

Heat Transfer in Noble Gases Using Direct Simulation Monte Carlo Technique (DSMC)

¹Mohamed M. Elafify, ²Khalil M. Elawadly, ³Sherif G. Elsharkawy and ³M. Bassiouny

¹Department of Nuclear Engineering, ²Department of Math and Engineering physics
Faculty of Engineering, Alexandria University, Alexandria 21544

³College of Engineering and Technology, Arab Academy for Science and Technology (AAST)
Alexandria, Egypt

Abstract: Heat flow, temperature and density distributions in rarefied gas between two plates at rest with different Knudsen number values are analyzed using Direct Simulation Monte Carlo technique. The molecules are considered as hard sphere ones while the gas boundaries are diffusive surfaces. The results of the technique are compared to different methods. A sample problem of Helium gas between two plates at rest is used as basis for such comparison. The temperature ratio had been taken as 1.3265. The heat flow comparison shows a good agreement with 4-moment and Ohwada methods for Knudsen numbers higher than 0.2. The Direct Simulation Monte Carlo results fluctuate around the continuum solution for Knudsen numbers lower than 0.2. These statistical fluctuations were less than 15%. The temperature and density profiles show the wall jumps for Knudsen numbers higher than 0.2. These non-continuum effects are noticeable for Knudsen number equal to 1.0. For Knudsen numbers lower than 0.2, these non-continuum effects disappear.

Key Words: Direct Simulation Monte Carlo, Heat Flow, Temperature Distributions, Knudsen Number, Thermal Conductivity

Introduction

The heat transfer through gas is an important process in discussing many engineering applications. The gas may be treated on a continuum level or on molecular level depending on the value of Knudsen number ($Kn = \lambda/L$). For example, in nuclear reactors, the gas gap between the fuel and clad represents a thermal resistance to heat flow from fuel to clad. This gas gap affects the maximum temperature at fuel center especially at hot spot points in the reactor. The determination of the equivalent thermal conductivity of gas in the gap is an important issue for reactor safety. The gap conductance may be affected by two factors, namely, the molecular motion and the surface roughness. D. A. Wesley *et al.*, (1986) proposed a new gaseous gap conductance relationship to discuss the effect of surface roughness on the gap conductance. They used a closed mathematical form introduced by Kennard (1938) to represent thermal conductivity in gas due to molecular motion. The closed form assumes continuum behavior of gas molecules. Song *et al.*, (1989) discussed the effects of gas pressure and mechanical load on thermal gap conductance. They assumed a gaussian distribution of surface roughness. They discussed the conductance as a function of relative contact pressure.

Yovanovich (1982) Integral Gap Conductance (YIGC) model takes the variation in the local gap thickness into consideration due to the surface roughness. This model assumes that the temperature of the two surfaces under consideration are uniform at T_1 and T_2 and the entire interface gap consists of many elemental fluxes tubes of different thermal resistances. On the other hand, a number of different mathematical models have been introduced to represent the effect of molecular motion such as the moment method (full

range 4-moment and half range 8-moment methods), hard sphere, Maxwell-type boundary conditions and linearized BGK model equation (James *et al.*, 1978 and Carlo, 1975). The results obtained for the BGK model solution for Maxwell molecules are close to the Boltzmann solution for hard sphere molecules (Ohwada, 1996). Most of these models were concerned with molecular motion or they used the continuum closed mathematical form of the conductance. Harayama *et al.*, (1991) discussed the effect of eccentricity on the gap conductance. An experimental study of the gap heat transfer between boron carbide and cladding was performed by Kaminaga *et al.*, (1992).

For small gas gap dimension at high temperature, the mean free path of the molecule is comparable to the characteristic length of the gap. This effect limits the use of continuum model to represent gas conductivity. The gas molecules lie in between the continuum level representation and the free molecular level, i.e. in the transition region where Kn ranges from 0.1 to 0.2. To represent the behavior of these molecules, the transport Boltzmann equation is used.

There are two techniques for solving this equation. The first one is concerned with establishing the governing equation mathematically using a set of suitable assumptions, then solving the governing equations either analytically, numerically or using both. The other technique is concerned with statistical representation of the governing equation through simulation of motion and behavior of molecules. Direct Simulation Monte Carlo (DSMC) method introduced by Bird (1967) is an example of the second technique. In this work, direct simulation method is used to discuss the thermal conductivity of gases in the transition regime for different Knudsen numbers to evaluate the thermal resistance of gas gap in nuclear fuel.

Materials and Methods

For a simple dilute gas, the Boltzmann equation could be written in the form:

$$\frac{\partial}{\partial t}(nf) + \mathbf{V} \cdot \frac{\partial}{\partial \mathbf{r}}(nf) + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{V}}(nf) = \int_{-\infty}^{\infty} \int_0^{4\pi} n^2 (f^* f_1^* - f f_1) v_r \sigma d\Omega dV_1 \tag{1}$$

Where :

- \mathbf{V}_r : is the relative speed = $|\mathbf{V} - \mathbf{V}_1|$
- f, f_1 : are the distribution functions of colliding particles before collision
- f^*, f_1^* : are the distribution functions of colliding particles after collision
- n : is the molecular density
- \mathbf{F} : is the external force
- σ : is the collision cross section
- Ω : is the solid angle
- \mathbf{V}, \mathbf{V}_1 : are the velocity vectors of the collision partners
- t : is the time, and
- \mathbf{r} : is the position vector.

