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DSMC Simulations of the Gas Mass Flow Rate in a Microscale Tube

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Albuquerque, New Mexico, USA

Direct Simulation Monte Carlo 2011:

Theory, Methods, and Applications

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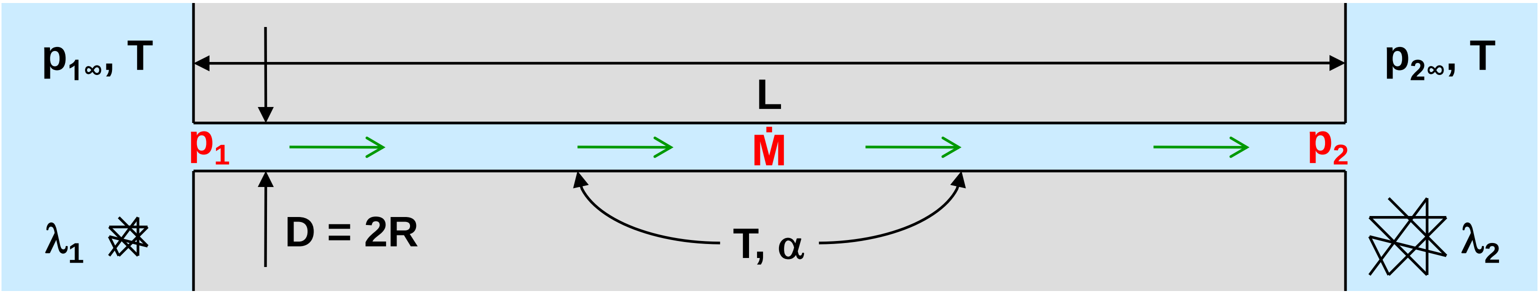
Gas Flow in a Microscale Tube



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

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Classic Study: Knudsen (1909)

Martin Knudsen, Annalen der Physik

- Circular tube with length >> diameter
- Pressure difference << mean pressure
- Mean free path arbitrary w.r.t. diameter
- Reflections with *unity accommodation*

Developed closed-form expression for steady isothermal mass flow rate

- Based on *empirical interpolation* between known free-molecular & continuum limits
- Uncertain accuracy away from limits

Discovered 'Knudsen minimum'

- For intermediate pressures, actual mass flow rates < free-molecular values

5. ***Die Gesetze der Molekularströmung und der inneren Reibungsströmung der Gase durch Röhren; von Martin Knudsen.***

1 **Einleitung.**

Für die Strömung der Gase durch lange, enge Röhren ist es, wie bekannt, möglich, Poisseuilles Gesetz zu verwenden, wenn die mittlere Weglänge der Gasmoleküle im Vergleich mit dem Durchmesser der Röhre verschwindend klein ist. Aus den Versuchen, welche Kundt und Warburg[1]) und später Warburg[2]) ausgeführt haben, geht hervor, daß Poisseuilles Gesetz nicht mit voller Genauigkeit gilt, wenn die Röhre so eng ist, daß die mittlere Weglänge der Gasmoleküle im Vergleich mit dem Durchmesser der Röhre nicht als verschwindend klein betrachtet werden kann. Die Abweichungen vom Gesetze gaben Anlaß zur Überführung der Begriffe von äußerer Reibung und Gleitung auf die Bewegung eines Gases längs einer festen Wand; die Gleitungserscheinung ist aber doch nicht so eingehend untersucht worden, daß diese Untersuchungen zu viel mehr als zu Korrektionen geführt hahen, wenn man aus Strömungsversuchen oder Versuchen mit schwingenden Platten den Koeffizienten der inneren Reibung berechnete. Der einzige, der soviel mir bekannt, in bezug auf die Strömung von Gasen durch sehr enge Kanäle entscheidende Versuche ausgeführt hat, ist C. Christiansen[3]), welcher zeigte, daß Poisseuilles Gesetz, für die Strömung zwischen parallelen Wänden modifiziert, seine Gültigkeit verliert, wenn der Abstand der Wände sehr klein gemacht wird. Christiansen wies außerdem nach, daß das Gesetz für die Strömung dann mit Grahams Gesetz für die Diffusion von Gasen durch Körper wie künstlichen Graphit stimmt, indem

1) A. Kundt u. E. Warburg, Pogg. Ann. **155.** p. 337, 525. 1875.
2) E. Warburg, Pogg. Ann. **159.** p. 399. 1876.
3) C. Christiansen, Wied. Ann. **41.** p. 565. 1890.

Classic Study: Smoluchowski (1910)

Marian Smoluchowski, Annalen der Physik

- Circular tube with length >> diameter
- Pressure difference << mean pressure
- Mean free path arbitrary w.r.t. diameter
- Reflections with *sub-unity accommodation*

Developed closed-form expression for steady isothermal mass flow rate

- Modification of Knudsen's *interpolation* between free-molecular and continuum
- Uncertain accuracy away from limits

Accommodation factor $(2 - \alpha)/\alpha$ derived

- Knudsen minimum at all accommodations

1559

22. ***Zur kinetischen Theorie der Transpiration und Diffusion verdünnter Gase; von M. v. Smoluchowski.***

(Bearbeitet nach einer am 4. Juli 1910 der Krakauer Akademie der Wissenschaften vorgelegten Abhandlung.)

I.

Die Erscheinungen der Zähigkeit in verdünnten Gasen und der thermischen Transpiration, welche vor etwa 30 Jahren allgemeines Interesse erregten und welche bei der Entwickelung der kinetischen Gastheorie eine bemerkenswerte Rolle gespielt haben, sind seitdem vollständig unbeachtet geblieben; erst in der letzten Zeit ist auf diesem Gebiet ein erheblicher Fortschritt zu verzeichnen, indem Knudsen[1]) sie in dem bisher wenig bearbeiteten Bereich sehr niedriger Drucke genauer studierte.

Ohne in eine Diskussion des experimentellen Teiles dieser bemerkenswerten Arbeiten einzugehen, möchte ich einige theoretische Bemerkungen vorbringen, um gewisse Mängel der theoretischen Überlegungen Knudsens zu beheben.

Knudsen verwendet die alte, von Maxwell in seinen ersten Arbeiten benutzte, und ebenso auch von Clausius, O. E. Meyer u. a. angewendete Methode, welche auf der Annahme elastischer Kugelmoleküle und auf der Einführung des Begriffs der mittleren Weglänge basiert, sowie auf der Voraussetzung, daß das Maxwellsche Geschwindigkeitsverteilungsgesetz in seiner normalen Form bestehen bleibt.

