SAND2011-5643P

An Expression for the Gas Mass Flow Rate through a Tube from Free-Molecular to Continuum Conditions

John R. Torczynski and Michael A. Gallis

Engineering Sciences Center

Sandia National Laboratories

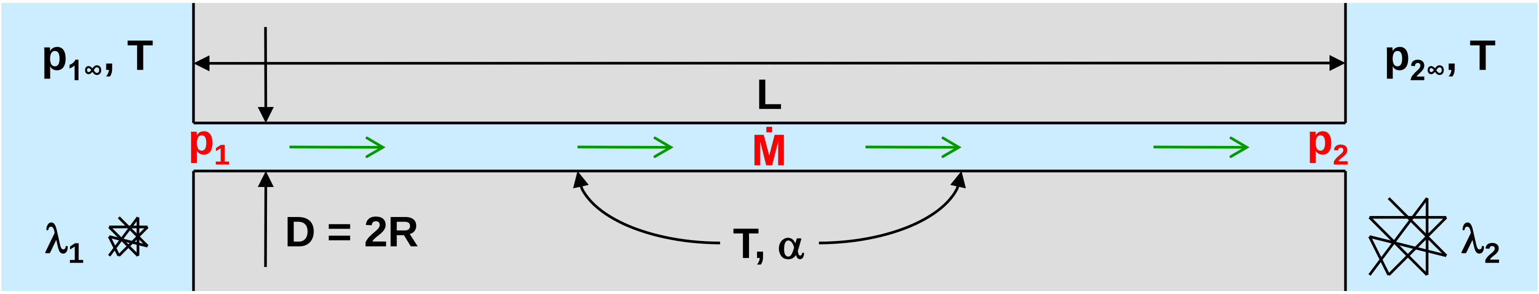
Albuquerque, New Mexico, USA

American Physical Society Division of Fluid Dynamics DFD11

64th Annual Meeting; Baltimore, Maryland; November 20-22, 2011

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Gas Flow in a Microscale Tube



Investigate steady isothermal gas flow in microscale tube

- Tube is long and thin (L >> D) with circular cross section
- Tube joins gas reservoirs at different pressures ($p_{1\infty} \geq p_{2\infty}$)
- Tube and reservoirs have same temperature (T)
- Molecules partially accommodate ($\alpha \leq 1$) when reflecting
- Flow speed << molecule speed, laminar, no turbulence

Determine the mass flow rate and the pressure profile

- General physics-based closed-form expressions
- Free-molecular to continuum (arbitrary mean free path λ)
- Theory and molecular-gas-dynamics simulations

Tube Mass Flow Rate – Classic Studies

M. Knudsen (1909)

- Interpolation between free-molecular and continuum flow for long tubes (L >> D) and accommodation $\alpha = 1$
- Knudsen minimum: actual value < free-molecular value

M. Smoluchowski (1910)

- Extension of Knudsen's expression for long tubes (L >> D) with accommodation $\alpha \leq 1$
- Free-molecular accommodation factor $(2 - \alpha)/\alpha$

P. Clausing (1932)

- Rigorous integral equation for free-molecular flow for arbitrary length with accommodation $\alpha = 1$

E. H. Kennard (1938)

- Free-molecular expression for arbitrary cross section for long tubes (L >> D) with accommodation $\alpha \leq 1$

Sandia National Laboratories

Tube Mass Flow Rate – Recent Studies

F. Sharipov and Collaborators (1990+)

- BGK-based analytical methods for long tubes (L >> D) with accommodation $\alpha = 1$, and some simulations
- Extensive tables of mass flow rate for all regimes

G. E. Karniadakis and A. Beskok (1990+)

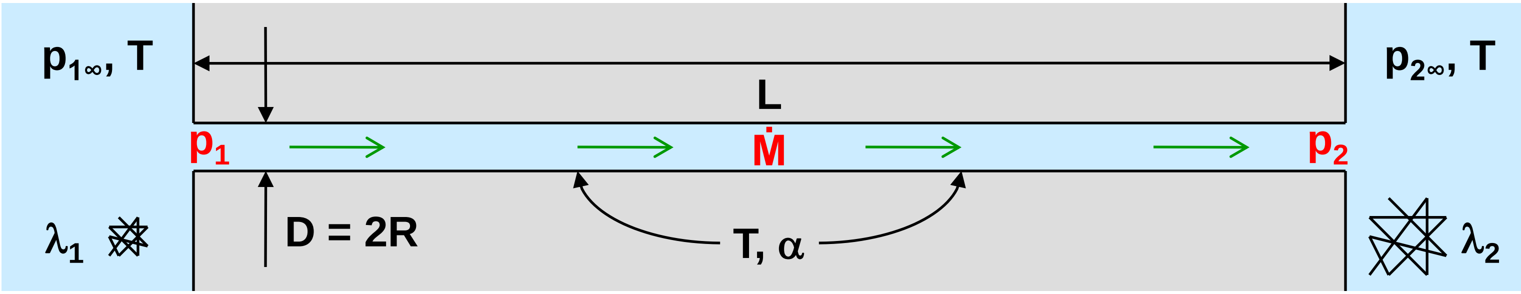
- More accurate velocity profiles through better slip boundary conditions for Navier-Stokes equations
- More accurate mass flow rate into transition regime

M. A. Gallis, D. J. Rader, and J. R. Torczynski (2000+)

- Transport rate more important than related spatial field
- Construct boundary conditions to give accurate rates in all regimes when used with Navier-Stokes equations
- Works well for energy, momentum, & mass transport between parallel plates (Fourier, Couette, Fickian flow)

Sandia National Laboratories

Tube-Flow Application



Ideal Gas

$$\rho = \frac{mp}{k_B T}, \quad \mu = \mu[T]$$

Boundary Condition at $r = R$

$$-\lambda \frac{\partial u}{\partial r} = \frac{\alpha}{2-\alpha}\left(\frac{1+b_2(\lambda/D)}{1+b_1\alpha+\varepsilon b_0 b_2(\lambda/D)}\right)u$$

$$b_0 = \frac{16}{3\pi}, \quad b_1 = 0.15, \quad b_2 = \frac{0.7\alpha}{2-\alpha}$$

$$\delta = \frac{4}{3}(2-\alpha), \quad \kappa = \frac{\delta-1}{\delta}\frac{\alpha L}{D}, \quad \varepsilon = \frac{1+\kappa}{\delta+\kappa}$$

Navier-Stokes

$$\frac{dp}{dz} = \frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)$$

Mean Free Path

$$c = \sqrt{\frac{8k_B T}{\pi m}}, \quad \lambda = \frac{2\mu}{\rho c}, \quad p_\lambda = \frac{p\lambda}{D}$$

Knudsen Number

$$p_m = \frac{p_1+p_2}{2}, \quad \mathrm{Kn}_m = \frac{\lambda_m}{D} = \frac{p_\lambda}{p_m}$$

