



The Contradicting Results of different Methods of Calculation for Solving Same Problem of Flow in a Microchannel in Fluid Mechanics. And Solving Same Problem Using Dynamic Universe Model. Find that Flow is almost near Walls at Molecular Level

Satyavarapu Naga Parameswara Gupta (S N P Gupta)^{1*} and SS Vamsi Krishna²

¹Retired Assistant General Manager, Bhilai Steel Plant, India

²H O D Mech Engineering, IIT Bhilai, India

³Data Brics, 33532 Stephano ct, Fremont, CA

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Abstract

In this paper comparison of solving flow problems in a Microchannel using different methods of a problem mentioned by Niraj et al using Nitrogen gas along with Dynamic Universe Model's SITA simulations. We used commercially available common pure nitrogen gas with 2% to 5% impurities. Though 99.999% pure nitrogen is available, which is very expensive to procure and experiment. The theoretical results are discussed in this paper. It also may be worth mentioning that the output of Microchannel is in three dimensional i.e., in all xyz axes in this simulation, instead of single axis flow mentioned by Niraj et al. Boundary conditions are not required in this SITA simulation, as this method gives unique solution.

***Corresponding author:** Satyavarapu Naga Parameswara Gupta (S N P Gupta), Retired Assistant General Manager, Bhilai Steel Plant, India.

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Introduction

Let's dive into the fascinating world of microfluidics! In Fluid Mechanics, especially on the study of flow in Microchannels, problem can be solved in multiple ways. Sometimes we will obtain different numerical solutions using some simple methods even. We study some of them here. There are wide variety of methods used by different authors. We tried some of them in the problem solving in this paper. We added a new method: SITA simulations of Dynamic Universe Model. We will compare all the methods.

Niraj et al [1] compared various boundary conditions inside of micro channel as assumed by various authors. We did not specify any boundary inside Microchannel in this SITA simulation. We allowed molecules hitting the walls of the micro channel and inter-molecule hitting's due to flow velocities under the given pressure and the imposed flow conditions of flow stated. We also allowed mutual inter-gravitational attraction forces between molecules and influence of earth gravitation on these molecules. Here we don't want to neglect any force. In these conditions we tried to solve this problem. Here outgoing velocities came in all three dimensions.

We introduce and tried to solve this problem using our Dynamic Universe Model's SITA solution. Boundary conditions are not required in this SITA simulation; Dynamic universe model gives unique solution as it was a n-body problem solution. It solves complex problems. May be this is a better solution as we calculate at molecular level; molecular wall hitting's, inter-molecular hitting's in the flow are considered and calculated. Individual molecules velocities are found; the molecular paths are traced. Some of the first author published papers can be found in ref [22-26]. Advantages are many.

Using Boundaries

When we are using numerical approaches, boundary conditions are a must. These are the best solutions at present. We require boundary conditions to solve differential equations. Otherwise, innumerable solutions are possible. Boundary conditions are essential because they provide the necessary physical context to find a unique solution to the fluid flow equations. Without them, the equations could have an infinite number of solutions. They define how the fluid interacts with its surroundings and are critical for accurately predicting flow characteristics such as velocity profiles, pressure drop, and mass flow rate.

The DSMC (Direct Simulation Monte Carlo) Method and Some Earlier Work

Niraj et al [1] in his 'Comparison of Various Pressure Based Boundary Conditions for Three-Dimensional Subsonic DSMC Simulation' compared various boundary conditions inside of micro channel as assumed by various authors. Jana Wedel et al. [2] gave in the no-slip and slip flow regimes. T. J'unemann et al [3], discussed 'Maxwell velocity slip and Smoluchowski temperature jump boundary condition'

Now let's see some earlier work using boundaries. For us base problem was taken from Niraj et al, so some of the important references were taken accordingly. This method was initially used for solving supersonic or hypersonic flow problems. For simulating such external or internal flows, stream and vacuum boundary conditions are widely used [4--9]. Both these schemes were proposed by Bird [10]. The stream boundary conditions are the Dirichlet type in which the density, velocity, and temperature are known in advance and used to determine the number flux of the molecules entering the boundary. Lilley and Macrossan [11] proposed the implementation of stream boundary condition for high-speed flows with an alternative method to the acceptance rejection procedure proposed by Bird [10] to decide entry of molecules in the computational domain from the boundary. It was found that the alternative method is only efficient for the upstream boundaries [11]. And to deal with the shock structure in supersonic flows, the stream boundary condition is used at the upstream side, whereas moving piston type boundary condition [10, 12, 13] is [14] applied at the downstream side. A periodic boundary condition [10] is used in many simulations [15,16,17] where the flow pattern is of

a periodically repeating nature.

How did we solve this problem using the SITA simulations?

We used the following procedure that we discussed in this paper. We used nitrogen gas with a purity of 95% in this SITA simulation. Estimated impurities are given in the table.1. We have given the uses of such nitrogen gas below. Masses of all these molecules /atoms are given in Table 2.

Procedure

Take 95% Pure nitrogen gas, find most probable Composition. Take molecular weights of constituent elements and compounds and estimate / simulate the space distribution of these molecules N₂, O₂, Ar, CO₂, H₂O. Find the minimum possible intermolecular distances, Radii are not minimum distances, Diameters of the molecules are the minimum distances, in N₂, O₂, Ar, CO₂, H₂O at the pressure and volume set given by Niraj et al [1]. We will work-out the problem discussed by Niraj et al simulation for Microchannel by different methods and ultimately by SITA simulations of Dynamic Universe Model.

Then we proceeded for simulation. We took 6 small slices of Microchannel, took 133 molecular weights of 95 % Nitrogen in the first slice or box, simulated xyz positions distributed as distances from centerline. We did not simulate different sets of XYZ coordinates in each separate box. Same set of molecules were taken throughout simulation, without altering their XY coordinates. The Z coordinate show the flow from input end and displacement throughout the channel and then to exit.

Simulate using the starting velocities according to flow velocities calculated approximately. Note that the Molecular velocities are maximum at centerline and not zero on the walls of Microchannel. There will be some slip at the boundary walls, as indicated by Knudsen number in the problem

From one slice the flow goes next slice in a way the outgoing going velocities & directions become incoming velocities & directions to the next slice. Continue this way till the end of Microchannel reached. Starting turbulent flow and Steady state flow variations and calculation of individual velocities & directions of molecules throughout the channel length.

See section 9 for the remaining final procedure after finding mass flow rates, velocities and velocity distribution across cross section etc., of individual molecules.

95% to 98%Pure nitrogen Gas Composition

High commercial-grade nitrogen used for food packaging typically has impurities, though in very small percentages. Food-grade nitrogen is generally 99% or more pure, with impurities such as oxygen, carbon dioxide, and water being present in trace amounts. These impurities are kept below certain limits to ensure the safety and effectiveness of the nitrogen in preserving food. The specific composition of impurities can vary based on the production method (e.g., air separation) and handling practices. For certain applications, such as in pharmaceuticals or electronics manufacturing, even small amounts of impurities can be problematic, so higher purity grades (e.g., 99.999%) may be necessary.

Table 1: 95% Pure nitrogen Gas Composition

Impurity	95%	95% to 98%	Average %	Rounded %	This simulation uses 133 mol	Rounded for this simulation
Oxygen (O ₂)	3.0 - 3.5%	0.5 - 3.5%	3.5	4	5.32	5
Argon (Ar)	1.0 - 1.5%	0.0 - 0.5%	1	1	1.33	1
Carbon Dioxide (CO ₂)	0.1 - 0.5%	0.1 - 0.5%	0.5	1	1.33	1
Water Vapor (H ₂ O)	0.1 - 0.5%	0.1-0.5%	0.5	1	1.33	1
Hydrocarbons (C _x H _y)	<0.05 %	<0.5%	0.05	0	0	0
Other trace gases (e.g., H ₂ , CO)	<0.05 %	<0.1%	<0	0	0	0
remaining are N ₂						125

Masses of all these molecules /atoms are here in Table.2.

(Weights per atom or Molecule in Kg:)

- N₂: (4.65×10^{-26}) {kg} per molecule
- O₂: (5.31×10^{-26}) {kg} per molecule
- CO₂: (7.31×10^{-26}) {kg} per molecule
- CO: (4.65×10^{-26}) {kg} per molecule
- H₂O: (2.99×10^{-26}) {kg} per molecule
- Ar: (6.63×10^{-26}) {kg} per atom

It may please be noted Argon (Ar) occurs only in monoatomic state. It is an inert gas, never combines with any other element. All the others are molecular weights. All are in KG. In this paper we followed uniform MKS system of units.

Diameters of Molecules of N₂, O₂, Carbon Dioxide, Carbon Monoxide, Argon, Water Vapor in Meters

We need these diameters to find inter molecular hits and hits with micro channel walls.

Here are approximate molecular diameters for the molecules you listed, given in meters:

- N₂ (Nitrogen): $\sim 0.3 \text{ nm} = 3 \times 10^{-10} \text{ m}$
- O₂ (Oxygen): $\sim 0.3 \text{ nm} = 3 \times 10^{-10} \text{ m}$
- Carbon Dioxide (CO₂): $\sim 0.33 \text{ nm} = 3.3 \times 10^{-10} \text{ m}$
- Carbon Monoxide (CO): $\sim 0.3 \text{ nm} = 3 \times 10^{-10} \text{ m}$
- Argon (Ar): $\sim 0.3 \text{ nm} = 3 \times 10^{-10} \text{ m}$
- Water vapor (H₂O): $\sim 0.28 \text{ nm} = 2.8 \times 10^{-10} \text{ m}$

These are approximate values based on typical molecular sizes.

Problem Statement

Niraj et al simulation problem statement for the Microchannel.

Validation: Flow of nitrogen through a microchannel is simulated with inlet

Knudsen number of 0.053 and pressure ratio of 2.5. The microchannel size is $2\mu\text{m} \times 0.4\mu\text{m} \times 2\mu\text{m}$. Flow inlet temperature and wall temperature are kept as 300K. The pressure at the outlet of channel is kept as 100 kPa.

Ours is a simulation of gas flow in a microchannel, which falls under the regime of slip flow since the Knudsen number ($Kn = 0.053$) is between 0.01 and 0.1. In this regime, the continuum assumption of Navier-Stokes equations needs to be modified with slip boundary conditions at the walls.