Nun sind aber alle derartigen Berechnungen, soweit Zähigkeit, Wärmeleitung und Diffusion in Betracht kommen, unrichtig. Maxwell und Boltzmann haben bewiesen[2]), daß daß das Geschwindigkeitsverteilungsgesetz in diesen Fällen

1) M. Knudsen, Ann. d. Phys. **28.** p. 75. 1909; **31.** p. 205, 633. 1910.
2) J. Maxwell, Phil. Trans. **170.** p. 231. 1879; L. Boltzmann, Wiener Ber. **81.** p. 117. 1880; **84.** p. 40, 1230. 1881.

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Classic Study: Clausing (1932)

961

Pieter Clausing, Annalen der Physik

- Tube with *arbitrary length* w.r.t. diameter
- Pressure difference << mean pressure
- Mean free path >> diameter
- Reflections with *unity accommodation*

Developed integral expression for steady isothermal mass flow rate

- Expression is *not closed-form*
- Limited to free-molecular flow

Rigorous free-molecular mass flow rate

- Length is finite relative to diameter

Über die Strömung sehr verdünnter Gase durch Röhren von beliebiger Länge

Von P. Clausing[1]

(Natuurkundig Laboratorium der N. V. Philips' Gloeilampenfabrieken Eindhoven-Holland)

(Mit 1 Figur)

Inhalt: § 1. Die Formeln von Knudsen, v. Smoluchowski und Dushman für die stationäre Molekularströmung. — § 2. Transformation der Formeln auf kinetische Veränderliche; Durchlaufswahrscheinlichkeit. — § 3. Ableitung der Dushmanschen Formel. — § 4. Das Problem der kurzen runden Zylinderröhre. — § 5. Das Problem der langen runden Zylinderröhre. — § 6. Die Anwendung der Strömungsformeln in der Hochvakuumtechnik. — Zusammenfassung.

§ 1. Die Formeln von Knudsen, v. Smoluchowski und Dushman für die stationäre Molekularströmung

Knudsen[2]) hat für die stationäre Strömung eines sehr verdünnten Gases durch eine zylindrische Röhre mit beliebig geformtem Querschnitt die folgende Formel gegeben:

$$J = \frac{8}{3}\sqrt{\frac{2}{\pi}} \cdot \frac{S^2}{s L} \cdot \frac{1}{\sqrt{d}}\,(p_1 - p_2). \qquad (1)$$

J = Menge des durchgeströmten Gases pro Sekunde, gemessen durch das Volumen, daß sie beim Druck = 1 beanspruchen würde.
d = Dichte des Gases beim Druck = 1.
S = Durchschnitt der Röhre.
s = Umriß des Durchschnitts.
L = Länge der Röhre.

1) Die Hinweise A bis H in den Noten beziehen sich auf die folgenden Arbeiten des Verfassers: A. Verslagen Amsterdam **35.** S. 1023. 1926; B. Leidener Dissertation, Amsterdam 1928; C. Physica **9.** S. 65. 1929; D. Ann. d. Phys. [5] **4.** S. 533. 1930: E. Ann. d. Phys. [5] **4.** S. 567. 1930; F. Ann. d. Phys. [5] **7.** S. 489. 1930; G. Ann. d. Phys. [5] **7.** S. 569. 1930; H. Ztschr. f. Phys. **66.** S. 471. 1930.

2) M. Knudsen, Ann. d. Phys. [4] **28.** S. 75. 1909.

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Classic Text: Kennard (1938)

Earle Kennard, Kinetic Theory of Gases

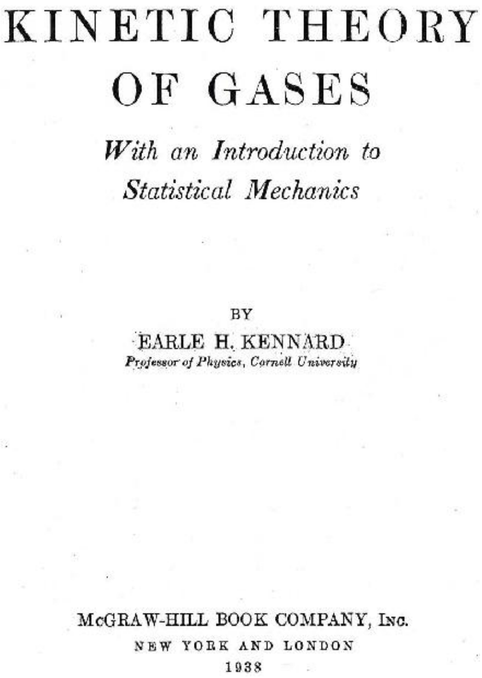
- Tube of *arbitrary cross section* << length
- Pressure difference << mean pressure
- Mean free path >> diameter
- Reflections with *sub-unity accommodation*

Developed 'closed-form' expression for steady isothermal mass flow rate

- Factor contains *complicated integrals*
- Limited to free-molecular flow

Rigorous free-molecular mass flow rate

- Long tubes with arbitrary cross section
- Generalizes classic studies to date



KINETIC THEORY OF GASES

With an Introduction to Statistical Mechanics

BY

EARLE H. KENNARD

Professor of Physics, Cornell University

McGRAW-HILL BOOK COMPANY, INC.

NEW YORK AND LONDON

1938

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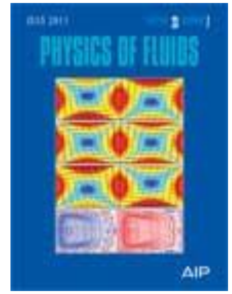
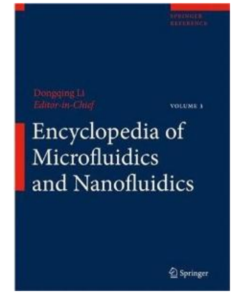
Recent Work: Sharipov & Coworkers (1990+)

$$\frac{df}{dt} \to \nu\left(f_0 - f \right)$$

analysis with BGK collision operator





Felix Sharipov

Felix Sharipov et al. have studied tube flow extensively

- Coworkers include Seleznev, Kalempa, Loyalka, Siewert, Thomas, Valougeorgis, Varoutis, Cercignani, …
- Two encyclopedic reviews in J. Phys. Chem. Ref. Data and many other articles, chapters, and books

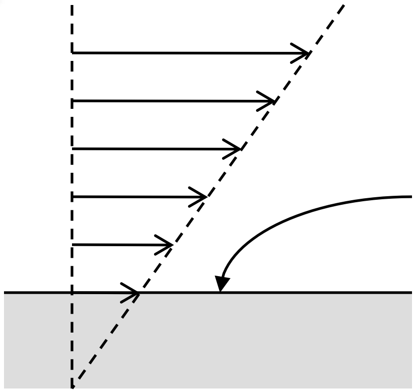
Sharipov has emphasized BGK-based analytical methods

- Focused mainly on long tubes with unity accommodation
- Provided extensive tables of mass flow rate for all regimes

