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Understanding the Transition Flow region through COMSOL Multiphysics modeling

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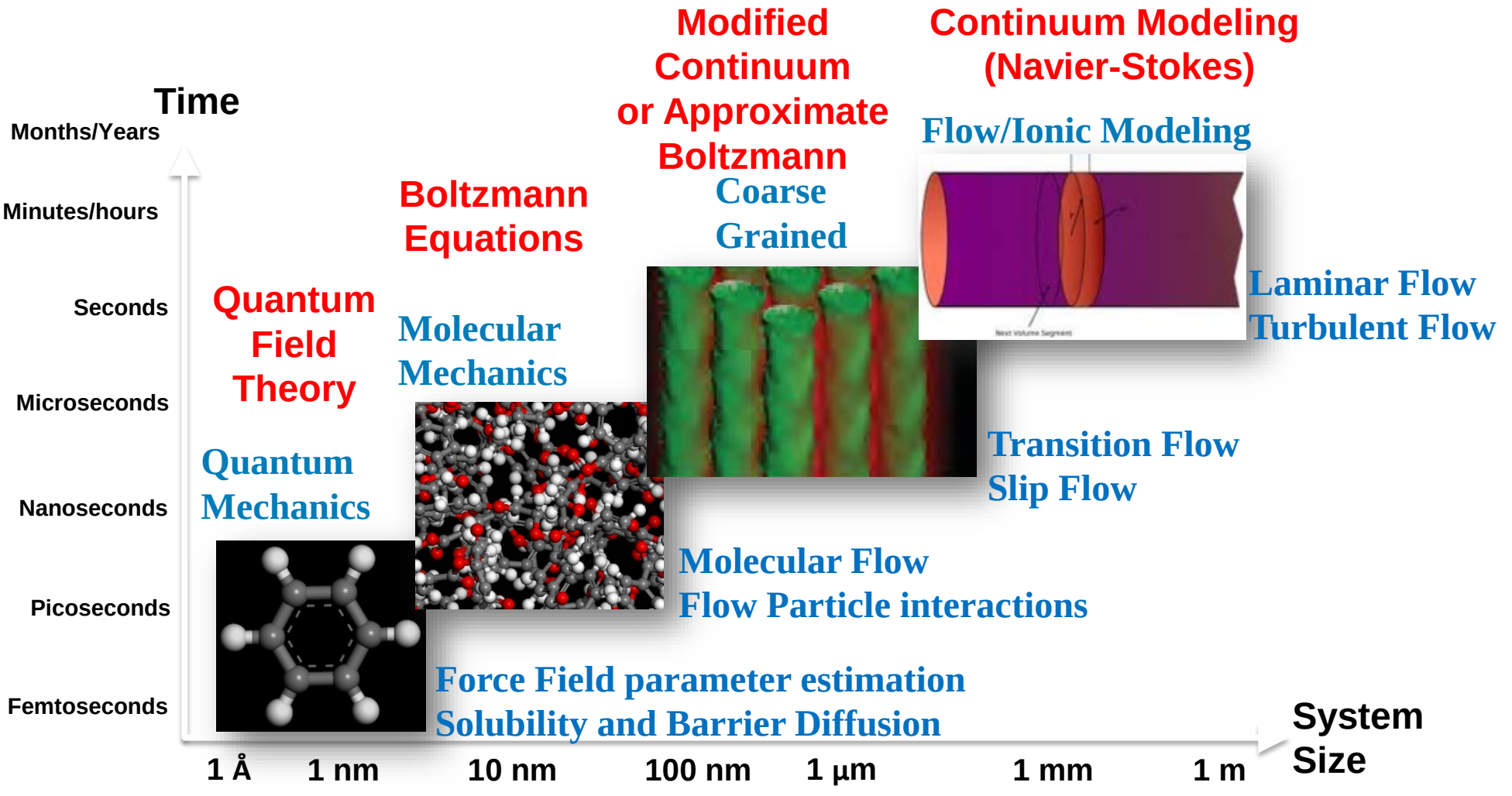
Outline

- Background
  - Scale in Flow Modeling
  - Knudsen Number and Flow Equations
  - Influences at Different Scale
  - Different Approaches to Modeling Transition Flow
- Examples of Modeling Transition Flow of Gases
  - Higher Order Slip Flow
    - » Flow profile – pressure dependence (first order and second order slip approximation)
    - » Validating the model through standard flow (helium and nitrogen)
    - » Variation of Knudsen flow along the pore
  - Self Diffusion modification of Navier Stokes Equation
  - Example of binary flow
- Summary
- Other Approaches

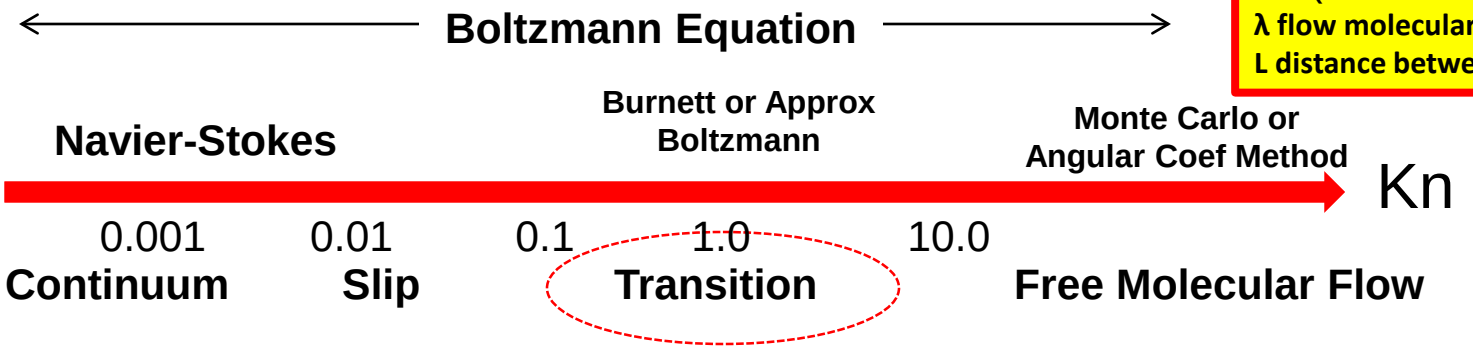
Scales in Flow Modeling



Knudsen Number and Flow Equations

- Scale is important to Flow Modeling
  - Continuum Flow is the result of average behavior of huge number of particles
  - At smaller scale, there is significant variation from averaging assumptions
  - Boltzmann Equation is difficult to solve for large Scale
  - Transition Flow regime can use approximations of Boltzmann Equation to solve
  - Knudsen Number provides indication of range of Equation validations

Kn (Knudsen Number) = **λ/L**
λ flow molecular mean free path length
L distance between boundaries



Transition between Laminar N-S Equation

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=-\nabla p+\nabla\cdot\left(\mu\cdot\left(\nabla\mathbf{v}+(\nabla\mathbf{v})^{\mathrm{T}}\right)\right)+\nabla\left(\frac{2}{3}\mu\nabla\cdot\mathbf{v}\right)+\rho\mathbf{g}$$

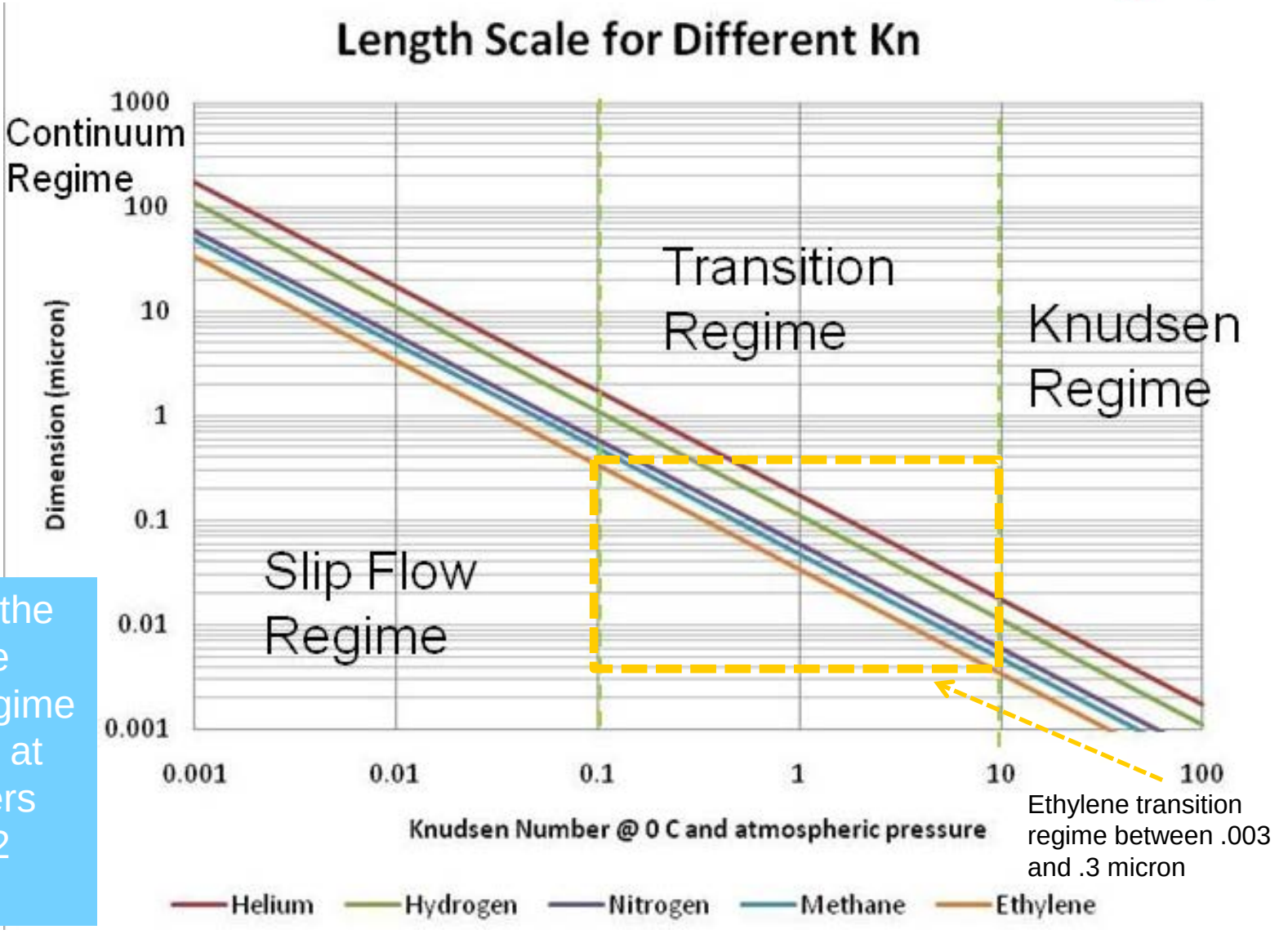
$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\mathbf{v})=0$$

