STUDY OF FLOW IN MICRO-CHANNELS USING DSMC APPROACH

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AHMEDABAD-382481

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Major Project Report

Submitted in partial fulfillment of the requirements

For the Degree of

Master of Technology in Mechanical Engineering (Thermal Engineering)

By

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Guided By

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MAY 2014

Declaration

This is to certify that

1. The thesis comprises my original work towards the degree of Master of Technology in Mechanical Engineering (Thermal Engineering) at Nirma University and has not been submitted elsewhere for a degree or diploma.

2. Due acknowledgement has been made in the text to all other material used.

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Undertaking for Originality of the Work

I,Jalpan Y. Dave, Roll. No. 12MMET32, give undertaking that the Major Project entitled "**STUDY OF FLOW IN MICRO-CHANNELS USING DSMC APPROACH** " submitted by me, towards the partial fulfillment of the requirements for the degree of Master of Technology in Mechanical Engineering (Thermal) of Nirma University, Ahmedabad, is the original work carried out by me and I give assurance that no attempt of plagiarism has been made. I understand that in the event of any similarity found subsequently with any published work or any dissertation work elsewhere; it will result in severe disciplinary action.

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Place: Nirma University, Ahmedabad.

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(Signature of Guide)

Certificate

This is to certify that the Major Project Report entitled " **Study of flow in micro channels using DSMC approach**" submitted by **Mr. Jalpan Y Dave (12MMET32)**, towards the partial fulfillment of the requirements for the award of Degree of **Master of Technology in Mechanical Engineering (Thermal Engineering)** of Institute of Technology, Nirma University, Ahmadabad is the record of work carried out by him under our supervision and guidance. In our opinion, the submitted work has reached a level required for being accepted for examination.The result embodied in this major project, to the best of our knowledge, has not been submitted to any other University or Institution for award of any degree.

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As the time marches,opportunities arise,obligated to the time for opportunity.

JALPAN Y.DAVE

Abstract

The recent advancements in the technology which has the obvious direction towards the miniaturization of electronics devices has led many researches and also has opened many branches towards such technologies.The usage of MEMS is the essential part of the recent chunk which has acquired by human intellgence.The MEMS are per say miniature version of the battery cells which has the dimensions in microns and inside the MEMS device there are many micro channels in which the fluid flaw must be studied in order to achieve better performance.

Keeping that in mind,here we have taken a 2D rectangular geometry which is the typical channel shape in most MEMS like MOSFET and others.The flow inside that channel is studying with certain assumptions and boundary condtitions and some pre-requisites as well.The reference fluid here taken is Argon(Ar) and the temperature is taken at 300k and adiabatic conditions are assumed.

The different parameters are varied according to the requirement of the study and different juxtapose of parameters has been used .We have varied Aspect ratio of a channel,different knudsen numbers,different TMAC values and studied the effect on the macroscopic quantities like velocity,pressure and temperature.

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Nomenclature

MEMS	=	Micro Electro Mechanical Syestems
DSMC	=	Drect Simulation Monte Carlo
ρ	=	Density (kg/m^3)
P	=	Pressure (Pa)
μ	=	Viscosity (kg/m.s)
CFD	=	Computation of Fluid Dynamics
λ	=	Mean Free Path(μm)
VHS	=	Variable Hard Sphere
VSS	=	Variable Soft Sphere
HS	=	Hard Sphere
GHS	=	Generelized Hard Sphere
L-B	=	Lattice-Boltzmann
MOSFET	=	Metal Oxide Semi conductor Field Effect Transistor
L	=	Characteristic Length
r	=	Space co ordinate
p	=	Momentum Co ordinate
$\triangle P$	=	Pressure Drop(Pa)
t	=	Time co ordinate(sec)
N	=	Number of Particles
NTC	=	No Time Counter
Fnum	=	Number of Simulated Particles
C_r	=	Reflected velocity of a molecule(m/s)
V_{mp}	=	Most Probable Speed of molecule(m/s)
TMAC	=	Tangential Momentum Accomodation Co-efficient
PR	=	Pressure Ratio(Pa)
AS	=	Aspect Ratio(Height:Length)
Kn	=	Knudsen Number
u_r	=	Velocity of a molecule after reflection
u_i	=	Velocity of a molecule before reflection
U_w	=	Velocity of molecule at wall
T	=	Temperature(K)
X_{new}	=	Position of a molecule after collision
X_{old}	=	Position of a molecule before collission

Chapter 1

INTRODUCTION

The objective of this chapter is to build the context to the exact problem definition as well as the methods and techniques used for simulating the flow in micro-channels and the overview of the Direct Simulation Monte Carlo Method.This chapter also contains the problem which is to be studied,the objective of the project and the outline of the report.

The classical physics which deals with the behaviour of the flow has certain assumptions regarding to the quonta of the properties.The local values are often taken as an average of the relatively small amount of qounta and the properties around the wall is taken same as the flow with no slip conditions.Now when the dimensions get smaller,the qounta gets smaller and the local value gets bigger as the qounta becomes more in proportion with the dimensions and we no longer can achieve the objective.So when there is a small dimension of a geometry as to the level of microns,or the low density flows,we assume there is a slip between the wall and the flow quantities and so that the flow behaviour can not be studied using the conventional Navier-Stoke or CFD;this is where the DSMC OR Lattice Boltzman approach or particle based methods be used.[1]

The micro-gas flows are often used in modern day devices such which are very popular for example MEMS; and the classical laws of physics can not be applied to study the behaviour of the flow as in the micro channel the continuum does not hold and the numerical tchniques such as CFD can not be applied either.Therefore,the gas flow in microchannels and micro-geometries are investigated using Direct Simulation Monte Carlo method.Direct Simulation Monte Carlo (DSMC) method uses probabilistic (Monte Carlo) simulation to solve the Boltzmann equation for finite Knudsen number fluid flows.The DSMC method was proposed by Prof. Graeme Bird, Emeritus Professor of Aeronautics, University of Sydney. DSMC is a numerical method for modeling rarefied gas flows, in which the mean free path of a molecule is of the same order (or greater) than a representative physical length scale (i.e. the Knudsen number Kn is greater than 1). In these rarefied flows, the Navier- Stokes equations can be inaccurate. The DSMC method has been extended to model continuum flows (Kn is very less than 1) and the results can be compared with Navier stokes solutions.DSMC method models fluid flows using simulation molecules which represent a large number of real molecules in a probabilistic simulation to solve the Boltzmann equation. Molecules shall be moved through a simulation of physical space in a realistic manner that is directly coupled to physical

time such that unsteady flow characteristics can be modeled.[1] Intermolecular collisions and molecule-surface collisions are calculated using probabilistic, phenomenological models. Common collision models include the Hard Sphere model, the Variable Hard Sphere (VHS) model, and the Variable Soft Sphere (VSS) model. The fundamental assumption of the DSMC method is that the molecular movement and collision phases can be decoupled over time periods that are smaller than the mean collision timeCurrently the DSMC method is being applied to the solution of flows ranging from estimation of the Space Shuttle re-entry aerodynamics, to the modeling micro-electro-mechanical systems(MEMS).In the analysis of the heat and fluid flow in a micro scales, a particular type of theoretical method should be chosen depending on the range of Knudsen number, Kn, because the molecular characteristics of the flow become more vulnerable as the characteristic length L becomes smaller as compared with the mean free path.In slip flow,analysis based on the momentum and energy conservation equation for slip flow, analysis based on the momentum and energy conservation equations are still valid as long as such rarefaction effects as velocity slip and temperature jump are included. The conventional boundary conditions containing these phenomena are usually referred to as the Maxwell/Smoluchowski relations. Therefore,it is absolutely necessary to investigate the reliability of these relations before performing the continuum-based analysis using conservation equations. The continuum-based approach is no longer valid in the transition flow because of the stronger molecular characteristics of the flow. In this case, the direct simulation Monte Carlo (DSMC) can be a good alternative. Moreover, the DSMC can be applied to all types of flows. For this reason, an attempt to analyze the micro flow by employing the DSMC is quite popular now.

1.1 MEMS an overview:

The Micro Electro Mechanical Systems are the "it" technology of today's electronics as well as the automation industries.They are also referred as micro machines in Japan.They are separate from molecular mechanics or molecular elctronics,for the change they are as real as they get.Now the motivation of the present study lies somewhere in the global interest and upwind towards the MEMS and for the better understanding of the thesis one should understand the significance of those and their working.MEMS are made up of components between 1 to 100 micrometers in size and mems devices generally range in size from 20 micrometers to a millimitre.They usually consist of a central unit that processes data and several components components that interact with the surroundings such as microsensors.MOSFET is such device which is the key part of our wireless communication systems and it is being used in all the electronics devices virtually like mobile handsets,walkie-talkies,laptops etc.

MOSFET are the micro chip which works like a miniature version of the electric cell and the flow of elcetrons from the source to the drain is controlled by the voltage applied to the gate.A positive viltage applied to the gate,attracts the electrons to the inerface between the gate dielectric and the semiconductor. The figure of the MOSFET is shown below.[2]

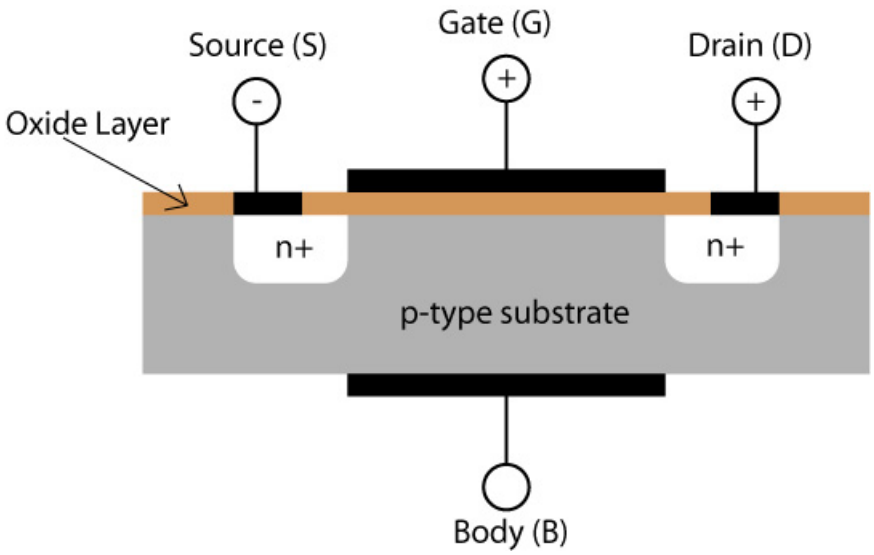


Figure 1.1: The MOSFET Chip[2]

the channels shown in the figure are typically of the scale of micro meters and the flow inside these channels can be studied for the further modification and better effectiveness.

1.2 Significance of the Knudsen Number(Kn):

The study of the flow in very small channels for the purpose of elucidating rarefied phenomena is not unheard of. In 1909 Knudsen carried out some experiments using micro cappilarries and studied the flow regimes from continuum to free molecular flow and introduced the significance of the ratio of mean free path to characteristic dimension, now known as the Knudsen number (Kn)

$$Kn = \frac{\lambda}{L} \tag{1.1}$$

This knudsen number signifies the range which can help us analyse the flow patterns using the knudsen number as the parameter.[4]

Table 1.1: The Knudsen number [4]

Knudsen Number	Type of flow	Solution Methods
Kn$\longrightarrow 0$	Inviscid FLow	Euler Equation
Kn$\leq 10^{-3}$	continuum flow	Euler/Navier Stokes Equations
$10^{-3} \leq$Kn$\leq 10^{-1}$	Slip Regime	Boltzmann Equation/DSMC method
$10^{-1} \leq$Kn≤ 10	Transition Flow	DSMC/L-B Method
Kn $\geq$1	Free Molecular Flow	DSMC/Modified DSMC/L-B Method

1.3 Boltzmann Generic Equation:

In physics,specially in non-equillibrium statistical mechanics,the Boltzmann transport equation describes the statistical behaviour of thermodynamic system.It was devised by Ludwig Boltzmann in 1872.The

equation arises not by statistical analysis but of all the individual positions and momenta of each molecule in the fluid by considering the probability that a number of particles all occupy a very small region of the space and denotes the change in quantity at a very small instant of time. [3][3]

The set of all possible positions r and momenta p is called the phase space of the system,i,e three co ordinates for each position co ordinate x,y,z and three more for each momentum component p_x,p_y,p_z.The entire space is 6 dimensional,a point in space is (r,p)=(x,y,z,p_x,p_y,p_z) and each co ordinate is parameterized by time t.The small volume is written d^3rd^3p=dxdydzdp_xdp_ydp_z.Since the probability of N molecules which all have r and p within d^3rd^3p is in question, at the heart of the equation is a quantity f which gives this probability per unit phase-space volume, or probability per unit length cubed per unit momentum cubed, at an instant of time t. This is a probability density function: f(r, p, t), defined so that[3][5],

$$dN = f(r, p, t)d^3rd^3p \tag{1.2}$$

which is the number of molecules which all have positions lying within a volume element d3r about r and momenta lying within a momentum space element d3p about p, at time t. Integrating over a region of position space and momentum space gives the total number of particles which have positions and momenta in that region:

$$N = \int_{positions} d^3r \int_{momenta} d^3pf(r, p, t) = \int\int_{positions} \int\int\int_{momenta} \int f(x, y, z, p_x, p_y, p_z, t)dxdydzdp_xdp_ydp_z \tag{1.3}$$

which is a 6-fold integral. While f is associated with a number of particles, the phase space is for one-particle (not all of them, which is usually the case with deterministic many-body systems), since only one r and p is in question. It is not part of the analysis to use r_1, p_1 for particle 1, r_2, p_2 for particle 2, etc. up to r_N, p_N for particle N.It is assumed the particles in the system are identical (so each has an identical mass m). For a mixture of more than one chemical species, one distribution is needed for each which is not discussed as we are using monoatomic gases only.