Mass Flow Rate, Pressure Profile

$$\frac{\dot{M}}{\dot{M}_C} = 1+\frac{8p_\lambda}{p_m}\varpi[p_1,p_2], \quad \dot{M}_C = \frac{D^4 p_m(p_1-p_2)}{16\mu c^2 L}$$

$$\frac{z}{L} = \frac{p_1^2 - p^2 + 16p_\lambda(p_1-p)\varpi[p_1,p]}{p_1^2 - p_2^2 + 16p_\lambda(p_1-p_2)\varpi[p_1,p_2]}$$

$$\varpi[p_A,p_B] = \frac{2-\alpha}{\alpha}\left\{1+b_1\alpha+(\varepsilon b_0-1-b_1\alpha)\frac{b_2 p_\lambda}{p_A-p_B}\ln\left[\frac{p_A+b_2p_\lambda}{p_B+b_2p_\lambda}\right]\right\}$$

$$F = \frac{3\pi D}{32L}\left(1+\frac{16p_\lambda}{q_1+q_2}\left(\varpi[p_1,p_2]-\frac{3}{4}\right)\right), \quad q = p+6p_\lambda$$

$$q_1 = \sqrt{\frac{(1+F)q_{1\infty}^2+Fq_{2\infty}^2}{1+2F}}, \quad q_2 = \sqrt{\frac{(1+F)q_{2\infty}^2+Fq_{1\infty}^2}{1+2F}}$$

Boundary condition yields closed-form expressions for mass flow rate and pressure profile covering all regimes

- Parameters b_0, b_1, b_2, and ε are specified to ensure accuracy in free-molecular, slip, and transition regimes
- Mass flow rate has Knudsen minimum: $\varepsilon b_0 > 1 + b_1\alpha$

Mass Flow Rate Has Correct Limits

Approximate Closed-Form Expression

$$\dot{M} = \dot{M}_C\left(1+\frac{8p_\lambda}{p_m}\varpi[p_1,p_2]\right),\quad \varpi[p_A,p_B] = \frac{2-\alpha}{\alpha}\left\{1+b_1\alpha+(\varepsilon b_0-1-b_1\alpha)\frac{b_2 p_\lambda}{p_A-p_B}\ln\left[\frac{p_A+b_2 p_\lambda}{p_B+b_2 p_\lambda}\right]\right\}$$

Continuum

$$\dot{M}_C = \frac{D^4 p_m (p_1-p_2)}{16\mu c^2 L}$$

Slip

$$\dot{M}_S = \dot{M}_C\left(1+\frac{8p_\lambda}{p_m}\varpi_S\right),\quad \varpi_S = \frac{2-\alpha}{\alpha}(1+b_1\alpha)$$

Free-Molecular

$$\dot{M}_F = \dot{M}_C\left(\frac{8p_\lambda}{p_m}\varpi_F\right),\quad \varpi_F = \frac{2-\alpha}{\alpha}\varepsilon b_0$$

Continuum Orifice

$$\dot{M}_{OC} = \frac{R^3\rho_{m\infty}}{3\mu}(p_{1\infty}-p_{2\infty})$$

Free-Molecular Orifice

$$\dot{M}_{OF} = \pi R^2 \frac{mc}{4}(n_{1\infty}-n_{2\infty})$$

Free-Molecular Short Tube

$$\dot{M}_{TF} = \dot{M}_{OF}\Big/\big(1+(\alpha L/D)\big),\quad \alpha L/D \ll 1$$

Expression reproduces known limits correctly

Continuum	Not affected by ε, b_0, b_1, b_2
Slip	Determined by b_1
Free-Molecular	Determined by ε, b_0
Orifice/Short-Tube	Determined by ε, b_0

Sandia National Laboratories

How Parameters Are Specified

Approximate Closed-Form Expression

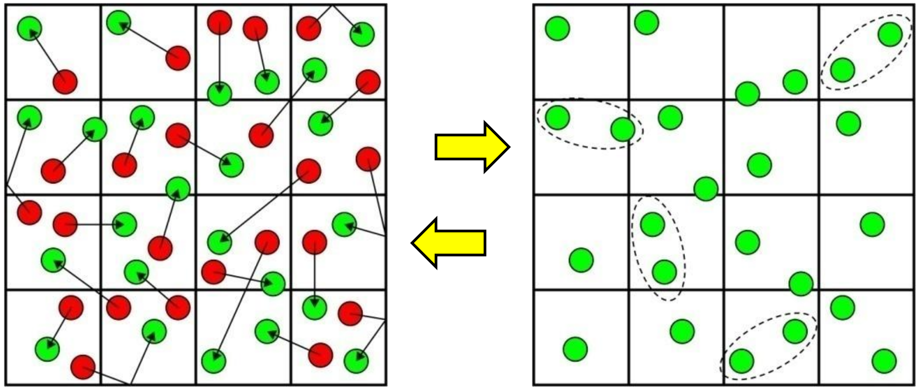
$$\dot{M} = \dot{M}_C \left(1 + \frac{8p_\lambda}{p_m} \varpi[p_1, p_2]\right), \quad \varpi[p_A, p_B] = \frac{2-\alpha}{\alpha}\left\{1 + b_1\alpha + (\varepsilon b_0 - 1 - b_1\alpha)\frac{b_2 p_\lambda}{p_A - p_B}\ln\left[\frac{p_A + b_2 p_\lambda}{p_B + b_2 p_\lambda}\right]\right\}$$

Mass flow rate and pressure profile contain 4 parameters

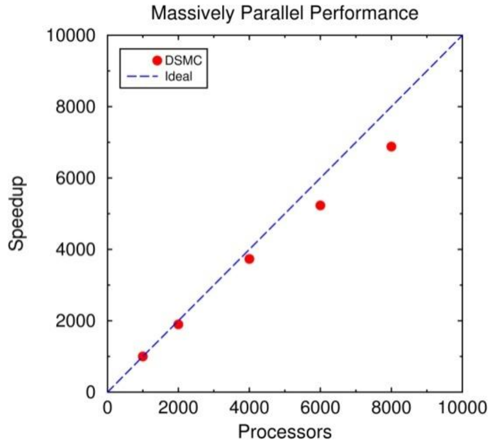
- Product εb_0 controls behavior in free-molecular regime
  - Choose $b_0 = 16/3\pi$ to match Knudsen-Smoluchowski formula
  - Choose ε to match Clausing-Kennard inlet-outlet resistances
- Parameter b_1 controls behavior in slip regime
  - Loyalka, Siewert, and coworkers suggested $(1 + b_1\alpha)$ form
  - Gallis and coworkers showed common gases have $b_1 \approx 0.15$
- Parameter b_2 controls behavior in transition regime
  - Cannot be determined from above known limits
  - May depend on accommodation coefficient

Determine b_2 using molecular-gas-dynamics simulations

Molecular-Gas-Dynamics Simulations



molecules move ballistically   molecule pairs collide



Direct Simulation Monte Carlo (DSMC) method of Bird uses computational molecules to simulate gas flows

- Each computational molecule ('simulator') represents a very large number of real molecules
- Simulators move, reflect from boundaries, and collide with each other so as to reproduce statistics of real molecules
- Flow field is found by averaging the (stationary) properties of the simulators in each cell over many time steps

DSMC scales well on massively parallel computers

- Essential for simulations in slip regime

Sandia National Laboratories

Simulation Conditions

DSMC simulation parameters

- Tube radius: 10 μm
- Tube length: 10 and 1 mm
  - Length/radius = 1000 and 100, long and short
- Accom: 1.00, 0.75, 0.50, 0.25
  - Most gases/surfaces are ~0.8, but helium/metal can be ~0.4
- Inlet pressure: 1-10,000 Pa
  - Free-molecular to slip regime
  - Kn = 1 at $p = p_\lambda$ = 316.4 Pa
- Outlet pressure: (0.0-0.5) inlet
  - 0.5 is weak gradient; 0.0 is strong gradient

