0.2%
2	0.69803	2.3056×10^{-5}	0.09	1.0	6.40×10^{-6}	6.43×10^{-6}	0.5%
3	0.79142	1.7600×10^{-5}	0.07	0.8	6.40×10^{-6}	6.42×10^{-6}	0.3%
4	0.74247	2.4112×10^{-5}	0.10	0.8	6.40×10^{-6}	6.45×10^{-6}	0.7%
5	0.68743	2.4112×10^{-5}	0.10	1.0	6.41×10^{-6}	6.45×10^{-6}	0.6%
6	0.74273	1.8814×10^{-5}	0.08	1.0	6.40×10^{-6}	6.42×10^{-6}	0.3%
7	0.83100	1.7600×10^{-5}	0.07	0.6	6.40×10^{-6}	6.42×10^{-6}	0.3%

Channel flow with Random Boundary Conditions

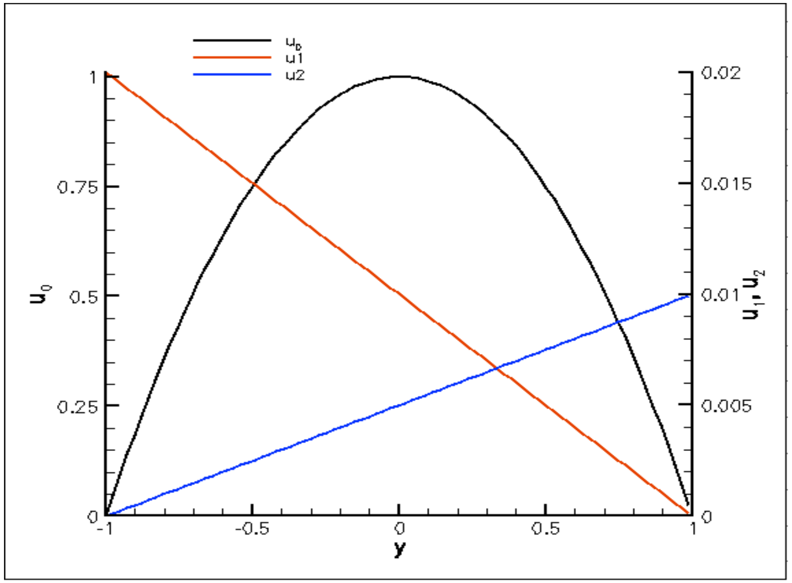


Exact solution (uniform BCs):