Assumed Distribution of Molecules in the Microchannel

1 molecule at center, which is in middle of all axis (X, Y, Z) = (0, 0, 0)

33 in each quadrant

X axis is width = $2 \mu\text{m} = 2\text{E-}6 \text{ m}$

Y axis is Height = $0.4 \mu\text{m} = 0.4\text{E-}6 \text{ m}$

Z axis is length = $2 \mu\text{m} = 2\text{E-}6 \text{ m}$

Z axis length is divided into 100 parts/slices so each length = $2 \mu\text{m} / 100 = 2\text{E-}6 / 100 \text{ m} = 2\text{E-}8 \text{ m}$.

That is, Z axis is length = $2 \mu\text{m} / 100 = 2\text{E-}6 / 100 \text{ m} = 2\text{E-}8 \text{ m}$

Height-to-width ratio = $0.4/2 = 0.2$

Quarter wise distribution of molecules

Ist Quadrant Number of molecules = 33

X positive = 0 to $1 \mu\text{m} = 0 \text{ to } 1.0\text{E-}6 \text{ m}$

Y positive = 0 to $0.2 \mu\text{m} = 0 \text{ to } 0.2\text{E-}6 \text{ m}$

Z axis is length = $2 \mu\text{m} / 100 = 2\text{E-}6 / 100 \text{ m} = 2\text{E-}8 \text{ m}$

IInd Quadrant Number of molecules = 33

X positive = 0 to $1 \mu\text{m} = 0 \text{ to } 1.0\text{E-}6 \text{ m}$

Y Negative = 0 to $-1 \mu\text{m} = 0 \text{ to } -1.0\text{E-}6 \text{ m}$

Z axis is length = $2 \mu\text{m} / 100 = 2\text{E-}6 / 100 \text{ m} = 2\text{E-}8 \text{ m}$

IIIrd Quadrant Number of molecules = 33

X negative = 0 to $1 \mu\text{m} = 0 \text{ to } 1.0\text{E-}6 \text{ m}$

Y positive = 0 to $0.2 \mu\text{m} = 0 \text{ to } 0.2\text{E-}6 \text{ m}$

Z axis is length = $2 \mu\text{m} / 100 = 2\text{E-}6 / 100 \text{ m} = 2\text{E-}8 \text{ m}$

IVth Quadrant Number of molecules = 33

X negative = 0 to $1 \mu\text{m} = 0 \text{ to } 1.0\text{E-}6 \text{ m}$

Y negative = 0 to $-1 \mu\text{m} = 0 \text{ to } -1.0\text{E-}6 \text{ m}$

Z axis is length = $2 \mu\text{m} / 100 = 2\text{E-}6 / 100 \text{ m} = 2\text{E-}8 \text{ m}$

Different Methods

Let's examine different procedures possible (we thought) at present. We got different numerical answers by using these simple procedures. First, we will calculate Mass flow rate and later we will see incoming and outgoing velocities.

Calculating the Mass Flow Rate

1st Method (Better)

Calculating the mass flow rate for this problem involves several steps due to the compressible and slip flow nature. We'll need to consider the average velocity across the channel and the density of the gas, which changes along the length.

The general formula for mass flow rate ($\dot{m}$) is:

$$\dot{m} = \rho \bar{u} A$$

Where:

- ρ is the density of the gas.
- $\bar{u}$ is the average velocity of the gas in the cross-section.
- A is the cross-sectional area of the channel.

The challenge is that ρ and $\bar{u}$ are not constant along the length of the channel due to the pressure drop. For compressible flow, mass flow rate is conserved along the channel, meaning $\dot{m}$ should be constant.

Let's estimate the mass flow rate using properties at the inlet and outlet, and then discuss how to get a more accurate value.

Given Data

- Fluid: Nitrogen (N_2)
- Inlet Pressure (P_{in}): 250 kPa
- Outlet Pressure (P_{out}): 100 kPa
- Channel Dimensions: $h=0.4\mu m$, $w=2\mu m$
- Length (L): $2\mu m$
- Temperature (T): 300 K (isothermal flow assumed)
- Knudsen Number (Kn): 0.053 (slip flow regime)

Calculate Cross-sectional Area (A):

$$A = h \times w = (0.4 \times 10^{-6} \text{ m}) \times (2 \times 10^{-6} \text{ m}) = 0.8 \times 10^{-12} \text{ m}^2$$

Calculate Densities at Inlet and Outlet (using Ideal Gas Law)

For an ideal gas, $\rho = P / RT$.

The specific gas constant for Nitrogen (R_{N2}) is approximately

$$R_{N2} = 296.8 \text{ J/(kg} \cdot \text{K)}$$

Inlet Density (ρ_{in}): $P_{in}=250\text{kPa}=2.808 \text{ kg/m}^3$

$P=\rho RT$ Rearranging to solve for density: $\rho = P / RT$

Inlet pressure (P_{in}) = 250kPa = $250 \times 10^3 \text{ Pa}$

Inlet temperature (T) = 300K

Substituting the values: $\rho_{in} = 250 \times 10^3 \text{ Pa} / (296.8 \text{ J/(kg} \cdot \text{K)} \times 300 \text{ K})$ Inlet density of nitrogen is approximately 2.808 kg/m^3 .

Outlet Density (ρ_{out}):

The density at the outlet (ρ_{out}) is calculated using the ideal gas law: $\rho = P / RT$ Given:

Outlet pressure $P_{out} = 100 \text{ kPa} = 100 \times 10^3 \text{ Pa}$

Specific gas constant for Nitrogen (R) = $296.8 \text{ J/(kg} \cdot \text{K)}$

Outlet temperature (T) = 300K

Substituting the values: $\rho_{out} = 100 \times 10^3 \text{ Pa} / (296.8 \text{ J/(kg} \cdot \text{K)} \times 300 \text{ K})$ Outlet density of nitrogen is approximately 1.123 kg/m^3 .

Estimate Average Velocity

A precise average velocity is hard to calculate without simulation due to compressibility and slip. However, we can use an analytical model for compressible slip flow in a rectangular microchannel to get an approximate mean velocity.

For compressible flow in microchannels, various models exist. One common approach is to use a corrected form of the Poiseuille flow, often integrating along the channel length. For isothermal compressible flow, the mass flow rate can be given by a generalized form:

The derivation of the compressible Poiseuille flow equation, which we've provided in a generalized form, is a good exercise in fluid dynamics. It accounts for the effects of pressure and density changes along the length of a channel, which are significant in high-velocity or long-channel flows.

Derivation Steps

The derivation starts with the fundamental equation for incompressible Poiseuille flow and then adapts it for compressible fluids. Here is a step-by-step breakdown:

Incompressible Poiseuille Flow: We begin with the well-known Hagen-Poiseuille equation for incompressible, laminar flow through a circular pipe. This equation relates the pressure drop (ΔP) to the volumetric flow rate (Q):

$$Q = \frac{\pi R^4}{8\mu} \frac{\Delta P}{L}$$

where R is the pipe radius, μ is the dynamic viscosity, and L is the pipe length.

Accounting for Compressibility: For compressible flow, the fluid density (ρ) changes with pressure along the length of the pipe. Therefore, the volumetric flow rate (Q) is not constant. However, the mass flow rate ($\dot{m}$) is constant. The relationship between mass flow rate and volumetric flow rate is $\dot{m} = \rho Q$. Substituting this into the Poiseuille equation, we get:

$$\frac{\dot{m}}{\rho} = \frac{\pi R^4}{8\mu} \frac{dP}{dx}$$

Here, we've used differential terms (dP/dx) because the pressure gradient is no longer uniform along the pipe due to density changes.

Applying the Ideal Gas Law: For an isothermal compressible flow, the ideal gas law states that $P = \rho RT$, where R is the specific gas constant and T is the temperature. We can rearrange this to express density in terms of pressure:

$$\rho = P / RT$$

Now, substitute this expression for ρ into the modified Poiseuille equation:

$$\frac{\dot{m}}{P/RT} = \frac{\pi R^4}{8\mu} \frac{dP}{dx}$$

Simplifying this gives:

$$\frac{\dot{m}RT}{P} = \frac{\pi R^4}{8\mu} \frac{dP}{dx}$$

Integration: The next step is to separate the variables and integrate the equation over the length of the channel. We want to integrate from the inlet ($x=0, P=P_1$) to the outlet ($x=L, P=P_2$).

$$\int_0^L \frac{8\mu\dot{m}}{\pi R^4 RT} dx = \int_{P_1}^{P_2} P dP$$

The left-hand side is straightforward, as $\dot{m}$, μ , R , R , and T are all constants. The righthand side is a simple polynomial integral.

Solving the Integrals

Left side:
$$\frac{8\mu\dot{m}}{\pi R^4 RT} \int_0^L dx = \frac{8\mu\dot{m}L}{\pi R^4 RT}$$

Right side:
$$\int_{P_1}^{P_2} P dP = \left[\frac{1}{2} P^2 \right]_{P_1}^{P_2} = \frac{1}{2} (P_2^2 - P_1^2)$$

Final Equation: Equating the results of the two integrals gives:

$$\frac{8\mu\dot{m}L}{\pi R^4 RT} = \frac{1}{2} (P_2^2 - P_1^2)$$

Finally, we can rearrange this equation to solve for the mass flow rate ($\dot{m}$).

$$\dot{m} = \frac{\pi R^4}{16\mu L R T} (P_1^2 - P_2^2)$$

This is the corrected form for isothermal, compressible Poiseuille flow, which matches the generalized equation you provided.

Analogy: River Flow

Think of a river. In an incompressible flow (like water), the volume of water passing any point in the river is the same, assuming no tributaries. The pressure drop is due to friction with the riverbed and banks. For a compressible flow (like air), it's more like a gas flowing through a long, narrow pipe. As the gas expands, its velocity increases, and its density decreases. The mass of gas passing any point is constant, but the volume is not. The pressure drop is now not only due to friction but also due to the expansion of the gas. The derived equation accounts for this expansion, making it a more accurate model for real-world scenarios.

Fully Developed Isothermal Compressible Slip Flow

The derivation of the mass flow rate for fully developed isothermal compressible slip flow in a rectangular microchannel involves several key steps. The final equation you provided is a simplified approximation for channels where the height h is much smaller than the width w ($h \ll w$).