and Full Boltzmann

$$\frac{\partial f}{\partial t}+\xi_i\cdot\nabla f_i=\frac{f_i-f_i^{eq}}{\tau}+\left(\frac{\partial f}{\partial t}\right)_{coll}$$

f is a distribution function of particle positions and velocity

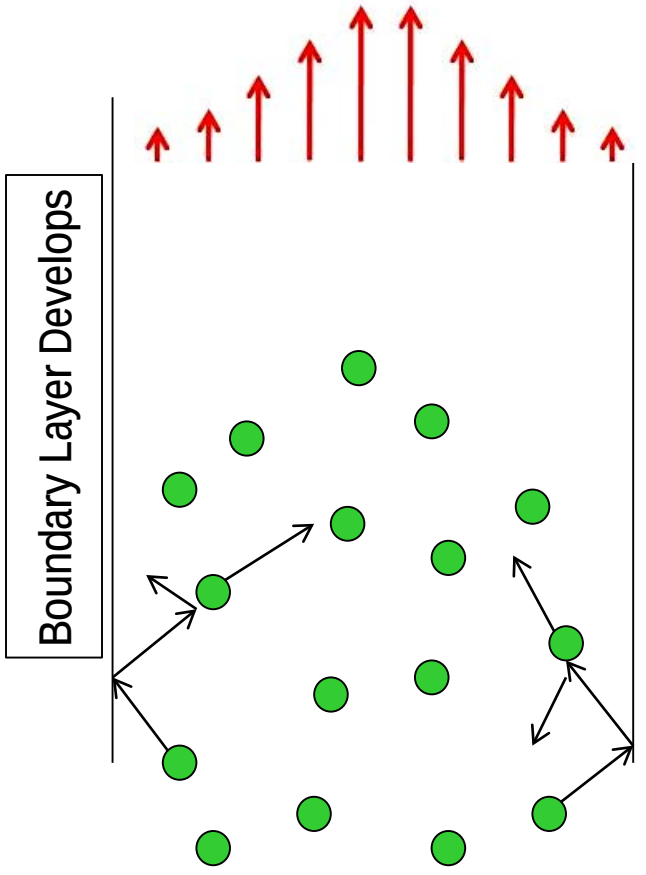
Transition Regime



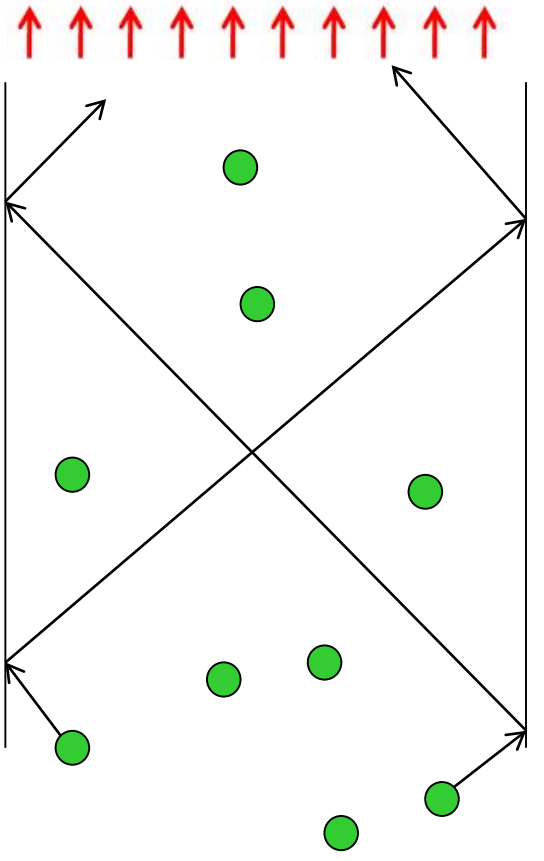
For Helium, the effects of the transition regime can be seen at wall diameters as large as 2 microns

Ethylene transition regime between .003 and .3 micron

Momentum Transfer



In **continuum regime**, the momentum reflected off the wall is transferred towards the center of the fluid by molecular collisions and reducing the forward momentum near the wall resulting in a parabolic forward momentum distribution



In **Knudsen regime**, the momentum reflected off the wall is transferred to the other wall keeping the forward momentum uniform across the channel diameter

For perfectly reflecting wall, velocity at wall is the amount of velocity change which can be moved to the wall in the mean free path distance

$\lambda \, \partial v / \partial n$

Slip Flow through Channel

Assuming narrow gap through parallel plates, perfect gas, dynamic viscosity is pressure independent

$$Q_m = \frac{\Delta P\, P_m\, w\, b^3}{12\,\mu\, R\, T\, L}\,(1 + 6\,A_1 K_n)$$

where Q_m volumetric flow rate at outlet
ΔP = Difference between Outlet and Inlet Press
P_m = Average of Outlet and Inlet Press
w = channel width
b = channel gap (height)
μ = dynamic viscosity
R = gas constant
T = Absolute Temperature
L = Length of channel
A1 = Reflectivity Factor (typically between 1 to 1.4)

Wall boundary condition

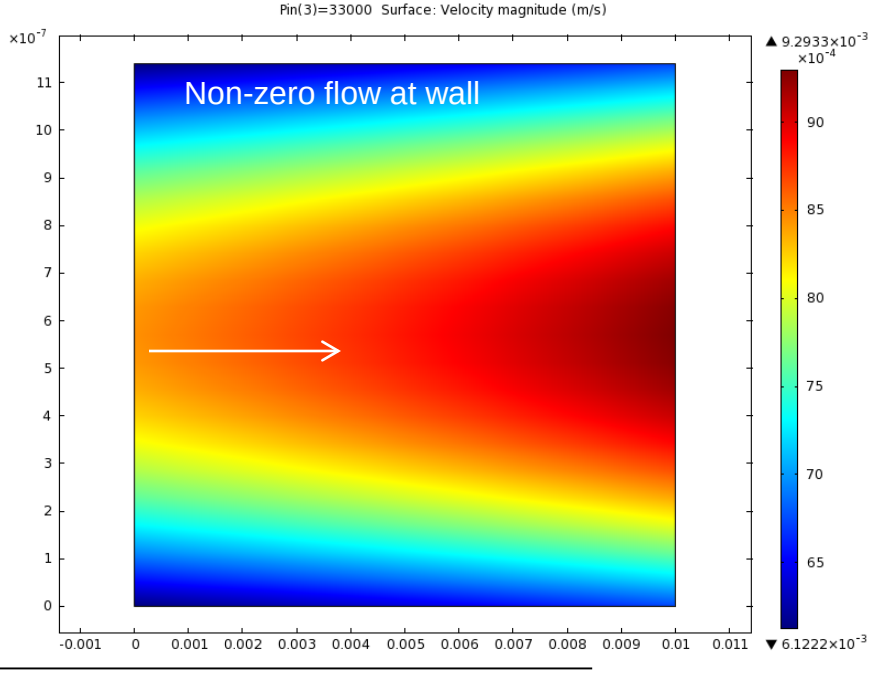
$$v = A_1 \lambda \frac{\partial v}{\partial n}$$

where $\frac{\partial v}{\partial n}$ is the derivative of velocity normal to boundary,

$A_1 = \frac{2-\sigma}{\sigma}$, and σ diffusive reflection fraction

Slip factor can be used to indicate the increase of the flow against nonslip flow

