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DSMC-Based Shear-Stress/Velocity-Slip Boundary Condition for Navier-Stokes Simulations

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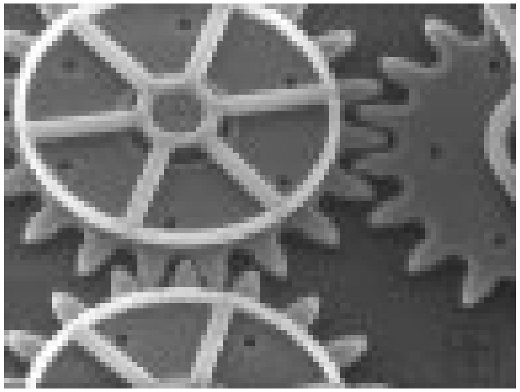
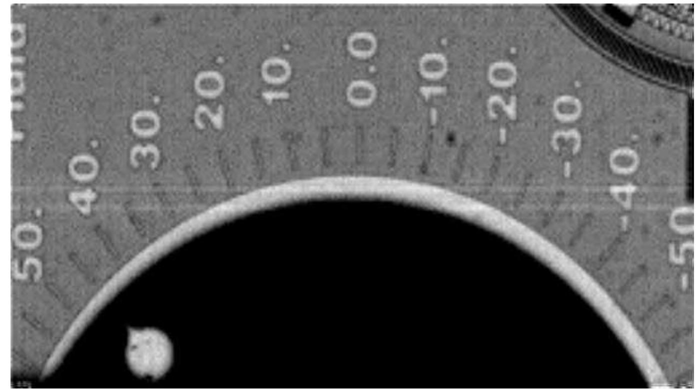
Motivation



MEMS gears (disks)

Gap L ~ 2 μm
MFP λ ~ 0.07 μm
Kn = λ/L ~ 0.03



Torsionally-oscillating disk

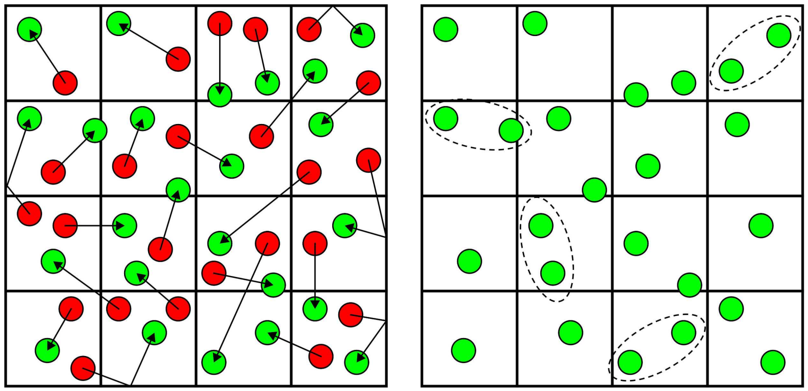
Compute gas force on MEMS disk from adjacent substrate

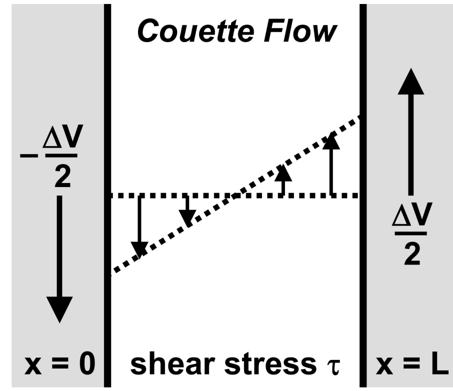
- Disk and substrate are separated by few-micron gap
  - Comparable to mean free path, especially if pressure reduced
- Disk is parallel to substrate and 100s-1000s microns wide
  - Gap region is very long and wide compared to height
- Disk has tangential velocity (substrate is stationary)
  - Couette-flow geometry: parallel surfaces move tangentially
- Gas shear stress transmits force between substrate & disk

Need accurate model for noncontinuum Couette flow

- Predict shear stress accurately in all regimes

Approach





Develop shear-stress model for isothermal Couette flow

- Linear in gas-wall velocity difference
  - Low speeds relative to molecules, very small gaps
- Based on DSMC simulations
  - Wide ranges of pressures and accommodation coefficients
- Accurate in all flow regimes
  - Free-molecular, transitional, near-continuum, continuum
- Suitable for Navier-Stokes (NS) and dynamics simulations
  - Slip-jump (SJ) boundary conditions for NS equations

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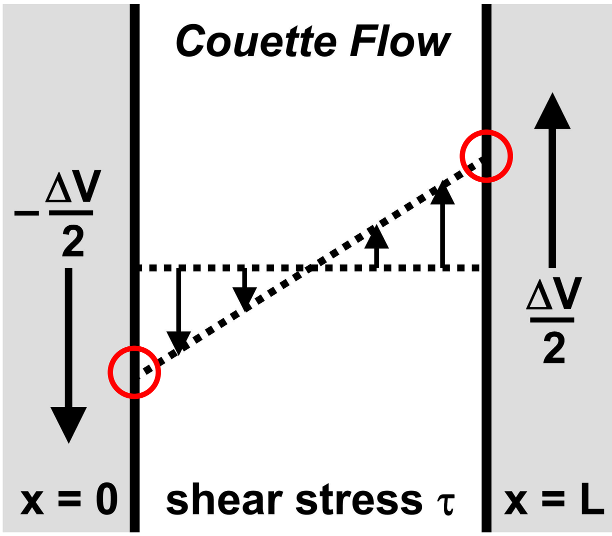
Model