Governing Equations

The starting point is the Navier-Stokes equation for steady, one-dimensional, fully developed flow in the z -direction (Let's start with similar equation):

$$0 = -\frac{dP}{dz} + \mu \left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} \right)$$

This equation relates the pressure gradient (dP/dz) to the viscous forces. For a microchannel with a very large aspect ratio ($w/h \gg 1$), we can assume that the velocity profile is primarily a function of the height, so we simplify the equation to:

$$0 = -\frac{dP}{dz} + \mu \frac{d^2 u_z}{dy^2}$$

Slip Boundary Conditions

Unlike classical fluid dynamics, microscale flow exhibits slip at the walls. This means the fluid velocity at the wall is not zero. The first-order slip boundary condition is given by:

$$u_z|_{wall} = \lambda \left. \frac{du_z}{dn} \right|_{wall}$$

where λ is the mean free path and n is the direction normal to the wall. For our simplified geometry, the walls are at $y = \pm h/2$. The boundary conditions become:

$$\begin{aligned} \text{At } y = -h/2: u_z &= \lambda \left. \frac{du_z}{dy} \right|_{y=-h/2} \\ \text{At } y = +h/2: u_z &= -\lambda \left. \frac{du_z}{dy} \right|_{y=+h/2} \end{aligned}$$

Integrating the Navier-Stokes Equation

We integrate the simplified Navier-Stokes equation twice with respect to y .

First integration:

$$\frac{du_z}{dy} = \frac{1}{\mu} \frac{dP}{dz} y + C_1$$

Second integration:

$$u_z = \frac{1}{2\mu} \frac{dP}{dz} y^2 + C_1 y + C_2$$

Now, we apply the slip boundary conditions to solve for the constants C_1 and C_2 . Due to the symmetry of the velocity profile, we find that $C_1=0$. Using the boundary condition at $y=+h/2$:

$$u_z|_{h/2} = \frac{1}{2\mu} \frac{dP}{dz} \left(\frac{h}{2} \right)^2 + C_2 = -\lambda \left(\frac{1}{\mu} \frac{dP}{dz} \frac{h}{2} \right)$$

$$C_2 = -\frac{1}{8\mu} \frac{dP}{dz} h^2 - \frac{\lambda h}{2\mu} \frac{dP}{dz}$$

Solving for C_2 :

Solving the integral:

$$-\frac{wh^3}{12\mu} \left[\frac{P^2}{2} + \frac{6\lambda_{ref}P_{ref}}{h}P \right]_{P_1}^{P_2} = -\frac{wh^3}{12\mu} \left[\left(\frac{P_2^2 - P_1^2}{2} \right) + \frac{6\lambda_{ref}P_{ref}}{h}(P_2 - P_1) \right]$$

Since $P_2 < P_1$, we can flip the sign to make the terms positive, giving:

$$\frac{wh^3}{12\mu} \left[\frac{P_1^2 - P_2^2}{2} + \frac{6\lambda_{ref}P_{ref}}{h}(P_1 - P_2) \right]$$

Finally, we solve for the mass flow rate $\dot{m}$:

$$\dot{m} = \frac{wh^3}{24\mu LRT} \left[(P_1^2 - P_2^2) + \frac{12\lambda_{ref}P_{ref}}{h}(P_1 - P_2) \right]$$

This can be written in a more compact form using the average pressure $P^- = (P_1 + P_2)/2$ and the pressure drop $\Delta P = P_1 - P_2$.

$$\dot{m} = \frac{wh^3}{12\mu LRT} (P_1^2 - P_2^2) \left(1 + \frac{12\lambda_{ref}P_{ref}}{h} \frac{P_1 - P_2}{P_1^2 - P_2^2} \right)$$

Simplifying the last term using $P_1^2 - P_2^2 = (P_1 - P_2)(P_1 + P_2)$:

$$\dot{m} = \frac{wh^3}{12\mu LRT} (P_1^2 - P_2^2) \left(1 + \frac{12\lambda_{ref}P_{ref}}{h} \frac{1}{P_1 + P_2} \right)$$

$$\frac{12\lambda_{ref}P_{ref}}{h(P_1 + P_2)}$$

This matches the form of the equation provided. The term is the Knudsen number correction factor. The Knudsen number is defined as $Kn = \lambda/h$.

This derivation showcases how classical fluid mechanics equations are adapted for microscale flow by incorporating the effects of rarefaction and gas compressibility.

So, for fully developed isothermal compressible slip flow in a rectangular microchannel, the mass flow rate can be approximated by (based on integrations of the Navier-Stokes equations with slip boundary conditions, often simplified for specific aspect ratios):

$$\dot{m} = \frac{1}{2\mu R T L} \left(\frac{wh^3}{12} (1 + \alpha_{slip,h} Kn_h) + \frac{hw^3}{12} (1 + \alpha_{slip,w} Kn_w) \right) (P_{in}^2 - P_{out}^2)$$

This expression is for channels where $h \gg w$ or $w \gg h$, and involves constants α_{slip} related to the slip coefficient and aspect ratio corrections.

A commonly cited formula for mass flow rate in a rectangular microchannel for isothermal compressible flow with first-order slip, which is integrated along the length, is:

$$\dot{m} = \frac{wh^3}{12\mu RT L} \left[\frac{P_{in}^2 - P_{out}^2}{2} + \frac{6\mu\sigma_v}{P_{avg}h} \left(\frac{\pi RT}{2} \right)^{1/2} \frac{P_{in}^2 - P_{out}^2}{2} \right]$$

This is sometimes simplified and adapted to a form that resembles:

$$\dot{m} = \frac{wh^3}{12\mu L} \frac{P_{in}^2 - P_{out}^2}{2P_{avg}RT} \left(1 + 6 \frac{2 - \sigma_v}{\sigma_v} Kn \right)$$

Where $P_{avg} = (P_{in} + P_{out})/2$ and Kn is based on the hydraulic diameter or height. Let's use the average pressure as a characteristic pressure for a simplified Kn calculation.

Let's use an average Knudsen number based on the average pressure:

$$P_{avg} = (250 + 100)/2 = 175 \text{ kPa}$$

$$P_{avg} = (250 + 100)/2 = 175 \text{ kPa}$$

Mean free path (λ) for nitrogen at STP (101.325 kPa, 273.15 K) is about $0.065 \mu\text{m}$.

The mean free path scales with $1/P$ (and slightly with $T^{1/2}$). So, at 300 K and 175 kPa:

$$\lambda \approx 0.065 \times \frac{101.325}{175} \times \sqrt{\frac{300}{273.15}} \approx 0.038 \mu\text{m}.$$

Characteristic length: Hydraulic diameter

$$D_h = \frac{2hw}{h+w} = \frac{2 \times 0.4 \times 2}{0.4+2} = \frac{1.6}{2.4} \approx 0.667 \mu\text{m}$$

$Kn_{avg} = \lambda/D_h = 0.038 / 0.667 \approx 0.057$ (consistent with our given Kn of 0.053).

Let's use a simpler, common form that combines the effects:

Mass flow rate for compressible flow in a rectangular microchannel with slip:

$$\dot{m} = \frac{(P_{in}^2 - P_{out}^2) A_{channel}^2}{2\mu RT L} \times F_{geo} \times F_{slip}$$

Where:

- F_{geo} is a geometric factor for rectangular channels (related to Poiseuille number for rectangular ducts, often $1/K$ where K is related to fRe).
- F_{slip} is a slip factor, often of the form $(1 + \alpha Kn)$.

For a rectangular channel, the shape factor needs to be considered. Without a precise complex analytical solution, a common simplified approach is to use the hydraulic diameter D_h and a correction for rectangular channels, or use models specifically for rectangular channels.

Let's try a simplified approximation by first estimating an average velocity in the channel.

Let's take an average cross-sectional velocity over the length of the channel to be approximately 150 m/s.

Now, we need a representative density for the mass flow rate calculation. Since the density changes along the channel, we can use the average density, or acknowledge that the mass flow rate is constant throughout. So,

we can use the outlet density and outlet velocity, or inlet density and inlet velocity (if we knew them). Let's use the average density from our inlet and outlet density calculations to get a value form.

Average density (ρ_{avg}) = (2.808+1.123)/2 $\approx$ 1.966kg/m³ Now, estimate mass flow rate:

$$\dot{m} = \rho_{avg} \times \bar{u}_{avg} \times A$$

$$\dot{m} \approx 1.966 \text{ kg/m}^3 \times 150 \text{ m/s} \times 0.8 \times 10^{-12} \text{ m}^2 \quad \dot{m} \approx 294.9 \text{ kg/(m}^2\text{s)} \times 0.8 \times 10^{-12} \text{ m}^2$$

$$\dot{m} \approx 235.92 \times 10^{-12} \text{ kg/s}$$

$$\dot{m} \approx 2.36 \times 10^{-10} \text{ kg/s}$$

Let's try a more robust approach using a typical mass flow rate formula for compressible slip flow:

A common form for isothermal compressible slip flow in a 2D channel (or using hydraulic diameter for rectangular) is given by a modified Darcy's Law or Poiseuille-like equation:

$$\dot{m} = \frac{C_D A}{RT P_{avg} L} (P_{in}^2 - P_{out}^2) (1 + \alpha Kn)$$

Where C_D is a constant related to the Poiseuille number, and α is related to the slip coefficient. For a rectangular channel with aspect ratio $\epsilon = h/w = 0.4/2 = 0.2$: The Poiseuille number fRe for no-slip rectangular channels is dependent on aspect ratio. For $\epsilon = 0.2$, $fRe \approx 72.9$. This corresponds to $C_D = D_{h2} / 32$.

$$C_D = \frac{D_h^2}{32}.$$

The correction factor $(1 + \alpha Kn)$ for slip, where α is often around 4 to 6 for first-order slip. Let's use $\alpha \approx 4$.

Let's use a standard formula for isothermal flow in a microchannel with slip. For a rectangular channel, the mass flow rate is given by:

$$\dot{m} = \frac{1}{\mu R T L} \left[\frac{w h^3}{12} \left(1 + 6 \frac{2 - \sigma_v}{\sigma_v} K n_h \right) + \frac{h w^3}{12} \left(1 + 6 \frac{2 - \sigma_v}{\sigma_v} K n_w \right) \right] \frac{P_{in}^2 - P_{out}^2}{2}$$

This formula is significantly more complex than the simplified multiplicative form we discussed earlier because it's a more direct solution to the Navier-Stokes equations with slip boundary conditions.