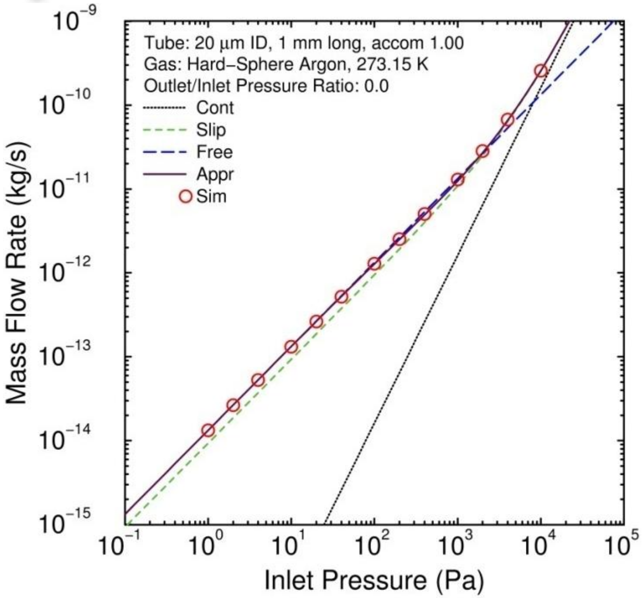
Mass flow rate uncertainty ~1%

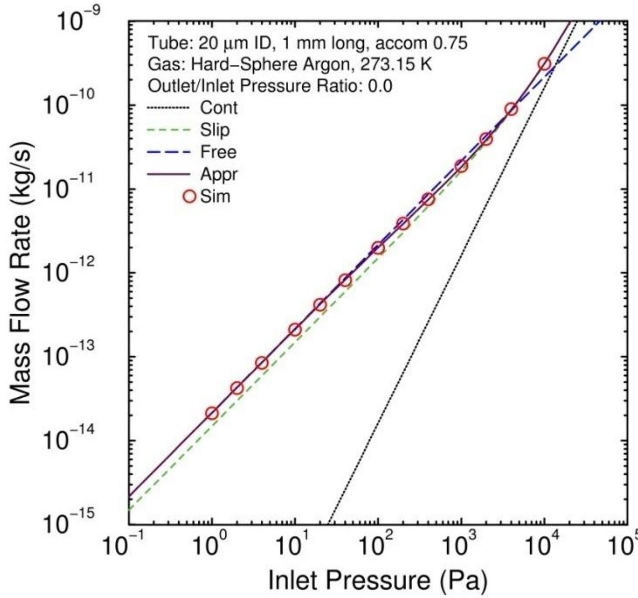
Quantity	Symbol	Value
Boltzmann constant	k_B	1.380658×10^{-23} J/K
Gas, interaction	Ar, HS	Argon, hard-sphere
Mass, molecular	m	6.63×10^{-26} kg
Temperature, wall	T	273.15 K
Viscosity	μ	2.117×10^{-5} Pa·s
Pressure, inlet	p_1	10^0-10^4 Pa
Pressure, outlet	p_2	$(0\text{-}0.5)\,p_1$
Mean molecular speed	c	380.6 m/s
Mean free path	λ	0.6328 μm at 10^4 Pa
Radius, tube	R	10 μm
Length, tube	L	1 or 10 mm
Square side, plenum	S	50 μm
Accommodation	α	1.00, 0.75, 0.50, 0.25
Pressure, Knudsen	p_λ	316.4 Pa
Time step	Δt	0.5 ns
Cell size, radial	Δr	0.2 μm
Cell size, axial	Δz	$L/500 = (10\text{-}100)\Delta r$
Cell size, plenum	Δs	1 μm
Molecules per cell	N_S	30 (average)
Time step, normalized	$c\Delta t/\lambda$	≤ 0.30
Cell size, normalized	$\Delta r/\lambda$	≤ 0.32

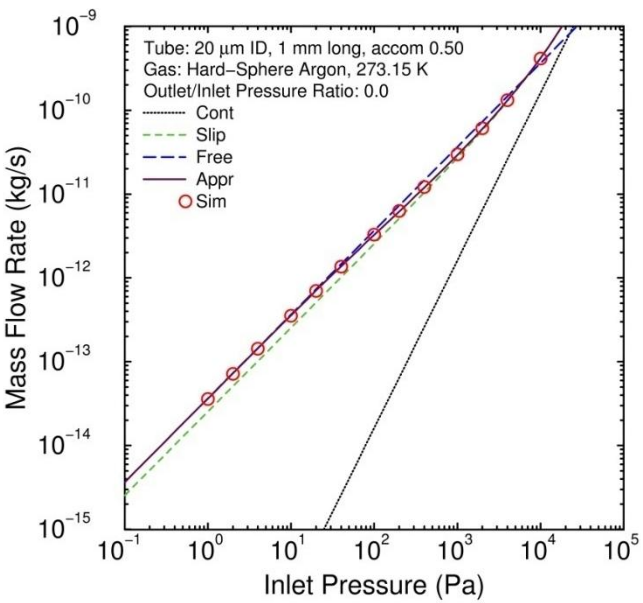
Simulations take ~1 processor-year on a massively parallel computer