1.4 Lattice-Boltzman Method:

Lattice-Boltzmann method has been applied to many fluid flow problems and was proven to serve as a CFD tool alternative to the methods that solve Navier-Stokes equations such as Finite Volume, Finite Element and Finite Difference methods.LBM has the advantage to handle simulations with arbitrary complexed geometries like as flow through porous media, ocean modeling etc. The governing equation is a simplified Boltzmann equation and due to the intrinsic kinetic nature of LBM, it can be used in microscale flow simulations where knundsen number is greater than zero.[6][6]

1.5 Direct Simulation Monte-Carlo Method:

The DSMC method is a technique for the computer modeling of a real gas flow by simulated molecules whose number has ranged from the order of hundreds in early calculations to millions in some contemporary simulations. The DSMC method employs simulated molecules of correct physical size and their number is reduced to a manageable level by regarding each simulated molecule as representing a fixed number of real molecules. This is typically a large number and advantage can sometimes be taken of its

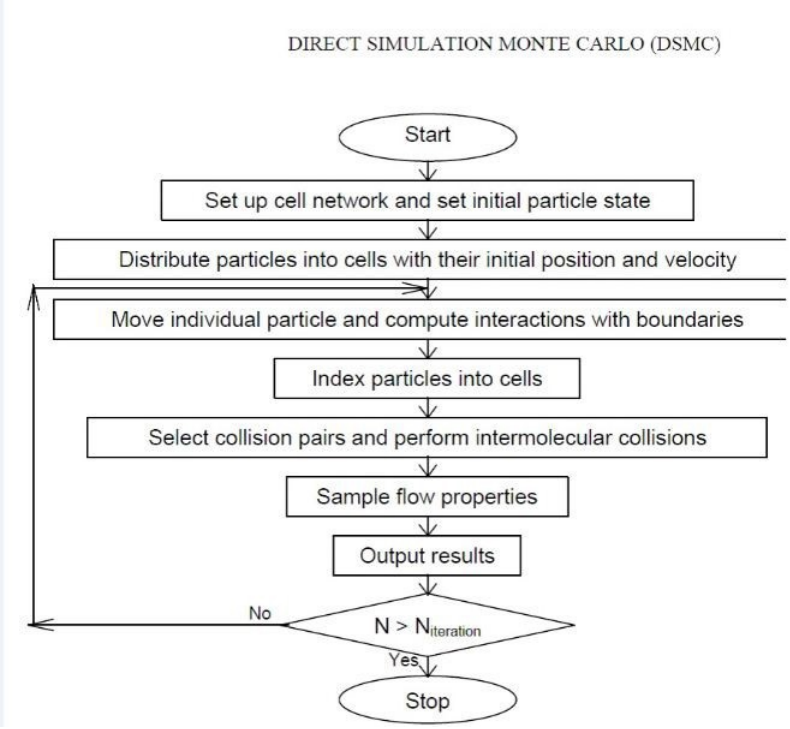


Figure 1.2: Flow chart of DSMC algorithm
[6][5]

size to specify some properties through a distribution of values instead of a single value for each simulated molecule. The velocity components, position coordinates and internal states of simulated molecules are stored in the computer and are modified with time, as the molecules are concurrently followed through representative collisions and boundary interactions in simulated physical space. The velocityspace information is contained in the positions and velocities of simulated molecules. These positions and velocities are continuously distributed and the velocity-space is unbounded.The conservation of mass, momentum, and energy are imposed to within the round-off error of the compiler.[6][5]

The process of DSMC follows the above flowchart.A computational cell network which represents the physical space is first set up for the requirement of the selection of collision and the sampling of flow properties. The initial states of the gas such as vacuum and uniform equilibrium flow are prescribed. After the position and velocity of each particle is set, the method proceeds the iteration: (1) given a time step Dt, particles along their trajectories are displaced and interactions with boundary are calculated as they occur; (2) particles are sorted and their cell locations are rear- ranged; (3) collision pairs are selected and intermolecular collisions are performed on a probabilistic basis; (4) flow properties such as velocity, temperature, are obtained by sampling the microscopic state of particles in each cell. The computational approximations associated with DSMC method are the ratio of the number of simulated molecules to the number of real molecules, the time step over which the molecular motion and collisions are uncoupled, and the finite cell and sub-cell sizes in physical space. The fundamental requirements are that the linear dimensions of the cells should be small in comparison with the scale length of the macroscopic flow gradients in the streamwise direction, which generally means that the cell dimensions should be of the order of the local mean free path, and the time step should be much less than the local mean collision time. Theoretically, the DSMC becomes more exact when the cell size and the time step tend to zero.[5]

So,lest we can say that the process mainly follows 4 steps:

1. Move the partical into specifed grid
2. Index and cross reference the particles
3. Simulate the collisions
4. Sample the flow field

Step:1 In the first process, all the molecules are moved through distances appropriate to their velocity components and the discrete time-step. Appropriate action is taken if the molecule crosses boundaries representing solid surfaces, lines or surfaces of symmetry, or the outer boundary of the flow. As for the boundary conditions, the microscopic boundary conditions are specified by the behaviour of the individual molecules according to the conservation laws, rather than in terms of the distribution function. Collisions with surfaces can be treated as being either fully specular, fully diffuse, or some combinations of the two.

Step: 2 For every molecule, the index of cell to which the molecule belongs is calculated (indexing of molecules).At a time step, only collisions between molecules belonging to the same cell are taken into account. Every collision is considered as a random event occurring with some probability of collisionIn every cell, pairs of colliding molecules are randomly sampled (collision sampling in a cell). For every pair of colliding molecules, pre-collisional velocities are replaced by their post-collisional values The second DSMC process involves indexing and tracking the particles. A scheme for molecular referencing is the prerequisite for the next two steps: modeling the collisions and sampling the flow field

Step 3: The third step, simulating the collisions, is a probabilistic process that sets DSMC apart from deterministic simulation methods such as molecular dynamics. The probability of a collision between two molecules in a homogenous gas is proportional to the product of their relative speed and total collision cross-section. The mean value of the product is calculated for each cell, and the maximum value is also recorded. The collision pairs could then be chosen by the acceptance-rejection method; the probability of a particular pair being chosen depends on the ratio of their product to the maximum product. However, this procedure would have a computation time directly proportional to the square of the total number of molecules in the cell. So the no-time-counter technique was introduce in order to obtain a computation time directly proportional to the number of molecules. When used in conjunction with the subcell technique, it ensures that collisions occur only between near neighbours and thereby improves the accuracy of the simulations. An appropriate number of representative collisions between randomly selected pairs of molecules within each cell is simulated .

Step 4: Final process is sampling the macroscopic flow properties. The spatial coordinates and velocity components of molecules in a particular cell are used to calculate macroscopic quantities at the geometric centre of the cell.

The DSMC procedure is explicit and time marching and it always produces a flow simulation that is unsteady. For an unsteady flow application, an ensemble of many computations may be assembled and averaged to obtain final results with an acceptable statistical accuracy. To simulate a steady problem, each independent computation proceeds until a steady flow is established at a sufficiently large time, and the desired steady result is time average of all values calculated after reaching the steady state. As a steady flow gets developed through a physically real unsteady flow, there are minimal problems with boundary conditions. There is no need for an initial estimate of the flow-field and there is no artificial iteration process. The DSMC, rather than solving an average description of macroscopic flow properties

represented by partial differential equations, deals with gas flows at a molecular level. This allows the inclusion of chemical reactions and non equilibrium effects into the methodology in a direct and physical manner. This has made the DSMC technique a very popular methodology for the simulation of flows when the continuum holds off.[1]

1.5.1 Random Numbers:

As its name implies, Direct Simulation Monte Carlo uses random numbers. Unlike other Monte Carlo schemes, such as Metropolis MC or Quantum MC, DSMC uses a wide variety of probability distributions for different purposes. For example, to initialize particles in a volume we might first determine the number of particles to be inserted by choosing the value from a Poisson's distribution. If the particles are distributed uniformly then their coordinates are generated from the uniform distribution; their velocity components are usually generated from the Maxwell-Boltzmann distribution, which is equivalent to a normal or Guassian distribution. As described below, at various stages of the [processes like advection and collision processes more random variables are used from various distributions. Given the importance of the Monte Carlo elements in DSMC it is essential to use a high-quality random number generator. Simple generators that were adequate a decade ago are obsolete today because, with increased computer power, modern DSMC calculations can cycle throughout the entire period of a simple generation in a matter of seconds. Although DSMC generates random values from a variety of distributions, the program only needs one generator that produces the uniform distribution in (0,1); all other distributions are obtained by transformation (usually inversion of the cumulative distribution) or iteration (typically an acceptance / rejection scheme). There are several modern generators for the uniform distribution to choose from; the author's current favourite is the Mersenne Twister. One final note regarding the use of random number generators: for the purpose of debugging the initial state (or seed) should be recorded so that a calculation that fails can be repeated exactly.[6]

1.5.2 Boundary Condition:

Once the particles have been initialized the DSMC calculation advances in the time steps Δtalternating between ballistic motion of the particlesand collision amongst the particles. Typically the particles simply are displaced by a distance$\triangle r = v\triangle t$ but if there is a body force, such as gravity, then the motion is slightly more complicated. The particles move without interaction and can even overlap; the only place in DSMC where the particles' cross-section is used is in determining the collision rate. For transient flows, on the first time step one should use $\frac{1}{2}\triangle t$ (Strang splitting) to maintain temporal accuracy. If measuring non-conserved variables (e.g., fluxes) then one should also time-center the sampling (half move, sample, half move, collisions) for all steps.

During their motion some of the particles will reach boundaries, either at the periphery of the computational domain or at the surfaces of objects within the domain. One of the strengths of DSMC is the ease with which boundary conditions may be imposed. For periodic boundaries a particle crosses one boundary and re-enters at the periodic mirror boundary. For specular boundaries a particle reflects off the surface with the perpendicular component of velocity reversed. nflow/outflow boundary conditions are commonly treated as a reservoir with given density, fluid velocity, temperature. Particles in the main system are removed if they cross the boundary into the reservoir. Particles are injected from reservoir to main system by either: Surface generator - From the number flux determine number to be injected during a time step and then generate particle velocities from surface distribution (e.g., inflow Maxwellian); Volume generator

- Fill a "ghost cell" with particles before the ballistic move and discard any that do not cross the boundary into the main system during the move phase. Efficient schemes are available for both types of generators. [13]

1.5.3 Collision Selection:

To evaluate collisions the domain is partitioned into cells and the particles are sorted into them; the algorithm then loops over cells evaluating collisions independently in each cell. A maximum collision rate, R_{max} is calculated in each cell based on the number of particles, the cell volume, the collisional cross-section for the particles, and the (estimated) maximum relative speed. The explicit form for this function depends on the interaction potential; for example.[13]

Once a pair is accepted for a collision all that remains is the calculation of the particles' post-collision velocities (if there are also internal degrees of freedom or chemistry then there are addition steps). By conservation of momentum the center-of-mass velocity is constant; for particles of equal mass, conservation of energy implies that the magnitude of the relative velocity is unchanged. These constraints fix four of the six unknowns; the remaining two are set by the direction angle for the relative velocity. Because DSMC does not use the actual particle trajectories to evaluate collisions this direction angle is selected at random. For hard-sphere collisions the direction angle is chosen as uniformly distributed in the unique pattern.[13]

1.5.4 DSMC-A global application:

The direct simulation Monte Carlo method (DSMC) has grown for more than 40 years into a powerful analysis tool for computation of kinetic nonequilibrium hypersonic types of entry flows inside a geometry. The heart of the technique is its detailing in the treatment of collisional phenomena including relaxation of internal energy modes, chemistry, radiation, and gas-surface interaction. Assessment of the DSMC technique for hypersonic flows using ground-based experimental measurements has been limited to conditions without chemistry due to the technical challenges of generating high-energy, rarefied flows. The DSMC method has been validated by using flight simulation data for slender bodied vehicles based on measurements of radiation emission and plasma density. The DSMC technique has also been applied to analyze the entry into Earths atmosphere of several different blunt body configurations including comparisons with flight measurements for the Space Shuttle, space station Mir and Stardust. The DSMC technique generally provides excellent comparisons done with most of the measured data sets. The confidence obtained in the physical accuracy of the DSMC method has led to its application to analyze the aerothermodynamic performance of proposed vehicles such as ballutes and to aid in the design of entry flight sided experiments. The DSMC technique has played a key role in the design and flight analysis of several NASA Mars entry missions including the entry of Pathfinder and the aerobraking of Mars Global Surveyor. Further notable applications of the DSMC technique to planetary entries include analysis of the aerobraking maneuver of the Magellan spacecraft in the atmosphere of Venus, and entry into Jupiter of the Galileo probe. [13]

1.6 Definition of Problem:

In this problem we have a simple geometry in the scale of micro measurements.This geometry has been created with the help of some graphical softwares,then the exact emulation of the process and the geometrical conditions are implemented.The assumption to be made is that the geometry is perfectly finished

and in 2D.As we can observe that the geometry is rectangular in shape,which we can say is a symmetrical shape.