Here's a breakdown of the terms:

- $u(x,y)$: The local velocity in the z-direction (flow direction) at a point (x,y) in the cross-section. The origin (0,0) is typically at the center of the rectangular crosssection.
- μ : Dynamic viscosity of the fluid (nitrogen in our case).
- $(-dP/dz)$: The constant pressure gradient along the flow direction (since it's a pressure-driven flow). Note that for flow in the positive z direction, dP/dz will be negative, so $-dP/dz$ will be positive.
- h : Height of the channel (along the y-axis).
- w : Width of the channel (along the x-axis).
- ζ_v : Velocity slip coefficient (or slip length). This is a crucial term that incorporates the slip effect. For first-order slip, it's defined as:

$$\zeta_v = \frac{2 - \sigma_v}{\sigma_v} \lambda$$

where σ_v is the tangential momentum accommodation coefficient (between 0 and 1, typically 0.8-0.9 for gases on engineering surfaces), and λ is the mean free path of the gas molecules.

- The terms involving the infinite series account for the complex 2D nature of the velocity profile in a rectangular duct, especially the influence of the corners and the aspect ratio.
- cosh and cos: Hyperbolic cosine and cosine functions.
- n: An integer that takes odd values (1, 3, 5, ...) for the sum.

How this formula relates to our problem and why it's still an approximation

Direct Incorporation of Slip (ζ_v): This formula directly includes the slip coefficient ζ_v , which depends on the mean free path (λ) and the tangential momentum accommodation coefficient (σ_v).

More Accurate for Rectangular Geometry: The infinite series inherently captures the 2D variations in velocity across the rectangular cross-section more accurately than a simple product of two 1D parabolic-like profiles.

Still Assumes Incompressible Flow: Despite its complexity, this formula is still fundamentally derived for incompressible flow. Our problem has a pressure ratio of 2.5, meaning it's highly compressible. This is the biggest limitation for applying this exact formula to our specific scenario.

Fully Developed Flow: It also assumes fully developed flow, where the velocity profile does not change along the length of the channel. With a 2 μm length, this might not be the case.

Requires Iteration/Numerical Summation: To use this formula, you would need to sum a sufficient number of terms in the infinite series to achieve convergence, which can be computationally intensive if done manually.

In summary

This more detailed formula is a better analytical representation of incompressible slip flow in a rectangular microchannel. It clearly shows how the slip length (ζ_v) modifies the velocity profile,

leading to a non-zero velocity at the walls and a flattened profile. However, due to the significant compressibility of nitrogen flow and the short channel length, directly using this formula will still provide an approximation rather than a precise solution for our problem. Numerical simulation remains the most reliable method. For further details see [19] Shah, R. K., & London, A. L. (1971), while focused on heat transfer, the fundamental fluid dynamics solutions for various duct geometries are covered. And a book specifically addresses rarefied gas dynamics and microfluidics, and have detailed analytical and numerical solutions for slip flow is by Karniadakis, G.

E., & Beskok, [20]; and the book by A. Nguyen, N. T., & Wereley, S. T. (2002). Fundamentals and applications of microfluidics. Artech House, [21].

For Mass flow rate Calculations

First Approach Results of Niraj et al simulation as given in their paper and Analytic calculation of results

The simulated mass flow rate ($1.24 \times 10^{-10} \text{ kg/s}$) is found to compare very well with that obtained from the analytical formulation [42] ($1.26 \times 10^{-10} \text{ kg/s}$), the difference being only 1.6%

Calculated Mass flow rate is $\dot{m} \approx 9 \times 10^{-14} \text{ kg/s}$ or $\dot{m} \sim 9 \times 10^{-14} \text{ kg/s}$

Another method: Calculated Mass flow rate is $\dot{m} \approx 3.55 \times 10^{-16} \text{ kg/s}$ or $\dot{m} \sim 3.55 \times 10^{-16} \text{ kg/s}$ There is a large difference.

Second Approach (assume an average velocity): We have to use velocity after knowing velocities

The mass flow rate of nitrogen through a microchannel depends on several factors, including the Knudsen number, pressure ratio, channel dimensions, and boundary conditions. Based on the parameters you provided, the flow falls within the slip flow regime (Knudsen number of 0.053), where rarefaction effects like velocity slip and temperature jump become significant.

Rarefaction effects like velocity slip and temperature jump become significant when the characteristic length of a system approaches the mean free path of the gas molecules. This typically occurs in microchannels or low-pressure environments, where the continuum assumption starts to break down.

- **Velocity Slip:** Instead of adhering to the no-slip boundary condition, gas molecules exhibit a finite velocity at the solid surface. This effect is more pronounced at higher Knudsen numbers.
- **Temperature Jump:** The temperature of the gas molecules near the surface differs from the wall temperature due to incomplete energy exchange during molecular collisions.

These effects influence heat transfer, fluid flow behavior, and pressure distributions, making them crucial in microfluidic applications and MEMS devices to calculate the mass flow rate, you would typically use numerical methods such as the Direct Simulation Monte Carlo (DSMC) method or modified Navier-Stokes equations tailored for microchannel flows. These methods account for rarefaction effects and the specific boundary conditions.

To calculate the mass flow rate of nitrogen through the microchannel, we can use the following simplified equation:

$$\dot{m} = \rho \cdot A \cdot v$$

Where:

$\dot{m}$ = The mass flow rate (kg/s), ρ = The density of nitrogen (kg/m³), A = The cross-sectional area of the microchannel (m²), V = The average velocity of nitrogen (m/s).

Step-by-Step Calculation

Cross-sectional Area: The microchannel dimensions are $2 \mu\text{m} \times 0.4 \mu\text{m} \times 2 \mu\text{m}$.

$$A = 8 \times 10^{-13} \text{ m}^2$$

Density of Nitrogen: At 300 K and 100 kPa, the density of nitrogen can be approximated using the ideal gas law: $\rho = P / (R \times T)$

Where--

P is the pressure (Pa),

R is the specific gas constant for nitrogen (296.8 J/kg·K), T is the temperature (K).

Substituting the values:

$$P = 100,000 / (296.8 \times 300) = 1.125 \text{ kg / m}^3$$

Velocity: The velocity can be estimated using numerical methods or experimental data for slip flow conditions. Here we assume an average velocity of 0.1 m/s (a typical value for microchannel flows).

Mass Flow Rate: Substituting values into the equation:

$$= 1.125 \times 8 \times 10^{-13} \times 0.1 = 0.9 \times 10^{-13} = 9 \times 10^{-14} \text{ kg/s}$$

This is a simplified calculation. For more accurate results, numerical simulations like DSMC or modified Navier-Stokes equations are recommended.

Third Approach

To calculate the mass flow rate of nitrogen through the specified microchannel, we can use the following formula derived from the ideal gas law and assuming isothermal flow:

$$\dot{m} = \{(P_1 \times A) / (R \times T)\} \times \text{Sqrt} \{(2 \times k) / (k-1)\} \times (R \times T) / P_1 \} \text{ Where: } \dot{m} = \text{mass flow rate (kg/s)}$$

P_1 = inlet pressure (Pa)

A = cross-sectional area of the microchannel (m^2)

R = specific gas constant for nitrogen (approximately $296.8 \text{ J/kg}\cdot\text{K}$)

T = absolute temperature (K)

K = specific heat ratio for nitrogen (approximately 1.4) Given Data:

- Inlet Pressure: To find P_1 , we can calculate it from the outlet pressure and the pressure ratio:
- $P_1 = \text{Pressure Ratio} \times P_{\text{outlet}} = 2.5 \times 100 \text{ kPa} = 250,000 \text{ Pa}$ - Temperature: $T = 300 \text{ K}$ - Channel Dimensions: Length = $2 \mu\text{m}$
Height = $0.4 \mu\text{m}$ Width = $2 \mu\text{m}$
- Cross-sectional Area:

$$A = \text{Height} \times \text{Width} = (0.4 \times 10^{-6} \text{ m}) \times (2 \times 10^{-6} \text{ m}) = 0.8 \times 10^{-12} \text{ m}^2$$

Calculating the Mass Flow Rate:

Insert values into the equation:

$$k = 1.4$$

$$\dot{m} = \{(P_1 \times A) / (R \times T)\} \times \text{Sqrt} \{(2 \times k) / (k-1)\} \times (R \times T) / P_1 \} \text{ i.e., } \dot{m} = \{250000 \times 0.8 \times 10^{-12} / (296.8 \times 300)\} \times \text{Sqrt} \{(2 \times 1.4) / (1.4 - 1)\} \times (296.8 \times 300) / 250000 \}$$

$$\dot{m} = (\text{approx.}) 3.548 \times 10^{-16} \text{ kg/s}$$

Important Considerations in the above Method

- **Compressibility:** For gases with significant pressure drops and Mach numbers, the flow becomes compressible. The Mach number needs to be checked. For nitrogen at 300 K, the speed of sound is approximately 353 m/s. Our calculated velocities are subsonic, but the variation along the channel suggests that a fully incompressible model is an approximation.
- **Isothermal vs. Adiabatic:** The problem states constant inlet and wall temperatures (300K), suggesting an isothermal assumption.
- **Flow Profile:** The above calculations give average velocities. The actual velocity profile in a microchannel in the slip flow regime is not parabolic like in continuum flow. There's a non-zero slip velocity at the walls.
- **Advanced Models:** For higher Knudsen numbers (approaching the transition regime like at the outlet), more advanced models beyond first-order slip (e.g., second-order slip models or direct simulation Monte Carlo (DSMC)) might be necessary for higher accuracy. The problem is simplified by asking for velocities, implying a simplified approach is expected.
- **Channel Geometry:** The formula used is for a parallel plate channel. For a rectangular channel, a shape factor may be needed, but for a height-to-width ratio of $0.4/2 = 0.2$, the parallel plate approximation might be acceptable.

Let's calculate the average velocity at the inlet and outlet using their respective local mean free paths.