$$S = 1 + 6\,A_1 K_n$$



Approaches to Transition Flow

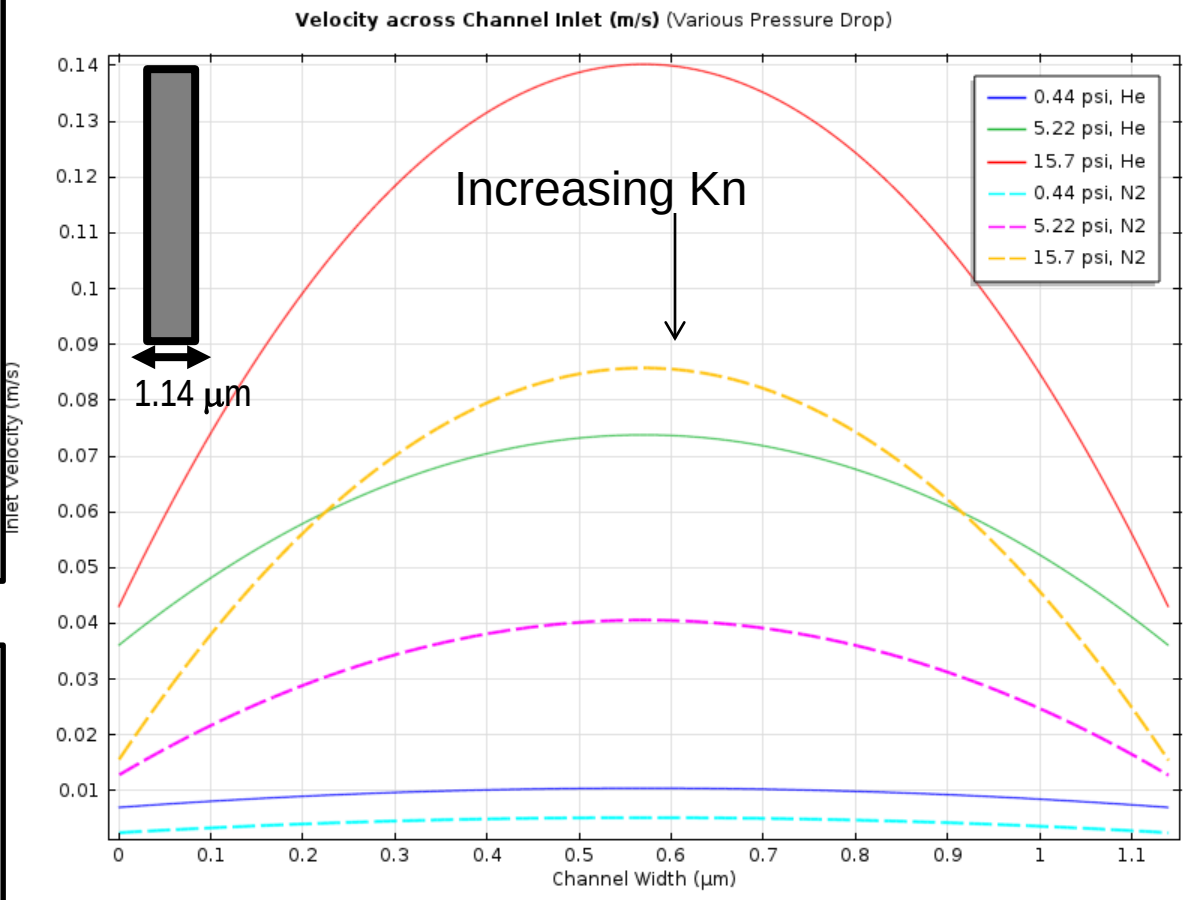
Transition Flow is still an area of active research

- Higher Order Slip Flow
  - Boundary Condition $v = A_1\lambda\frac{\partial v}{\partial n} + A_2\lambda^2\frac{\partial^2 v}{\partial n^2}$
- Diffusion Modified Navier Stokes Equation
  - Introduces a self diffusion term $\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = -\nabla\dot{m}^D$
- Burnett Equation
  - Approximate Boltzmann Equation to 2nd order in Kn
- Molecular Dynamics
- Direct Simulation Monte-Carlo
- Boltzmann BGK
  - COMSOL method – Simplifies Collision Operator term $\left(\frac{\partial f}{\partial t}\right)_{coll}$
- Dusty Gas

2nd Slip: Impact of Pressure on Pure Gases

As the average pressure goes down, the Knudsen number goes up and molecules are able to recoil further from the walls. This results in less drag on the wall, so the velocity profile flattens.

Helium has higher Knudsen number than Nitrogen so for the same conditions it has more slip on the wall



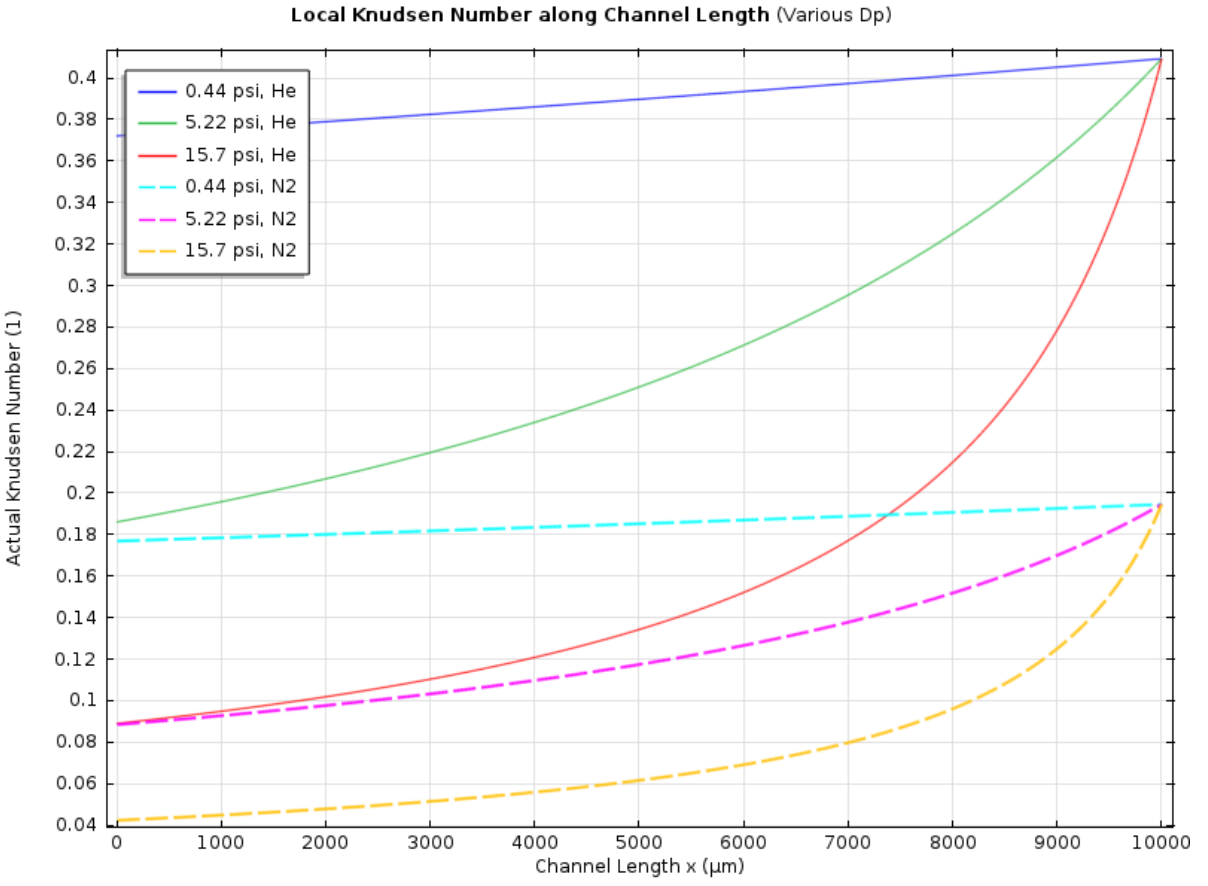
Channel width: 1.14 **µm**
Outlet pressure: 4.35 psia

Local Knudsen Number

- Knudsen Number is Pressure Dependent
  - Knudsen Number at Average Pressure is Often Used
  - Amount of Slip at the Wall depends on the local Pressure

Local Knudsen number varies inversely with the Local Pressure

The greater the pressure drop, the greater the variation of the Slip



Slip Order and Slip Coefficient

- 2nd Order Slip factor increases for larger Knudsen #

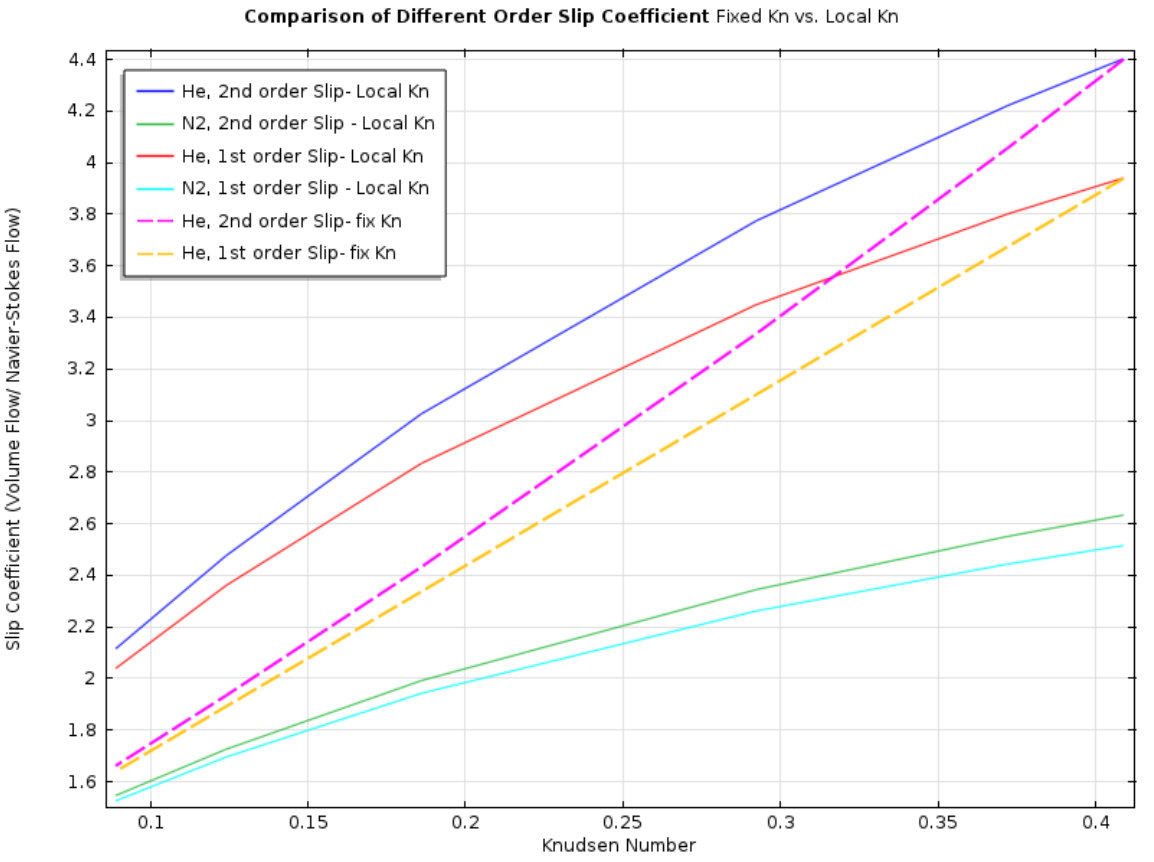
$$S \approx 1 + 6 A_1 K_n + 12 A_2 K_n^2$$ *