$$u(y) = (1 - y^2) + \frac{1-y}{2}\sigma_1\xi_1 + \frac{1+y}{2}\sigma_2\xi_2$$

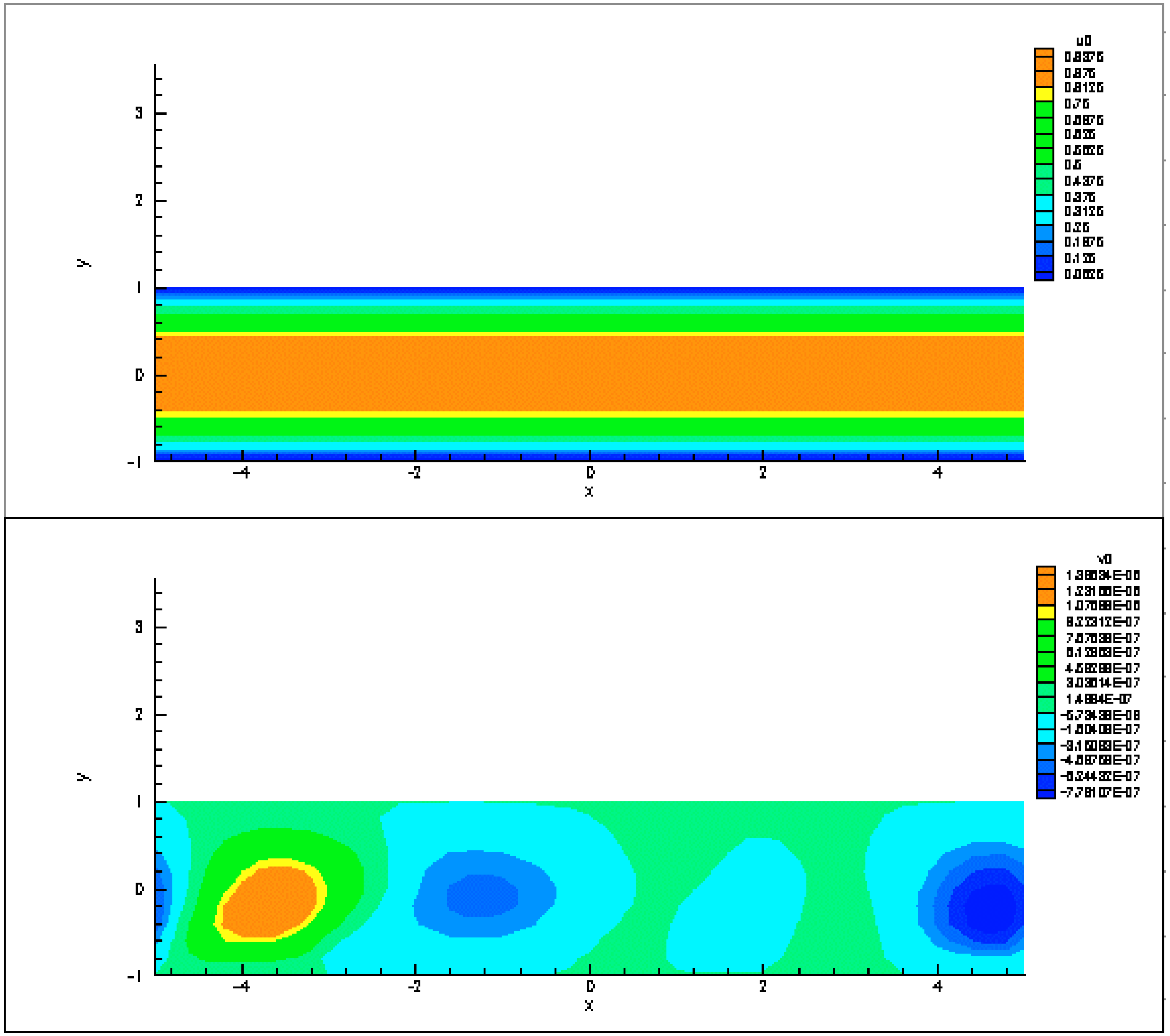
- Two-dimensional PC expansion
- Gaussian inputs :