- **Velocity at the Inlet:** $U_{\text{inlet}} = -12 \times (1.78 \times 10^{-5} \text{ Pa s})(0.4 \times 10^{-6} \text{ m})^2 \times (-7.5 \times 10^{10} \text{ Pa/m}) \times (1 + 60.4 \times 10^{-6} \text{ m} / 2.12 \times 10^{-9} \text{ m} / 0.91.1)$
 $U_{\text{inlet}} = (7.49 \times 10^{-10}) \times (7.5 \times 10^{10}) \times (1 + 0.388) U_{\text{inlet}} = 56.175 \times 1.388 U_{\text{inlet}} \approx 77.9 \text{ m/s}$
- $U_{\text{inlet}} \approx 77.9 \text{ m/s}$
- **Velocity at the Outlet:** $U_{\text{outlet}} = -12 \times (1.78 \times 10^{-5} \text{ Pa s})(0.4 \times 10^{-6} \text{ m})^2 \times (-7.5 \times 10^{10} \text{ Pa/m}) \times (1 + 60.4 \times 10^{-6} \text{ m} / 53 \times 10^{-9} \text{ m} / 0.91.1)$
 $U_{\text{outlet}} = (7.49 \times 10^{-10}) \times (7.5 \times 10^{10}) \times (1 + 6 \times 0.1325 \times 1.222) U_{\text{outlet}}$

$$=56.175 \times (1+0.97)U_{\text{outlet}} = 56.175 \times 1.97U_{\text{outlet}} \approx 110.6 \text{ m/s}$$

- $U_{\text{outlet}} \approx 110.6 \text{ m/s}$

From the above calculations (Approximate Numerical Values):

- Inlet Velocity (U_{inlet}): 77.9 m/s
- Outlet Velocity (U_{outlet}): 110.6 m/s

These are approximate values. A detailed numerical simulation would be required for more precise results, considering the compressibility and the varying Knudsen number along the channel. The values indicate a significant increase in velocity from inlet to outlet due to the decreasing pressure and the effect of rarefaction.

Velocities Calculation

Calculation of Velocities of Nitrogen

To calculate the velocities of nitrogen flow in the microchannel, we need to consider the slip flow regime (Knudsen number of 0.053) and the pressure-driven flow characteristics. Here's a simplified approach:

Formula for Velocity

The average velocity in the microchannel can be estimated using the Hagen-Poiseuille equation, modified for rarefied gas flow:

$$v = \Delta P h^2 / 12 \mu L$$

Where:

v --is the average velocity (m/s),

ΔP --is the pressure difference 150000 (Pa), h --is the height of the microchannel 0.4 micro (m), μ --is the dynamic viscosity of nitrogen 1.76×10^{-5} (Pa·s), L --is the length of the microchannel 2.0 (m).

Step-by-Step Calculation

Pressure Difference: $\Delta P = P_{\text{inlet}} - P_{\text{outlet}}$ Given the pressure ratio of 2.5 and outlet pressure of 100 kPa:

$P_{\text{inlet}} = 2.5 \times 100,000 = 250,000 \text{ Pa}$. $\Delta P = 250,000 - 100,000 = 150,000 \text{ Pa}$. 7.3.1.2. Dynamic Viscosity: The dynamic viscosity of nitrogen at 300 K is approximately $\mu = 1.76 \times 10^{-5} \text{ Pa}\cdot\text{s}$.

Channel Dimensions

o Height $h = 0.4 \mu\text{m} = 0.4 \times 10^{-6} \text{ m}$, o Length $L = 2.0 \mu\text{m} = 2 \times 10^{-6} \text{ m}$.

Average Velocity: Substituting values into the equation:
$$v = \frac{150,000 \times (0.4 \times 10^{-6})^2}{12 \times (1.76 \times 10^{-5}) \times (2 \times 10^{-6})} \quad /$$

$$= (\text{approx.}) 0.568 \text{ m/s}$$

This is a simplified calculation. For more accurate results, numerical simulations like DSMC or modified Navier-Stokes equations are recommended.

Calculation of velocities of nitrogen in another method

To find the velocities of nitrogen flowing through a microchannel given the conditions you've mentioned, we can use some fundamental principles of fluid mechanics.

Parameters

- **Inlet Knudsen Number (Kn):** 0.053
- **Pressure Ratio (P_{ratio}):** 2.5
- **Microchannel Size:** $2 \mu\text{m} \times 0.4 \mu\text{m} \times 2 \mu\text{m}$ (converted to consistent units, assuming $\mu\text{m} = \text{micrometers}$)
- **Inlet Temperature (T):** 300 K
- **Outlet Pressure (P_{out}):** 100 kPa

Key Formulae and Concepts

Knudsen Number (Kn):

$$Kn = \lambda L$$

Where:

- λ is the mean free path of the gas
- L is the characteristic length of the microchannel
- The mean free path for nitrogen at 300 K can be estimated using:

$$\lambda \approx \frac{2}{\pi} \frac{d^2 P k T}{\sqrt{2}}$$

Where:

- k is the Boltzmann constant (1.38×10^{-23} J/K)
- d is the molecular diameter (for nitrogen, approx. $0.364 \text{ nm} = 3.64 \times 10^{-10} \text{ m}$)
- P is the pressure (converted to Pa)

Average Velocity of Gas Flow

The average velocity (V_{avg}) can be calculated using the following equation derived from the ideal gas law and continuity equation:

$$V_{avg} = \frac{Q}{A}$$

Where:

- Q is the volumetric flow rate
- A is the cross-sectional area of the microchannel

The volumetric flow rate can also be related to the inlet/outlet pressures and other properties using the following:

$$Q = C_d A^2 (P_{in} - P_{out}) \rho$$

Where:

- C_d is the discharge coefficient (typically around 0.61 for laminar flow).
- ρ is the density of nitrogen at the inlet conditions.

Density of Nitrogen (ρ): Using the ideal gas law:

$$\rho = \frac{P}{R T}$$

Where:

- R is the specific gas constant for nitrogen ($R \approx 296.8 \text{ J/(kg K)}$)

Cross-sectional Area (A) of the microchannel:

$$A = h w$$

Where:

- h and w are the height and width of the channel respectively.

Calculations

Calculate Cross-Sectional Area:

$$A = 0.4 \times 2 \mu\text{m}^2 = 0.8 \mu\text{m}^2 = 0.8 \times 10^{-12} \text{ m}^2$$

Calculate Density (ρ)

Convert pressures to Pa:

$$\begin{aligned} P_{in} &= P_{out} \times \text{Pratio} = 100 \text{ kPa} \cdot 2.5 = 250 \text{ kPa} = 250,000 \text{ Pa} \\ \rho &= 250,000 \times 296.8 \times 300 \approx 2.506 \text{ kg/m}^3 \end{aligned}$$

Estimate Flow Rate (Q)

Using a typical value for Cd: $Q \approx C_d A^2 (P_{in} - P_{out}) \rho$

Calculate the flow rate Q first.

$$\begin{aligned} Q &\approx 0.61 \times 0.8 \times 10^{-12} \times 2 \times (250,000 - 100,000) \times 2.506 \\ &= 3.66878 \times 10^{-7} \end{aligned}$$

Calculate Average Velocity

$$V_{avg} = QA = 0.8 \times 10^{-12} \text{ m}^2 \times 3.66878 \times 10^{-7} = 2.93502 \times 10^{-19} \text{ m/s}$$

Calculation of Average Velocity by a Third Method

To determine the velocities, we need to calculate the mean free path of nitrogen and then apply a suitable slip flow model.

Properties of Nitrogen at 300 K:

- Gas Constant (R): For Nitrogen (N₂), R = 296.8 J/(kg·K) (from ideal gas properties at 300K).
- Molar Mass (M): M = 28.013 kg/kmol.
- Boltzmann Constant (k_B): 1.380649×10^{-23} J/K
- Kinetic Diameter of Nitrogen (d): Approximately 3.7×10^{-10} m (This value can vary slightly depending on the source, but it's a common approximation for nitrogen).
- Viscosity (μ): At 300 K, the dynamic viscosity of nitrogen is approximately 1.78×10^{-5} Pa·s (This can be found in thermophysical property tables for nitrogen).

Mean Free Path (λ)

The mean free path (λ) is the average distance a molecule travels between collisions. It

$$\lambda = k_B T / [\sqrt{2} \times \pi d^2 P]$$

Where:

- k_B is the Boltzmann constant.
- T is the temperature in Kelvin.
- d is the kinetic diameter of the gas molecule.
- P is the pressure in Pascal.

Given:

- T = 300 K
- Outlet pressure (P_{outlet}) = 100 kPa = 100×10^3 Pa
- Inlet pressure (P_{inlet}) = Pressure ratio $\times$ P_{outlet}

$$= 2.5 \times 100 \text{ kPa} = 250 \text{ kPa} = 250 \times 10^3 \text{ Pa} \text{ Let's calculate the mean free path at the inlet and outlet:}$$

$$\text{At the inlet (} P_{inlet} = 250 \text{ kPa): } \lambda_{inlet} = [(1.380649 \times 10^{-23} \text{ J/K}) \times 300 \text{ K}] / [\sqrt{2} \times \pi \times (3.7 \times 10^{-10} \text{ m})^2 \times (250 \times 10^3 \text{ Pa})]$$

$$\lambda_{inlet} \approx 0.65 \times 10^{-7} \text{ m} = 65 \text{ nm}$$

$$\text{At the outlet (} P_{outlet} = 100 \text{ kPa): } \lambda_{outlet} = [(1.380649 \times 10^{-23} \text{ J/K}) \times 300 \text{ K}] / [\sqrt{2} \times \pi \times (3.7 \times 10^{-10} \text{ m})^2 \times (100 \times 10^3 \text{ Pa})]$$

$$\lambda_{outlet} \approx 1.63 \times 10^{-7} \text{ m} = 163 \text{ nm}$$

The characteristic length (L_c) for the Knudsen number is typically the smallest dimension of the channel, which is $0.4 \mu\text{m} = 0.4 \times 10^{-6} \text{ m}$.

Let's verify the inlet Knudsen number provided:

$$\text{Kn}_{\text{inlet}} = \lambda_{\text{inlet}} / L_c = (65 \times 10^{-9} \text{ m}) / (0.4 \times 10^{-6} \text{ m}) = 0.1625$$

The provided inlet Knudsen number is 0.053. This discrepancy might arise from a different definition of the characteristic length (e.g., hydraulic diameter) or a different method for calculating the mean free path. Assuming the given Knudsen number (0.053) is accurate, we can back-calculate the mean free path at the inlet for consistency.

$$\text{If } \text{Kn}_{\text{inlet}} = 0.053 \text{ and } L_c = 0.4 \mu\text{m}, \text{ then: } \lambda_{\text{inlet}} = \text{Kn}_{\text{inlet}} \times L_c = 0.053 \times (0.4 \times 10^{-6} \text{ m}) = 0.0212 \times 10^{-6} \text{ m} = 21.2 \text{ nm}$$

This value of λ_{inlet} (21.2 nm) is significantly smaller. This suggests that either the characteristic length used to calculate the given Kn is different (e.g., twice the height, or hydraulic diameter), or the mean free path used was calculated with a more precise model, or a different kinetic diameter.