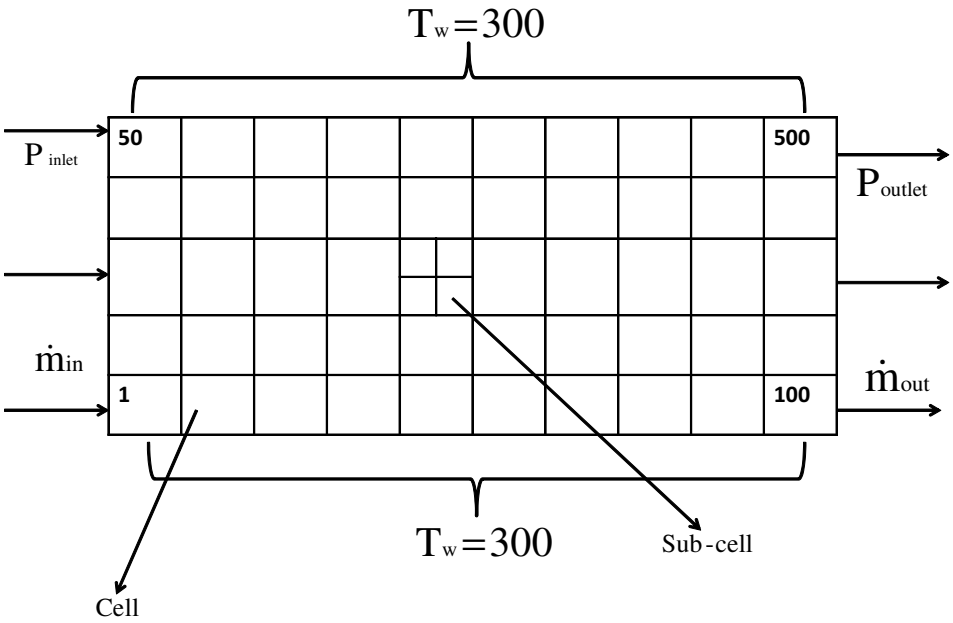


Figure 1.3: Problem line diagram

The flow inside this geometry is to be simulated with certain assumptions and given properties.In this case we have taken the Argon(Ar) as the reference fluid,we have assumed the pressure ratio as 5 and the reference height(h) of the channel as 1 μmwhich is to be constant and keeping that value constant we are varying the length of the channel(L),Pressure ratio,Knundsen number,and Tmac.After varying above parameters we are studying the effects of variance with certain quantities like,centrline pressure,velocity,temperature,mass flux etc.The objective of these parametric jumble is to achieve the definite pattern of flow quantities and identify the amount of rarefaction achieved.

1.6.1 Objective of the Project:

To analyse the flow inside the micro channels stands a greater value these days as the usage of MEMS are widening and the world has been getting used to such innovations which increases compactibility.Lest we shall analyse the diverse effects of the diiferent parameters inside a given geometry to create some basic calculations and to predict the behaviour.The main objective is to establish the behaviour of flow inside a micro channel which is rectangular shaped with different parameters jumbled and those parameters are enlisted below:

- Different aspect ratio
- Different Knudsen numbers
- Different Tmac for different Knudsen numbers

- Different pressure ratio

1.6.2 Outline of Report:

The first chapter as shown discussed about the DSMC as the abstract,the overview of the process itself and its application and the context building towards the basic outline of the DSMC method and its application.

The second chapter which is for the personal understanding and in depth understanding towards the problem,its fundamentals and such research if done in the past.The literature survey is done with this objective baring in mind and the list and summery of different literature studies has been given.Followed by the conlcuding of the survey with respect to the problem and its application.

This chapter which says the mathematical modeling and numerical techniques which includes the main mathematical formula used to analyze the problem,the basic assumptions,the flow of calculations and the logic behind the formula and the conditions regarding to the problem.

The fourth chapter carries the weight of the unique work done by the author and its conclusion and to the what extent the work is successful or has struck to a dead end.In short the summery of the work carried out followed by the conlcusion of the whole process.

Chapter 2

Literature Review

This chapter consists of the literature survey carried out for the problem solution.The survey consists the study of different research papers published,books as well as the internet resuorces,this is to enhance the horizon about the DSMC,Rarefied Gas Dynamics,Coding methods and analytical approcahes regarding to DSMC.

The literature surveyed so far can be subcategorized in three major categories.

1. Study of rarefied gas dynamics
2. The DSMC process
3. Coding methods

2.1 Study of rarefied gas dynamics:

Nobuyuki Satofuka et al[7] carried out the experiment to establish the rarefaction existance inside a MEMS(Micro Electro Mechanical Systems) even at the normal operating pressures.They used the conventional DSMC process to analyze the flow inside the channels of MEMS and as it operates between very low Mach number range and very low Reynold's number range and due to very low velocity gradients they encountered a problem and could not distinguish between very low velocity gradient and statistical noise.

Nevena Stevanovic[8] et al in their research paper "Low Mach number High Order rarefied gas flow in microchannels" contains the isothermal rarefied gas flow in micro-channels of slowly varying cross section. It is assumed that the ratio of the reference Mach number square and the reference Reynolds number is a small quantity, so that inertia can be neglected and the effect of viscosity is spread over the whole cross-section of the channel. Higher order slip boundary condition on the wall is used for the solution of governing equations. Gas rarefaction leads to increase of mass flow rate for the same inlet and outlet pressure ratio.

The book by S.A. Schaff[9] has the introduction of the dynamics of the rarefaction as well as the concerned mathematics related to that.The review of this reference was to get acquainted to the mechanics of rarefied fluids and gain some knowledge related to that.

Ibramovic G N carried[10] out severel experiments involving different rarefied gas dynamics model on jet engines and applied the gas dynamics principles of the theory of jet engines and similar systems are outlined, and the theory of one-dimensional gas streams, which forms the basis for modern approaches to the design of jet engines, rotating machines, ejectors, wind tunnels, and test stands is covered in detail. Special chapters are devoted to boundary layer theory and jet theory, and the use of these theories in the determination of the friction drag and velocity and temperature fields in nozzles, ejectors, combustion chambers, etc. Chapters dealing with hypersonic flows, rarefied gas flows, and with the elements of magnetohydrodynamics are included with a view toward space applications.

2.2 The DSMC Process:

P S.Prashanth et al.[5] conducted their study of different numerical methods including DSMC in the transition flow regime.This paper gives the overview of the basic DSMC numerical technique,its mathematical modeling ,its limitations and recent advancements in DSMC as well.The review included the computational error involving DSMC and the basic coding as well.

Bird G A [1]has authored a book "Molecular Gas Dynamics and Direct Simulation of Gas Flows"which is literally the thesaurous of the numerical methods,the molecular gas dynamics and all the basics of boltzman equation's applications,and the whole basic structure of the study.

Alejandro L Garcia[6] noted the basic theory methods for the Direct Simulation Monte Carlo (DSMC) algorithm. Some of the open challenges in the treatment of complex, multi-scale flows are also discussed. It also involves the outline about stochastic and hybrid PDE(Partial Differential Equation) solvers,their errors and limitations.

Seckin Gokaltun [11]et al. in paper "Statistical Modelling of Rarefied Gas FLows in Microchannels" compares the Lattice Boltzman method and DSMCmetohds.The Lattice Boltzmann method (LBM) and direct simulation Monte Carlo (DSMC) method are used for analysis of moderate Knudsen number phenomena. Simulation results are presented for pressure driven isothermal microchannel flow at various pressure ratios. An- alytical equations for non-linear pressure distribution and velocity profiles along the channel axis are used to verify the present LBM and DSMC results. It was concluded that the LBM method can be used as an alternative model to DSMC simulations.

J.S. Wu et[13] al did the analysis of micro scale gas flows with pressure boundaries using DSMC method.The development of a two-dimensional direct simulation Monte Carlo program for pressure boundaries using unstructured cells and its applications to typical micro-scale gas flows are described. For the molecular collision kinetics, variable hard sphere molecular model and no time counter collision sampling scheme are used, while the cell-by-cell particle tracing technique is implemented for particle movement. The applicability of the treatment of pressure boundaries using the equilibrium Maxwell/Boltzmann distribution function is discussed in terms of the magnitude of the local Knudsen number at the pressure boundary for micro-nozzles and slider air bearing applications is also discussed.

2.3 Coding Methods:

The Direct Simulation Monte Carlo method is the improvisation of the generic equation called Boltzman equation.To use it to its maximum effects one needs to understand the working of the equation and code it accordingly for more iterations.More the iterations,more fruitful the work.To hand the different coding

techniques is the pre-requisite though and hence the effort to understand the fundamentals of coding,C programming and C++ using NICE handbook for beginners.

Keith Christopher Kennenberg [13][13]worked to develop the 3D code using DSMC logic and different computational techniques.The descrete codes are yet to be studied but the logic some how was articulated and understood.

The softwares which are available on the official website of G A.Bird were acquired and the literature regarding to those were studied extensively.The softwares which were there are listed below:

1. DSMC(X)
2. DS2V (Version 2.6)
3. DS3V

- DSMC(X) is the basic 1-D code which can simulate the flow at molecular levels,low density flows,bi-atomic fluids across the basic geometries like line,sphere,wedge,cone,square and rectangle.It involves basic near neighbour collision and the meshing or cell division is done by the software itself considering the inlet pressure and density of fluid.
- DS2V is a general programme for steady or unsteady one dimensional flows.The flows may be either plane,cylinderical or spherical and the gas options range from simple monatomic molecules to chemically reacting gas mixtures.Coutte flows,shock waves,combustion of homegeneous gas etc can be studied using this software.
- DS3V is the modified version of DS2V programme,apart from all the shapes that were in DS2V,it can analyse flows inside MEMS channels,channels with bends and complicated shapes.It also comprises the ghost cell division grid which has three invisible layers and it provides better accuracy as the molecular tracking is very sophisticated and it involves new ray tracing technique as well.[12]

2.4 Conclusion of the literature review:

From the previous researches one can conclude that many techniques have been compared to DSMC method when operating in micrometer ranges,using different inlet conditions,pressure boundary conditions and geometries as well and hence the conclusively the DSMC stands out as the simplest,most effective and most accurate method to simulate the flow inside the micro channels.The geometry creation and cell division is the complicated parts of the process but it is under research also the sophisticated softwares now a days provide the default values and shapes too which makes the computation and analysis part very easy.

Chapter 3

Mathematical Modelling and Engineering Parameters:

The chapter contains the logic behind the mathematical modeling and the calculation flow of the DSMC applied over the given geometry with certain assumptions as well as pre requisites matched. Different collision models are also discussed.

The basic DSMC process just follows the Boltzmann equation as discussed before,yet the improvisations or per say the suitable boundary conditions shall apply to acquire the desired results.In present case we have used the Maxwell-Boltzmann equation which is suited for pressure boundary conditions as well as the particle flux method.We are assuming thermal equillibrium here as well as mass conservation at each pressure boundary.Note that the assumption of thermal equilibrium at the pressure boundaries may not be holding good for very high local Knudsen number flow, which can be seen clearly from the results presented here and later for specifc test cases. However, we will show that the thermal equilibrium is correct for most MEMS related subsonic flows. For completeness, the implementation of updating the pressure boundary conditions has been briefly described,for further study refer paper by tseng[5]

3.1 Flow of Calculation:

For a given mean speed (V) and temperature (T), the particle flux across a boundary surface with area A in a particular direction h with the surface normal can be determined, assuming equillibrium Maxwell-Boltzmann distribution:

$$N/A = \frac{nV_{mp}\{exp(-q)^2 + \sqrt{\pi}q[1 + erf(q)]\}}{2\sqrt{\pi}} \tag{3.1}$$

where,

$$q = \frac{V}{V_{mp}} cos\theta \tag{3.2}$$

and

$$V_{mp} = \sqrt{\frac{2KT}{m}} \tag{3.3}$$

where,m is the molecular mass, n is the number density, $V_{mp}$is the most probable speed and k is the Boltzmann Constant.

At the inflow pressure boundary, in flow pressure p_i and temperature T_i are both known and thus the in flow number density n_i is known. By applying the particle flux conservation for each cell interface m (area A_m) at the in flow pressure boundary, the updated in flow streamwise velocity at cell m (outside the flow domain) is computed as,

$$(u_i)_m = \frac{N_+ - N_-}{n_i A_m} \tag{3.4}$$

where $N_+$is the particle flux coming in to the cell m ,$N_-$is the particle flux coming out of cell m,$A_m$is the area of the cell,$n_i$is the number density inside the cell m.The value of u_{i_m} and the sampled streamwise velocity for each inflow cell m will be varied during the simulation and eventually attain approximately the same value as steady state is reached.

At the outflow pressure boundary, all fluid properties except pressure are computed from the simulation. Again, we apply the concept of particle flux conservation rather than the theory of characteristics for each cell at the outflow pressure boundary. Then, a similar procedure treating in flow conditions is carried out for updating outflow streamwise velocity ue m (outside the flow domain) for each out flow boundary cell m. Note that the outflow temperature for each cell interface is not given in advance and is set to the temperature sampled inside for each out flow boundary cell m during simulation. Additionally, the out flow number density is computed using the equation of state.