$$\tau_{\text{wall}} = \mu \frac{\partial v}{\partial n} = k\left(v - V_{\text{wall}}\right) \qquad k = \frac{\sigma \rho c_0}{S_1 S_2}$$

$$S_1 = 2 - \sigma \qquad S_2 = 1 + \frac{d_1 \sigma}{1 + d_2 \text{Kn}} \qquad \text{Kn} = \frac{\lambda}{L}$$

$$\lambda = \frac{\mu}{\rho c_0} \qquad c_0 = \frac{\bar{c}}{2} = \sqrt{\frac{2 k_B T}{\pi m}} \qquad \rho = \frac{mp}{k_B T}$$

- **Shear stress τ equals product of velocity difference $v - V_{wall}$ and momentum transfer coefficient k defined as above**
  - **Boltzmann constant k_B, molecular mass m, temperature T, pressure p, mass density ρ, mean molecular 1D speed c_0, viscosity μ, mean free path λ, accommodation coefficient σ, gap height L (all gas quantities evaluated adjacent to wall)**
- **Two O(1) dimensionless model parameters d_1 and d_2**
  - **d_1 affects near-continuum regime, Knudsen layer**
  - **d_2 affects transitional regime, Kn = λ/L ~ 1**

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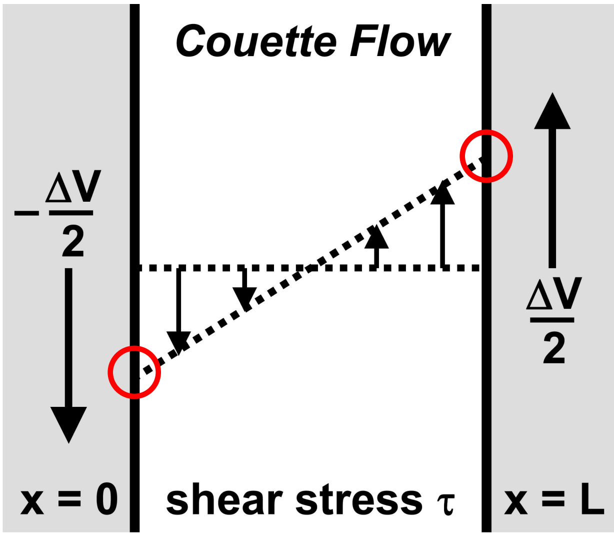
Model Limit: FM-AA Regime



Free-molecular (FM) flow with arbitrary accommodation (AA)

$$\mathrm{Kn} >> 1 \qquad 0 \le \sigma \le 1$$

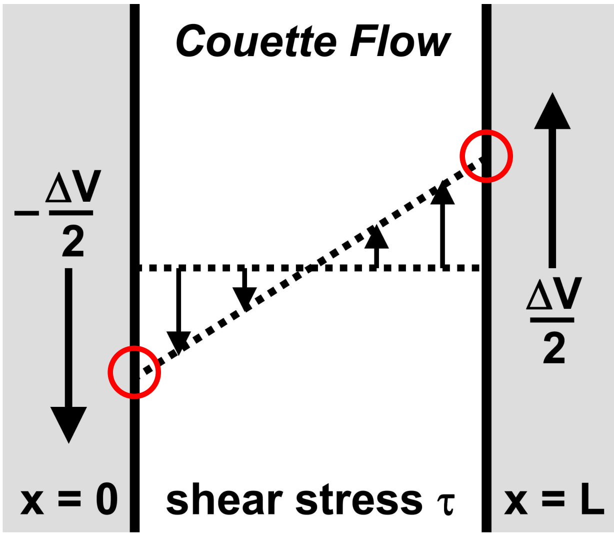
$$S_1 = 2 - \sigma \qquad S_2 = 1$$

$$\tau_{\text{wall}} = \left(\frac{\sigma}{2-\sigma}\right)\left(\frac{mn\bar{c}}{4}\right)\Delta V$$

Boundary condition has correct free-molecular limit

- Arbitrary fraction σ of half-range Maxwellian with –ΔV/2 reflects into half-range Maxwellian with ΔV/2 & vice versa
- Found by matching 2 rightward and 2 leftward half-range Maxwellians with ± ΔV/2 at right & left walls (no collisions)

Model Limit: NC-SA Regime



Near-continuum (NC) flow with small accommodation (SA)

$$\mathrm{Kn} << 1 \qquad \sigma << 1$$

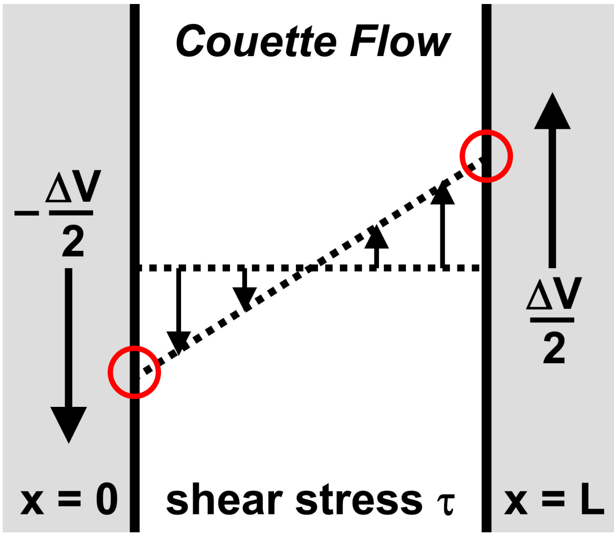
$$S_1 = 2 \qquad S_2 = 1$$

$$\tau_{\mathrm{wall}} = \sigma\left(\frac{mn\bar{c}}{4}\right)\left(v - V_{\mathrm{wall}}\right)$$