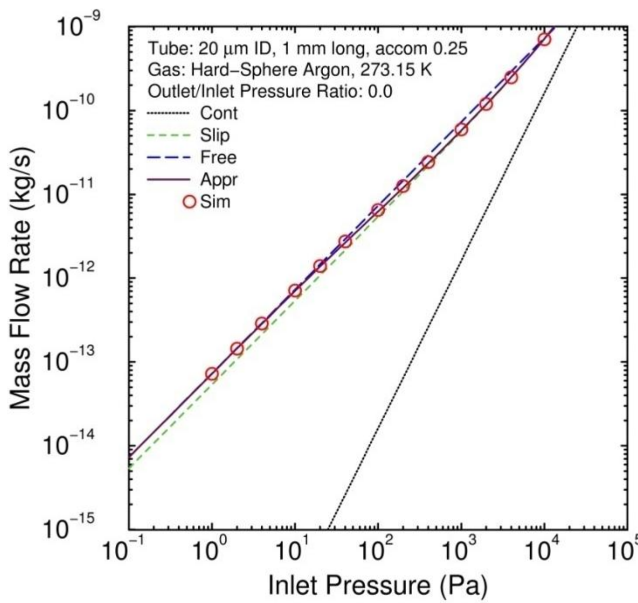
Sandia National Laboratories

Mass Flow Rate: Short Tube









Conditions

- **L/R = 100 (short)**
- **p_2/p_1 = 0.0 (strong)**

Expression agrees well with simulations

- **All inlet pressures p_1**
- **All accom. coeffs. α**

Expected behavior is observed in known limits

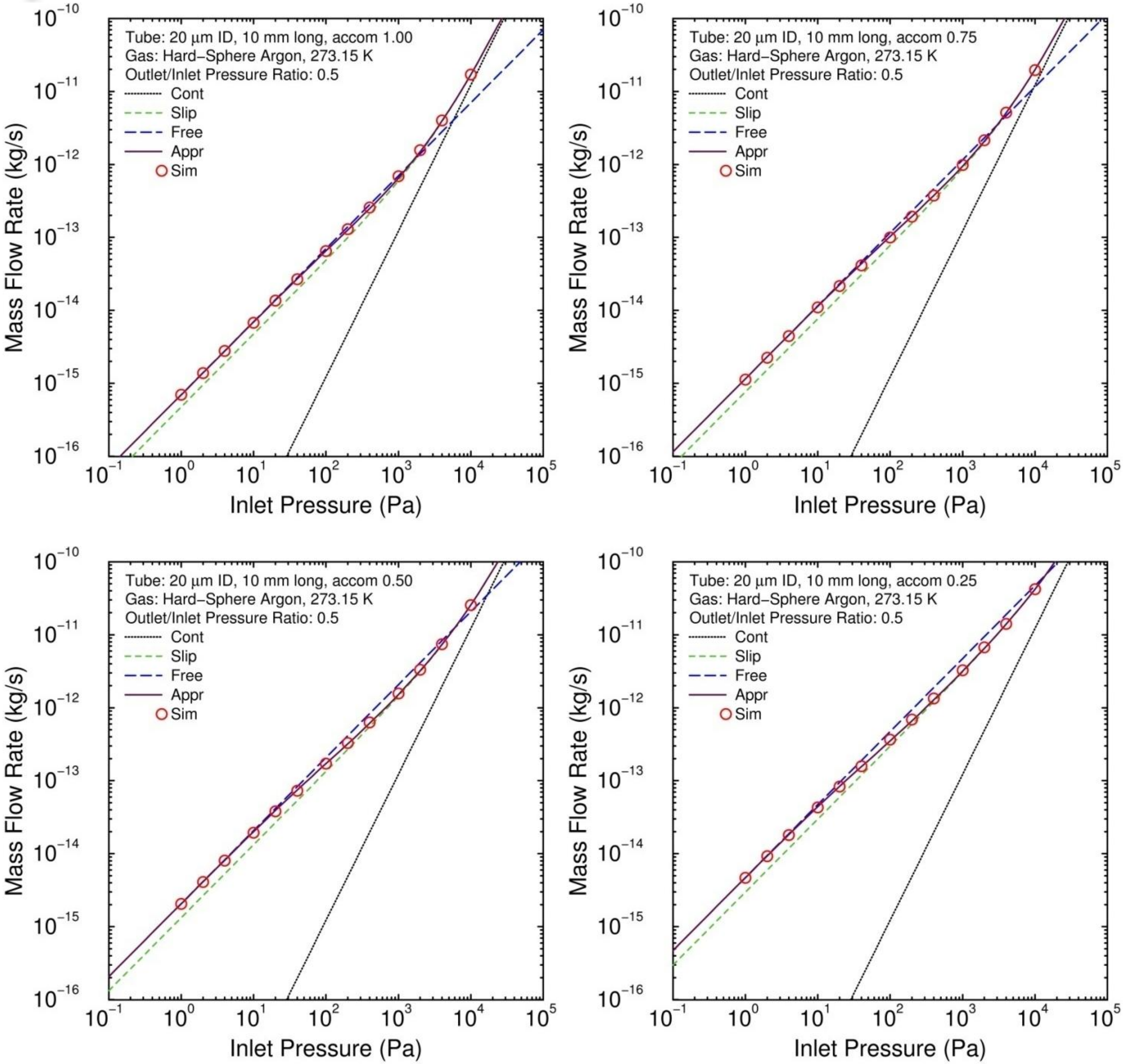
- **FM at low pressures**
- **Slip at high pressures**

Expression & simulations have Knudsen minimum

- **Accurate depth, breadth**
- **Reasonable ε, b_0, b_1, b_2**

Sandia National Laboratories

Mass Flow Rate: Long Tube



Conditions

- L/R = 1000 (long)
- $p_2/p_1 = 0.5$ (weak)

Expression agrees well with simulations

- All inlet pressures p_1
- All accom. coeffs. α

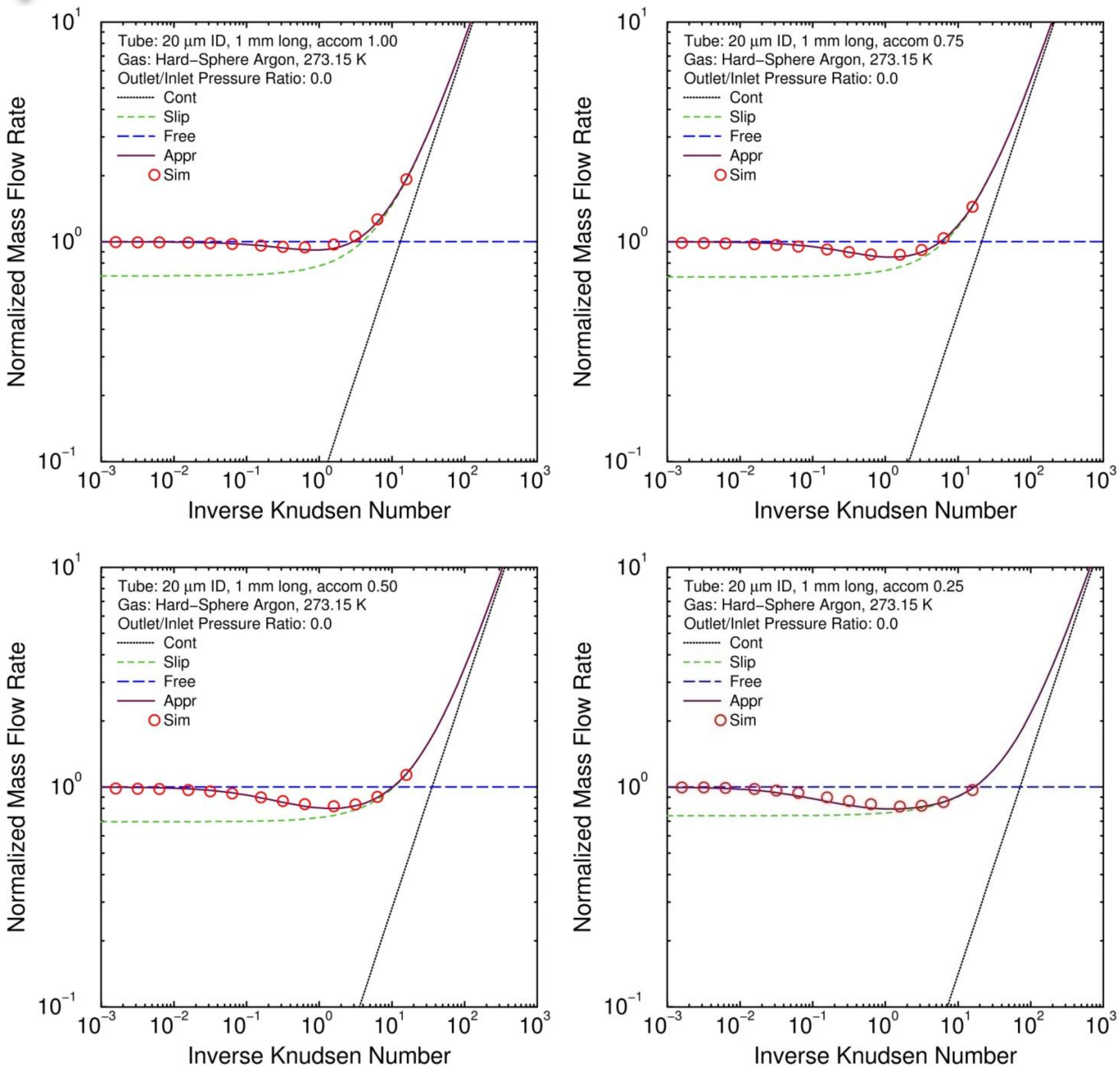
Expected behavior is observed in known limits