Here we have used the argon as the governing fluid inside a micro channel.The reason of choosing the monatomic gas was for the simplicity of the problem and for the less computational time as we speak and the parameters we wish to analyse.The geometry we have chosen is a simple 2 dimensional rectengular channel and for indexing the particles we will divide that geometry into number of cells.

The properties of argon is taken from the reference and listed below;

Table 3.1: Properties of Argon

[1]

Boltzmann Constant(K)	Wall Temperature(k)	Molecular Diameter(m)	Molecular mass(kg)	Kn_{inlet}
1.3806E-23	300	4.77E-10	66.32E-27	1(varied)

For the given case,this are the properties known,

now the parameters we have varied are;

- Knundsen Number
- Pressure Ratio
- Aspect Ratio
- Tmac regimes

suppose the given Kn_{inlet}=1,channel height is kept constant at $1\mu m$ and length is $5\mu m$ and the pressure ratio is 5.

$$Pressure\,Ratio = \frac{P_{inlet}}{p_{outlet}} \tag{3.5}$$

$$Kn_{inlet} = \frac{KT}{\sqrt{2}\pi d^2 L P_{inlet}} \tag{3.6}$$

As we can see,Inlet pressure and inlet knundsen number are inversly proportionated and all the quantities are constant so we can say if the pressure ratio is 5,kn_{outlet}=5 kn_{inlet}.

Now, we know Kn_{inlet}=1 and we know;

$$Kn = \frac{\lambda}{L} \tag{3.7}$$

Using equation 8,we can find out $\lambda(Mean$ free path),which will be equal to characteristic length(L) in case of kn=1.

Thus in this case,$\lambda = 1\mu m$ and we know that the size of cell must be lesser or equal to $\frac{\lambda}{3}$.

Hence,cell size=3.33E-7 in this case.

$$No\,of\,cells\,in\,direction = \frac{Length}{cellsize} \tag{3.8}$$

Similarly applicable for y direction as well.Now we will have to compute the timestep,Number Density,Number of simulated molecules.

To find out the value of time-step,we will have to compute the most probable speed of a moleculer.Which is formulated as below,

$$\nu = \sqrt{\frac{2KT}{m}} \tag{3.9}$$

with comes out as 1118.3717m/s with kn_{inlet}=1.

Now,Time step calculation is very essential for the simulation as we have to make sure that value of time step must not exceed the size of cell.

$$Time\,step = \frac{height}{most\,probable\,speed} \tag{3.10}$$

To find out the number density,

$$P_{inlet}=nKT \tag{3.11}$$

P_{inlet},K,T are known and thus we can calculate the value of n.

Which eventually will give the value of number of simulated molecules as

$$F_{num} = \frac{n}{cell\,volume} \tag{3.12}$$

The total number of cells will also be known as we know both num of cells in x dir as well as y dir.

$$Total\,number\,of\,cells = no.of cells\,in\,X\,direction \times no.of\,cells\,in\,Y\,direction \tag{3.13}$$

and

$$Total\,number\,of\,subcells = 4 \times total\,number\,of\,cells \tag{3.14}$$

For different knundsen number regimes,the values of above mentioned properties are listed below:

Table 3.2: Table of properties with different kn_{inlet}

Property	$Kn_{inlet} = 0.1$	$Kn_{inlet} = 1$	Kn_{inlet}=10
P_{inlet}(Pa)	53610.7821406113	5361.0782140611	536.1078214061
P_{outlet}(Pa)	10722.1564281223	1072.2156428122	107.2215642812
Number density(mols/volume)	2.58E24	2.58E23	2.58E22
Mean free path(m)	1.00E-07	1.00E-6	1.00E-5
cell width(m)	3.33E-08	3.33E-07	3.33E-06
No. of cells in X dir^n	2400	240	24
No. of cells in Y dir^n	30	3	1
Actual cells in X dir^n	800	100	100
Actual cells in Y dir^n	30	20	20
Actual cell length(m)	1.00E-07	8.00E-07	8.00E-08
Actual cell width(m)	3.33E-08	5.00E-08	5.00E-08
Fnum	431461217.67	517753461.20	51775346.12
Most Probable Speed(m/s)	353.470	353.470	353.470
Timestep(sec)	3.14343652443297E-011	1.4899379584746E-011	4.715154786649E-011
Total No of cells	24000	2000	2000
Total number of subcells	96000	8000	8000
Total SImulated Molecules	5760000	400000	400000

As shown in the table and previously mentioned formula,we can calculate different properties.

Now the question remains as to why the parameters has been changed? and if changed then how the calculations have been made.As mentioned above we know that 4 types of different parameters were changed for study ;knowingly the knundsen number regime,Tmac regime,aspect ratio regime and pressure ratio regime.

1. For different knundsen numbers the calculations shall be made using above equations.We know inlet knundsen number,temperature of wall,Boltzmann constant and so properties.

2. For different aspect ratio,we take different lengths of channels,which in this case is kept 10,40,80 and different knundsen numbered regimes as well.Aspect ratio 2 means the length of the channel is 2 times more than height,5 means it is 5 times more.The difference in length will acount for more number of cells,which means alteration in timesteps,total simulated particles and that will impact upon the behaviour of flow as well.That is discussed later in chapter 4 results and discussion.

3. As the Maxwell postulated that when molecules strike a surface some percentage of those rebound from the surface without transferring any of their streamwise momentum while others transfer all of their momentum and the ratio of the number of molecules rebounding without any streamwise momentum exchange to those that transfer all of their momentum is a physical characteristic based on surface and gas properties. In order to capture this effect in his analysis, the results of which are given above, Maxwell introduced the co eficient .

$$\frac{u_r - u_i}{U_w - u_i} = \sigma(Tmac) \tag{3.15}$$

thus we know that the Tmac denotes the ammount of molecules deflected without any momentum exchange and to vary this parameter has a fundamental effect upon the flow as well.We have taken the various values of Tmac which are 1,0.8,0.4 in three knudsen number regimes(0.1,1,10).

Different parameters varied to study the behaviour are tabulated below:

Table 3.3: Knudsen Numbers

Knudsen Number	Kn_{inlet}	Kn_{mean}	Kn_{outlet}
value set 1	0.1	0.3	0.5
value set 2	1	3	5
value set 3	10	30	50

Note:The pressure ratio has the direct effect upon the knudsen number values.Here the pressure ratio was kept 5 and we can observe the multiples of 5 in the table.

Table 3.4: Aspect Ratio

Aspect ratio	10	40	80
Length of the channel(μm)	10	40	80
Height of channel(μm)	1	1	1

Note:The analysis of different aspect ratio flow behaviour is done with the value of knudsen numbers 1,10,0.1.

Table 3.5: TMAC values

TMAC Values	1	0.8	0.4
Aspect Ratio	80	80	80
Knudsen Numbers	{0.1,1,10}	{0.1,1,10}	{0.1,1,10}
Number of iterations	3lacs	3lacs	3lacs

Note:The channel size is kept 80 because it was observed in the previous analysis that the flow gets fully developed around that length of channel.The objective was to analyse the effect of different TMAC values in long channels.

3.1.1 Collision Modelling in DSMC:

As the nature of the DSMC calculation is of probabilistic nature,the initialisation of the test molecules at open boundaries and the collision with other molecules or the wall are distributed randomly.

The movement of the test molecules is described as the simple change in the position:

$$x_{new} = x_{old} + \Delta t \xi \tag{3.16}$$

which shows the co ordinates of the molecules post collision,however these collisions are based of diiferent assupmtions as well as there are different molecule collision models like Hard Sphere model(HS), Variable Hard Sphere model(VHS),Variable Soft Sphere model(VSS) and latest Generelaised Hard Sphere model.

We have used the Variable Hard Sphere model here.The VHS model was introduced by Bird in 1981 to correct the primary deficiancy which was currently then used in Hard Sphere(HS) model.In the VHS model the molecule is the hard sphere with a diameter d which is a function of C_r.

$$d = d_{ref}(C_{r,ref}/C_r)^{\alpha} \tag{3.17}$$

$$\sigma_T = \sigma_{ref}(\frac{C_r^2}{C_{r,ref}^2})^{-\alpha} \tag{3.18}$$

for the gas in equillibrium,$C_r$is related to temperature by

$$C_r^2 = \frac{2(2-\alpha)kT}{m_r} \tag{3.19}$$

combining the equations 21 and 22,we get;

$$\sigma_T = \sigma_{ref}\left(\frac{m_r C_r^2}{2(2-\alpha)kT_{ref}}\right)^{-\alpha} \tag{3.20}$$

The VHS model denotes that the power law temperature depends upon the co-efficient of viscosity

$$\mu\alpha T^{\omega} \tag{3.21}$$

where $\omega = 0.5 + \alpha$, and the deflection angle

$$\chi = 2cos^{-1}\left(\frac{b}{d}\right) \tag{3.22}$$

VHS is an isotropic scattering law and does not correctly predict the diffusion flow of real gas,especially for gas mixtures anyhow though it works just fine for monatomic gas studies and hence it is used here.

The graphical representation of two sphere colliding is given below.

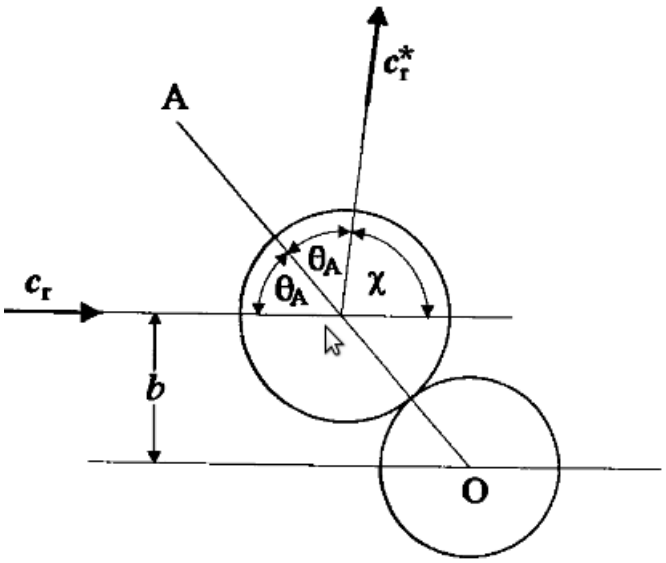


Figure 3.1: VHS collision
[6]

The figure 3.1 is the line diagram showing the collision of two spheres.The geometry is considered as per the figure in the calculations.

3.1.2 Boundary Conditions:

Collission sampling is carried out based on no time counter(NTC) technique described by bird.The treatment of pressure boundary condition at inlet and outlet is based on the implicit boundary conditions if Feng &Yiu[14]

Chapter 4

Results and Discussion:

This chapter contains the results acquired during the study.The flow of process to acquire the results and conclusions derived from those results.This one can say is the heartbeat of this thesis as we move forward to validate our efforts and conclude the work done.

The approach selected here was to establish the behaviour of the flow inside the given micro-channel having the geometrical essentials as shown in previous chapters.As one must have observed that the channel geometry we have used here is of the scale of microns.It shall be mentioned here as to build the outline the approach we have taken and that is, "we have varied different parameters to study the change in behaviour in the flow porperties such as velocity,temperature and pressure."

In the hindsight one shall describe about the route one has taken towards the research to make one understand the reasoning behind the particular analysis.The flow is as described below;

1. Study and validation of the mersenne twister used to generate the random numbers
2. Steady State Analysis
3. Knudsen number regimes study
4. Study of the behaviour of the flow using different aspect ratio
5. Study of the behaviour of the flow using different TMAC values

4.1 Random Number Generation:

As we know, we are carrying out the analysis inside very small or per say micro channel and the flow in question suspected to be rarefied one.As the mean free path or per say the characteristic length and the channel size of the scale of considerable comparison or in other words where the channel size is so small as it lies in the range of the characteristic lenght of the fluid in action,the continuum doesn't hold.It means that the slip in the values of the wall and the fluid quantities is there and the research carried out suggests that the classical newtonial physics doesn't apply here and it has to be studied using moleculer

approach.The moleculer approach takes virtually every molecule into account and traces its behaviour and using that information we shall be able to plot the behavioural study.

Now as described above,every molecule does count to achieve the better accuracy and for the better analysis.The molecular approach we are using will be DSMC and it is probablistic approach,i.e it counts for the probability of intermoleculer colissions and wall-moleculer colissions as well and using that probability and with the help of kinetic theory logic it is constructed to be the important tool to analyse the flows inside the micro channels.

Hence for the better accuracy of the prediction of the flow using DSMC we can simply say that we shall analyse different particles with less frequency of one's repetition.Especially when the DSMC is indexing the particles and it identifies the particles with different numbers,we are using mersenne twisters which are most efficient to generate the random numbers.

The small code was developed using mersenne and the limit was set between 0 to 1 and the aim to generate the 1000 different random numbers and to check for the validity and same was used to generate 100 random numbers.

With this code we use the mersenne file as the header and acquired some results which were indicating to the pattern that be the limits are very less and the ammount of random number to be generated are more of distinct values and tend to repeat less with given limits.The frequency graph is shown below.