Boundary condition has correct near-continuum limit with small accommodation

- Small fraction σ of half-range Maxwellian with v reflects into half-range Maxwellian with V_{wall}
- Small reflected fraction does not affect incident distribution (dilute assumption)

Model Limit: NC-UA Regime



Near-continuum (NC) flow with unity accommodation (UA)

$$\text{Kn} << 1 \qquad \sigma = 1$$

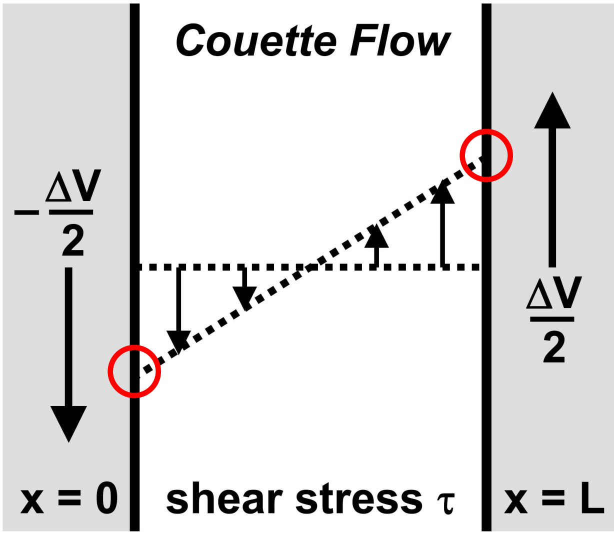
$$S_1 = 1 \qquad S_2 = 1 + d_1$$

$$(1 + d_1)\lambda \frac{\partial v}{\partial n} = v - V_{\text{wall}}$$

Boundary condition has correct near-continuum limit with unity accommodation

- Yields common form of velocity-slip boundary condition
- Suggests parameter d_1 = 0.1-0.2 based on Knudsen layer

Model Limit: Continuum Regime



Continuum flow with zero or nonzero accommodation

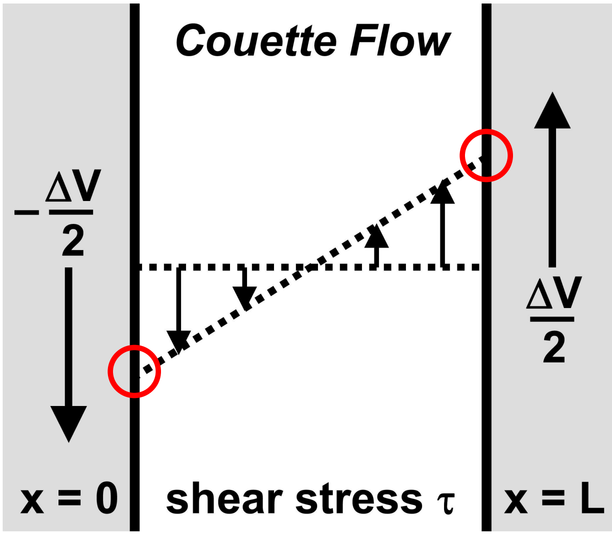
$$\mathrm{Kn} \rightarrow 0 \quad \sigma = 0 \quad \tau_{\mathrm{wall}} = \mu \frac{\partial v}{\partial n} = 0$$

$$\mathrm{Kn} \rightarrow 0 \quad 0 < \sigma \leq 1 \quad v = V_{\mathrm{wall}}$$

Boundary condition has correct continuum limit

- Yields zero-shear-stress (symmetry) condition when accommodation is zero
- Yields no-slip condition when accommodation is nonzero

Couette-Flow Solution



$$\frac{\tau_{\text{wall}}}{\tau_{\text{cont}}} = \frac{1}{1+\left(2S_1S_2\text{Kn}/\sigma\right)}$$

$$\tau_{\text{cont}} = \frac{\mu\Delta V}{L} \qquad \text{Kn} = \frac{\lambda}{L}$$

$$S_1 = 2-\sigma \qquad S_2 = 1+\frac{d_1\sigma}{1+d_2\text{Kn}}$$

Use Couette flow to determine model parameters d_1 & d_2

- Select a gas (Ar, He, N_2, Air)
- Perform DSMC simulations to determine shear stress τ
  - Pressure sets Kn: free-molecular to near-continuum
  - Accommodation coefficient σ: 1.00, 0.50, 0.25
- Adjust d_1 & d_2 for best fit by solution to DSMC values