He has also performed some numerical simulations

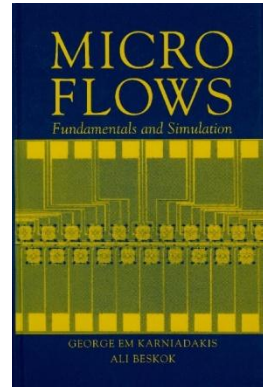
- Orifices, short tubes, arbitrary accommodation

Recent Work: Karniadakis & Beskok (2002)



slip velocity

$$U_S - U_W = \frac{2-\alpha}{\alpha}\left\{\frac{\mathrm{Kn}}{1-b\mathrm{Kn}}\left(\frac{\partial U}{\partial n}\right)_S\right\}$$

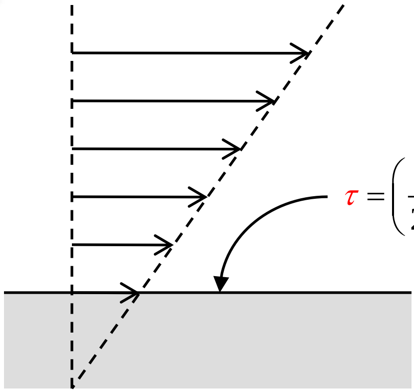


George Karniadakis

Ali Beskok

- Micro Electro Mechanical Systems (MEMS) reawakened interest in gas flow through long thin channels
  - Silicon channels of <10 μm height and >10 mm length
  - Mean free path at STP is 0.06 μm, large enough to matter
- George Karniadakis & Ali Beskok advocated new approach
  - Accurate mass flow rate needs accurate velocity profile
  - Improve slip boundary condition for Navier-Stokes equation
- Slip regime is more accurate; however, free-molecular and transition regimes are not directly addressed

Recent Work: Present Approach



shear stress

$$\tau = \left(\frac{\alpha}{2-\alpha}\right)\left(\frac{\rho c u}{2}\right)\left(\frac{1+d_2\left(\lambda/H\right)}{1+d_1\alpha+d_2\left(\lambda/H\right)}\right)$$

Michael Gallis

Dan Rader

John Torczynski

Gallis & coworkers (2007, 2008) adopt different philosophy

- Transport rates are of primary importance
  - Mass, momentum, energy
- Fields are of secondary importance
  - Concentration, velocity, temperature

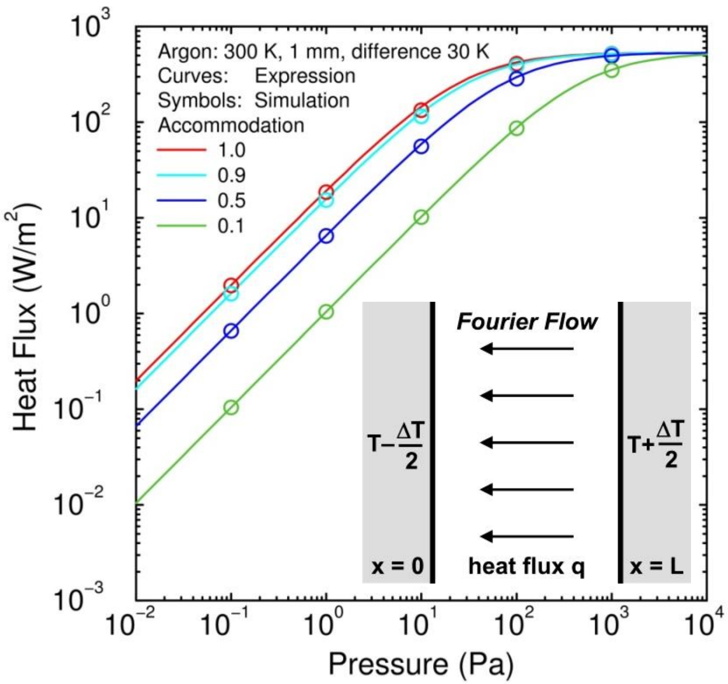
Construct boundary conditions to give accurate transport

- When used with Navier-Stokes equations
- For free-molecular, transition, slip, continuum

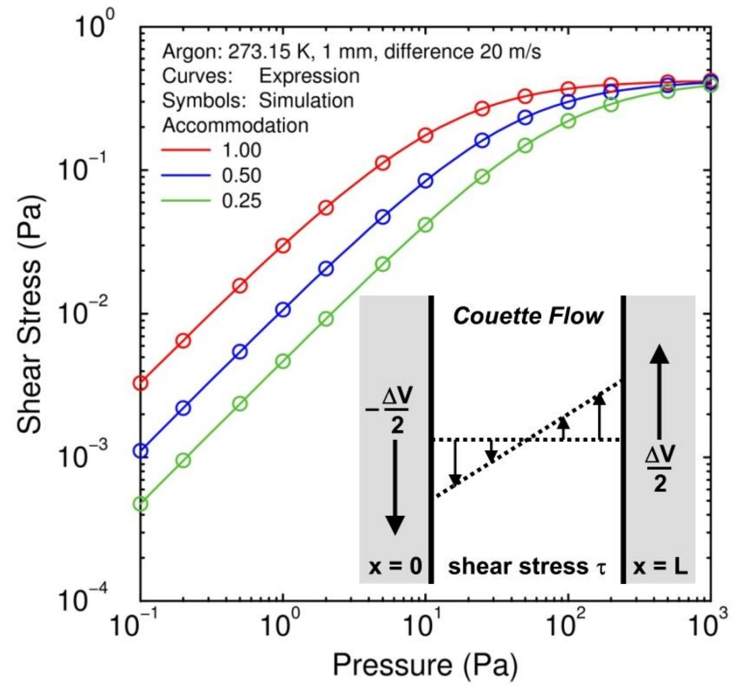
Resulting fields are only qualitatively correct

- Fields are accurate in continuum limit

Parallel-Plate Applications



$$q = \frac{\alpha}{2-\alpha}\left(\frac{1+c_2\left(\lambda/L\right)}{1+c_1\alpha+c_2\left(\lambda/L\right)}\right)\left(1+\frac{\zeta}{4}\right)\frac{pc}{T}\left(T-T_w\right)$$



$$\tau = \frac{\alpha}{2-\alpha}\left(\frac{1+d_2\left(\lambda/L\right)}{1+d_1\alpha+d_2\left(\lambda/L\right)}\right)\frac{\rho c}{2}\left(u-u_w\right)$$

Present philosophy works well for parallel-plate geometry

- Heat flux (Fourier flow): heat transfer
- Shear stress (Couette flow): momentum transfer