Nitrogen A_1= 1.3, A_2 =0.26

Helium A_1= 1.2, A_2 =0.23

A_1 determined by molecular spectroscopy techniques for glass and silicon
A_2 determined by fitting data

The Slip Coefficient is significantly increased when the Local Kn (instead of the Kn at average pressure) is used to solve for Flow

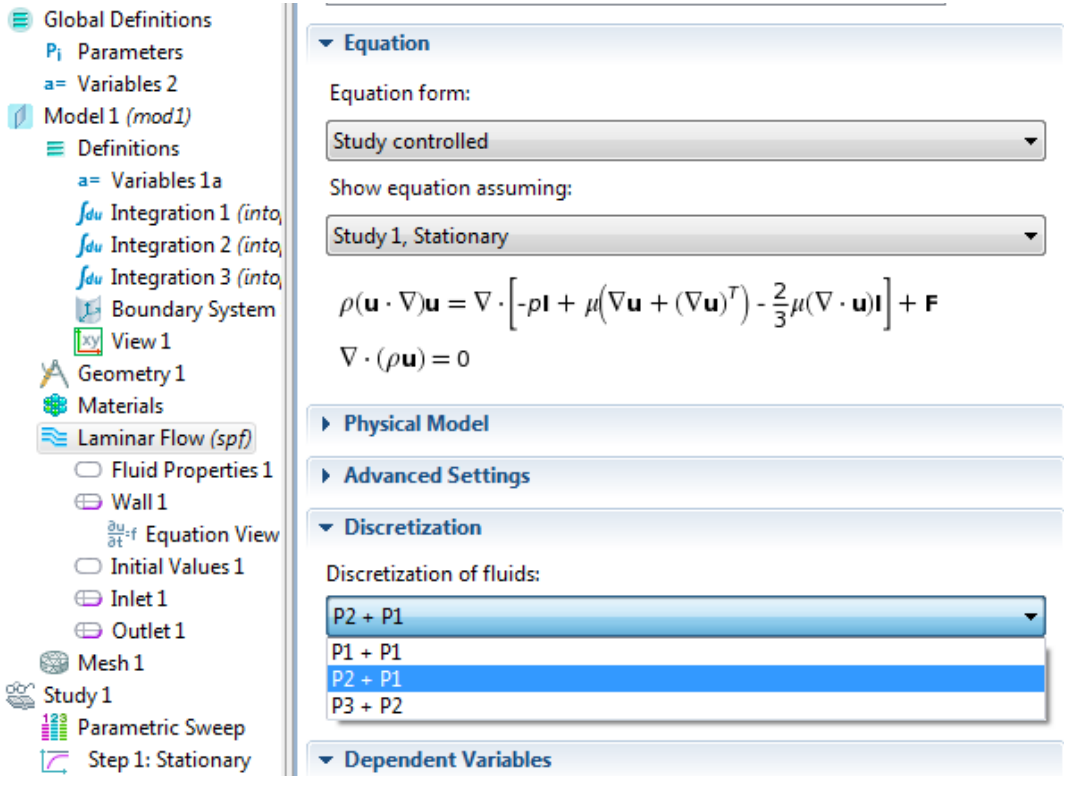


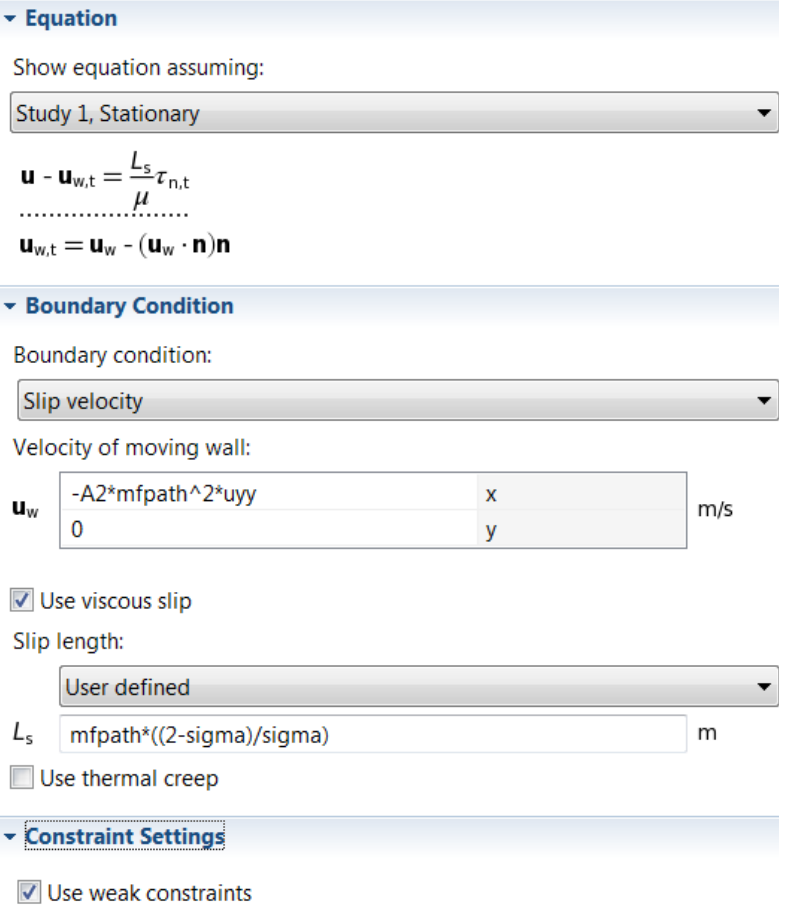
Channel width: 1.14 **µm**
Outlet pressure: 4.35 psia

*Maurer, J., Tabeling, P., Joseph, P. & Willaime, H. "Second-order slip laws in microchannels for helium and nitrogen" *Physics of Fluids* **15**, 2613-2621 (2003).

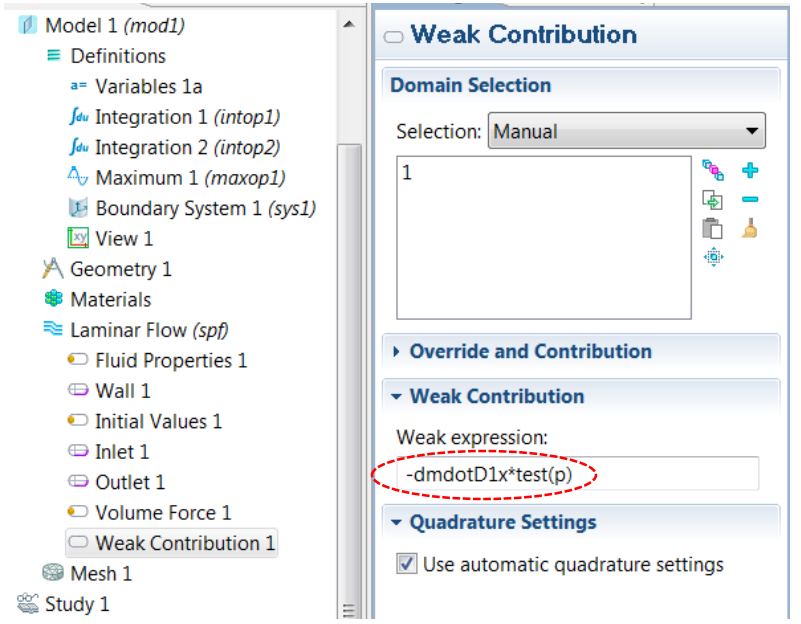
Second Order Slip in COMSOL

- Input 2nd Order as moving wall
  - Input 1st Order with Slip Length
  - Need to change discretization to calculate 2nd Derivatives
  - Flow in x-direction