Boundary condition is determined by d_1 & d_2

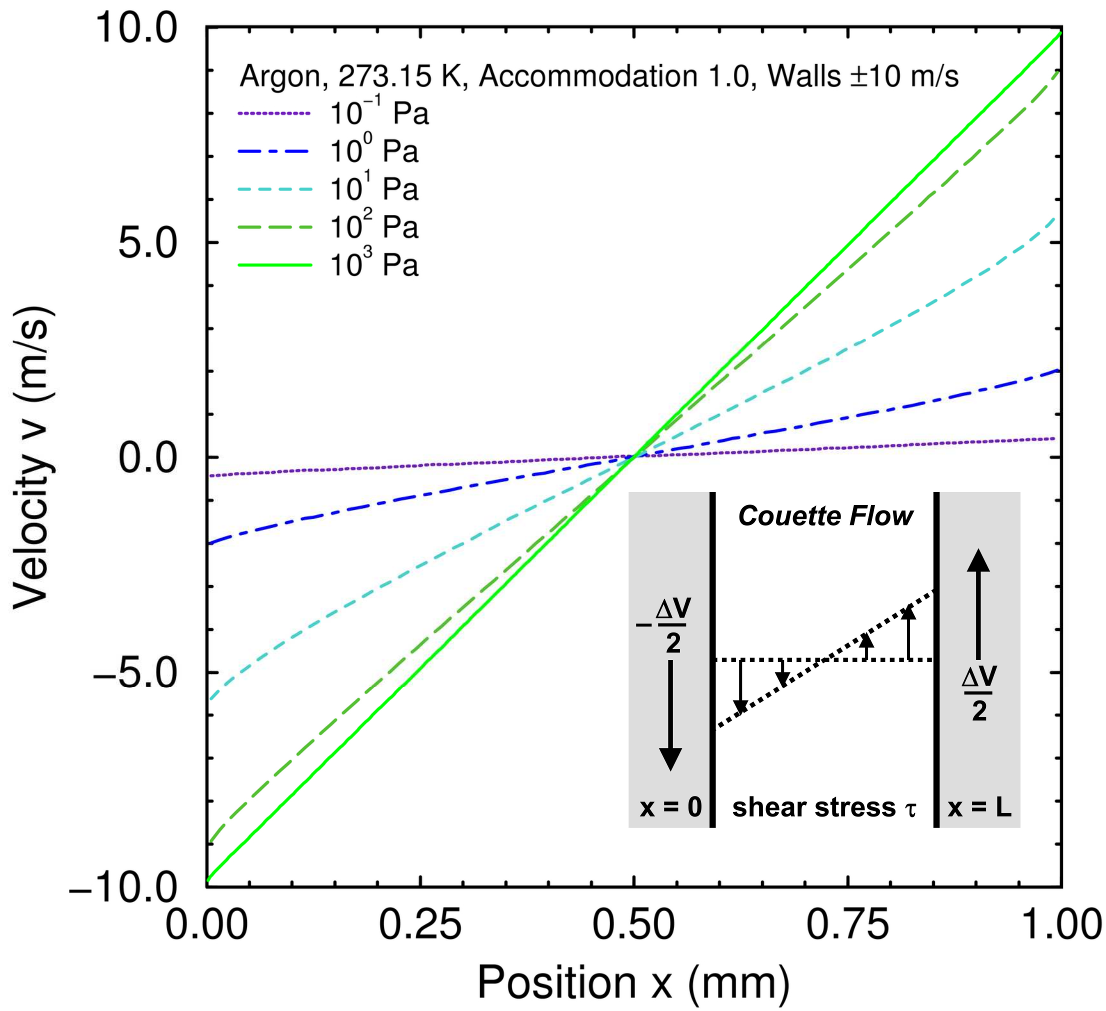
Couette-Flow Velocity Profiles

DSMC simulations

- Gas: argon
- Domain: 1 mm
- Temp: 273.15 K
- Pres (13): 10^{-1}-10^{3} Pa
- Accom: 1, 0.5, 0.25
- Walls: ±10 m/s

Velocity profiles

- Shown for $\sigma = 1$
  - Similar for other σ
- 10^3 Pa nearly linear
  - Near-continuum
- 10^{-1} Pa nearly flat
  - Free-molecular