Accurate for free-molecular through continuum

- Low to high pressures, all accommodations

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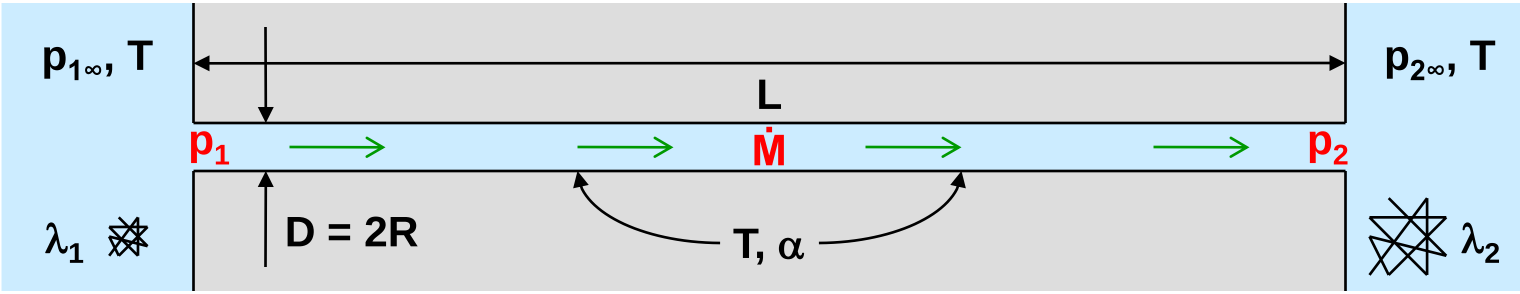
Tube-Flow Application



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

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**

How Parameters Are Specified

Approximate Closed-Form Expression

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

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

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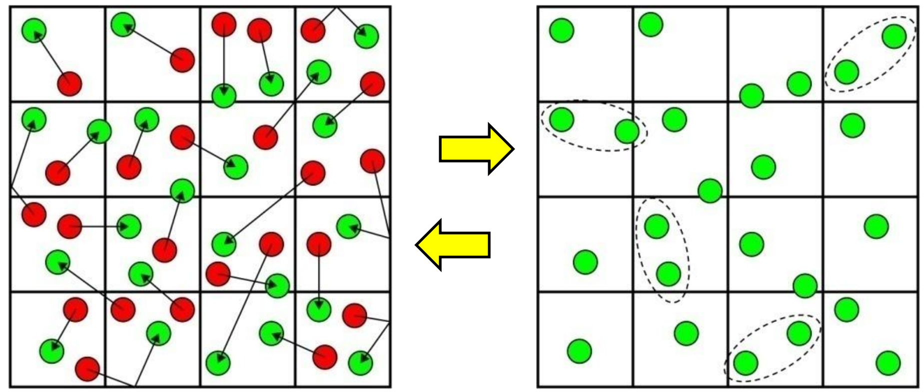
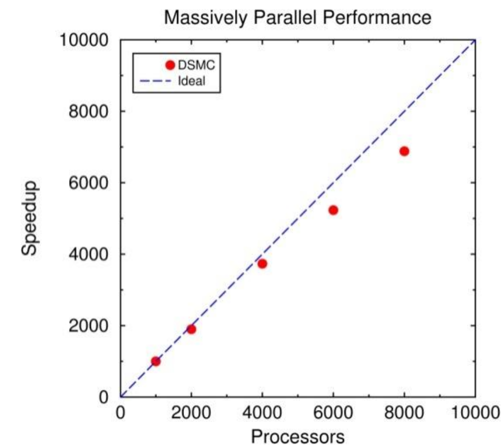
Molecular-Gas-Dynamics Simulations



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

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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_λ = 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

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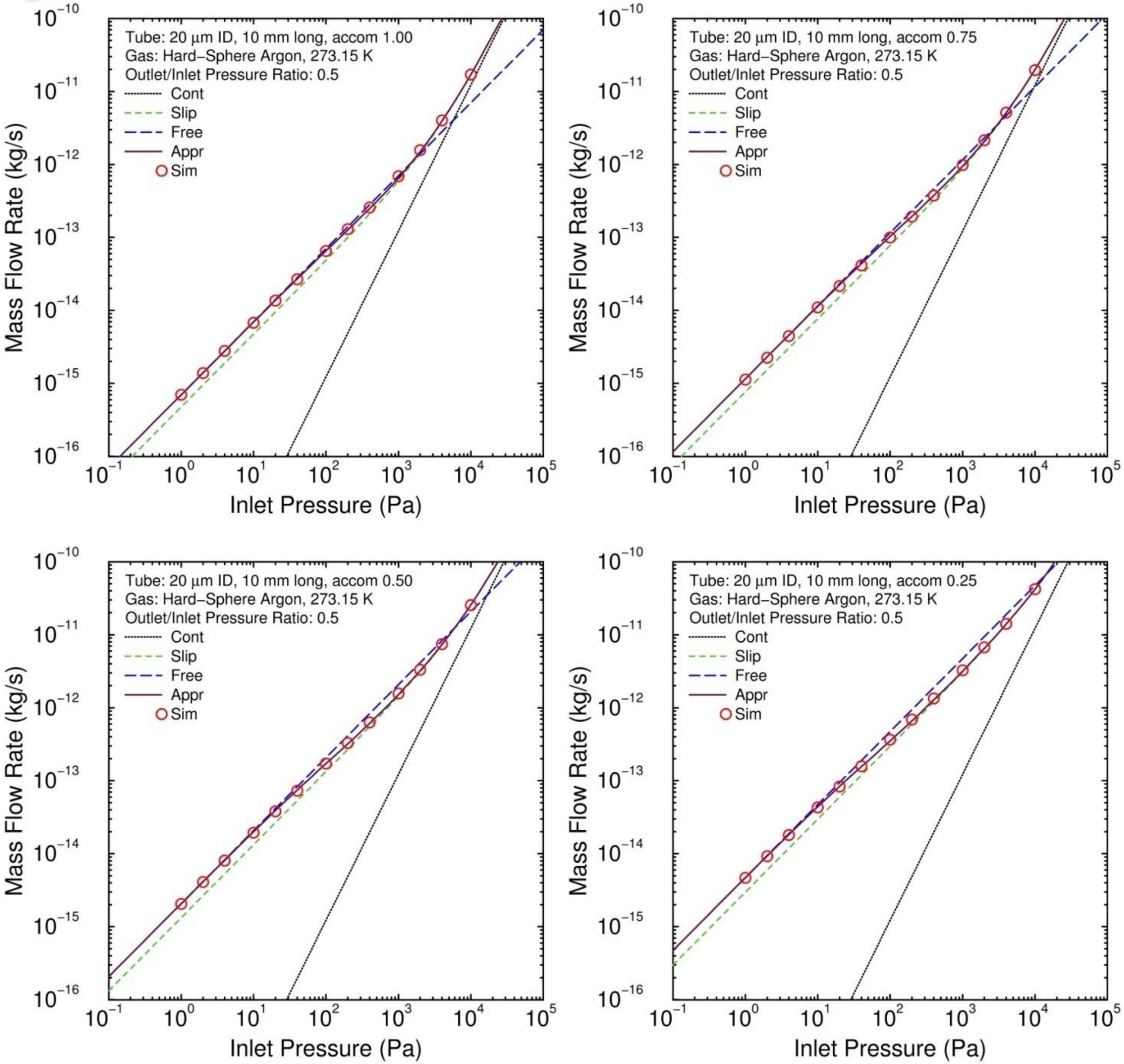
Mass Flow Rate: Long Tube