Self Diffusion Model in COMSOL

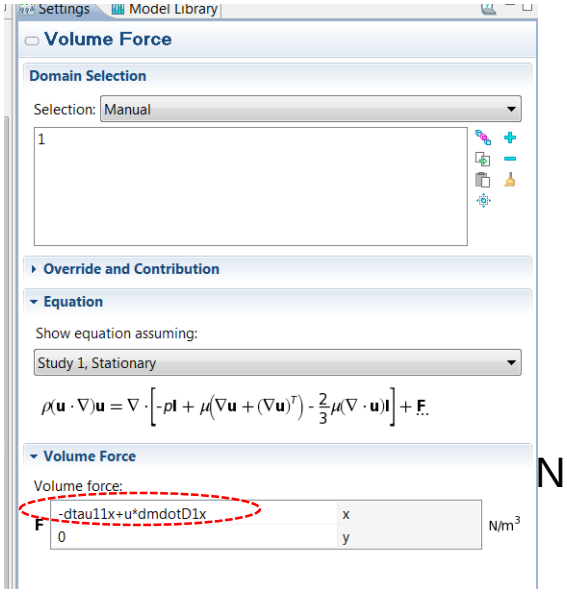


$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = -\nabla \dot{m}^D$$

Add as a weak contribution in Laminar flow model

Variables

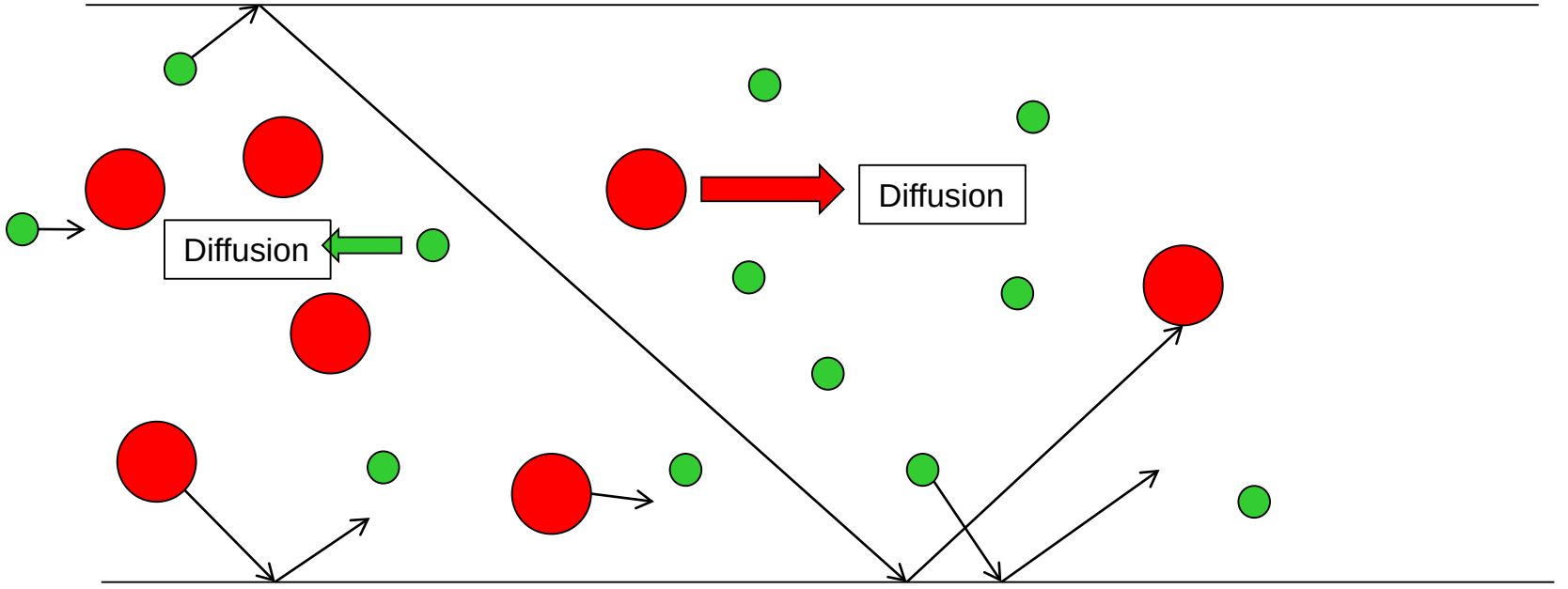
Name	Expression	Unit	Description
Df	spf.mu/spf.rho	m^2/s	
mdotD1	-spf.rho*Dfc*px/p	$kg/(m^2 \cdot s)$	Mass transport
tau11	4/3*mdotD1*u	Pa	MT diffusive xx term
dtau11x	d(tau11,x)	N/m^3	derivative of tau11 in x
dmdotD1x	d(mdotD1,x)	$kg/(m^3 \cdot s)$	derivative of Mass Transport
udiff1	mdotD1/spf.rho	m/s	Diffusion Velocity
utot	u+udiff1	m/s	Total Velocity



Need to introduce a volume force

Results similar to 2nd Order Slip

Dusty Gas: Binary Molecular Flow



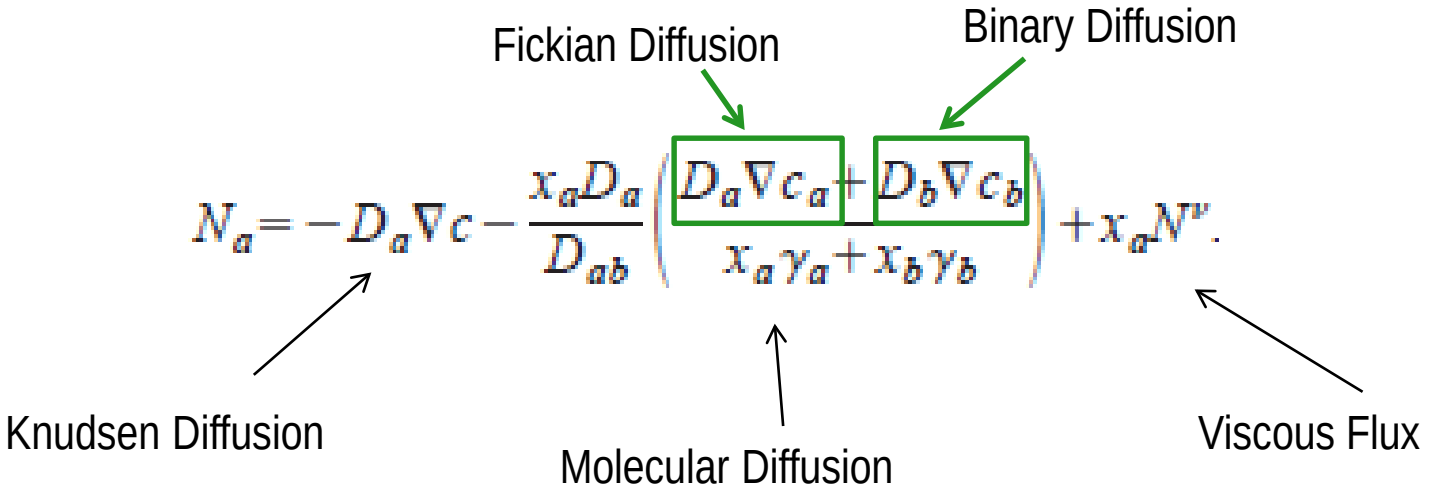
The larger particles are more likely to collide with other particles and transfer their momentum to other particles. The momentum transfer from the wall is more likely to be moved towards the center

Molecular diffusion will move the species toward the lower concentration, dragging some of the larger molecules forward and holding some of the smaller molecules back

Binary Flow through Pore

Dusty Gas Model

Flux of species “a” is given by



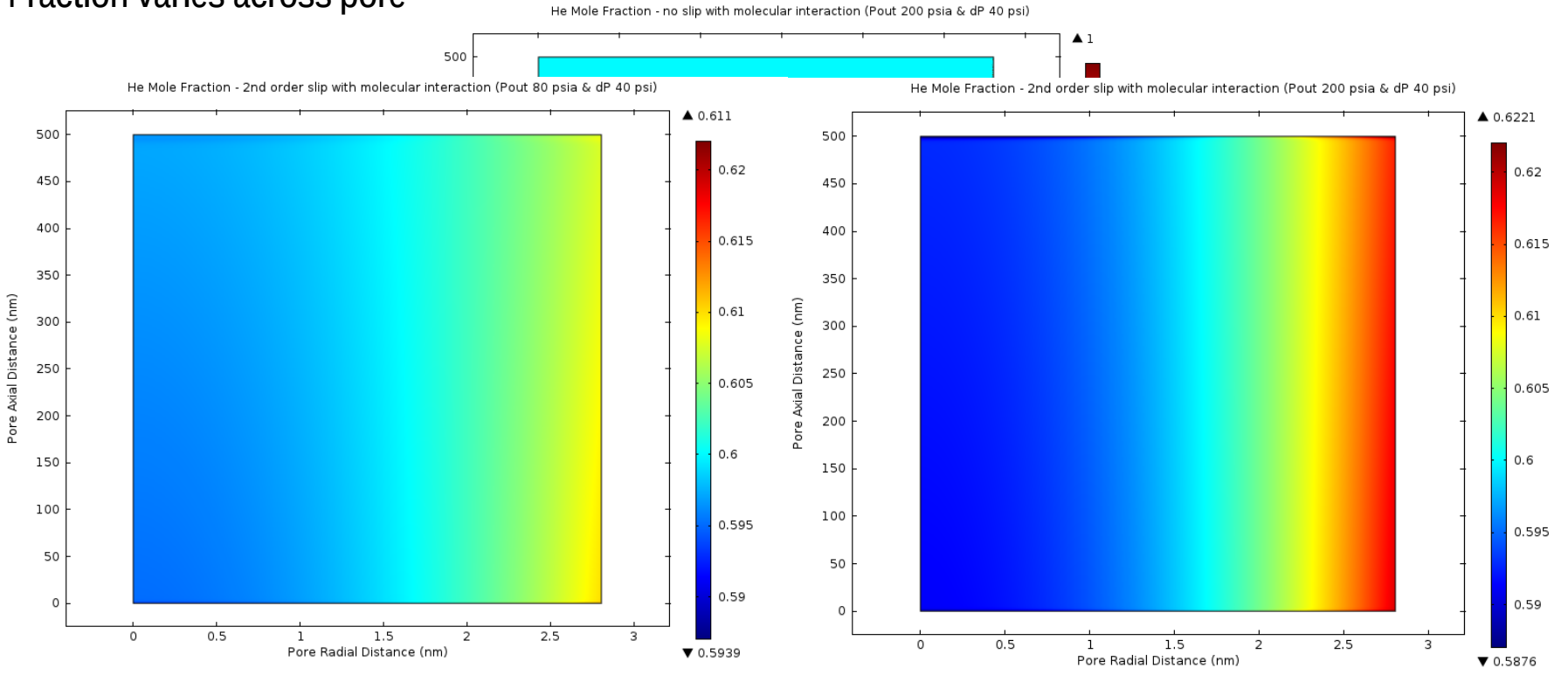
where c is the molar density of the gas mixture, the subscript a and b indicates the restrict to the particular species, x is the fraction, D is a diffusion coefficient, and γ are ratio of diffusion coefficients.