Argon Shear Stress

DSMC simulations

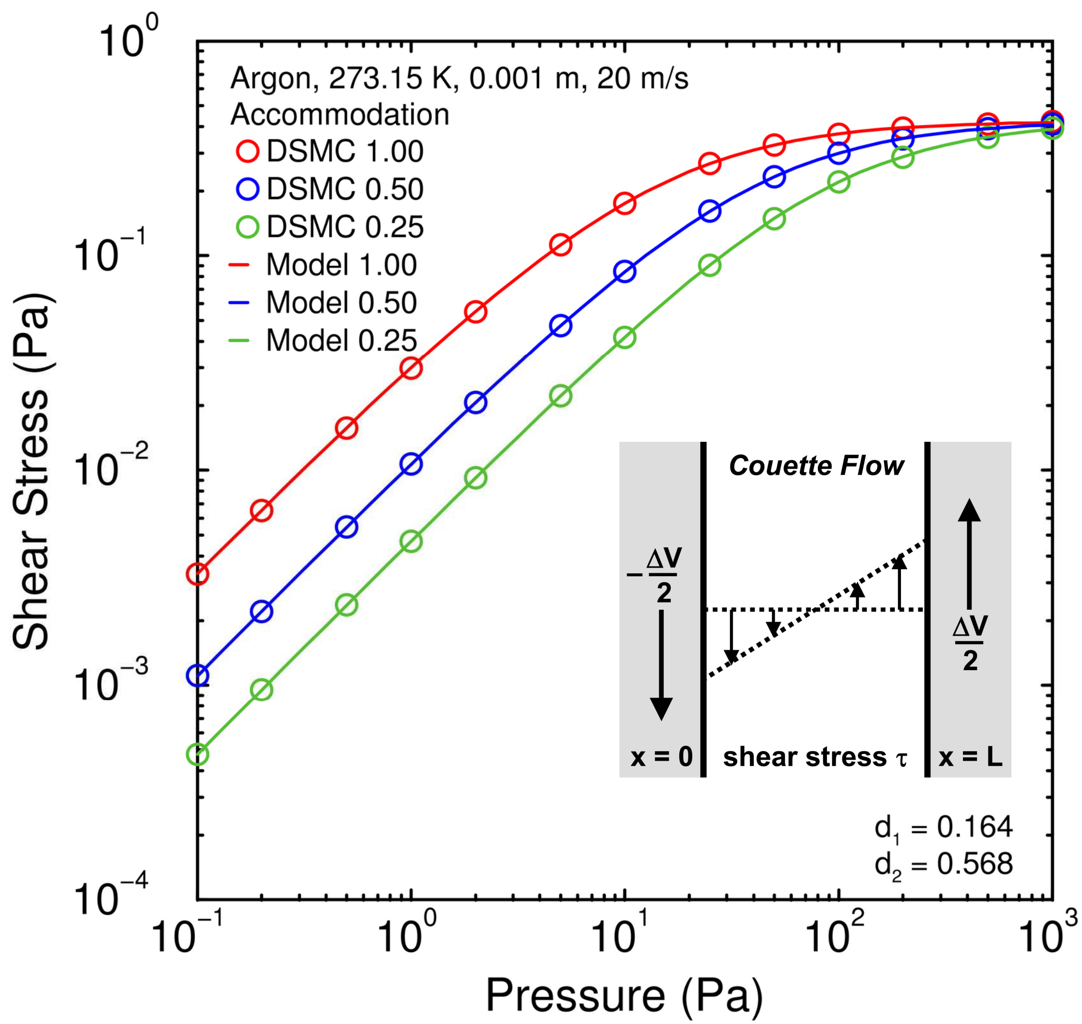
- Gas: argon
- Domain: 1 mm
- Temp: 273.15 K
- Pres (13): 10^{-1}-10^{3} Pa
- Accom: 1, 0.5, 0.25
- Walls: ±10 m/s

Shear stress (walls)

- 39 combinations of pressure & accom.
- Uncertainty ~0.2%

Argon parameters

- $d_1 = 0.16 \pm 0.02$
- $d_2 = 0.57 \pm 0.06$



Symbols: DSMC
Curves: Model

Shear Stress for All Four Gases

All gases are similar

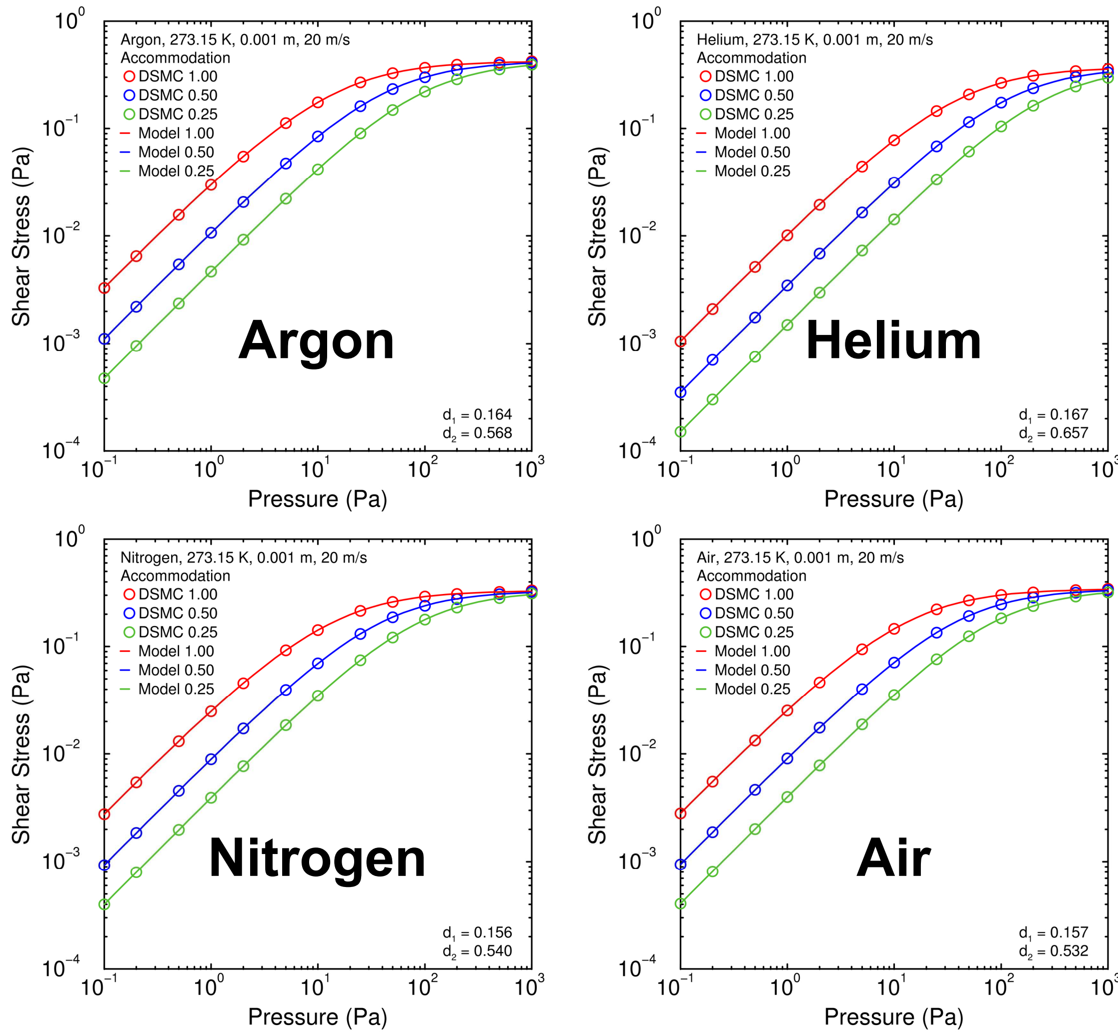
- 10^3 Pa nearly flat
  - Near-continuum
- 10^{-1} Pa nearly linear
  - Free-molecular