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

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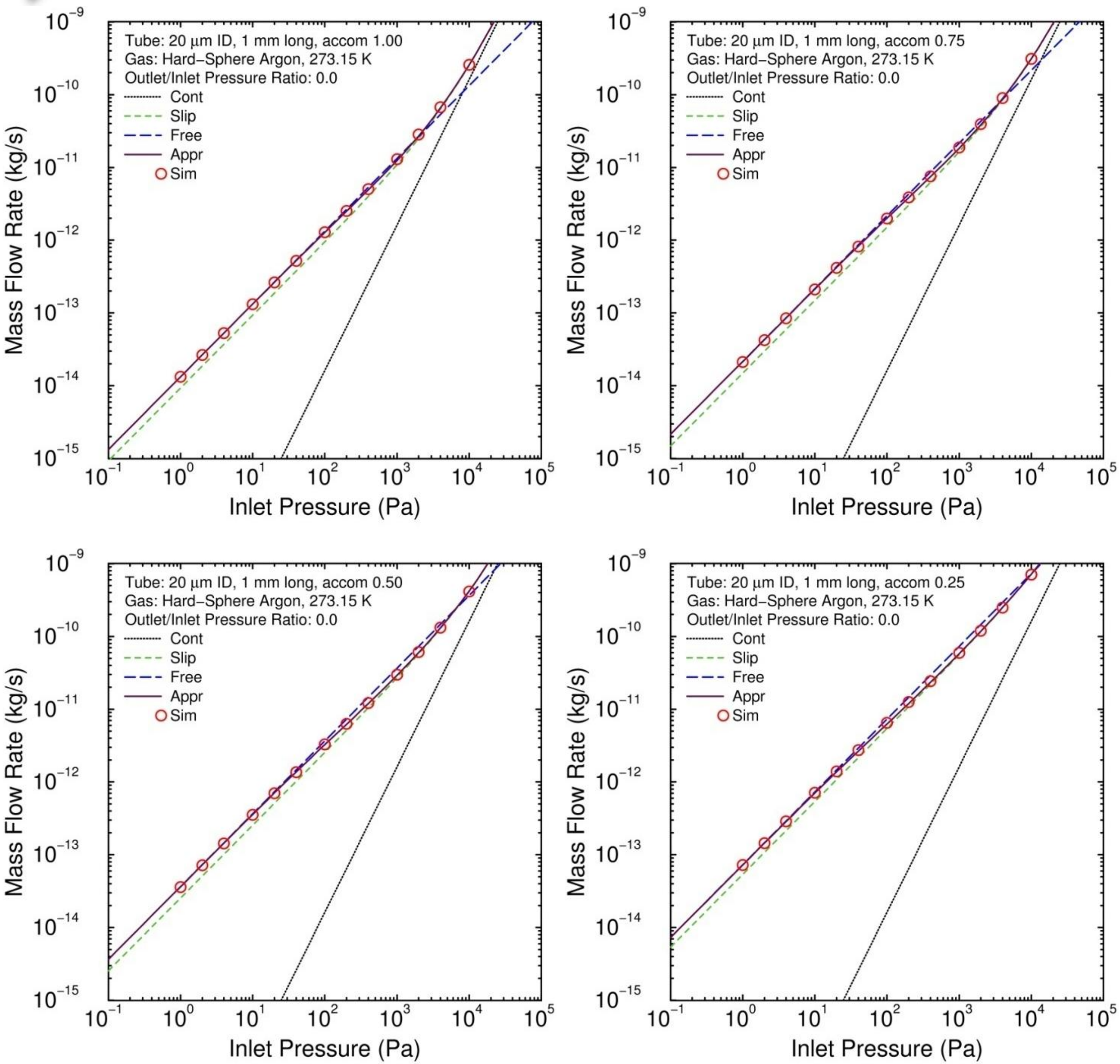
Mass Flow Rate: Short Tube



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**

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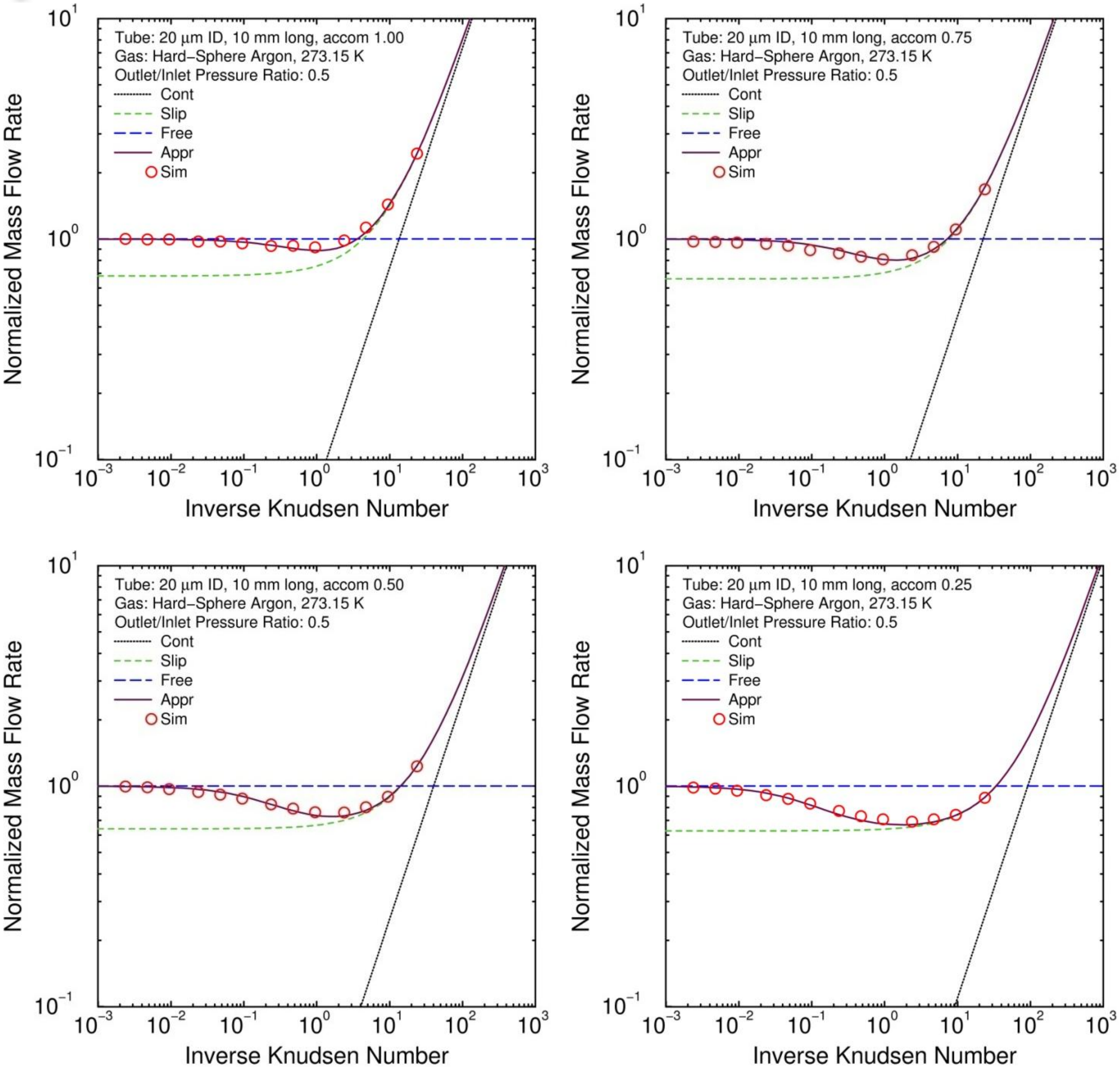
Normalized Mass Flow Rate: Long Tube