For the purpose of finding velocities, we will use the given Knudsen number and the associated flow regime. Since $0.01 < \text{Kn} < 0.1$, the flow is in the slip flow regime.

Velocity in Slip Flow Regime

For flow in microchannels in the slip flow regime, the classical Hagen-Poiseuille equation (for pressure-driven flow in a rectangular channel) needs to be modified with a slip velocity at the walls. The average velocity for a compressible gas flow in a rectangular microchannel under slip flow conditions can be approximated by:

$$U_{\text{avg}} = - (H^2 / 12\mu) \times (dP/dx) \times [(1 + (6\lambda / H) \times ((2 - \sigma_v) / \sigma_v))] \quad \text{Where:}$$

- U_{avg} is the average velocity.
- H is the channel height (which is the smallest dimension, $0.4 \mu\text{m}$).
- μ is the dynamic viscosity of the gas.
- dP/dx is the pressure gradient along the channel length.
- λ is the local mean free path.
- σ_v is the tangential momentum accommodation coefficient (TMAC). For most engineering surfaces, σ_v is often assumed to be 0.8 to 0.9 for nitrogen. A common value is $\sigma_v = 0.9$. If not specified, 1 (fully diffuse reflection) is also sometimes used for simplicity, which means $((2 - \sigma_v) / \sigma_v) = 1$. Let's use $\sigma_v = 0.9$, so $(2 - 0.9) / 0.9 = 1.1 / 0.9 \approx 1.222$. The pressure gradient can be approximated as:

$$dP/dx \approx (P_{\text{outlet}} - P_{\text{inlet}}) / L = (100 \text{ kPa} - 250 \text{ kPa}) / 2 \mu\text{m} \quad dP/dx = -150 \times 10^3 \text{ Pa} / 2 \times 10^{-6} \text{ m} = -7.5 \times 10^{10} \text{ Pa/m}$$

Since the pressure varies along the channel, the mean free path λ will also vary. For a first approximation, we can use an average mean free path or evaluate at the inlet and outlet.

$$\text{Let's use the given inlet Knudsen number } (\text{Kn}_{\text{inlet}} = 0.053) \text{ to find the mean free path at the inlet, which is } \lambda_{\text{inlet}} = \text{Kn}_{\text{inlet}} \times H = 0.053 \times (0.4 \times 10^{-6} \text{ m}) = 21.2 \text{ nm}.$$

$$\text{Now we need to estimate the mean free path at the outlet. We know that } \lambda \propto T/P. \text{ So, } \lambda_{\text{outlet}} = (\lambda_{\text{inlet}} \times P_{\text{inlet}}) / P_{\text{outlet}} = 21.2 \text{ nm} \times 250 \text{ kPa} / 100 \text{ kPa} = 21.2 \text{ nm} \times 2.5 = 53 \text{ nm}.$$

Therefore, $\text{Kn}_{\text{outlet}} = \lambda_{\text{outlet}} / H = (53 \times 10^{-9} \text{ m}) / (0.4 \times 10^{-6} \text{ m}) = 0.1325$. This value falls into the transition regime, implying that a simple first-order slip model might not be fully accurate throughout the channel. However, for a general estimation, we can proceed with the slip flow model.

Let's calculate the average velocity at the inlet and outlet using their respective local mean free paths, using above mentioned formulae.

The equations used in our calculations are based on a modified form of the HagenPoiseuille equation for microchannel flow. This form accounts for both the slip flow at the channel walls and the effects of compressibility, though the specific calculations are for the local average velocity.

The general equation for the average fluid velocity (U_{avg}) at a specific point in a rectangular microchannel with slip flow is:

$$U_{avg} = -\frac{h^2}{12\mu} \frac{dP}{dz} \left(1 + 6 \frac{\lambda}{h} \left(\frac{2-\sigma}{\sigma} \right) \right)$$

where:

- h is the channel height.
- μ is the dynamic viscosity of the fluid.
- dP/dz is the local pressure gradient along the length of the channel.
- λ is the local mean free path of the gas molecules.
- σ is the Tangential Momentum Accommodation Coefficient (TMAC), which is a value between 0 and 1 that characterizes the fluid-surface interaction. The term $2-\sigma / \sigma$ is a correction factor for the slip velocity. Our calculations use the absolute value of the pressure gradient, which is a common approach when the direction of flow is clear. The values for your specific calculations are:

Velocity at the Inlet

For the inlet, the equation is:

$$U_{inlet} = \frac{(0.4 \times 10^{-6} \text{ m})^2}{12 \times (1.78 \times 10^{-5} \text{ Pa} \cdot \text{s})} \times (7.5 \times 10^{10} \text{ Pa/m}) \times \left(1 + 6 \frac{1.2 \times 10^{-9} \text{ m}}{0.4 \times 10^{-6} \text{ m}} \frac{0.9}{1.1} \right)$$

- $h^2 = (0.4 \times 10^{-6} \text{ m})^2$
- $12\mu = 12 \times (1.78 \times 10^{-5} \text{ Pa} \cdot \text{s})$
- $|dP/dz| = 7.5 \times 10^{10} \text{ Pa/m}$
- $\Lambda_{inlet} = 1.2 \times 10^{-9} \text{ m}$

This yields the calculated value of approximately 77.9 m/s.

Velocity at the Outlet

For the outlet, the equation is:

$$U_{outlet} = \frac{(0.4 \times 10^{-6} \text{ m})^2}{12 \times (1.78 \times 10^{-5} \text{ Pa} \cdot \text{s})} \times (7.5 \times 10^{10} \text{ Pa/m}) \times \left(1 + 6 \frac{53 \times 10^{-9} \text{ m}}{0.4 \times 10^{-6} \text{ m}} \frac{0.9}{1.1} \right)$$

- $h^2 = (0.4 \times 10^{-6} \text{ m})^2$
- $12\mu = 12 \times (1.78 \times 10^{-5} \text{ Pa} \cdot \text{s})$
- $|dP/dz| = 7.5 \times 10^{10} \text{ Pa/m}$
- $\Lambda_{outlet} = 53 \times 10^{-9} \text{ m}$

This gives the calculated value of approximately 110.6 m/s.

The increase in velocity from the inlet to the outlet is due to the gas expanding as the pressure drops. The mean free path (λ) increases as the pressure decreases, which in turn leads to a larger slip correction factor and a higher local velocity.

To summarize from the above discussion:

Velocity at the Inlet:

$$U_{\text{inlet}} \approx 77.9 \text{ m/s}$$

Velocity at the Outlet:

$$U_{\text{outlet}} \approx 110.6 \text{ m/s}$$

General Approach with differential Equations

All these above are simplified methods, Now, let's go into a more research oriented method using partial differential equations and a bit rigorous mathematics. Simulating gas flow at the microscale requires considering the rarefaction effects that become significant when the characteristic length scale of the flow (like the channel dimensions) is comparable to the mean free path of the gas molecules.

The Knudsen number (Kn), which you've given as 0.053, neatly quantifies this. Given the Knudsen number (Kn=0.053), the flow regime likely falls within the slip flow regime ($0.001 < \text{Kn} < 0.1$). In this regime, the no-slip boundary condition typically used in macroscopic fluid mechanics no longer holds true at the walls. Instead, we observe a velocity slip.

To determine the velocities and provide the relevant formulae and numerical values, we'd typically rely on numerical simulations using computational fluid dynamics (CFD) software that can handle rarefied gas flows. These simulations would solve the governing equations, often the Navier-Stokes equations with slip boundary conditions, tailored for the specific geometry and flow conditions we've described.

Approach for Simulation

Governing Equations: For slip flow, the compressible Navier-Stokes equations are often used, incorporating modifications at the boundaries to account for velocity slip and temperature jump. These equations describe the conservation of mass, momentum, and energy.

- **Continuity Equation (Conservation of Mass):**

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

where ρ is the density and $\mathbf{u}$ is the velocity vector.

- **Momentum Equation (Conservation of Momentum):**

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

where p is the pressure, $\boldsymbol{\tau}$ is the viscous tensor, and $\mathbf{g}$ is the gravitational acceleration (which is often neglected in microchannel flows due to the small scale).

• **Energy Equation (Conservation of Energy):** $\frac{\partial (\rho e)}{\partial t} + \nabla \cdot (\rho e \mathbf{u}) = -p(\nabla \cdot \mathbf{u}) + \boldsymbol{\tau} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q} + \rho h$

where e is the internal energy, $\mathbf{q}$ is the heat flux vector, and h represents any heat sources.

- **Equation of State (for Nitrogen, an ideal gas can often be assumed):**

$$p = \rho R T$$

where R is the specific gas constant for nitrogen and T is the temperature.

Boundary Conditions: This is where the slip flow regime is specifically addressed.

- **Inlet:** We've specified an inlet Knudsen number of 0.053 and a pressure ratio of 2.5. Since the outlet pressure is 100 kPa, the inlet pressure (P_{in}) would be:
 $P_{in} = \text{Pressure Ratio} \times P_{out} = 2.5 \times 100\text{kPa} = 250\text{kPa}$ o The inlet temperature (T_{in}) is given as 300 K. Typically, you would also specify a velocity profile at the inlet (e.g., uniform).

- **Outlet:** The outlet pressure (P_{out}) is given as 100 kPa. A common boundary condition for the outlet is to assume a fully developed flow or a specified pressure.

- **Walls:** This is where the slip boundary conditions come into play. The most common form is the first-order slip boundary condition for velocity:

$$u_{wall} - u_{gas,wall} = \zeta_v \partial u_{gas} / \partial n |_{wall}$$

where u_{wall} is the velocity of the wall (which is 0 in this case), $u_{gas,wall}$ is the velocity of the gas at the wall, $\partial u_{gas} / \partial n |_{wall}$ is the velocity gradient normal to the wall, and ζ_v is the velocity slip coefficient. The slip coefficient is often related to the mean free path (λ) of the gas molecules and the tangential momentum accommodation coefficient (σ_v):

$$\zeta_v = [(2 - \sigma_v)\lambda] / \sigma_v$$

The mean free path can be estimated using the Knudsen number and a characteristic length scale (L_c , e.g., the hydraulic diameter of the channel):

$$Kn = \lambda / L_c \Rightarrow \lambda = Kn \times L_c$$

For a rectangular channel with dimensions $H \times W$, the hydraulic diameter (D_h) is given by:

$$D_h = 4 \times \text{Cross-sectional Area} / \text{Perimeter} = [4 \times (2 \times 10^{-6} \text{m} \times 0.4 \times 10^{-6} \text{m})] / [2 \times (2 \times 10^{-6} \text{m} + 0.4 \times 10^{-6} \text{m})] \quad \text{So, } \lambda = 0.053 \times 0.667 \times 10^{-6} \text{m} \approx 3.535 \times 10^{-8} \text{m}.$$

Similarly, a temperature jump condition can be applied at the walls:

$$T_{gas,wall} - T_{wall} = \zeta_T \partial T_{gas} / \partial n |_{wall}$$

where ζ_T is the temperature jump coefficient, related to the mean free path and the thermal accommodation coefficient (σ_T).