Ar, N_2, Air parameters

- $d_1 = 0.16 \pm 0.02$
- $d_2 = (0.53\text{-}0.57) \pm 0.06$

He parameters

- $d_1 = 0.17 \pm 0.02$
- $d_2 = 0.66 \pm 0.06$



Symbols: DSMC
Curves: Model

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Collision Parameters

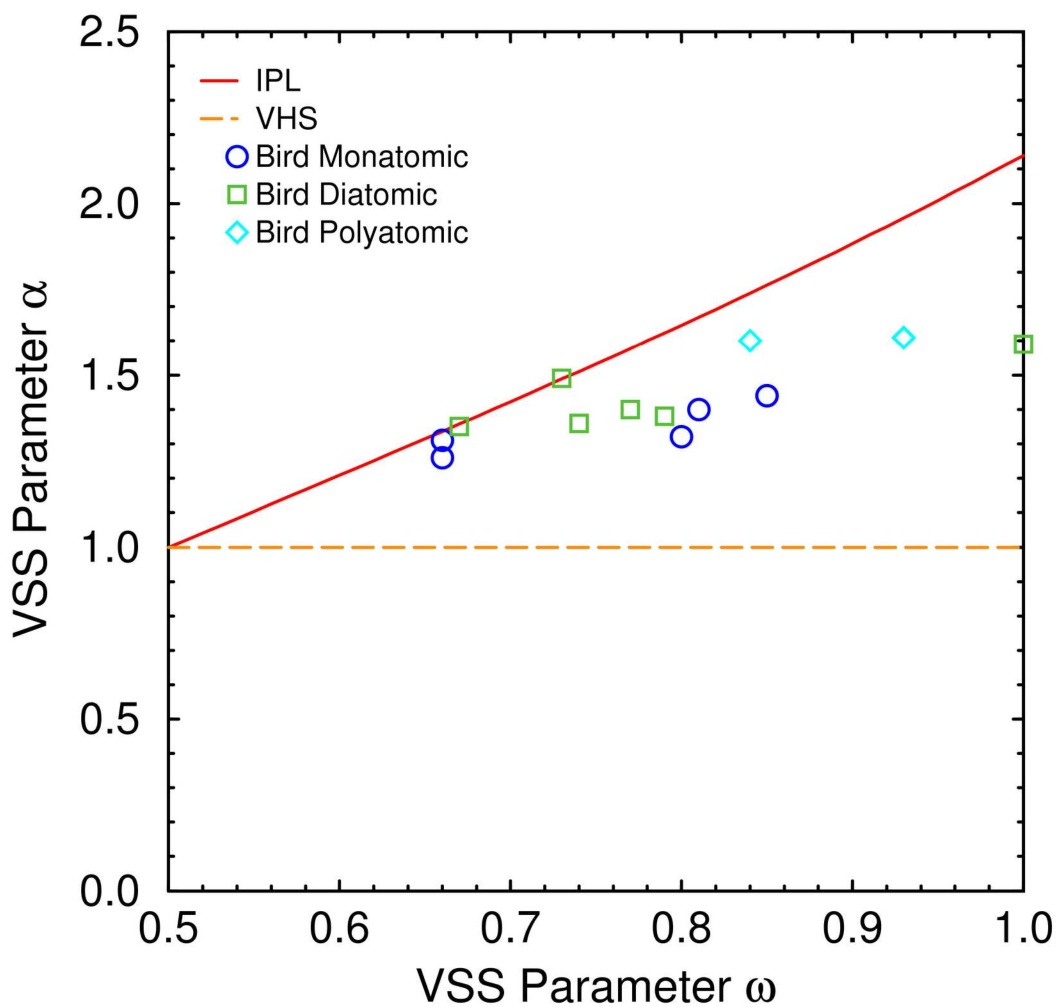
Variable Soft Sphere collision model

- **VSS parameters ω, α**

Bird (1994) values

- **Bounded above by Inverse Power Law**
  - **IPL: α = α[ω]**
- **Bounded below by Variable Hard Sphere**
  - **VHS: α = 1**