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**

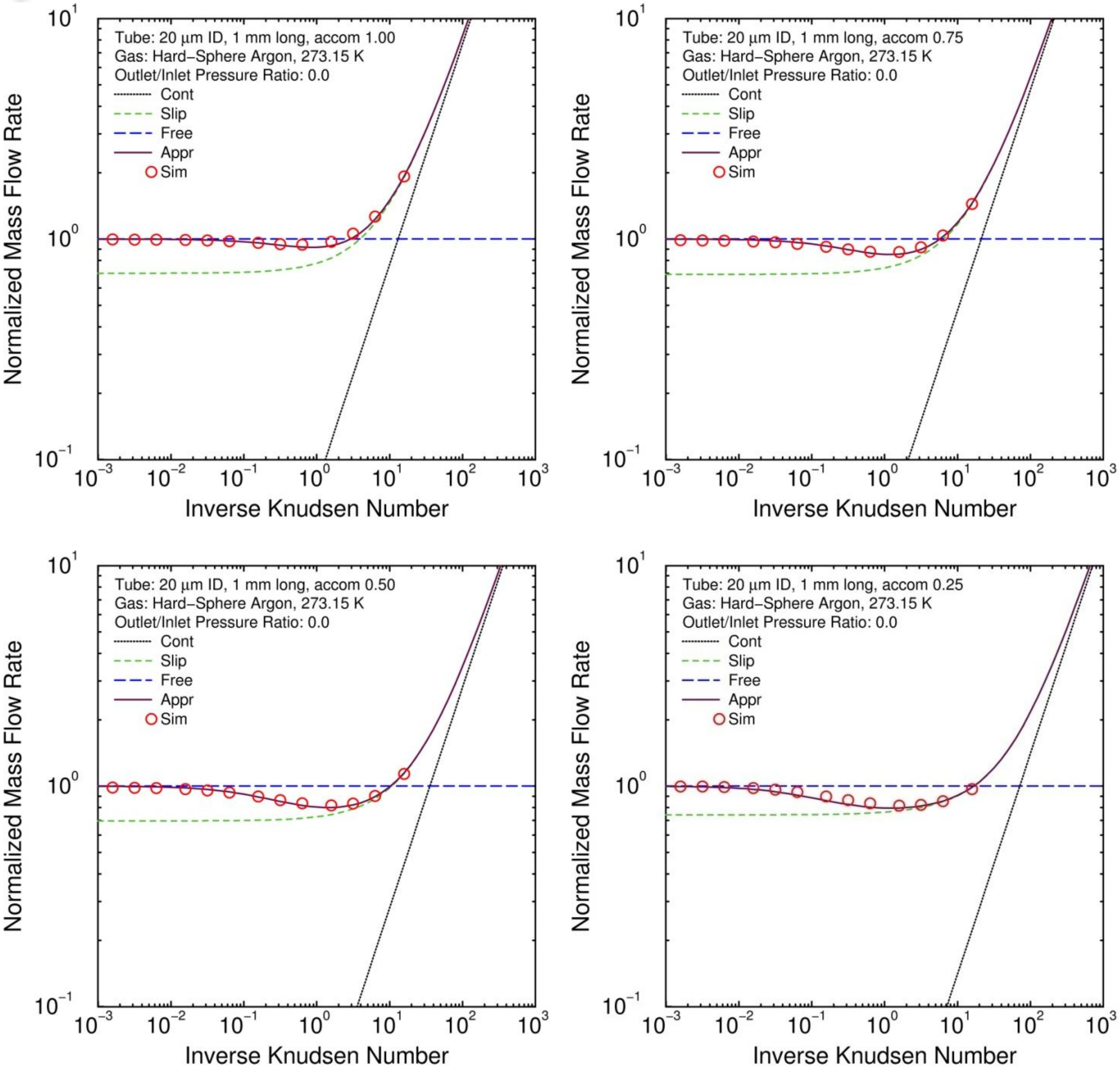
Normalized quantities facilitate comparison