$$\sigma_1 = 2\%, \quad \sigma_2 = 1\%$$



Solution profile across the channel

Non-Uniform Uncertainty at Wall



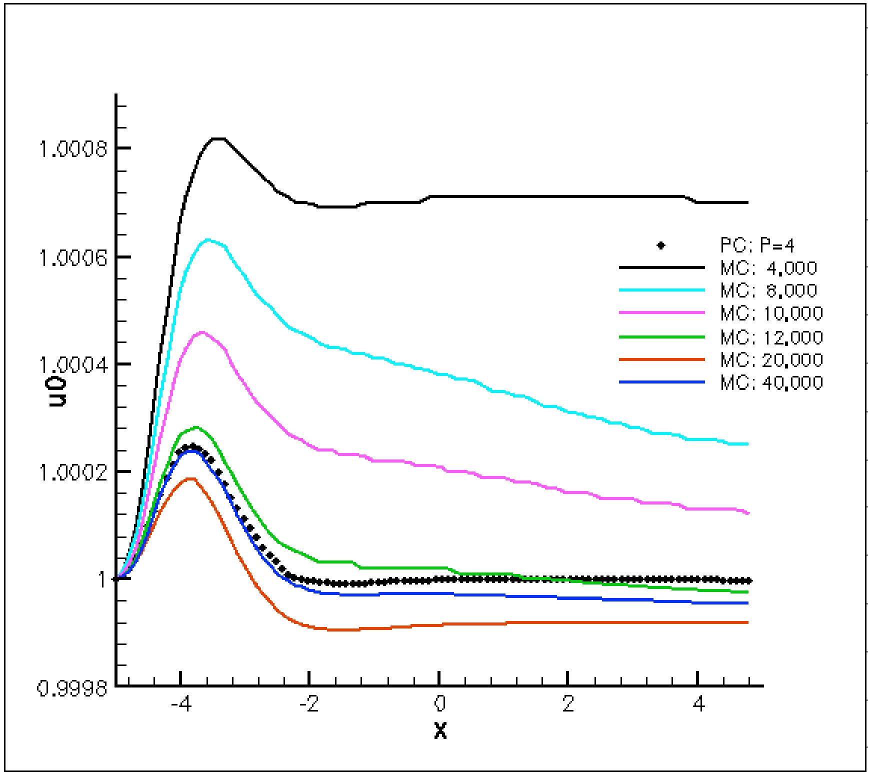
Non-uniform Gaussian Random BC

- Exponential correlation

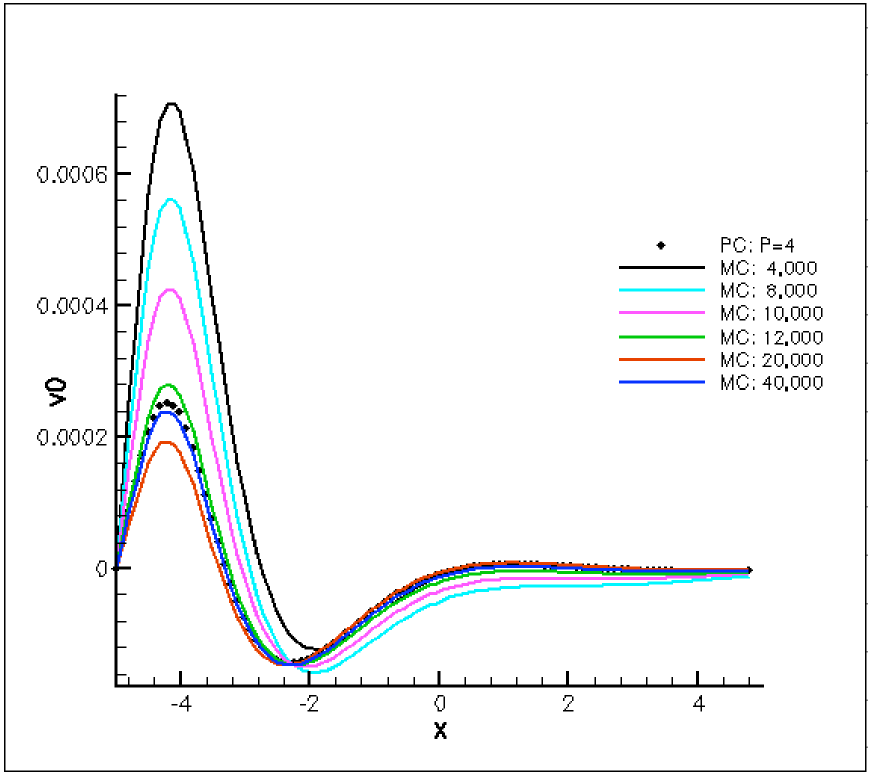
$$C(x_1, x_2) = \sigma^2 e^{-|x_1 - x_2|/b}$$

- Stochastic input: $\sigma = 0.1$

- 2D K-L expansion
- 4th-order Hermite-Chaos expansion
- 15-term expansion



U_{mean} along centerline



V_{mean} along centerline

Mode 1