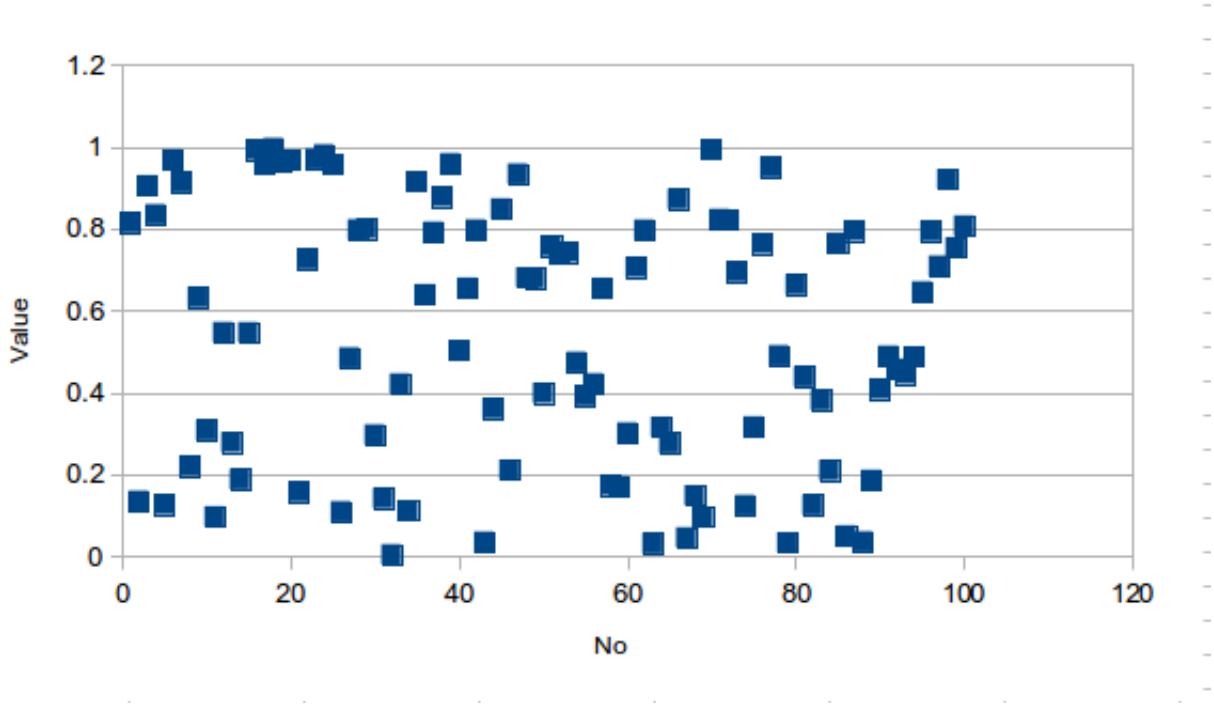


Figure 4.1: Random Number Generation Frequency
X Axis:Number of generated number
YAxis:Value of generated number

As it is shown in the figure,we can so far as conclude or state if not that the frequency of repetition of randomly generated numbers is very less per say.If we go out to connect the applicability with context to our case or the study carried out,we can correlate that the randomly generated numbers signifies the distinct numbered molecules being simulated and hence it accounts for the better accuracy as it covers the

maximum spread of fluid inside a geometry.

To make it simpler than it is,the author has taken liberty to give a pragmatic example as the heart of generic simulation lies in the distinct values being generalized in some pattern and as discussed earlier we have covered most molecules using mersenne twister and above code.Now imagine a classroom X no of students strong and the aim is to analyze the behaviour of each student in the academic year.We have to set the different parameters to examine the pattern and to choose that parameters we have to eye the ones which is seen in most students shall be selected and from that distinct data one shall proceed to generelise that data and it is mendatory for the better analysis to include more students and most common parameters.Consider this analogy as described here,students are molecules and parameters are the quantity we are to study.More random the student,more variety and more variety leads to better analysis.

4.2 Steady State Analysis:

Purpose: The purpose of the steady state analysis inside a cell geometry is to establish the verification of the code in question and to achieve the steady state inside a cell.The less variation or per say the steady state achievement will ensure the definite nature of the macroscopic quantities and the will show that the code written for given geometry holds well to the criterion of similitude to certain limits.

We are to analyse the macroscopic quantities inside a micro-channel.With reference to the research published earlier and mentioned in the chapter 2,the author fathoms the idea to ensure the steady state inside a geometry using temperature,velocity,pressure and mass balance verticals.

It is to be noted that the study has been carried out in various knudsen number regimes,pressure ratios,TMAC values and aspect ratio,yet the aim here is to ensure the verification of the code and to prove it using one example.Hence the author has taken the liberty to present one example and the details of the selected example is given in below table.

Table 4.1: Example Specifications

Type of Gas	Argon
Kn	1
Pressure Ratio	5
Aspect Ratio	1:80
Inlet Temperature	300K
No. of time steps	3lacs
Time-steps in an interval	20,000

Note:Remaining data calculated are shown in table 3.2.

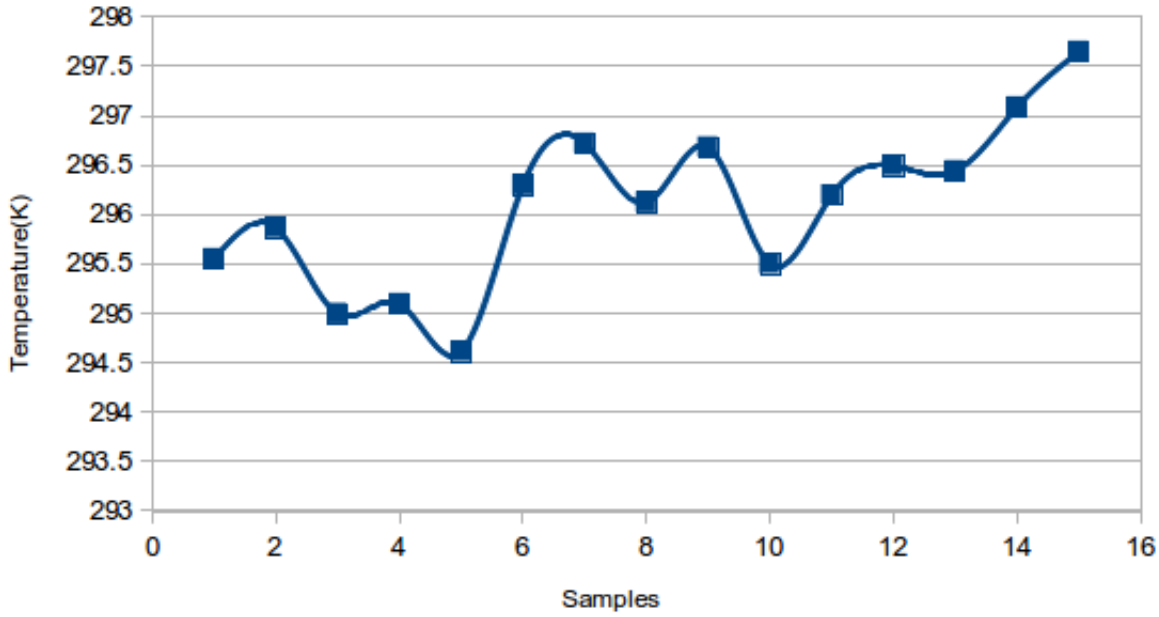
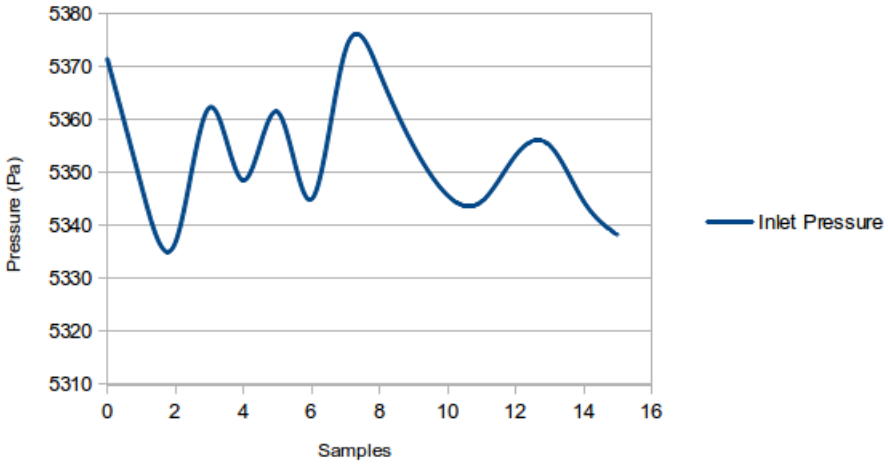


Figure 4.2: Temperature variance inside a cell

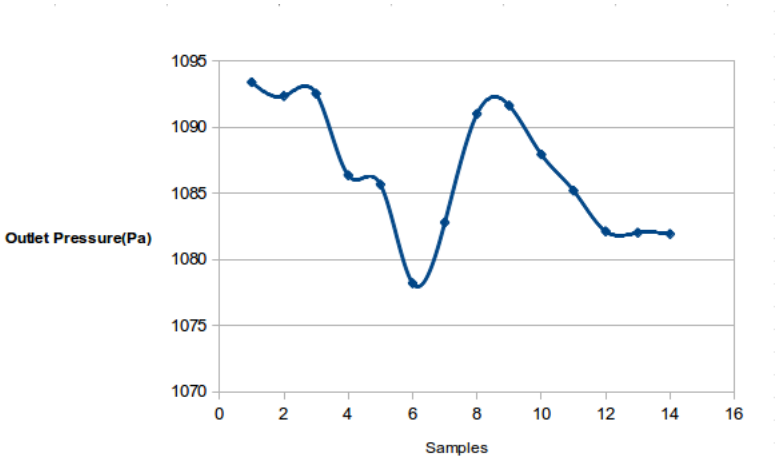
The graphs a,b,c and the figure 4.2 represents the variation of temperature,velocity and pressure with respect to sample numbers.It can be observed from the figure that the parameters are varying within the 1% of the quantities taken.So , it can be said that the steady state is achieved.Similar results details for simulated case is given in given.

Similar results were found for various simulated cases in which Knudsen number,aspect ratio,pressure and TMAC are varied.

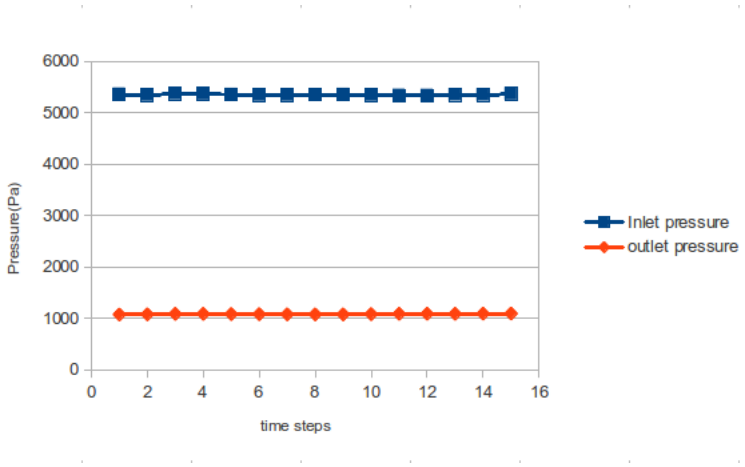
The conditions though suggests that other quantities shall also be in some sort of equillibiria inside a cell and one of those quantities being the velocity ,pressure and temperature and mass balance.The graphical presentation of those are given below.



(a) Variance of inlet pressure inside a cell



(b) Outlet Pressure Variance inside a cell



(c) Pressure ratio

The graphical representations do indicate that the pressure ratio is 5 and it holds as expected also to be noted inside the cell the variance is not of much intensity and the fluctuations are of smaller scale.Figure

(a) suggests that the inlet pressure variance inside a cell is not much and as per the inlet pressure input,the inlet pressure by calculation was found out to be 5361.07Pa(Table 3.2) and we can easily observe from the figure (a) that after 8 timesteps the variance is between 5340 and 5370 which is less than 1% of the calculated inlet pressure and also to be noted that after 8 time steps,it tends to fluctuate less,the steady state is achieved.

The figure(b) is the indicator of the variance inside a cell of outlet pressure.Physically one can say that if the pressure ratio is 5,the outlet pressure shall be 5th part of the inlet pressure amount and it holds out as it was predicted,the predicted value being 1072.21Pa and we can observe in the figure (b) that the variance lies between 1090 and 1060 and after 10 timesteps it steadies down at permissible limits and settles down that is the indication that it holds the steady state.However the figure (C) gives the actual scenario as to how small the fluctuations are and the pressure ratio conditions is being well fulfilled.