- **$\dot{M}/\dot{M}_F$, 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**

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

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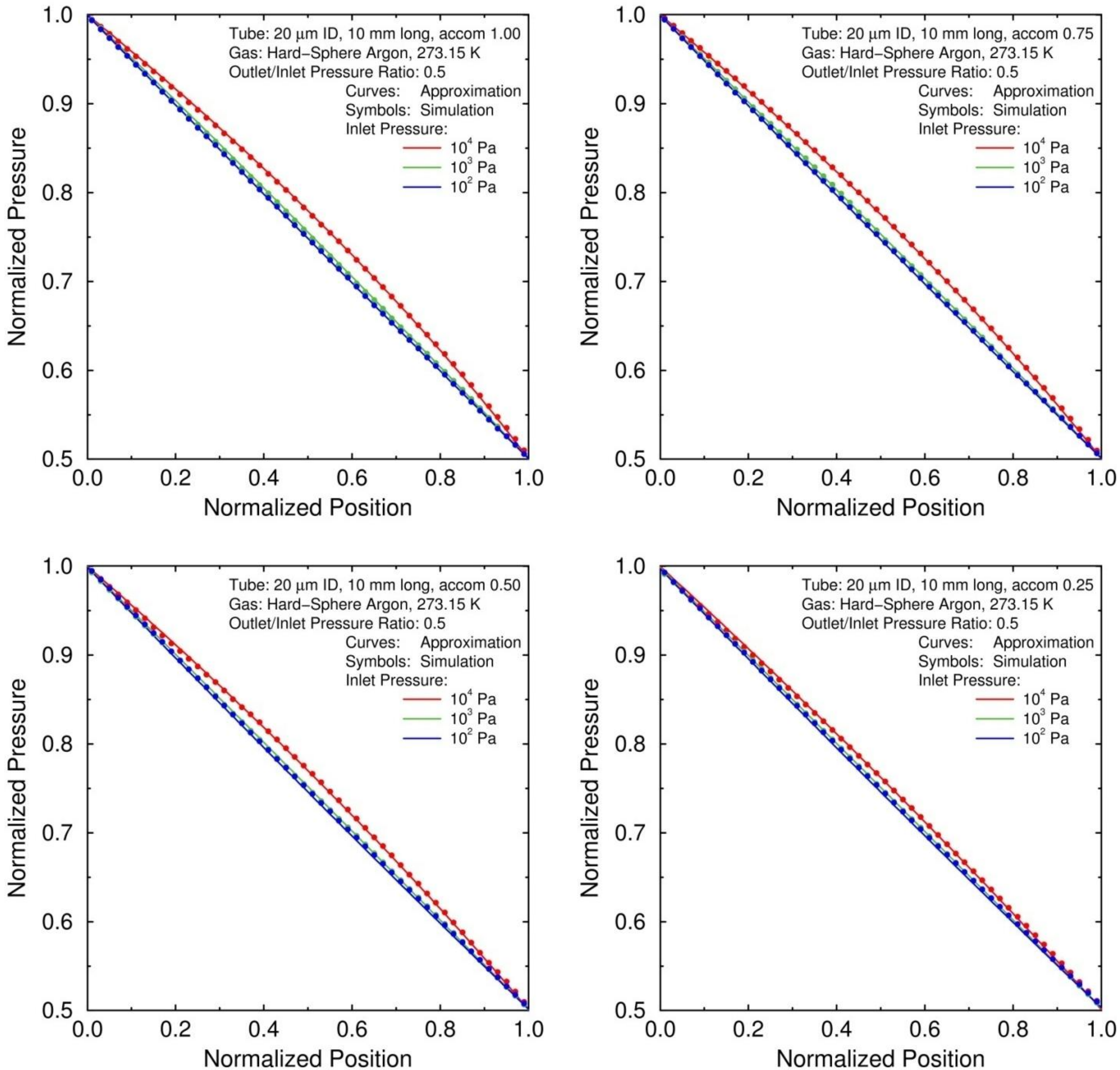
Normalized Pressure Profiles: Long Tube



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**

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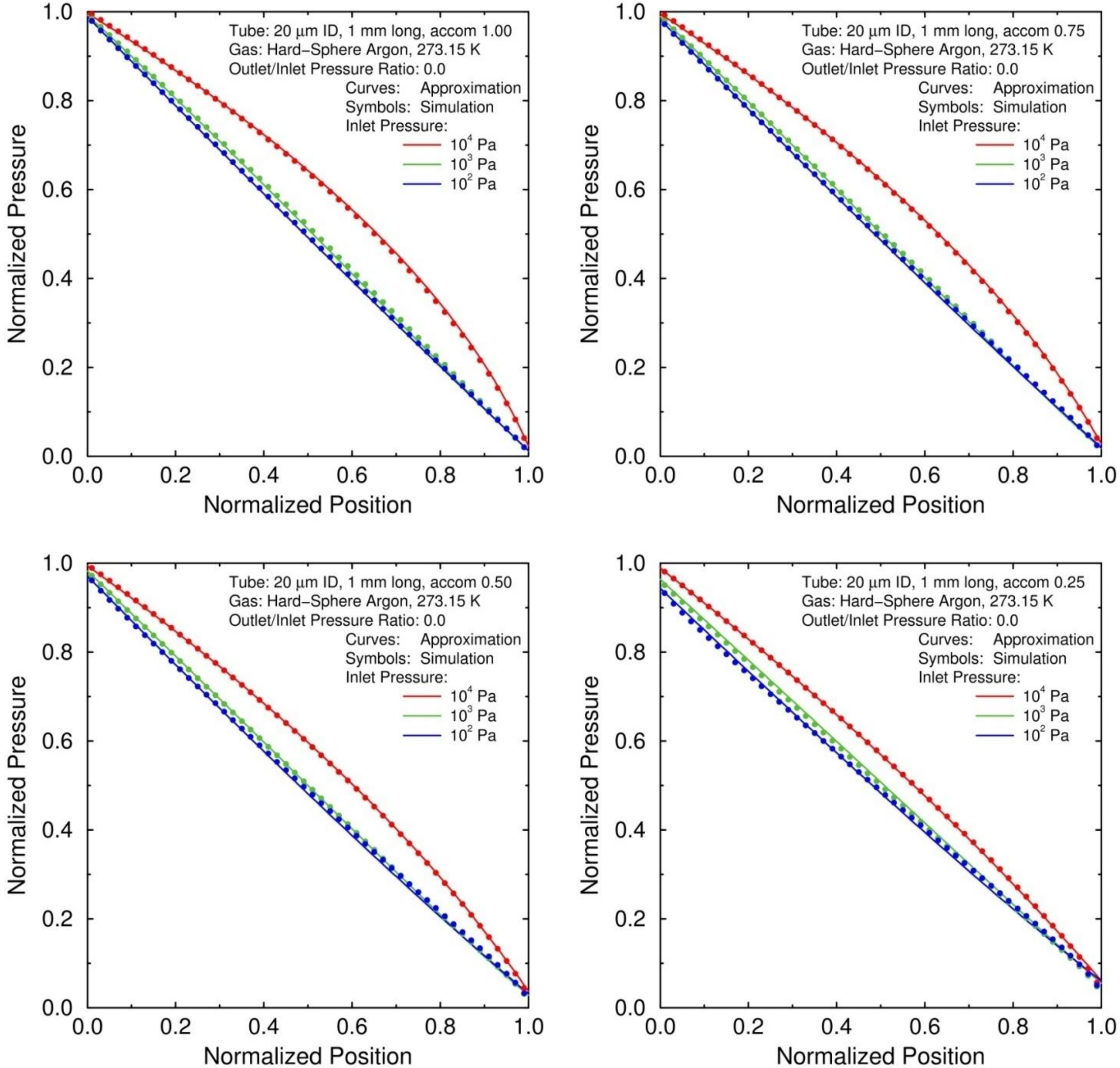
Normalized Pressure Profiles: Short Tube