- FM at low pressures
- Slip at high pressures

Expression & simulations have Knudsen minimum

- Accurate depth, breadth
- Reasonable ε, b_0, b_1, b_2

Normalized Mass Flow Rate: Short Tube



Conditions

- **L/R = 100 (short)**
- **p_2/p_1 = 0.5 (strong)**

Expression agrees well with simulations

- **All inlet pressures p_1**
- **All accom. coeffs. α**

Normalized quantities facilitate comparison

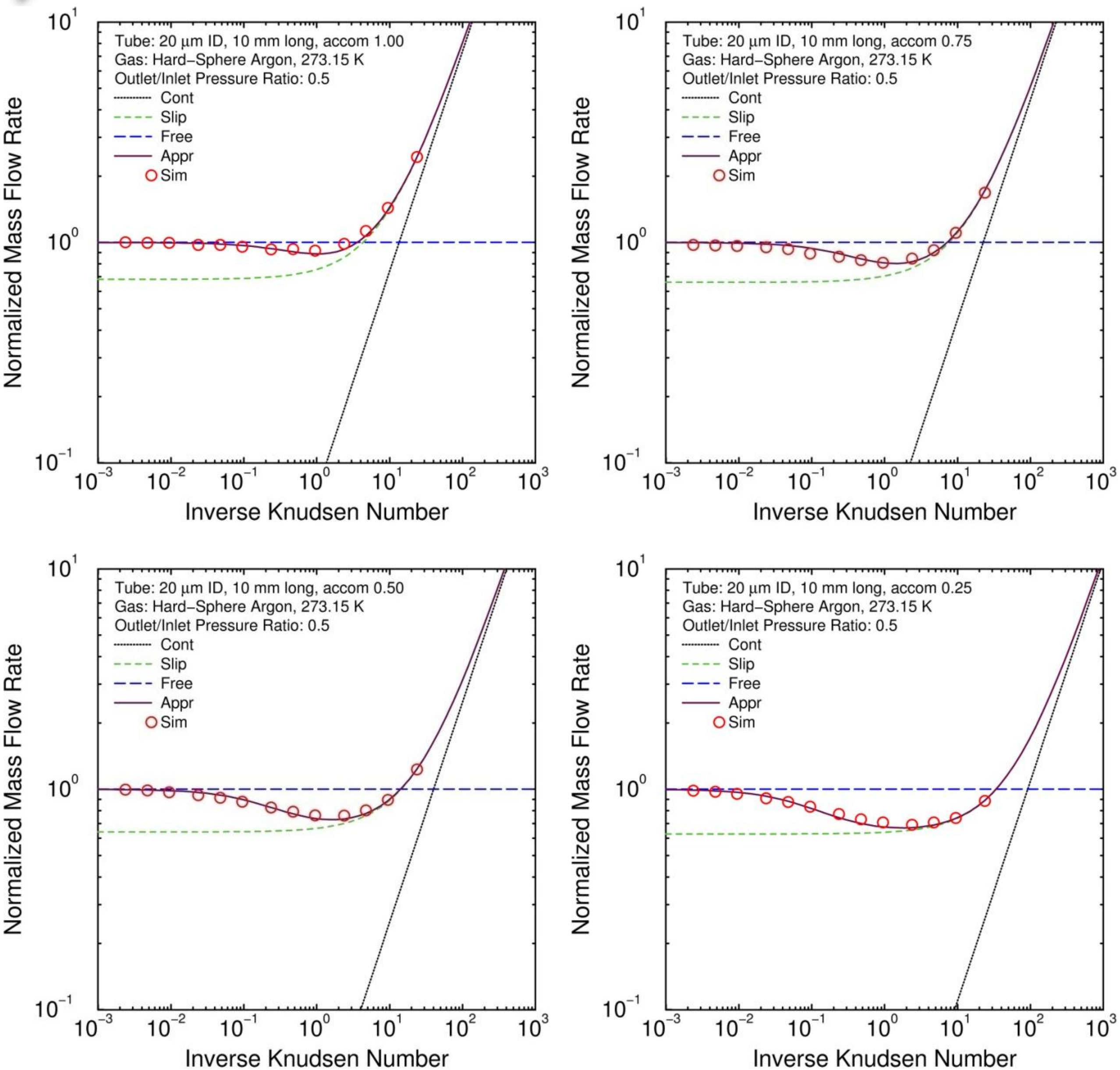
- **$\dot{M}/\dot{M}_F$, free-molecular**
- **$1/Kn_m = (p_1 + p_2)/2p_\lambda$**

Expression & simulations have Knudsen minimum

- **Accurate depth, breadth**
- **Reasonable ε, b_0, b_1, b_2**

Sandia National Laboratories

Normalized Mass Flow Rate: Long Tube



Conditions

- **L/R = 1000 (long)**
- **$p_2/p_1 = 0.5$ (weak)**

Expression agrees well with simulations

- **All inlet pressures p_1**
- **All accom. coeffs. α**

Normalized quantities facilitate comparison

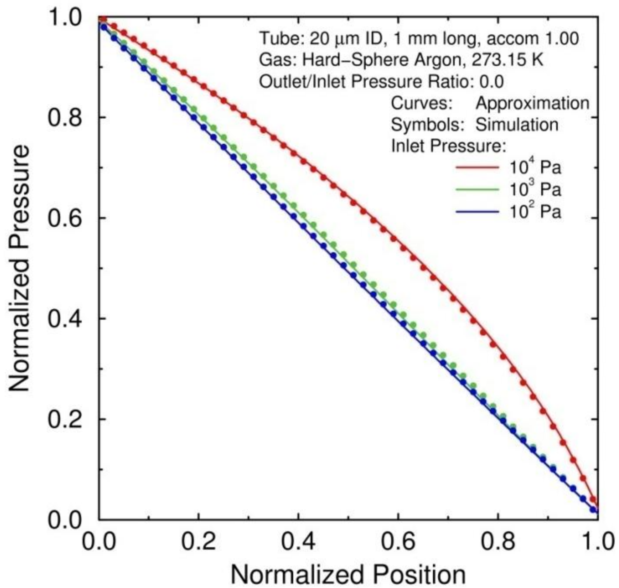
- **$\dot{M}/\dot{M}_F$, free-molecular**
- **$1/Kn_m = (p_1 + p_2)/2p_\lambda$**