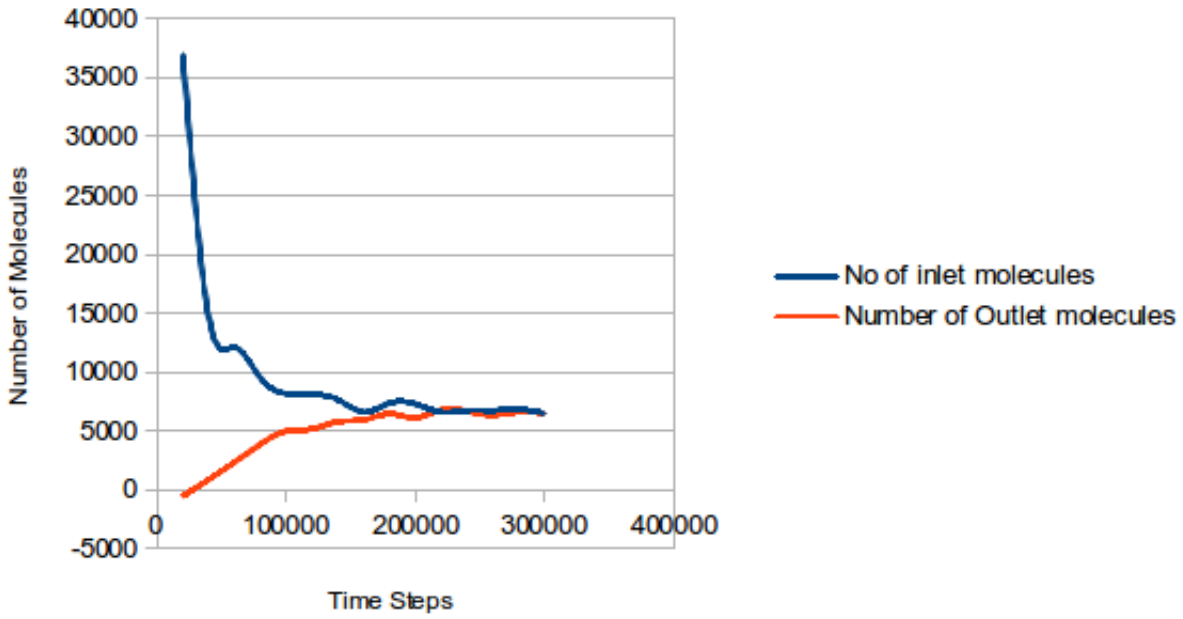


Figure 4.3: Mass Balance inside a cell geometry

From the graph,we can see that after 2,00,000 timesteps,number of molecules at inlet and number of molecules at outlet are found to be same.So , the simulations were carried out for 3 lac timesteps for all the conditions.

4.3 Knudsen Number Regime Study:

Purpose: The purpose of the knudsen number regime study is to analyse the effect of various knudsen numbers on centreline velocity,velocity contours,inlet temperature,outlet temperature,inlet pressure,outlet pressure,pressure contour.The validation of the variance is also presented here.The knudsen number has the major effect upon the behaviour of the study as we it is the ratio of mean free path to the characteristic length and we have discussed its effects on the flow earlier,this study however is with the eye to present and match the obvious.

4.3.1 Cetreline Pressure:

The centreline pressure trends are to be presented below.Now,the knudsen numbers are being varied here from 0.1,1,10 and the effect upon the centreline pressure is being shown here below.

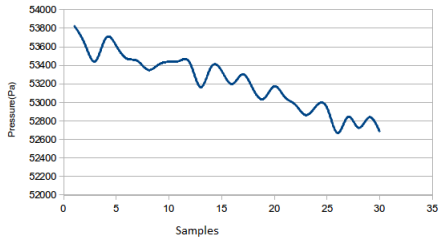
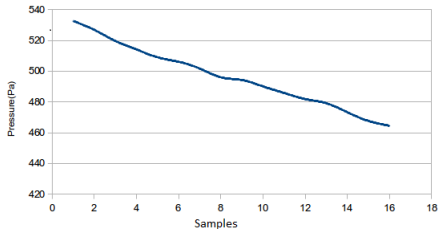
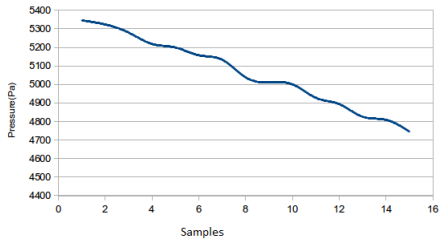


Figure 4.4: Behaviour of the centreline pressure (Kn 0.1)



(a) Behaviour of the centreline pressure(Kn 10)



(b) Behaviour of the centreline pressure(Kn 1)

Figure 4.5: Pressure Behaviour alnogside the centreline

The nature of the graph just by the observation looks like the continuous decrement.It was the nature observed in earlier reasearch works as well,the pressure ratio is 5 here,and because of the pressure difference inside a micro channel,the flow or the developement of flow is occuring.It is obvious that the flow direction will be from the higher pressure to lower pressure.Thus the velocity increases as we approach from inlet to outlet and as the velocity increases,the pressure shall decrease.Also one observes the increment in slope as the knudsen number increases,which indicates that that more the mean free path,more the pressure decrement along the centreline of the geometry as we have taken the aspect ratio same but varied the knudsen number.The velocity distribution and analysis has been presented in 4.3.2.It is to be noted from the graphs that the centreline pressure behaviour is not a linear one and this behaviour is due to the rarefaction encountered and the compressibility effects.

4.3.2 Centre line Velocity:

The nature of the velocity behaviour along the centreline is observed in kn 0.1,1,10 regimes.

As observed from the figures 4.9 (a),(b) and (c) the slope of the velocity behaviour alongside the centreline of the geometry is decreasing and the same pattern was observed in the centreling presssure behaviour with inverse effects,i.e slope was increasing as the knudsen number increases.Physical proof of this phenomenon being as the pressure increases the velocity decreases.You can also observe that the velocity of molecules is increasing,justification being as the knudsen number increases the mean free path increases lest it is just a more space to wander around for a molecule before colliding with fellow molecule or the wall.

4.3.3 Streamline velocity:

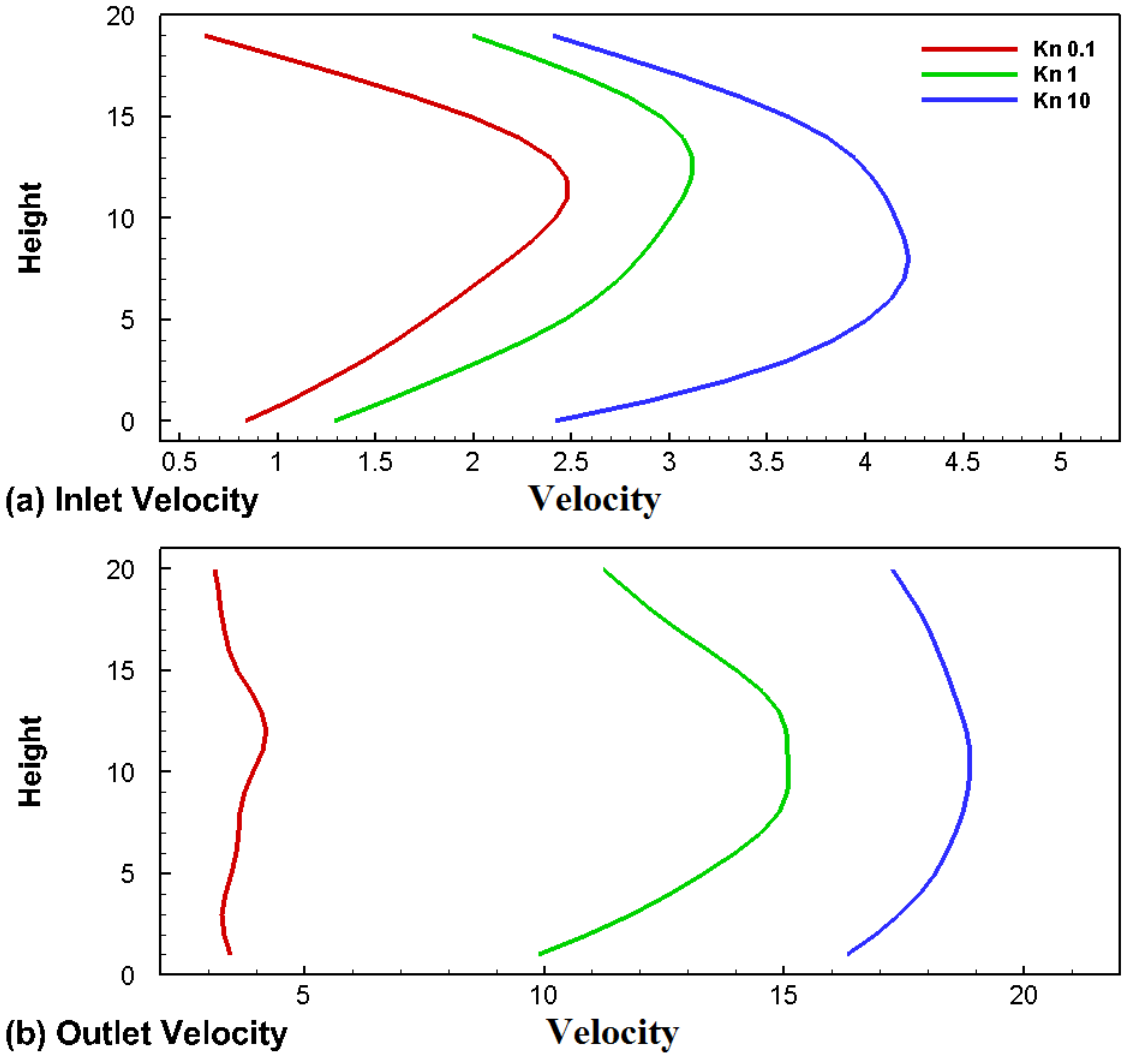
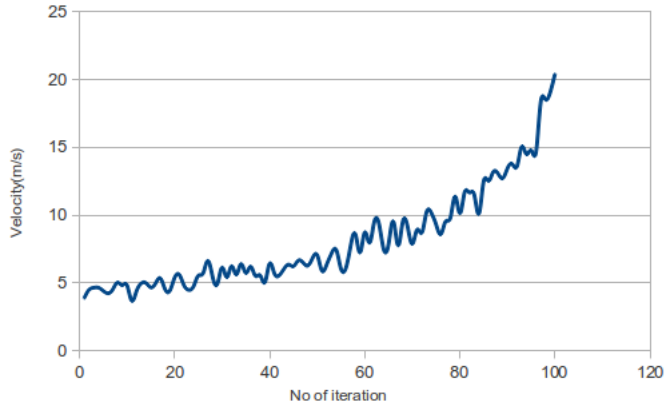
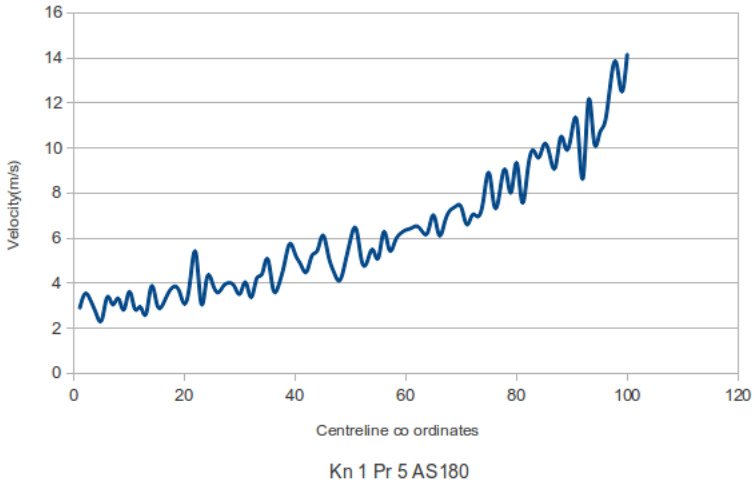


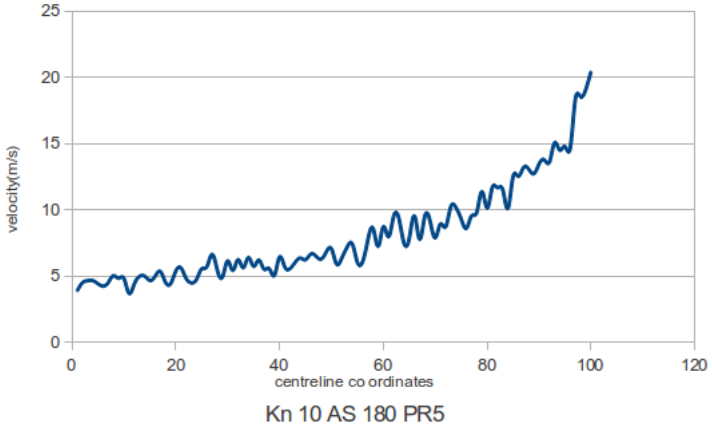
Figure 4.7: Stream line velocity comparison



(a) Kn 0.1



(b) Kn 1



(c) Kn 10

Figure 4.6: Velocity along the centreline

The effect of the knudsen number variance on the stream velocity values are depicted below.As one can observe that the velocity is increased as the knudsen number increases.The reason or the prime reason per say is being the pressure driven force and as the pressure ratio is kept same here (5) and the length and the height of the channel is kept the same as well i.e the aspect ratio is constant for the analysis.So one can identify the only reason is the pressure difference and only amicable explaination one can offer is that the mean free path of the molecules increases,the velocity as collective quantity increases .Yet the knudsen number gets too high,the free molecular flow happens.

4.3.4 Slip velocities:

In the macro scale flow regimes what typically is observed is the no slip condition between the cells nearby the wall and the wall which means the velocity of the molecules nearby the wall is zero in the macro scopic flows where the channel size are typically not in the microns but more.The indicative is the fact that the cells nearby the wall in the present case possess certain amount of velocity gradient.That is the obvious evidence of the rarefaction present in the micro channel.