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

Profiles have rather small discontinuities

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

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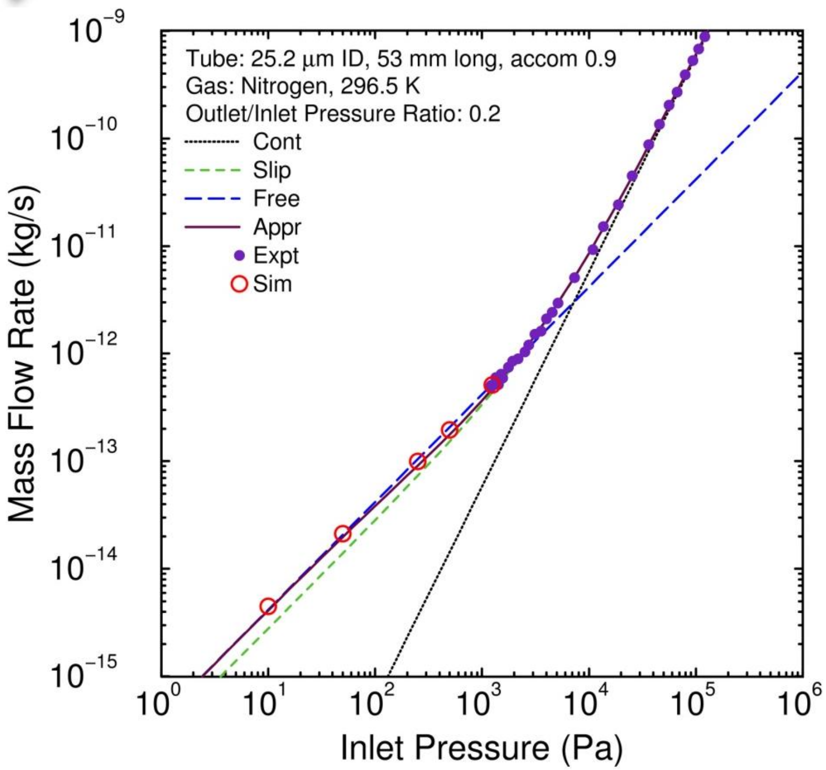
Ewart et al. (2006) Tube Experiments



Tube Mass Flow Rate

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

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

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

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

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**

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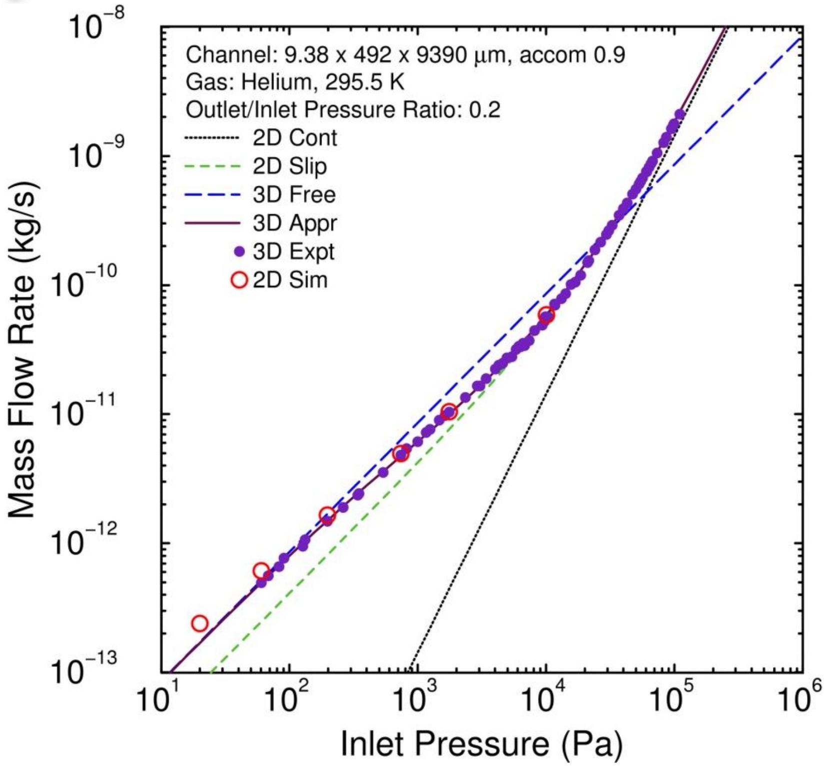
Ewart et al. (2007) Channel Experiments



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**

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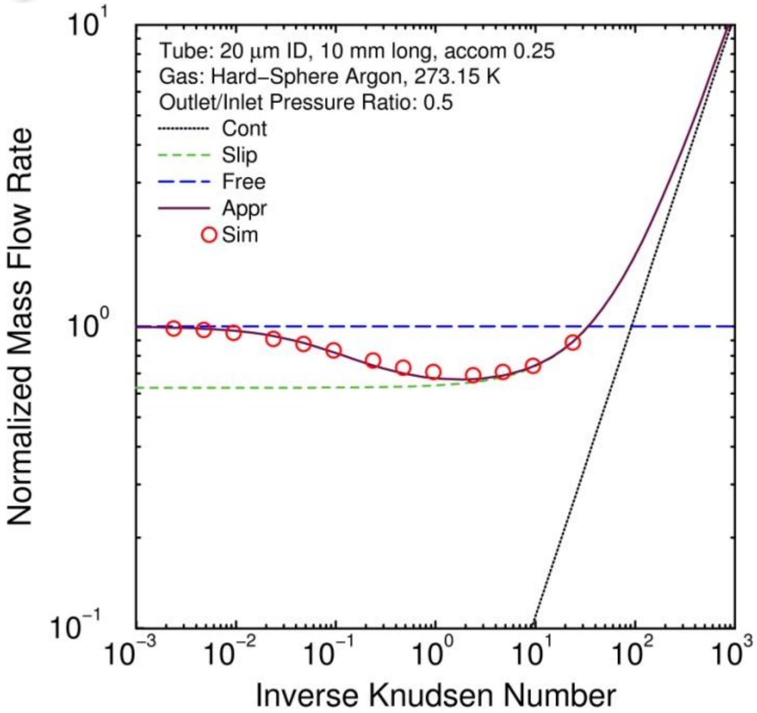
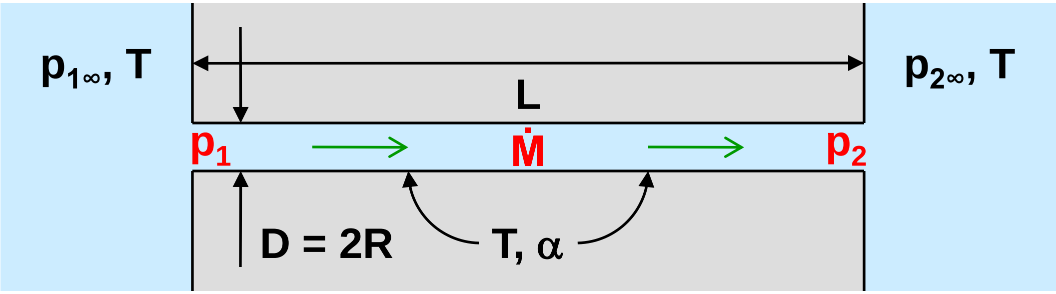
Conclusions





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

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

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

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

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

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