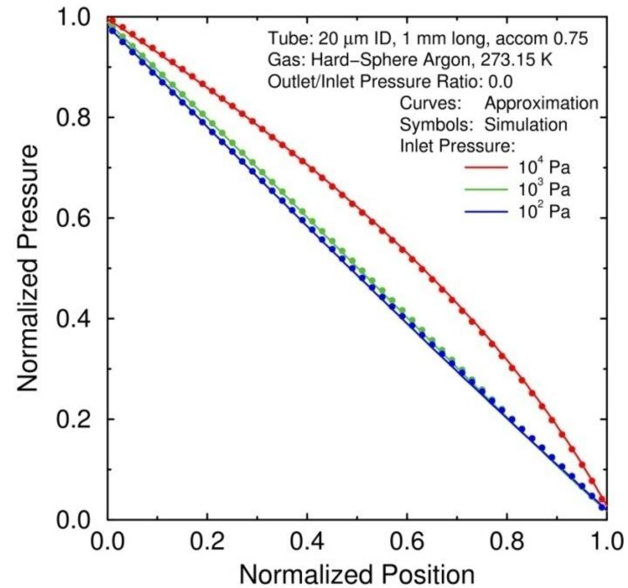
Expression & simulations have Knudsen minimum

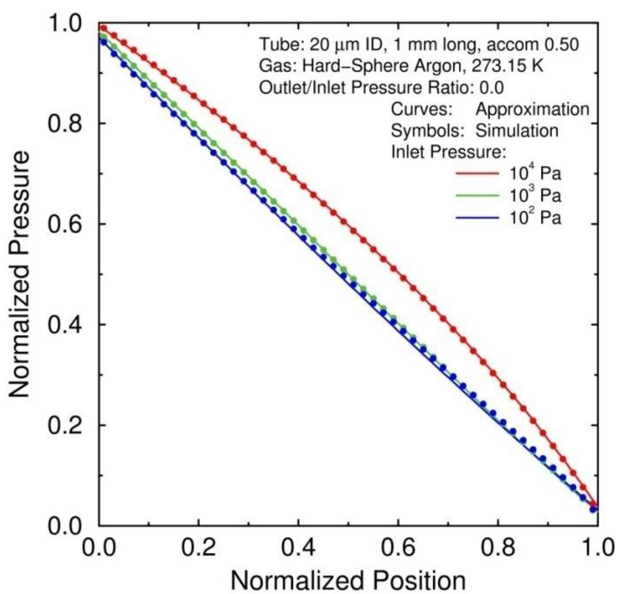
- **Accurate depth, breadth**
- **Reasonable ε, b_0, b_1, b_2**

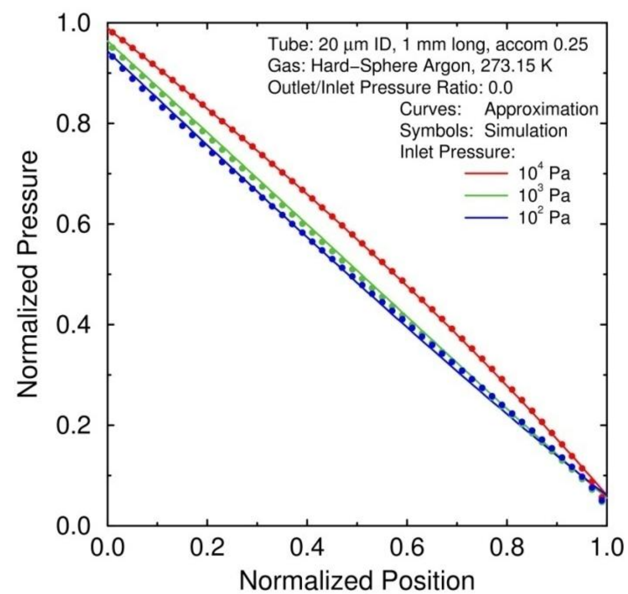
Sandia National Laboratories

Normalized Pressure Profiles: Short Tube









Conditions

- **L/R = 100 (short)**
- **p_2/p_1 = 0.0 (strong)**

Expression agrees well with simulations

- **All inlet pressures p_1**
- **All accom. coeffs. α**

Normalized quantities facilitate comparison

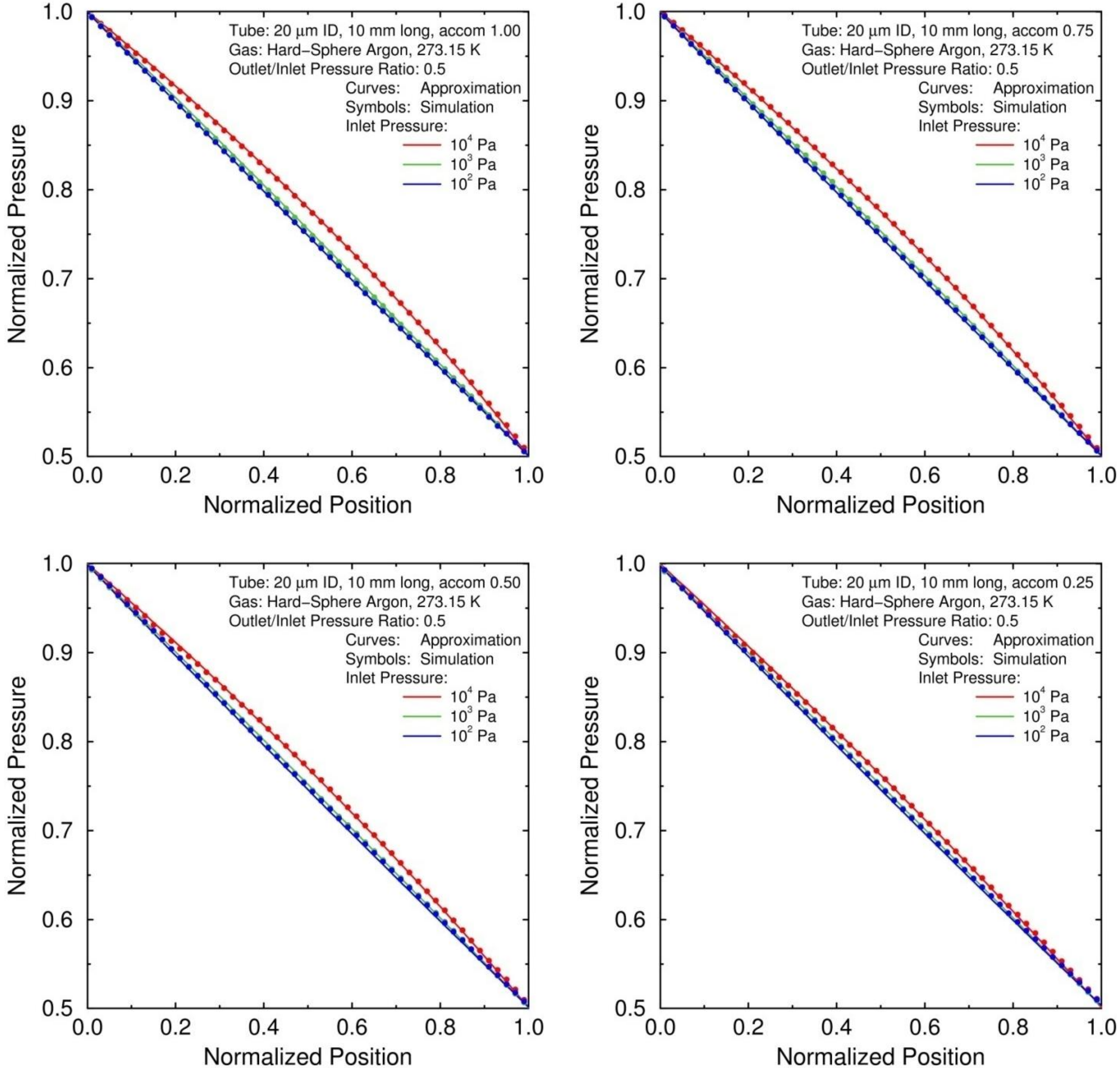
- **Pressure: $0 \leq p/p_1 \leq 1$**
- **Position: $0 \leq z/L \leq 1$**