Fickian Diffusion is partial pressure driven
Knudsen Diffusion adds a total pressure component

Modeling Binary Flow Model

- Each species separately modeled with their own CFD physics using the same mixture viscosity, but the gas densities are based on the individual molecular weight and the slip constants depend on the species.
- Flow of the gas mixture is weighted average of the flow of these individual components.
- Mole fraction approximated from relative velocity changes for each species (a PDE model of the mole fraction can be included for molecular diffusion effects)

With Slip Conditions, Mole Fraction varies across pore



Impact of Binary Mixture on Knudsen Number

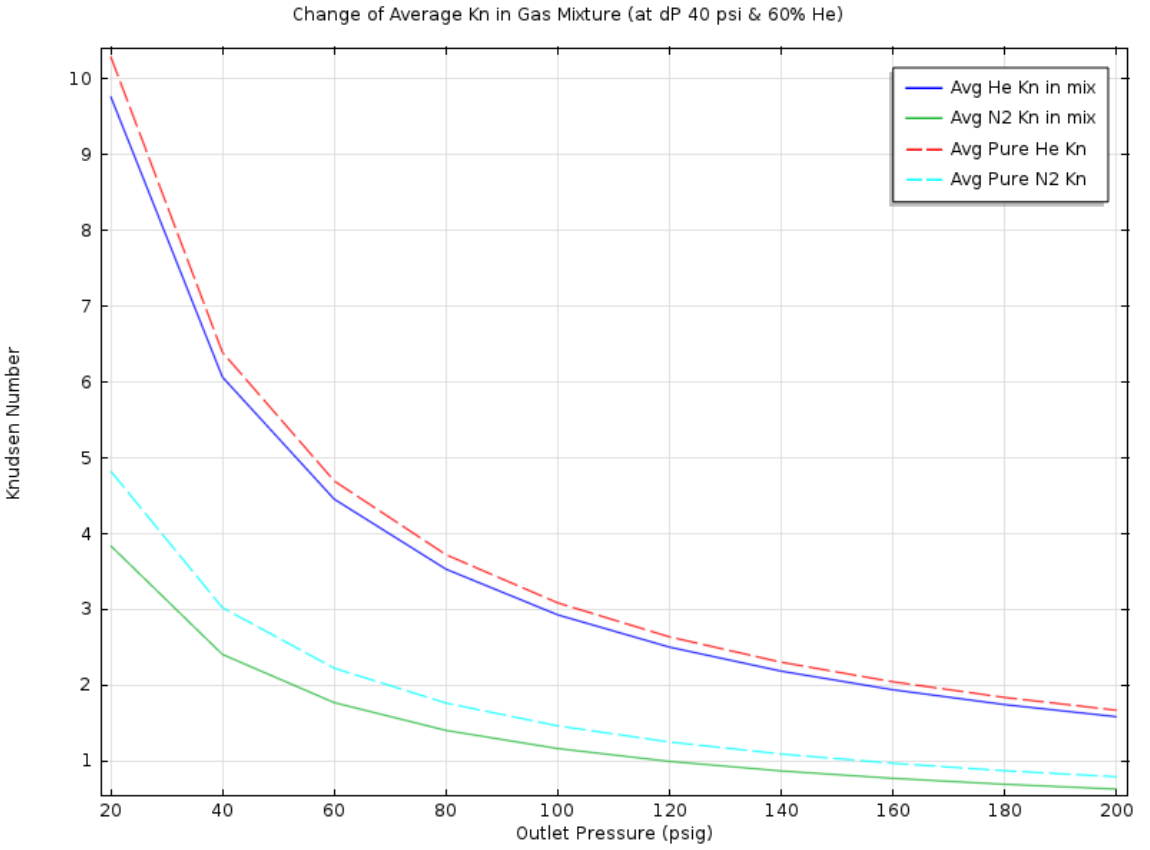
Mean Free Path of Gas Component in Mixture

For a molecule in a binary gas mixture, the mean free path is given by

$$\lambda_1 = \frac{1}{n_1 \pi \sigma_{11}^2 \sqrt{2} + n_2 \pi \sigma_{12}^2 \sqrt{1 + m_1/m_2}}$$

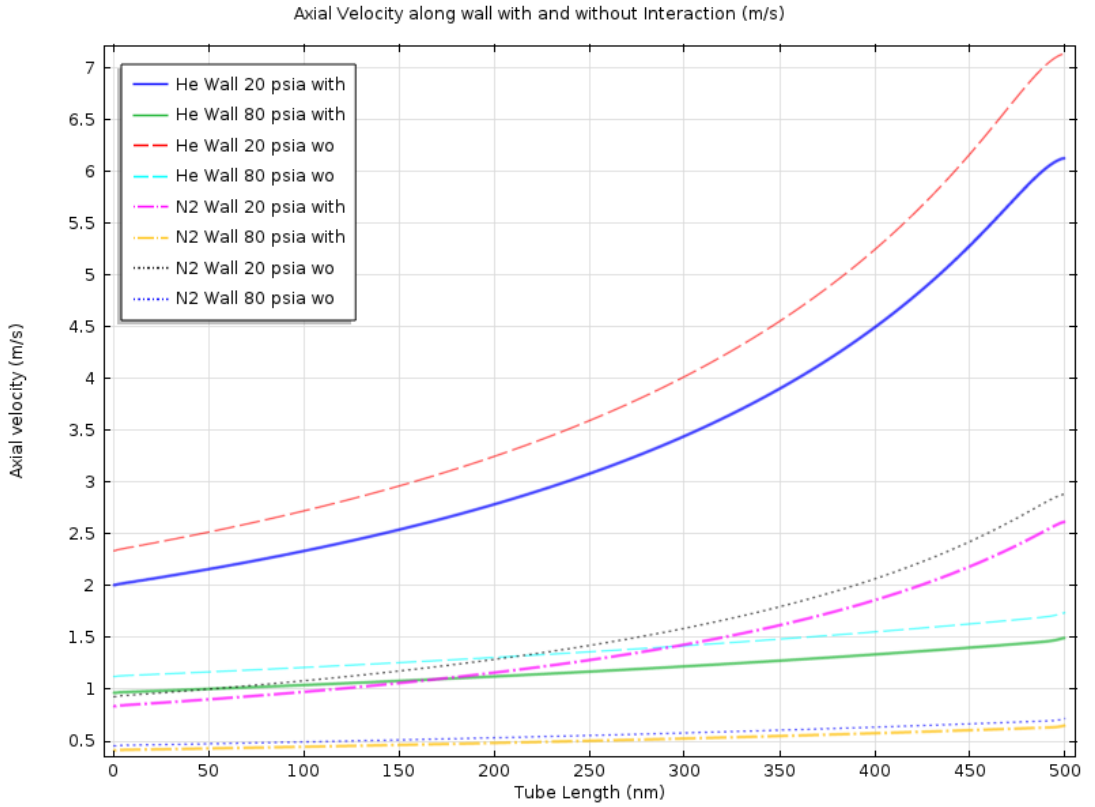
where n_i is the number density, σ_{ij} is the collision diameter, and m_i is the molecular weight.

In the Binary Mixture, the mean free path used in the wall boundary condition needs to be modified for the species interactions



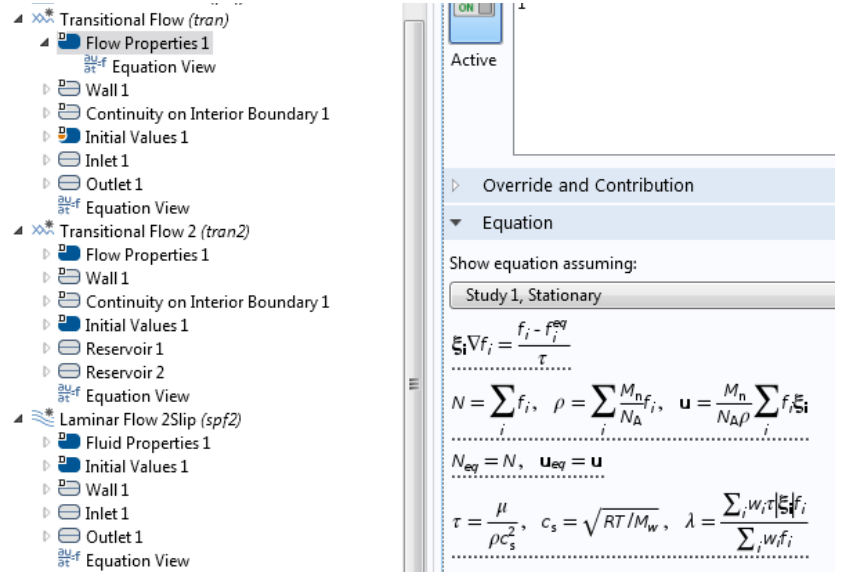
Impact of Molecular Interaction on Velocity

- The molecular interactions reduces the velocity of each species through the pore
  - Impacted by change in mean free path
- Higher Knudsen have higher speeds
  - Molecular interaction has greater impact for higher Knudsen Number
- Permeance of Gas Mixture is lower than weighted average permeance of species