Investigate how d_1 & d_2 depend on ω & α



Effect of VSS Parameters

VHS & IPL simulations

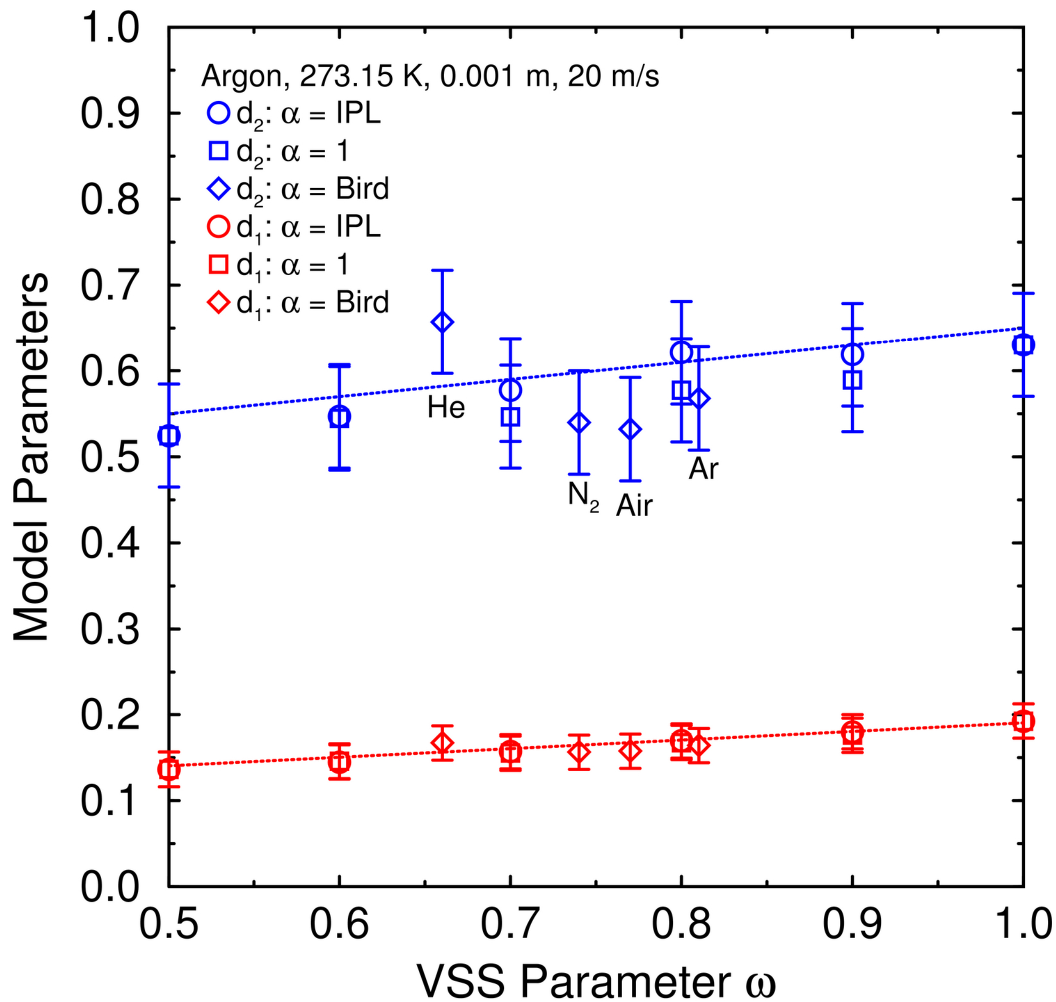
- All conditions same
- Argon-like properties
- Take ω = 0.5,0.6,...1.0
- VHS: $\alpha = 1$
- IPL: $\alpha = \alpha[\omega]$

Parameters d_1 & d_2 are almost constant

- All: $d_1 = 0.15 \pm 0.02$
- All: $d_2 = 0.59 \pm 0.07$
- Slight rise with ω lies within error bars

Four previous gases

- He seems high
- N_2 & air low, rotation?