Profiles have rather small discontinuities

- **At inlet and at outlet**
- **Increase as p_1 & α are decreased**

Sandia National Laboratories

Normalized Pressure Profiles: Long Tube



Conditions

- $L/R = 1000$ (long)
- $p_2/p_1 = 0.5$ (weak)

Expression agrees well with simulations

- All inlet pressures p_1
- All accom. coeffs. α

Normalized quantities facilitate comparison

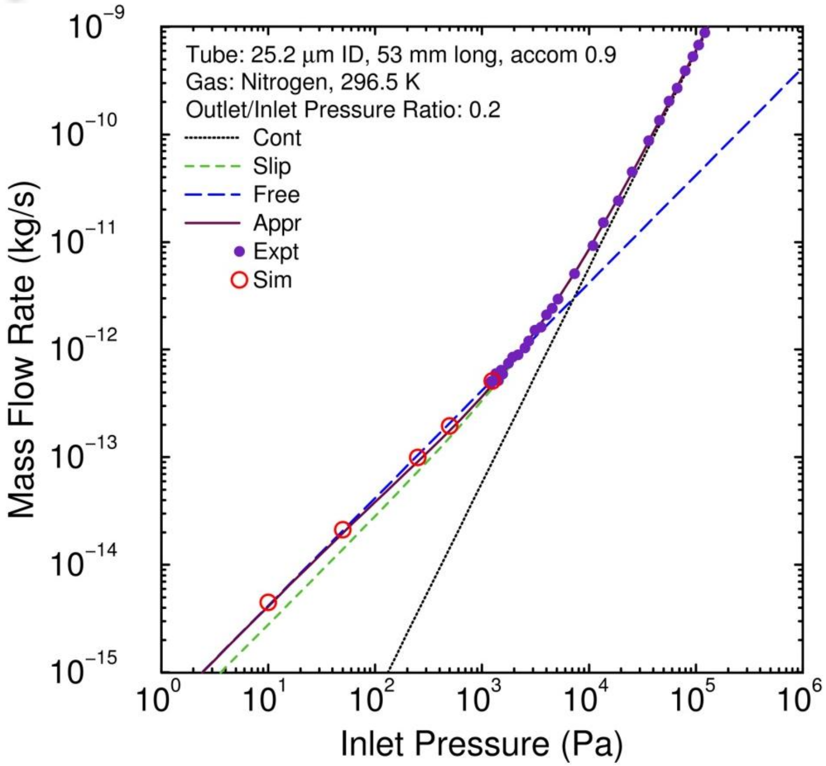
- Pressure: $0 \leq p/p_1 \leq 1$
- Position: $0 \leq z/L \leq 1$

Profiles have rather small discontinuities

- At inlet and at outlet
- Increase as p_1 & α are decreased

Sandia National Laboratories

Ewart et al. (2006) Tube Experiments



Tube Mass Flow Rate

$$\dot{M} = \dot{M}_C\left(1+\frac{8p_\lambda}{p_m}\varpi[p_1,p_2]\right),\quad \dot{M}_C = \frac{D^4}{16}\frac{p_m(p_1-p_2)}{\mu c^2 L}$$

$$\varpi[p_A,p_B] = \frac{2-\alpha}{\alpha}\left\{1+b_1\alpha+(\varepsilon b_0-1-b_1\alpha)\frac{b_2 p_\lambda}{p_A-p_B}\ln\left[\frac{p_A+b_2p_\lambda}{p_B+b_2p_\lambda}\right]\right\}$$

$$\rho=\frac{mp}{k_BT},\ \mu=\mu[T],\ c=\sqrt{\frac{8k_BT}{\pi m}},\ \lambda=\frac{2\mu}{\rho c},\ p_\lambda=\frac{p\lambda}{D},\ p_m=\frac{p_1+p_2}{2},\ \mathrm{Kn}_m=\frac{p_\lambda}{p_m}$$

$$\frac{\alpha L}{D}>10^3,\ \varepsilon\to 1,\ p_1\to p_{1\infty},\ p_2\to p_{2\infty};\ b_0=\frac{16}{3\pi},\ b_1=0.15,\ b_2=\frac{0.7\alpha}{2-\alpha}$$

Same values of ε, b_0, b_1, b_2 used for all circular tubes

- **Values are unchanged from previous cases (no adjusting)**
- **Relative to diameter, this tube length is essentially infinite**

Mass flow rate measured for silica microscale tube

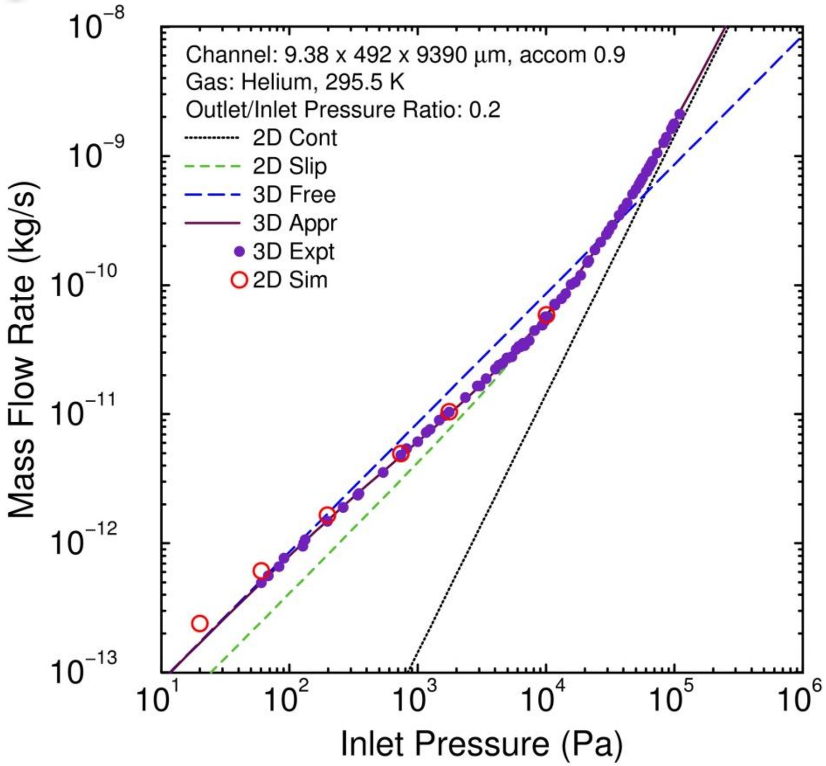
- **D = 25.2 μm, L = 53 mm, α = 0.9, N_2, T = 296.5 K, p_2/p_1 = 0.2**

Expression and simulations agree well with experiment

- **Lowest experiment pressure is above Knudsen minimum**
- **Highest simulation pressure reaches experiment**