5.6 nm pore with 40 psi pressure drop and 60 mole% Helium

Transition Flow in COMSOL

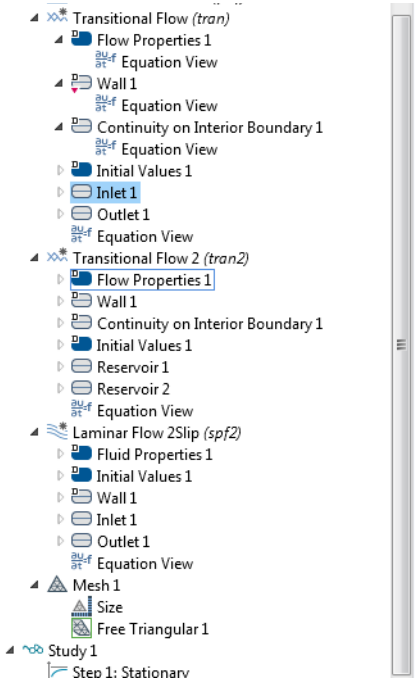


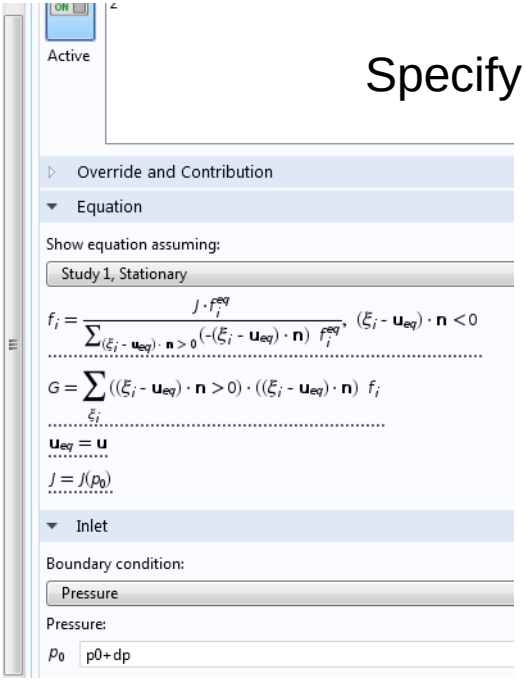
Based on

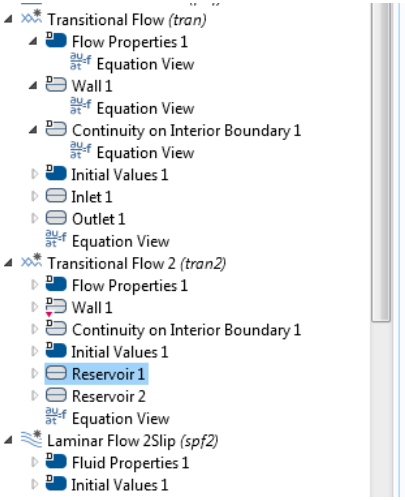
Boltzmann BGK

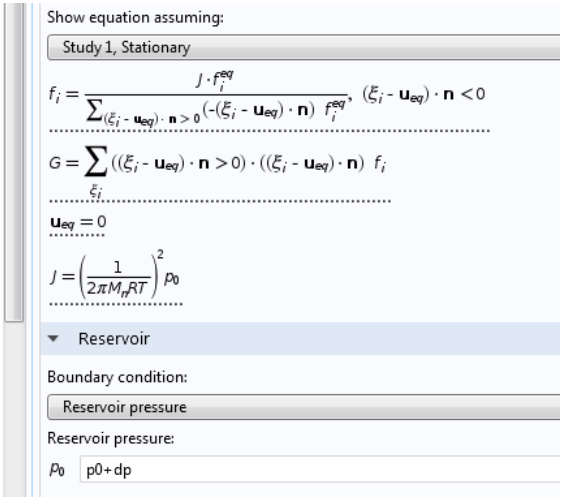
COMSOL method – Simplifies Collision Operator term $\left(\frac{\partial f}{\partial t}\right)_{coll}$

Specify boundary Conditions in Different way

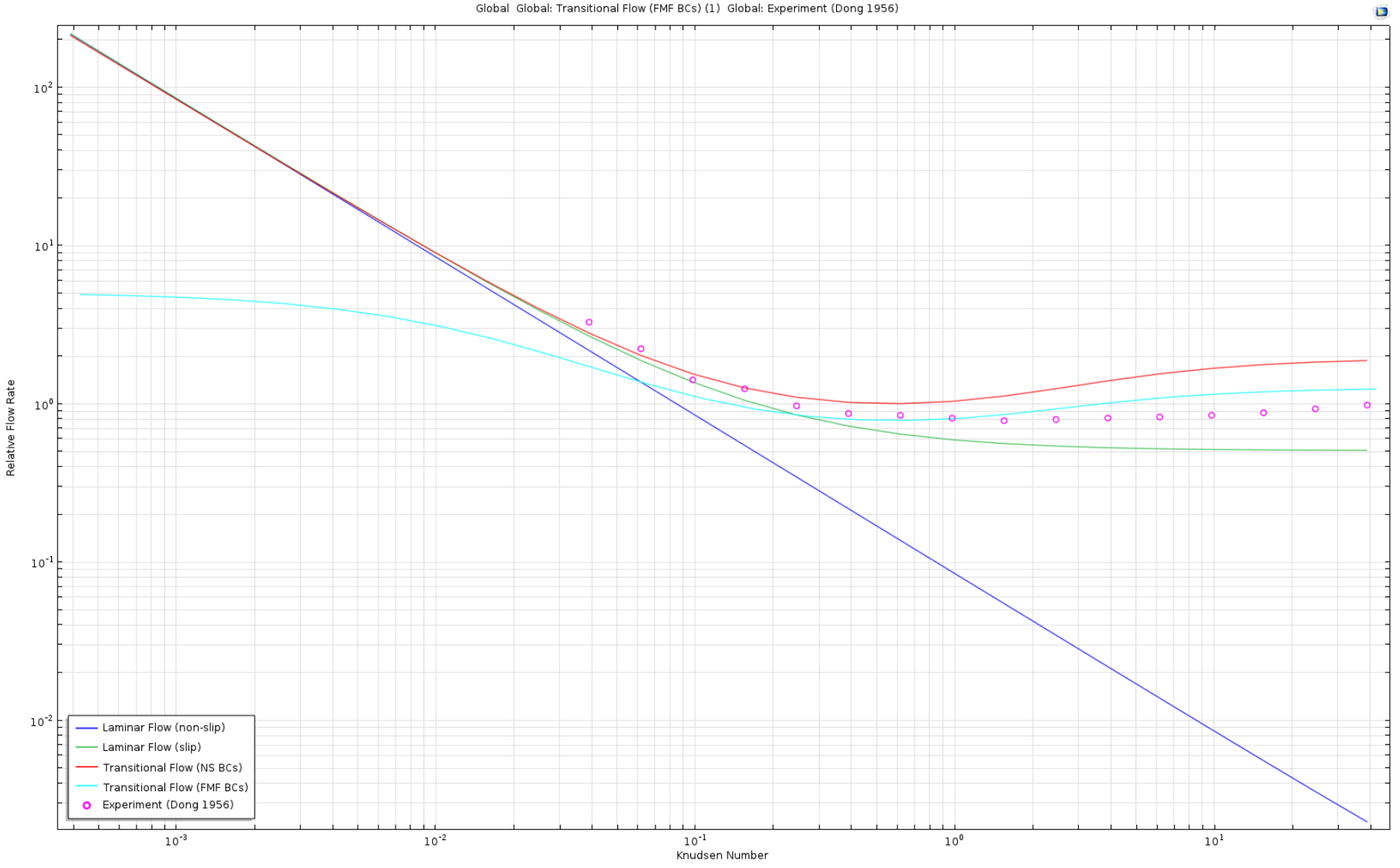








COMSOL models in the Transition Regime



From COMSOL's Knudsen_Minimum Example

Summary and Conclusions

- Transition flow Modeling can be done in Multiple Ways
  - Extension of Navier-Stokes (2nd Order Slip, Self Diffusion …)
  - Approximation of Boltzmann Equation
- Developed multi-physics model to understand influence of slip coefficient on single component flow
  - Comparison of 1st and 2nd Order Slip
  - Investigated the influence of pressure on local Kn
  - Investigated the relation between slip order and slip coefficient for helium and nitrogen flow
  - Implementing in COMSOL
- Binary flow modeling
  - Coupled the flow models of the individual species to get binary flow
  - Composition varies in pore with slip
  - Molecular interaction reduces velocity compared to individual species

Thanks to my Dow Collaborators

- Kishori Deshpande
  - Alexia Finotello
  - John Pendergast Jr
  - Mark Brayden

Back Up Slides

References

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- Dongari, N. & Agrawal, A. "Modeling of Navier–Stokes equations for high Knudsen number gas flows" *International Journal of Heat and Mass Transfer* **55**, 4352-4358 (2012)
- Agarwal, R.K., Yun, K.-Y. & Balakrishnan, R. "Beyond Navier--Stokes: Burnett equations for flows in the continuum--transition regime" *Physics of Fluids* **13**, 3061-3085 (2001).

Case Study: Single Component Diffusion

➢ Approach

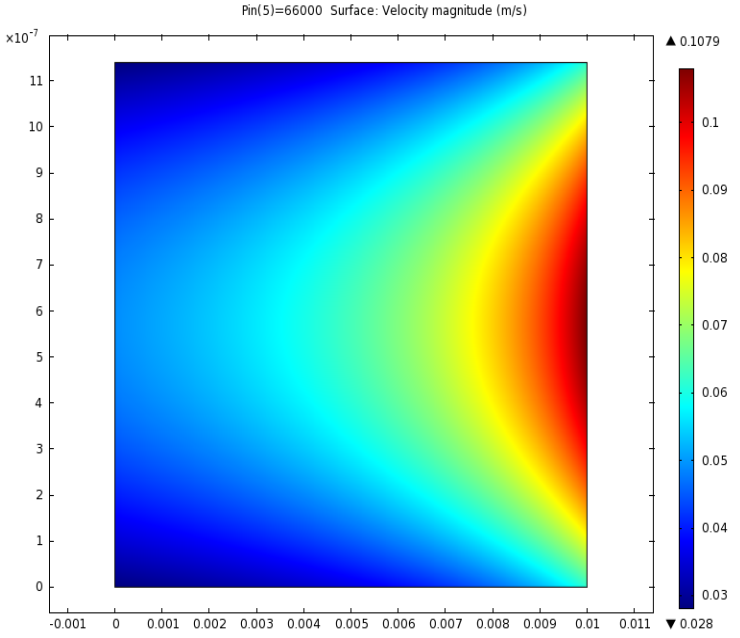
- Laminar Flow Physics in 2 dimensions assuming an infinitely wide channel
- Isothermal conditions, locally fully developed steady flow, and ideal gas behavior
- Maxwell's slip velocity equation