Hard-Sphere Comparison

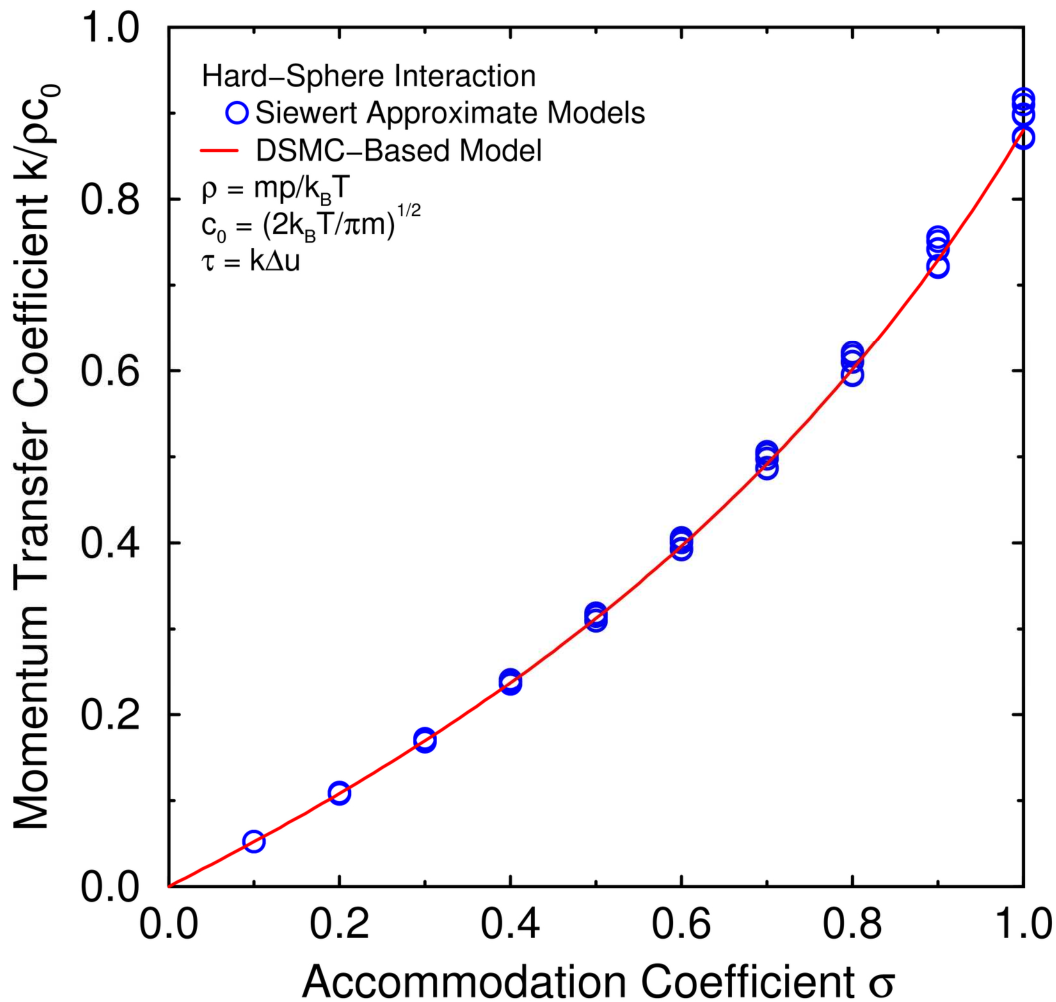
$$\tau_{\text{wall}} = k\left(v - V_{\text{wall}}\right) \qquad S_1 = 2 - \sigma$$

$$\frac{k}{\rho c_0} = \frac{\sigma}{S_1 S_2} \qquad S_2 = 1 + \frac{d_1 \sigma}{1 + d_2 \text{Kn}}$$

Mom. trans. coeff. k vs. accom. coeff. σ

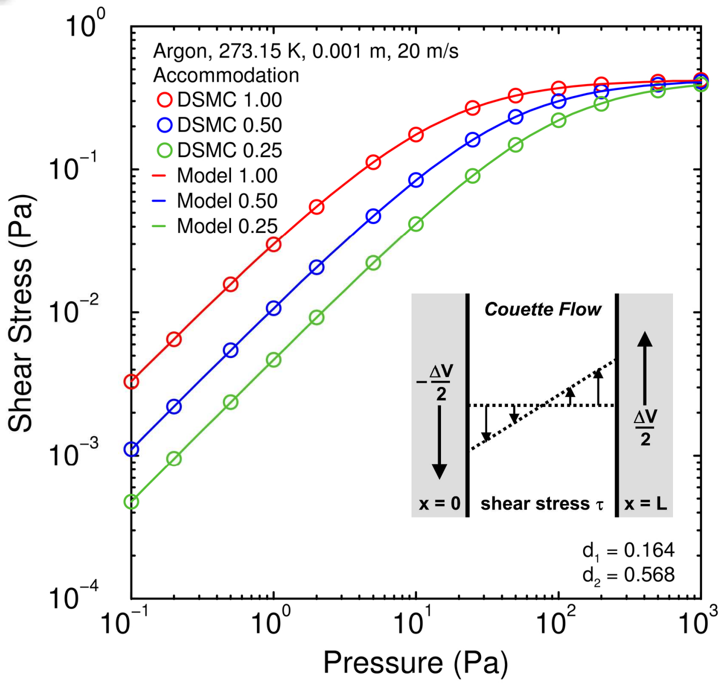
- DSMC-based model
- Siewert & Sharipov: 6 approximations
- Hard-sphere gas
- Kn → 0

Excellent agreement



Symbols: Approximations
Curve: DSMC model

Conclusions



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$$\lambda = \frac{\mu}{\rho c_0} \qquad c_0 = \frac{\bar{c}}{2} = \sqrt{\frac{2 k_B T}{\pi m}} \qquad \rho = \frac{mp}{k_B T}$$

DSMC-based shear-stress boundary condition developed

- Reproduces near-continuum and free-molecular limits
- Parameters depend only weakly on gas properties
- Agrees well with hard-sphere analytical approximations
- Suitable for Navier-Stokes and dynamics simulations