Sandia National Laboratories

Ewart et al. (2007) Channel Experiments



Channel Mass Flow Rate

$$\dot{M} = \dot{M}_C\left(1+\frac{6p_\lambda}{p_m}\varpi[p_1,p_2]\right),\quad \dot{M}_C = \frac{2WH^3}{3\pi}\frac{p_m(p_1-p_2)}{\mu c^2 L}$$

$$\varpi[p_A,p_B] = \frac{2-\alpha}{\alpha}\left\{1+b_1\alpha+(\varepsilon b_0-1-b_1\alpha)\frac{b_2 p_\lambda}{p_A-p_B}\ln\left[\frac{p_A+b_2p_\lambda}{p_B+b_2p_\lambda}\right]\right\}$$

$$\rho=\frac{mp}{k_BT},\ \mu=\mu[T],\ c=\sqrt{\frac{8k_BT}{\pi m}},\ \lambda=\frac{2\mu}{\rho c},\ p_\lambda=\frac{p\lambda}{H},\ p_m=\frac{p_1+p_2}{2},\ \mathrm{Kn}_m=\frac{p_\lambda}{p_m}$$

$$b_0=3.28457,\ b_1=0.15,\ b_2=0.194,\ \varepsilon=0.725$$

Channel-flow expression correlates experiment values well

- **Derived for L×W×H rectangular channel just like for tube**
- **b_0 from Kennard infinite-length free-molecular flow**
- **b_1 = 0.15 as before to match slip regime for most gases**
- **b_2 and ε selected to match transition regime: L/W = 19.1**

Mass flow rate measured for silicon microscale channel

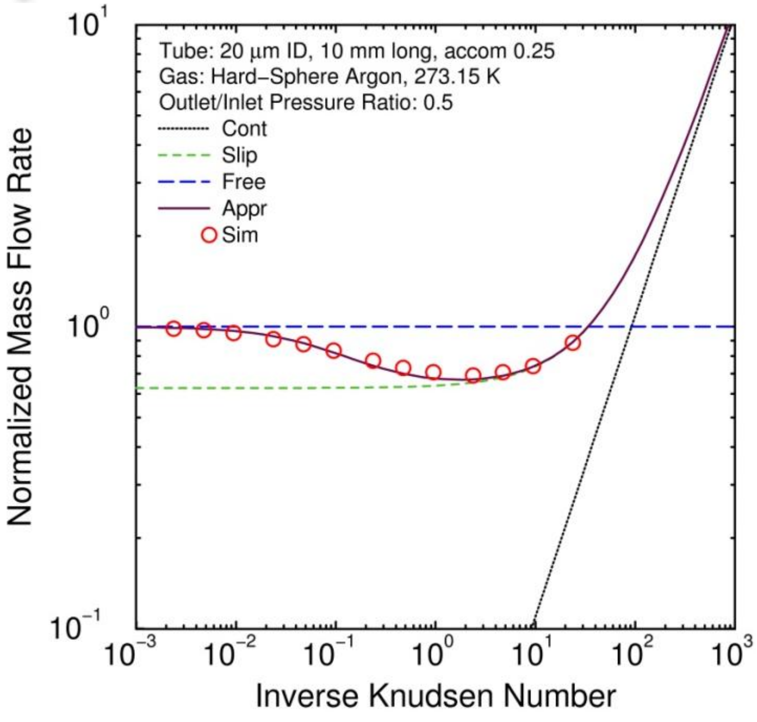
- **H,W,L = 9.38, 492, 9390 μm, α = 0.9, He, T = 295.5 K, p_2/p_1 = 0.2**

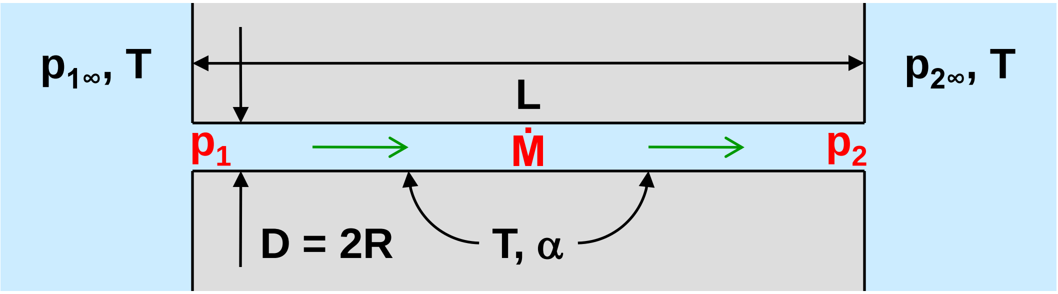
Expression and simulations agree with experiment

- **2D simulation overpredicts 3D experiment at low pressures**
- **b_2 and ε in channel expression are fit to experiment**

Sandia National Laboratories

Conclusions





$$\frac{\dot{M}}{\dot{M}_C} = 1 + \frac{8p_\lambda}{p_m}\varpi[p_1, p_2], \quad \dot{M}_C = \frac{D^4 p_m (p_1 - p_2)}{16\mu c^2 L}, \quad \frac{z}{L} = \frac{p_1^2 - p^2 + 16p_\lambda (p_1 - p)\varpi[p_1, p]}{p_1^2 - p_2^2 + 16p_\lambda (p_1 - p_2)\varpi[p_1, p_2]}$$

$$\varpi[p_A, p_B] = \frac{2-\alpha}{\alpha}\left\{1 + b_1\alpha + (\varepsilon b_0 - 1 - b_1\alpha)\frac{b_2 p_\lambda}{p_A - p_B}\ln\left[\frac{p_A + b_2 p_\lambda}{p_B + b_2 p_\lambda}\right]\right\}, \quad q = p + 6p_\lambda$$

$$F = \frac{3\pi D}{32L}\left(1 + \frac{16p_\lambda}{q_1 + q_2}\left(\varpi[p_1, p_2] - \frac{3}{4}\right)\right), \quad q_1 = \sqrt{\frac{(1+F)q_{1\infty}^2 + Fq_{2\infty}^2}{1+2F}}, \quad q_2 = \sqrt{\frac{(1+F)q_{2\infty}^2 + Fq_{1\infty}^2}{1+2F}}$$

$$\delta = \frac{4}{3}(2-\alpha), \quad \kappa = \frac{\delta - 1}{\delta}\frac{\alpha L}{D}, \quad \varepsilon = \frac{1+\kappa}{\delta+\kappa}, \quad b_0 = \frac{16}{3\pi}, \quad b_1 = 0.15, \quad b_2 = \frac{0.7\alpha}{2-\alpha}$$

$$\rho = \frac{mp}{k_B T}, \quad \mu = \mu[T], \quad c = \sqrt{\frac{8k_B T}{\pi m}}, \quad \lambda = \frac{2\mu}{\rho c}, \quad p_\lambda = \frac{p\lambda}{D}, \quad p_m = \frac{p_1 + p_2}{2}, \quad \mathrm{Kn}_m = \frac{\lambda_m}{D} = \frac{p_\lambda}{p_m}$$

Expressions for mass flow rate & pressure profile developed for isothermal steady flow in microscale tubes & channels

- **Covers free-molecular, transition, slip, & continuum regimes**
- **Treats all accommodation coefficients & tube aspect ratios**

Expression agrees with simulations & experiments

Sandia National Laboratories