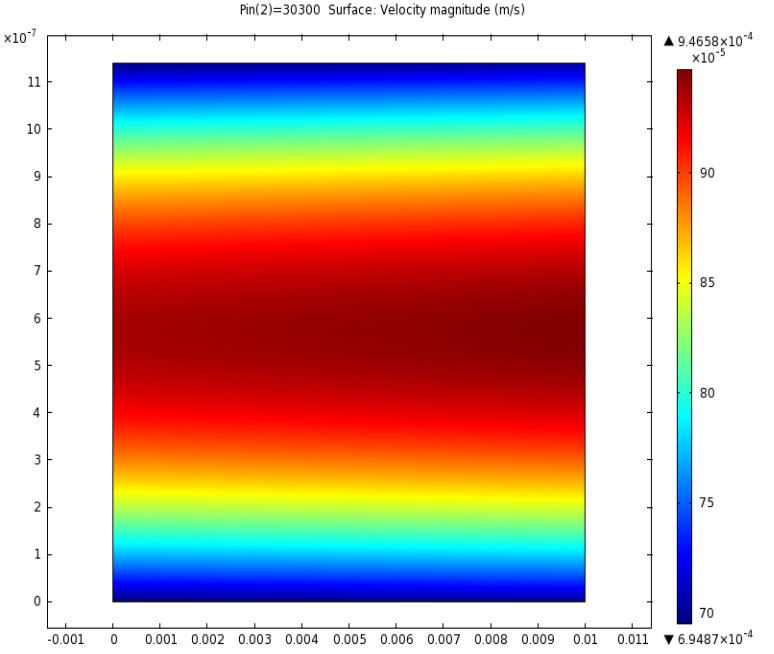
Parameters

Parameters

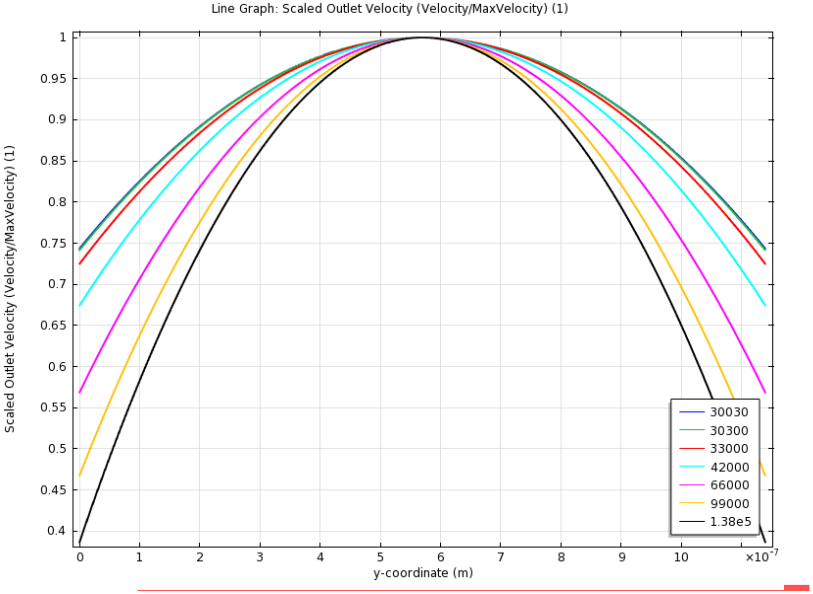
Name	Expression	Value	Description
hchannel	1.14[um]	1.14E-6 m	Channel Height
Lchannel	10000[um]	0.01 m	Channel Length
wchannel	200[um]	2.0E-4 m	Channel Width
Pin	.33[bar]	33000.0 Pa	Inlet Pressure
Pout	.3[bar]	30000.0 Pa	Outlet Pressure
Temp	293.15[K]	293.2 K	Temperature
Mn	4.0029[g/mol]	0.004003 kg/mol	Molecular Weight
Mdiam	210[pm]	2.1E-10 m	Molecular Diameter
mfpath	k_B_const*Temp/(sqrt(2)*pi*(Mdiam^2)*(Pin+Pout)/2)	6.558E-7 m	Mean Free Path
KnudsenN	mfpath/hchannel	0.5752	Knudsen Number
sigma	.91	0.91	Wall reflect fraction
A2	.23	0.23	2nd order slip coeff
PsqDiff	(Pin^2-Pout^2)/2	9.45E7 $kg^2/(m^2 \cdot s^4)$	Average Difference of Press Square

Single Component Diffusion: 1st order Slip

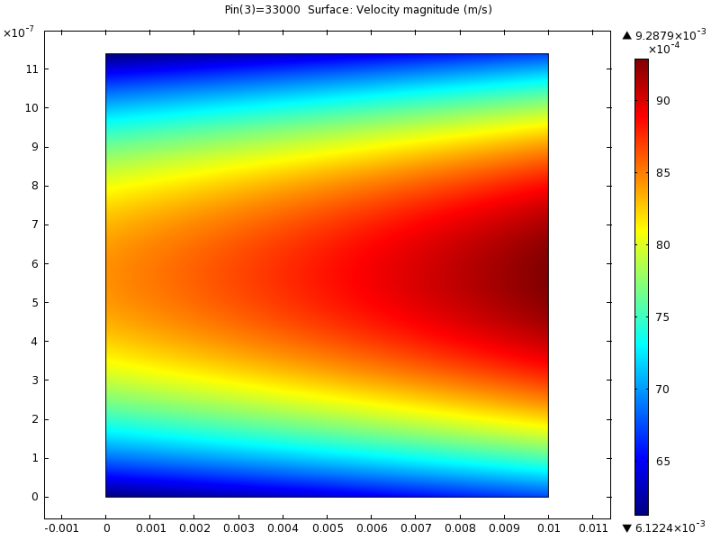




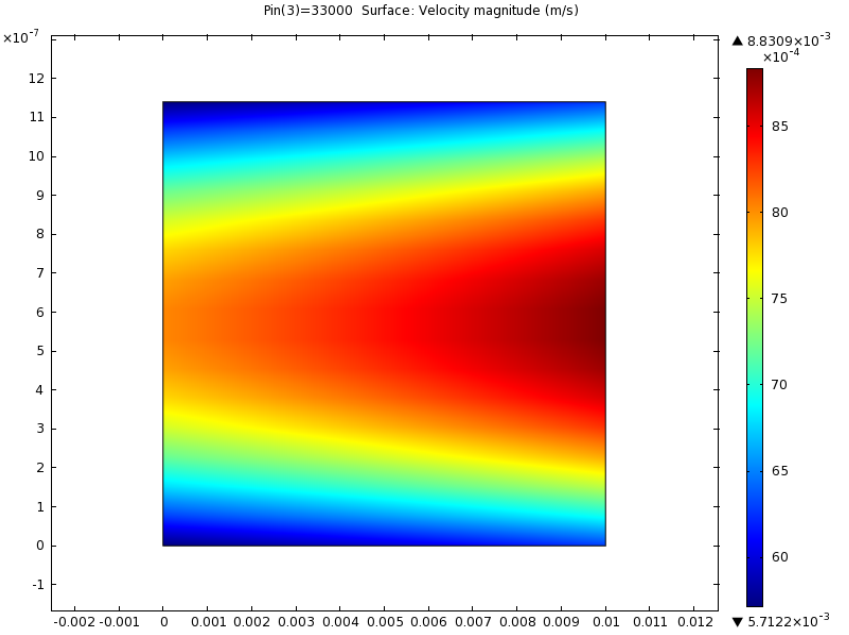
Velocity Profile with First Order Slip at Pin= .66 bar (L) and =.303 bar (R)



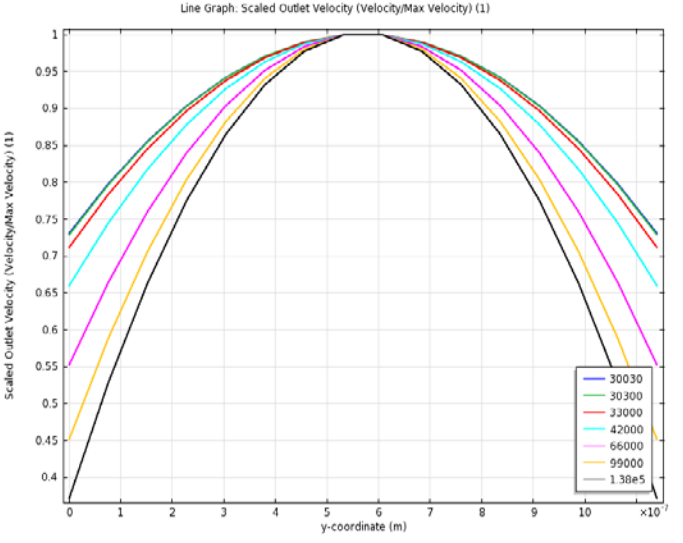
Single Component Diffusion: 2nd order Slip



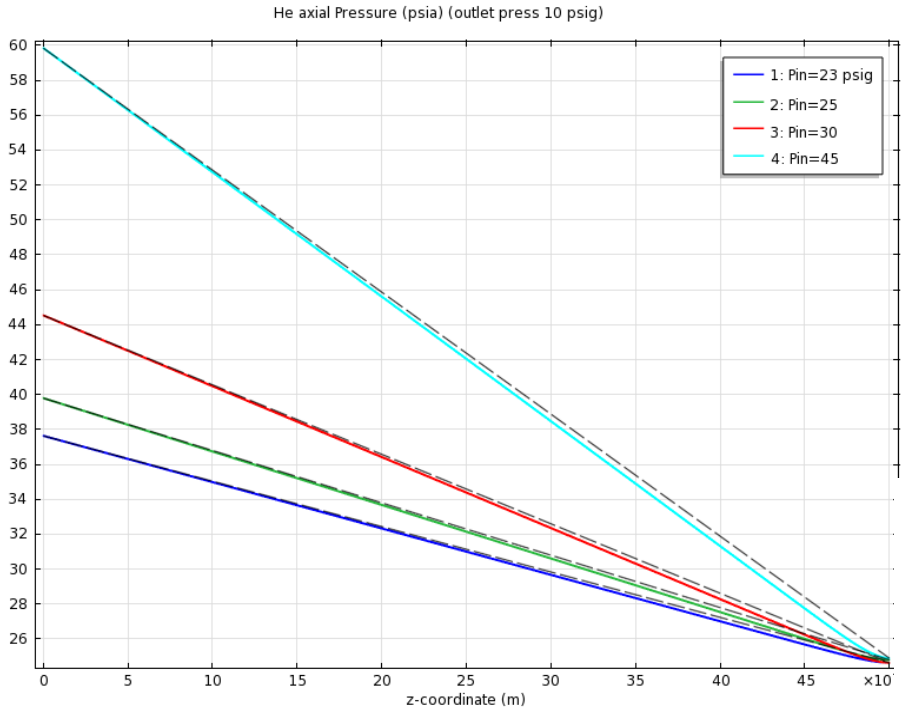
1st order Slip



2nd order Slip



Knudsen Number Variation down the Pore



As pressure drops along the length of pore, the Knudsen number changes. For high pressure drop, the flow can range from the slip flow regime to the Knudsen regime

With gas mixture, one component could be in the Knudsen regime while another is still in the transition regime

There are a number of competing models in the literature, so experimentation is critical