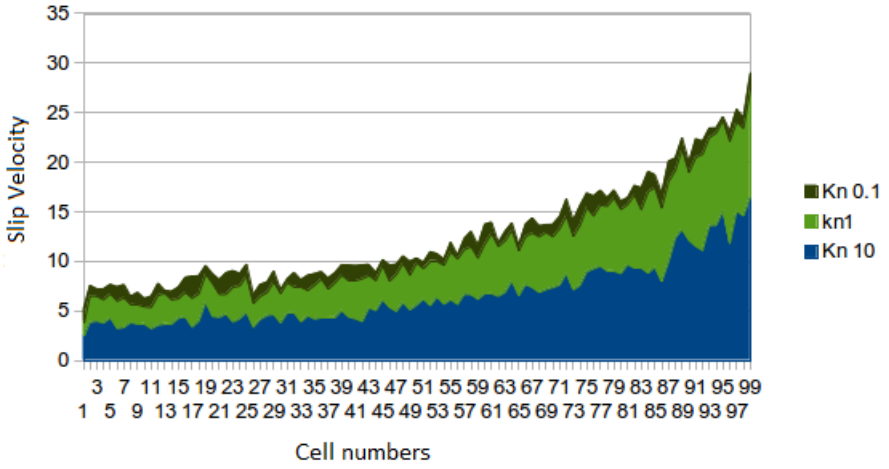


Figure 4.8: Rarefaction velocities near the wall in different knudsen numbers

Note shall say that as the knudsen number increases the velocity gradient decreases but the fluctuation in the range increases.It is due to the high mean free path or say the less pressure values as we move from low knudsen numbers to higher knudsen numbers.Though it is testimonial to the fact that there is some velocity gradient in all the knudsen number regimes and hence it is proved that the rarefaction is there.

4.4 Aspect Ratio:

Purpose: The aspect ratio means the ratio of the height of the geometry to length of the geometry.The aspect ratio variance is the very important vertical of the present study as the author wishes to establish the length when the flow is fully developed and the effect on the various properties as to how they change in short,long and very long channels.

To present the problem distinctly ,here one example is given where the Inlet knudsen number is taken 1 and the aspect ratio are varied from 1:10 to 1:80.Note that the height of the geometry is kept constant

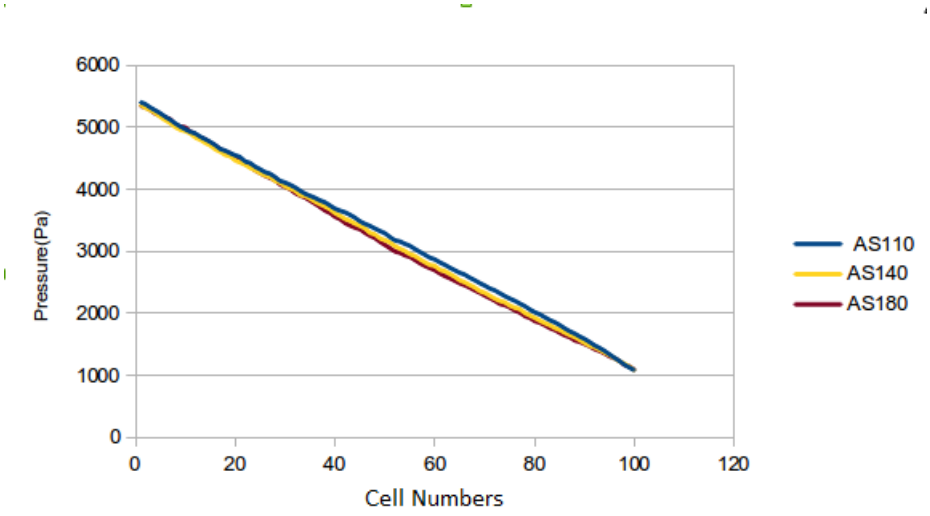


Figure 4.9: Cntreline pressure variance with different aspect ratio

and pressure ratio is taken as 5 .The above assumptions were taken to simplify the problem and to present it with common verticals.

The aspect ratio has been varied in the regime of 1:10,1:40 and 1:80.

4.4.1 Velocity Profiles:

The motivation to vary the aspect ratio of the micro channel was to establish the reference length or the length at which the flow is developing fully and to study the flow behaviour. To trace the velocity profile one has to track the cells corresponding to the percentage length and then find out their velocities and establish a curve suggesting the behaviour of the velocity at different locations of the geometry.

The centreline pressure at different channel size or say different aspect ratio is shown in the graph.

It is to note that the variance in centreline pressure with different aspect ratio is not much.

Now ; we will discuss the velocity profiles inside the micro channel with the aspect ratio 1:80.

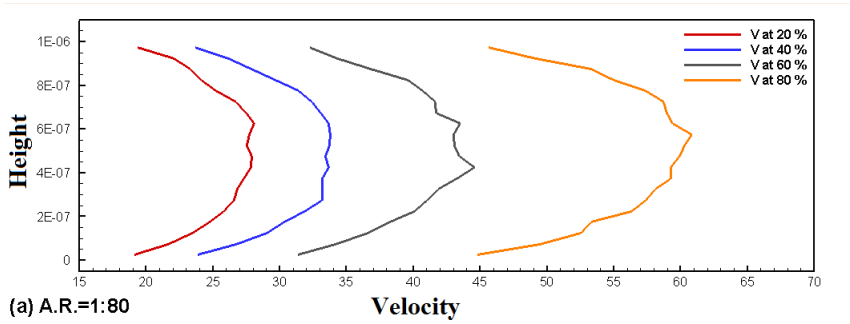


Figure 4.10: flow behaviour inside the geometry with aspect ratio 1:80

As one moves forward in the direction of the flow which in the figure the left to right direction,the profile of flow indicates it is slowly developing towards the end of the channel.It is clear from the figures presented above that the optimum length to develop a flow is $80\mu m$where as in the aspect ratio 1:40 the velocity compared to one with the aspect ratio of 1:80.Now earlier we have established the pattern that

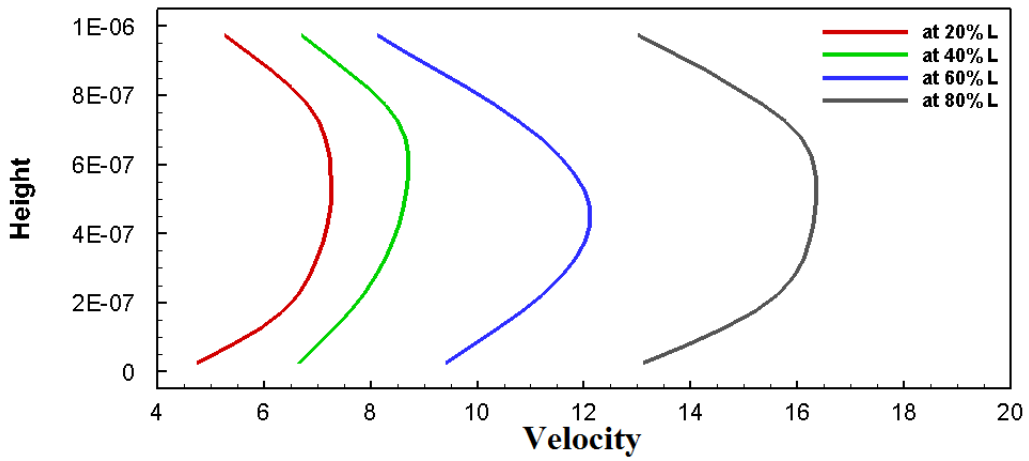


Figure 4.11: Flow development inside a geometry with aspect ratio 1:40

the centreline pressure is almost same for different aspect ratio channels.Yet one finds the difference in velocity gradient in above flow patterns.The velocity in bigger channel is more and that difference where the pressure is same but velocities are different is because of the rarefaction.

4.5 TMAC Analysis:

Purpose: The purpose of this analysis lies in the definition of the Tangential Momentum Accommodation Co efficient(TMAC) which is nothing but the ratio of number of molecules rebounding without any sort of energy exchange to the number of molecules who transports all of their energy at collision.So vaguely one can say that the if the TMAC be 1 there are same number of molecules which exchange all of their energy to the diffusive wall in typical gas surface interaction as the molecules which transport none.If TMAC value is to be 0.8,there are 25% more molecules which have transported their energy completely,and this certainly changes the whole ball game to some extent.Typically in MEMS the different metals,alloys are used and related TMAC value is to be taken into account for each material used,hence it is more need of the hour to analyse the effect of TMAC variance on the different parameters.

The present study has varied the TMAC with three different values which are TMAC 1,TMAC 0.8,TMAC 0.4 in the knudsen number 1.Yet for the exemplary reasons we have presented the case on kn1,AS 1:80,PR 5.We are to study the effect of variance in TMAC on Velocity,Slip velocity,Pressure,Temperature.

The graphical representation of the centreline pressure with different TMAC values suggests that there is not much of a difference when we are varying the TMAC values for the same knudsen numbers.It is to be studied with respect to the change in velocities value when the pressure is same.The difference in the velocity will give the amount of rarefaction happening inside a micro channel.

4.6 Effect of TMAC on velocity :

To analyze the effect on various TMAC,we have traced a velocity profiles at different sections of the micro channel,using same knudsen number and different TMAC values.The results were found to be like:

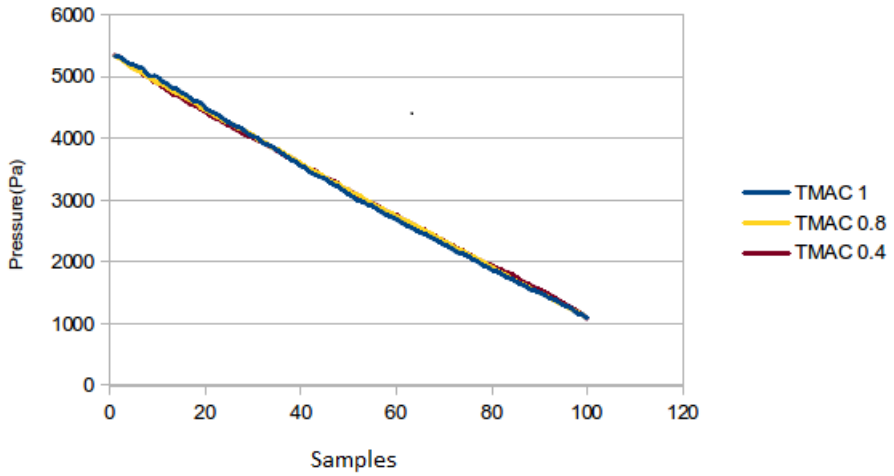


Figure 4.12: Effect of TMAC variance on centreline pressure

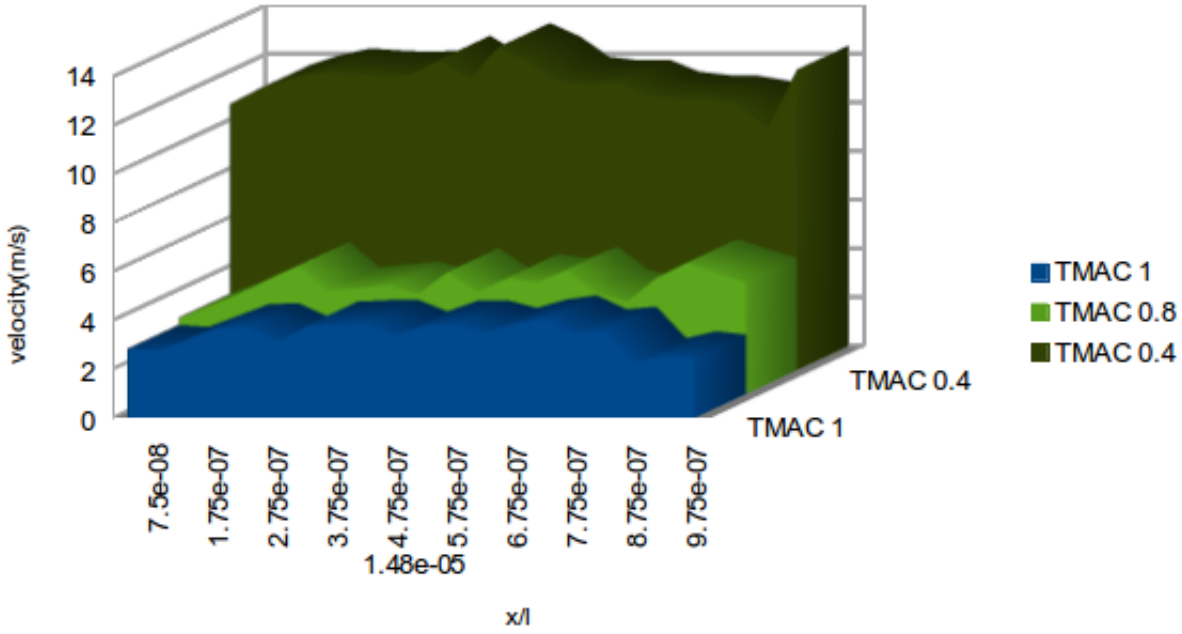


Figure 4.13: Velocity profile at 20% of length with different TMAC

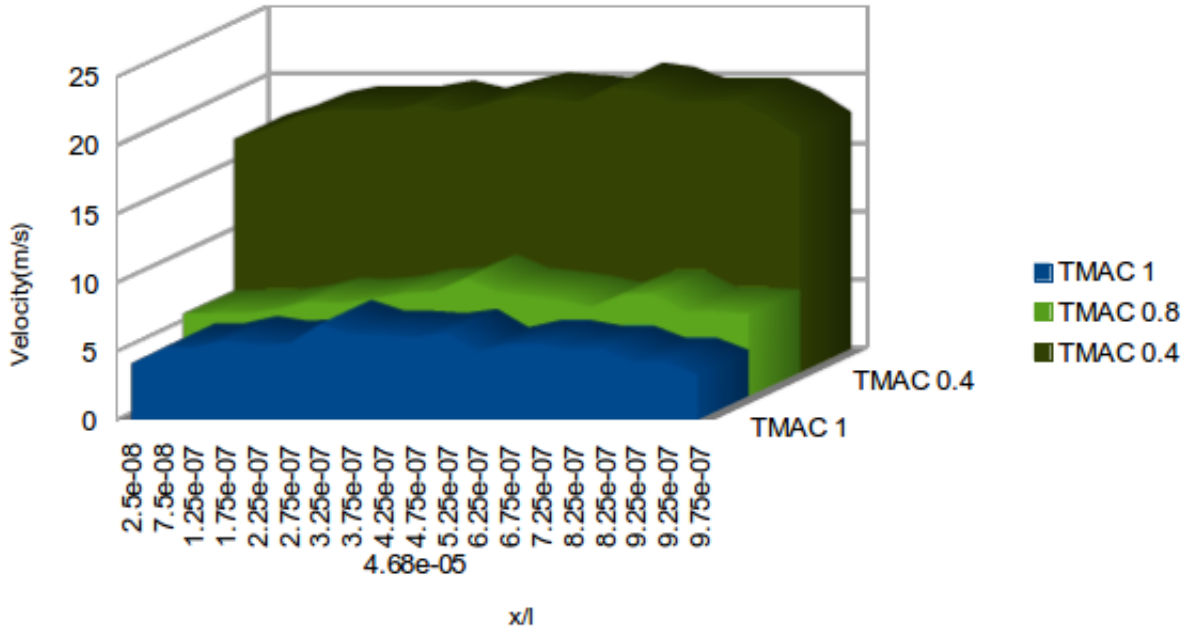


Figure 4.15: Velocity profile at 60% of length with different TMAC

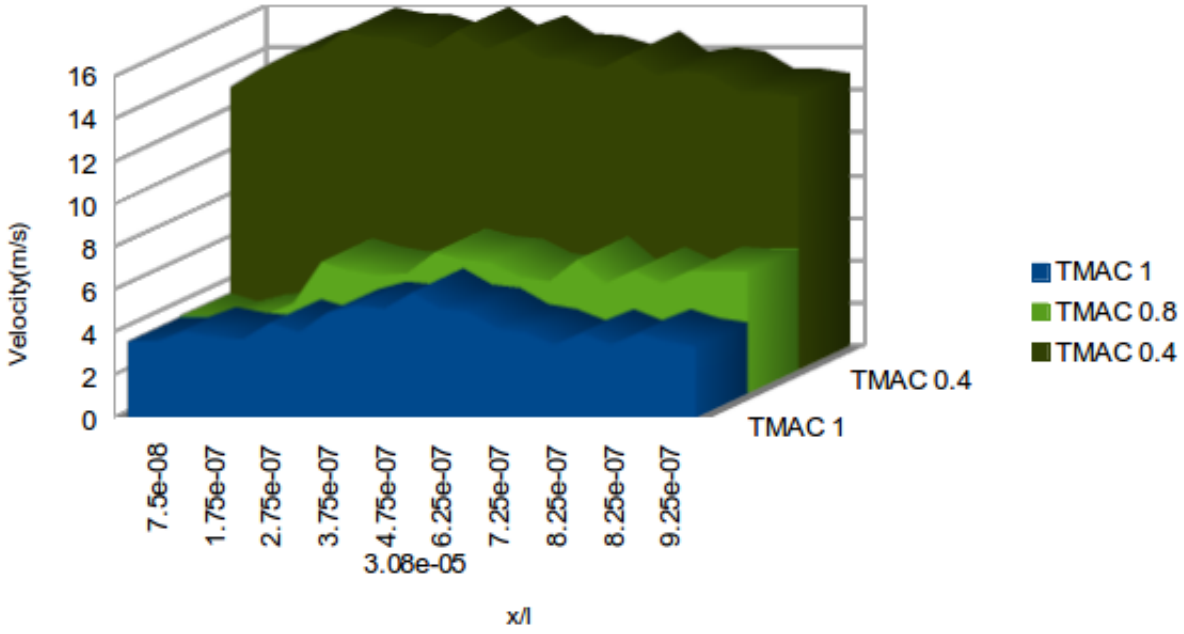


Figure 4.14: Velocity profile at 40% of length with different TMAC

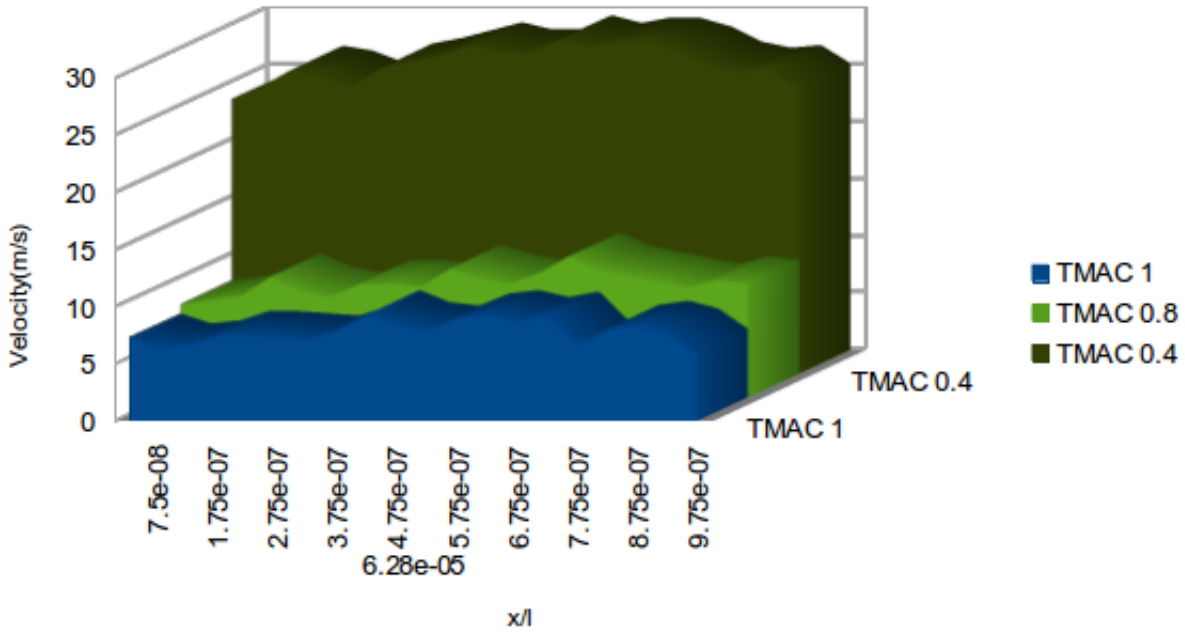


Figure 4.16: Velocity profile at 80%of length with different TMAC

From the figures 4.14,4.15 and 4.16 it is clear that the velocity of the flow is increasing with the reduction of TMAC values.It is to be noted that the velocity gradient at different section of the geometry is increasing,so one can say that the flow is developing inside a micro channel but as we have observed that the cetreline pressure with different TMAC was same so ideally the flow velocities should be the same but here it is not.

The reason is the amount of rarefaction.

4.6.1 Effect of TMAC on slip velocity:

Purpose: It is to be observed that the tangential momentum accommodation co-efficient has certain impact upon the various quantities.Its effect on the slip velocities is yet to be discussed in the present study and it is presented below.To present the comparison studies with varying TMAC,for the example kn 10 with different TMAC values is presented.

Above is the graphical representation of slip velocity on the boundary cells with different TMAC values.with just the visual observations,one can make out that TMAC value has impact on the slip velocity.

The observations are:

- Slip velocity gradient increases as the value of TMAC decreases in all the knudsen number regimes included in study i.e kn 0.1,1,10
- As the knudsen number increases from 0.1 to 10,the percentage increment in slip velocity with decrement of TMAC value is decreasing.

Offered reasons for above observation lies in the definition of the TMAC,as it indicates the ratio of number of molecules which transfers all the energy to the wall to the number of molecules which does not transfer

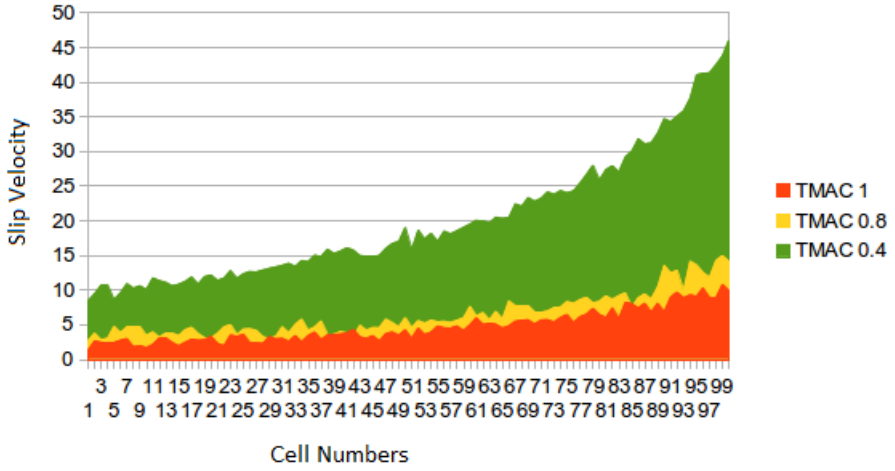


Figure 4.17: Slip velocity at the top edge of the domain

any energy to the wall.Less the TMAC,less the energy transfer and with low knudsen number and relatively higher mean free paths,the molecules have certain freedom to move around with less amount of energy transfer will give more rarefaction.

From the figure 4.17 and 4.18,we can infer that the slip velocity gradient increases as the TMAC value decreases.For all the TMAC value the slip velocity gradient is there and it is pretty suggestive of the earlier flow deflection with same centreline pressures.

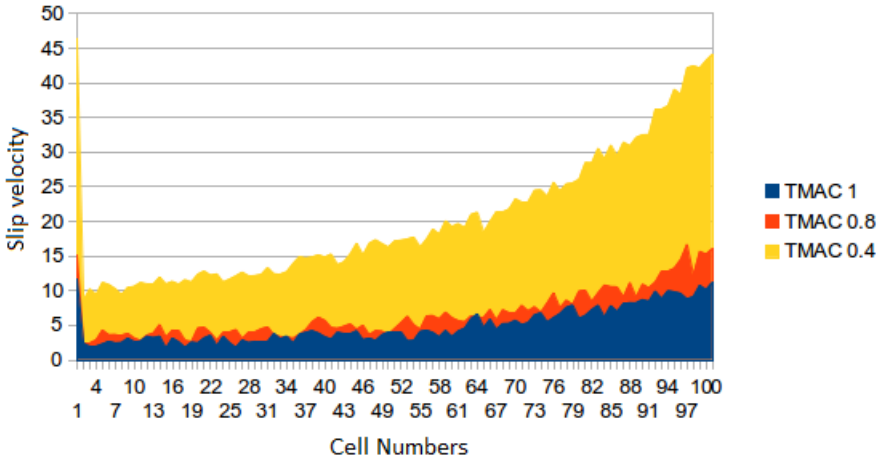


Figure 4.18: Slip Velocity at the bottom edge of the domain

Chapter 5

Conclusion and Futurework:

From the discussion in above chapters,one has establish certain amount of work and tried to present the analysis of the flow inside a micro channel and following conclusions were to be found while working:

- The steady state inside a cell domain was achieved by using the developed iterative mathematical model.Hence the model was found competent enough for the further analysis.
- The centreline pressure and the velocity profiles were found to be different when varying the knudsen numbers.From the variance in knudsen number regimes,the slope of centreline pressure was found to be increasing and yet the velocity was increasing too.This phenomena ensured the presence of rarefaction inside the geometry and from the further analysis we found that as the knudsen number increases,slip in velocity increases.
- The different aspect ratio flow analysis was suggestive of the increament in velocity gradient alongside the centreline while the cetreline pressure remained same.The ensurement of rarefaction lead to the inference that as the aspect ratio increases,the slip velocity near the boundary domains increases.
- Different TMAC values were introduced to study the effect of the same,the centreline pressure was found out to be same,TMAC variance did not have much effect on the centreline pressure yet the notable difference in velocity gradient at several sections .The velocity gradient of the flow having less TMAC value was found out to be highest and regarding slip velocity too was found to be highest when the TMAC value was lowest in tried permutation.

5.1 Futurework:

The flow analysis inside a micro channel so far establishes the basic context to study the further more complicated parameters such as flow with heat transfer,flow with different geometries,different cell geometry etc.The author wishes to pursue the topic and validate the efforts to the previous researches carried out at first then wishes to innovate the implicit solutions for different cases.

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