- **Symmetry:** If the flow and geometry exhibit symmetry, you can use symmetry boundary conditions to reduce the computational domain.
- **Numerical Solution:** The governing equations with the specified boundary conditions are then discretized and solved numerically using methods like the finite volume method. This would yield the velocity, pressure, temperature, and density fields throughout the microchannel.

Numerical Values and Formulae for Velocities:

Without running a full CFD simulation, it's challenging to provide precise numerical values for the velocity at every point in the microchannel. However, we can discuss some key aspects:

- **Average Velocity:** Due to the pressure difference between the inlet and outlet, there will be a net flow rate and hence an average velocity. This average velocity will be influenced by the channel dimensions, the pressure drop, the gas properties (viscosity), and the slip at the walls.
- **Velocity Profile:** In a typical pressure-driven flow through a rectangular channel under no-slip conditions, the velocity profile would be parabolic. However, with slip boundary conditions, there will be a non-zero velocity at the walls, leading to a flatter velocity profile compared to the no-slip case.
- **Maximum Velocity:** The maximum velocity will likely occur at the center of the channel cross-section.

Simplified Analytical Estimates (Illustrative)

For a fully developed, steady, incompressible flow in a rectangular channel under noslip conditions, the average velocity ($\bar{u}$) can be related to the pressure gradient ($\Delta P/L$) and the fluid viscosity (μ) through a shape factor that depends on the aspect ratio of the channel. However, our case involves compressible flow, slip conditions, and a significant pressure ratio, making such simplified incompressible flow analyses inaccurate.

For slip flow, the flow rate is generally higher compared to no-slip flow under the same pressure gradient due to the reduced resistance at the walls.

To get the numerical values of the velocities, you would need to perform a numerical simulation using software capable of handling compressible, rarefied gas flows with slip boundary conditions. This would involve:

- Creating a geometric model of the microchannel (2 μm x 0.4 μm x 2 μm).
- Meshing the computational domain.
- Setting up the physical model (compressible Navier-Stokes equations, ideal gas law for nitrogen).
- Defining the boundary conditions (inlet pressure of 250 kPa at 300 K, outlet pressure of 100 kPa, wall temperature of 300 K, and appropriate slip boundary conditions using a chosen tangential momentum accommodation coefficient for nitrogen on the channel walls – a common value is around 0.8-0.9).
- Running the simulation until convergence.
- Post-processing the results to extract the velocity field.
- The simulation would then provide you with detailed information about the velocity distribution within the microchannel, including the velocity vectors, velocity magnitudes, average velocity, and maximum velocity.

In summary, while I can provide the theoretical framework and the formulae involved in simulating this flow, obtaining the specific numerical values for the velocities necessitates a computational approach. The slip flow regime, characterized by the Knudsen number, requires the use of modified boundary conditions in the governing equations.

Velocity profile across XY plane in the Microchannel

A formula that incorporates the effects of slip for the variations in velocity. This velocity profile is applicable for compressible fluid slip flow through a rectangular Microchannel is generally not available, there are some analytical or semi-analytical solutions for incompressible slip flow in rectangular channels that can give you a qualitative idea.

One such form, derived by considering the slip boundary condition, modifies the no-slip solution. For a fully developed, steady, incompressible flow with first-order slip, the velocity profile can be expressed as:

$$u(x, y) = u_{max,slip} \left(1 - \left(\frac{2x}{w} \right)^2 + C_x Kn \right) \left(1 - \left(\frac{2y}{h} \right)^2 + C_y Kn \right)$$

Where:

- $u(x,y)$ is the velocity at (x,y) .
- $u_{max,slip}$ is the maximum velocity in the slip flow case (which will be different from the no-slip u_{max}).
- h and w are the height and width of the channel.
- Kn is the Knudsen number.
- C_y and C_z are constants that depend on the tangential momentum accommodation coefficient (σ_v) and are related to the slip coefficient. For firstorder slip, $C = [(2 - \sigma_v) / \sigma_v] \times (\text{factor})$. Often, for simplicity, a value around 4 is used for these constants for fully developed flow.

A widely used textbook that covers the fundamentals of microfluidics, including rarefied gas flows and slip boundary conditions. You'll likely find a discussion of slip flow velocity profiles in channels by Nam-Trung Nguyen and Steven T. Wereley [18].

Important Limitations of this Formula for our Case

Incompressible Assumption: This formula is derived assuming incompressible flow, which is not strictly valid for our case with a pressure ratio of 2.5.

Fully Developed Flow: It assumes a fully developed flow, which might not be the case in our short micro-channel.³

Simplified Slip Model: It typically uses a first-order slip boundary condition, which might not be accurate for all Knudsen numbers within the slip regime.

Influence of Compressibility on Slip: Compressibility can also affect the slip coefficient itself, which this formula doesn't explicitly account for.

What this Formula Qualitatively Tells us:

- **Non-zero velocity at the walls:** If you plug in $y=\pm h/2$ or $z=\pm w/2$, the velocity will not be zero due to the $+CKn$ terms. This represents the velocity slip.
- **Flattened profile:** The addition of the Kn terms generally leads to a less pronounced parabolic shape, indicating a flatter velocity profile. The higher the Knudsen number (and thus the slip), the flatter the profile becomes.

We can infer, while this formula offers a glimpse into how slip modifies the classic noslip velocity profile, it's crucial to remember its limitations, especially the incompressible flow assumption. For a more accurate representation of our nitrogen flow, a numerical simulation that accounts for both compressibility and slip is still the recommended approach.....

If you need to make some very rough estimates, you could potentially use this formula with a representative Knudsen number (0.053) and an assumed slip coefficient (which depends on the gas-surface interaction, often around 0.8-0.9 for common engineering surfaces). However, the numerical values you get should be treated with significant caution due to the neglected compressibility effects.

To summarize what we did till now for doing SITA simulations

For doing our SITA simulations, now we found inlet velocity and velocity distribution across the cross section. These are in addition to composition of commercially available 95% pure Nitrogen, its constituent other molecules like O_2 were discussed in section 3.2.1. Their molecular weights were discussed 3.2.2. Basis of quadrant wise assumed distribution of molecules was given in section 5.0. XYZ coordinates of all the 133 molecules are simulated. Their velocity distribution was also simulated. At this starting point only Z velocity of molecules will come. During the simulation process XY velocities also will be calculated for each molecule.

WE calculated the mass flow rate by different methods in 7.0. We gave all the derivation steps in different methods. Fully developed isothermal compressible slip flow and its derivation starting from Navier-Stokes equations can be found in section 7.1.6. Here we can see governing equations starting from Navier-Stokes equation. Define slip boundary conditions and integrating with Navier-Stokes equation. And finally find mass flow rate and calculate numerically as $2.36 \times 10^{-10} \text{ kg/s}$ approximately. Neeraj et al gave mass flow rate ($1.24 \times 10^{-10} \text{ kg/s}$) is found to compare very well with that obtained from the analytical formulation [42] ($1.26 \times 10^{-10} \text{ kg/s}$). We discussed this in section 7.2.1. In section 7.2.2. Second Approach gives $9 \times 10^{-14} \text{ kg/s}$. 7.2.3. Third Approach gives $3.55 \times 10^{-16} \text{ kg/s}$. Why so much variation?

For calculating XYZ velocities we use equations given in section 8.0. We assume flow is Z direction. In section 7.2.3. Third Approach of mass flow we found Inlet Velocity (U_{inlet}): 77.9 m/s, Outlet Velocity (U_{outlet}): 110.6 m/s also in a simple way. Now let us see the calculated results from some more different methods to find velocities as required for our SITA simulations. In section 7.3.0. we have done 3 types of Average Velocities Calculation. In 7.3.1. Calculation of velocities of nitrogen – First Method we got a result of 0.568 m/s. In section 7.3.2.2. the Average Velocity of Gas Flow found to be $2.93502 \times 10^{-19} \text{ m/s}$. In 7.3.3. we see Calculation of average velocity by a third method is as Velocity at the Inlet: $U_{\text{inlet}} \approx 77.9 \text{ m/s}$ Velocity at the Outlet: $U_{\text{outlet}} \approx 110.6 \text{ m/s}$. We can find all these are different.

We tried differential equations in section 7.4.0. and named it as General Approach with differential equations. For numerical simulations this method is generally used. This we can see in section 7.4.1.1. Governing Equations.

We discussed boundary conditions in section 7.4.2. We did not try for Numerical solution in section 7.5.0. We gave only procedure.

Niraj et al did Direct Simulation Monte Carlo Method or The DSMC technique in their paper. We did a different simulation called SITA simulation. That is the main difference.

A very rough estimate for the average velocity across the channel, considering a significant pressure drop and some rarefaction, might be in the range of 100 - 300 m/s. If the velocity profile is somewhat blunted due to slip, the $U_{\max, \text{slip}}$ might be 1.2 to 1.5 times the average velocity in that local cross-section. Therefore, for the maximum velocity ($u_{\max, \text{slip}}$) in some cross-section, a very loose estimate could be 110 m/s to 450 m/s, with the higher end of the range likely occurring near the outlet at the channel centerline.

Hence by seeing all these we will take after few other considerations like slip

$$U_{\max, \text{slip}} = 253.5 \text{ m/s}$$

Final procedure for doing SITA simulations:

Make slice widths as:

1st SLICE = 2 nano meters Z positive = 0 to 2 nano m = 0 to 2.0E-8 m

2nd SLICE = 398 n m Z positive = 2 to 398 nano m = 2.0E-8 m to 400.0E-8 m

3th SLICE = 600 nano meters Z positive = 400 to 1000 nano m = 400.0E-8 m to 1000.0E-8 m

4th SLICE = 600 nano meters Z positive = 1000 to 1600 nano m = 1000.0E-8 to 1600.0E-8 m

5th SLICE = 398 nano meters Z positive = 1600 to 1998 nano m = 1600.0 to 1998.0E-8 m

6th SLICE = 2 nano meters Z positive = 1998 to 2000 nano m = 1998.0E-8 to 2000.0E-8 m

Total = 2000 nano meters

Final Procedure

We remade this file Vak Niraj Nitrogen.xls from scratch, after this laptop disaster of hard-disk failure and repaired by putting new hard-disk & new battery about three months back. Last one-year hard work could not be retrieved.

We came to this stage after rebuilding whole work. Let us give iterations first today.

This SITA simulation was for a microchannel of total length 2 micro meters. We have to take a slice with different lengths as shown above. Calculate outgoing velocities from that slice. Do Sita Simulations, Inter molecular Hits, Boundary hits for every slice separately.

Then take next slice convert the out-going velocities of previous slice as incoming velocities for that slice. Make 5 iterations with that to stabilize in that situation.

Again, check out going velocities.

Then take next slice convert the out-going velocities of previous slice as incoming velocities for that slice. Make 3 iterations with that to stabilize in that situation.

Again, check out going velocities

Continue this cycle for a total of 6 slices (as shown above) to complete the length of 2 micro meters

Observations and Results

The following are tables (Table 2 to 5) showing output of SITA simulations of typical atoms or molecules. Here u_x , u_y & u_z show velocities; and s_x , s_y & s_z show positions with respect to central line of micro-channel in x, y & z axes. Velocities are in meters per second & positions are in meters. Here in Table 2 to Table 5 we are showing 4-digits accuracy only. We find that the variations are visible after 9-digits in x & y axes. We are giving one sample in Table 6, which is nothing but Table 2 with 10-digit accuracy. In z-axis atoms and molecules move fast so displacements are high; and z axis is having a pressure difference.

The first column in Table 2 gives slice number. The same is to be repeated in every table; but we did not repeat this column in every table, as it is well understood.

Coming to velocities, u_x Velocities increased after 12th digit slightly. The velocity u_y decreased after 9th digit slightly. The main u_z velocity was constant even at 13 digits. All these we are talking about atoms of element Argon.

Slice	Table 2: Output of SITA simulations for Argon					
No	u_x	u_y	u_z	s_x	s_y	s_z
1	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	7.53E-03
2	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	1.76E-02
3	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	2.76E-02
4	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	3.77E-02
5	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	4.77E-02
6	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	5.52E-02

Table 3: Output of SITA simulations for Nitrogen						
No	u_x	u_y	u_z	s_x	s_y	s_z
1	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	7.53E-03
2	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	1.76E-02
3	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	2.76E-02
4	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	3.77E-02
5	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	4.77E-02
6	2.36E-16	8.60E-17	2.51E+02	1.01E-07	4.65E-08	5.52E-02

Table 4: Output of SITA simulations for Carbon di oxide						
u_x	u_y	u_z	s_x	s_y	s_z	s_z
8.4858E-17	5.6438E-17	2.0928E+02	8.1238E-07	1.7154E-07	6.2784E-03	7.53E-03
8.4858E-17	5.6438E-17	2.0928E+02	8.1238E-07	1.7154E-07	1.4650E-02	1.76E-02
8.4858E-17	5.6438E-17	2.0928E+02	8.1238E-07	1.7154E-07	2.3021E-02	2.76E-02
8.4858E-17	5.6438E-17	2.0928E+02	8.1238E-07	1.7154E-07	3.1392E-02	3.77E-02
8.4858E-17	5.6438E-17	2.0928E+02	8.1238E-07	1.7154E-07	3.9763E-02	4.77E-02
8.4858E-17	5.6438E-17	2.0928E+02	8.1238E-07	1.7154E-07	4.6042E-02	5.52E-02

Table 6: Variations are visible after 9 digits

Argon	u y	u z	s x	sy	sz	sz
-1.2994E-16	5.3405E-16	2.6089E+02	7.0021E-07	1.8216E-07	7.8268E-03	7.53E-03
-1.2994E-16	5.3405E-16	2.6089E+02	7.0021E-07	1.8216E-07	1.8263E-02	1.76E-02
-1.2994E-16	5.3405E-16	2.6089E+02	7.0021E-07	1.8216E-07	2.8698E-02	2.76E-02
-1.2994E-16	5.3405E-16	2.6089E+02	7.0021E-07	1.8216E-07	3.9134E-02	3.77E-02
-1.2994E-16	5.3405E-16	2.6089E+02	7.0021E-07	1.8216E-07	4.9570E-02	4.77E-02
-1.2994E-16	5.3405E-16	2.6089E+02	7.0021E-07	1.8216E-07	5.7397E-02	5.52E-02

Table 5: Output of SITA simulations for Oxygen

u x	u y	u z	s x	sy	sz
2.36199078995 2E-16	8.60125099502 9E-17	2.510439798137 E+02	1.01201063393 1E-07	4.64826611483 3E-08	7.53133640119 3E-03
2.36199078995 4E-16	8.60125099486 9E-17	2.510439798137 E+02	1.01201063393 1E-07	4.64826611483 4E-08	1.75730955937 4E-02
2.36199078995 4E-16	8.60125099482 1E-17	2.510439798137 E+02	1.01201063393 1E-07	4.64826611483 4E-08	2.76148547862 9E-02
2.36199078995 4E-16	8.60125099480 3E-17	2.510439798137 E+02	1.01201063393 1E-07	4.64826611483 5E-08	3.76566139788 4E-02
2.36199078995 5E-16	8.60125099479 5E-17	2.510439798137 E+02	1.01201063393 1E-07	4.64826611483 5E-08	4.76983731713 9E-02
2.36199078995 5E-16	8.60125099479 1E-17	2.510439798137 E+02	1.01201063393 1E-07	4.64826611483 5E-08	5.52296925658 0E-02

Flow output is coming three dimensionally in all XYZ axes. Though the other two axes is small flow but exists.

One important observation is flow is MOSTLY near the walls. Mainly because the molecules are hitting the walls and bouncing with good enough inter molecular hits. Every molecule hit the wall. We also checked by clearing all the hits from the simulation for the next slot or box. Then also it confirmed above result that the flow is mostly near the box walls.

These can be experimentally verified with some right facilities.

In a new experiment to study above phenomena (BoxHits), in every iteration in that series of files, given the range BoxHits area was cleared manually before the start of that iteration. In the first slice only three HITS were observed. Later in the other four slices all the molecules HIT the walls of the slice. Five continuous iterations on the start file and compared TOTAL displacement in set of 5 different Excel files did not change and got the same result.

Various results with SITA

Average Velocity

From the following file and directory given below and the addresses noted given below we copied and gave the three axes average velocities from SITA simulations Dir....

D:\Vak NanoBio\Navier-Stokes\Temperature\Vak Micro channel\Slice
File

Vak support for paper MicroC FM SITA Boundary.xls

Average velocity x axis (BE141) = 1.55906×10^{-17} m/s

Average velocity y axis (BF141) = -1.50426×10^{-17} m/s

Average velocity z axis (BG141) = 199.9165997 m/s

10.2.2. Mass flow rate:

Inlet density of nitrogen is approximately 2.808 kg/m^3 from sec 7.1.2.1.

Outlet density of nitrogen is approximately 1.123 kg/m^3 from sec 7.1.2.2

Average density (ρ_{avg}) = $(2.808 + 1.123)/2 \approx 1.966 \text{ kg/m}^3$ from sec 7.1.6.5 Now, estimate mass flow rate:

$\dot{m} = \rho_{avg} \times u_{avg} \times A$

Taking velocities from

$\dot{m} \approx (1.966 \text{ kg/m}^3 \times 199.9165997 \text{ m/s} \times 0.8 \times 10^{-12} \text{ m}^2) +$

$(1.966 \text{ kg/m}^3 \times 1.55906 \times 10^{-17} \text{ m/s} \times 0.8 \times 10^{-12} \text{ m}^2) -$

$(1.966 \text{ kg/m}^3 \times -1.50426 \times 10^{-17} \text{ m/s} \times 0.8 \times 10^{-12} \text{ m}^2)$

$\approx 314.56 \times 10^{-12} \text{ kg/s}$ $\dot{m} \approx 314.56 \times 10^{-10} \text{ kg/s}$

(See section 7.1.6.4: Mass Flow Rate Calculation)

Future Plans

In a similar way we can develop the flow patterns of individual molecules for the divergent, convergent, oddly shaped micro channels. The programming is easy and there are no TIDIOUS programming and large computer requirements.

Error values are very less. There is no requirement of an error function. Normally 16digit accuracy we can get. Anybody and Everybody can repeat these. All programming was successfully done using Macros in Excel which is easily available with any PC.

Advantages of Using Nitrogen gas

- **Maintaining Food Freshness:**
Nitrogen is used in food packaging to displace oxygen, which can cause spoilage, rancidity, and nutrient loss. Even small amounts of oxygen can negatively impact the shelf life of certain products.
- **Preventing Microbial Growth:**
Nitrogen helps to create an oxygen-deprived environment that inhibits the growth of aerobic bacteria and molds.
- **Protecting Product Quality:**
By reducing oxygen levels, nitrogen helps to preserve the quality, flavor, and texture of packaged foods.

Advantages of Using Dynamic Universe Model:

- We introduce and tried to solve this problem using our Dynamic Universe Model's SITA solution. Initial formulation and adaptation of SITA equations, was a big and complex problem. In between another problem came. My laptop's hard disk burned and failed. First author was to replace it with a new SSD drive. All the data for one year was lost. Unfortunately, backups were not taken by me. Many things were forgotten by the first author and others. Everything was to be started from scratch.
- Boundary conditions are not required in this SITA simulation; Dynamic universe model gives unique solution as it was a n-body problem solution. Multiple solutions are not possible in this type of solution.
- It solves complex problems with complex partial differential equations with almost infinite solutions. It solved many such problems in many branches of Physics and engineering. Here we start from fundamentals, so automatically the complex partial differential equations were taken care of.
- May be this is a better solution as we calculate at molecular level.

- We considered molecular wall hitting's; and inter-molecular hitting's in the flow. These are considered and calculated.
- Individual molecules velocities are found.
- The molecular paths can be traced.
- Any complex shape of the Microchannel can be analyzed.

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