The Direct Simulation Monte Carlo (DSMC) method is a computer technique for modeling real gas flow by some thousands of simulated molecules. The velocity components and position coordinates are stored in the computer and modified with time as the molecules undergo representative collisions and boundary interactions in physical space. For one dimensional energy flow (which is used in this work), the temperature gradient is in x-direction. The velocity components are stored in the three dimensions of Cartesian coordinates. Three dimensional velocity components are stored because the collision phenomena must be treated as three-dimensional phenomena. Since the flow is always unsteady, the steady flow is achieved as the large time state of unsteady flow. The simulation field is divided into a network of cells with small dimensions. The dimension ΔX of each cell must be small such that the change in flow properties is negligible within the cell. The molecular motion and intermolecular collisions are uncoupled over time interval Δt_m which is small compared to the mean collision time per molecule. The uncoupling procedure follows the following steps:

Initially, all molecules are moved through a distance appropriate to their velocity component and time Δt_m . New molecules are generated at the boundaries across which there is an inward flux. In one-dimensional problems, the motion in x-direction of interest is enough for representing motion. Representative collisions between molecules are generated appropriate to Δt_m . The pre-collision velocity components are replaced with the values of post collision velocity components.

The time needed for re-ordering molecules is proportional to the number of molecules in the field. The collision time is taken from hard sphere model as (Springer, 1971):

$$\Delta t_c = \left(\frac{2}{N_m} \right) (\pi d^2 n V_r)^{-1} \tag{2}$$

where d is the effective molecular diameter.

Δt_c is essentially proportional to the inverse square of the number of molecules in the cell. The number of molecules per cell, N_m , must not be less than 20 molecules so that the number of collisions is significantly large. The cell network forms a suitable reference for sampling the macroscopic properties of the gas through the sampling time interval Δt_s . An advantage of DSMC method over other statistical methods is that it takes the interaction between molecules and the boundaries into consideration (boundary conditions) easily.

During molecule-molecule collision, the collision energy and momentum are conserved. Adequate collisions are calculated in each cell until the sum of many collision times, Δt_c 's, becomes just greater than Δt_m . Collision partners are chosen with probability of the relative speed distribution according to the hard sphere model. Random impact parameters are generated for the computation of each collision. After collision, the new velocity components are stored in place of the old ones. The number density in each cell is sampled to use for the next collisions computation. The macroscopic physical quantities such as temperature, average velocity, momentum, and energy fluxes can be sampled too. The heat flux can be sampled using the formula:

$$\mathbf{q}_x = \frac{1}{2} \rho \overline{V^2 \mathbf{V}_x} \tag{3}$$

where \mathbf{q}_x is heat flux in x-direction, \mathbf{V}_x is velocity component in the x-direction, and ρ is the density. The flow chart shown in Fig. (1) give a description of the procedures involves in the method.

In case of steady state flow, successive samples may be averaged after the establishment of steady flow in order to build up the sample size and reduce the statistical fluctuations in the final results. For inert gases, the energy flux is only the translational energy flux. This flux represents the heat flux from one side to another in the gap.

Calculations Procedure: In performing our calculations the following steps are applied:- The simulated region of physical space is divided into a network of cells with dimension ΔX . The number of these cells depends on the distance between the two plates, 50 cells per mean free path had been chosen to represent the gas gap. Each cell contains 30 simulating particles. The cells network usually forms a convenient reference for sampling the macroscopic gas properties. Each cell contains 30 molecules arranged in a single array in the order of their locations in the x-direction. The temperature and density distribution between the two plates are calculated for the Helium gas when the temperatures at the two boundaries are, T_H = temperature of the hot plate = 325.71 K and of the cold plate T_L = 245.71 K. The value of applied pressure is 1.013×10^4 Pa. These values are taken from Ohwada's work (1996) for the sake of comparison between the results of DSMC method and different methods. Different ratios between the size of the cells and the mean free path of the molecules (λ) are taken.

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The molecular motion and intermolecular collisions are uncoupled over the time interval Δt_m . All molecules are allowed to move through distances appropriate to their velocity components and time Δt_m . After that a series of collisions appropriate to Δt_m among molecules is computed. The pre-collision velocity components of the molecules involved in the collision are replaced with the post-collision values. The collision probability is proportional to the relative speed (V_r) between the two molecules, so, typical collision pairs are chosen on this basis. This is done through the acceptance-rejection technique (Bird, 1967). The fluxes of the various molecular quantities are sampled within each cell. The boundaries are assumed to be solid diffusive boundaries. The incident and reflected particles may be sampled in terms of the simulation of gas molecules-surface interaction. Sufficient collisions are calculated in each cell to keep the motion and collision time counters concurrent. When the steady state is reached, the physical quantities such as density, temperature profile and heat flux are obtained. Finally, the thermal conductivity of the gas under investigation can be calculated through the relation:

$$k = \frac{|q| \times L}{T_H - T_L} \quad (4)$$

Where L is the gas gap thickness.

The heat flux, q_r is averaged over space, and then sampled over time to determine the overall average thermal conductivity of the gas between the two walls. Another point concerns the ratio of the cell dimension ΔX to the time interval Δt_m . This ratio should not be large compared to the speed of propagation of acoustic disturbance and must be several times the shock wave speed ($\sqrt{\gamma RT}$ where γ is specific heat ratio, R is specific gas constant and T is the absolute temperature).

When these requirements regarding the sample size, cell dimensions, and the time steps are satisfied, the results are independent of these quantities and are within the expected statistical scatter. To avoid collisions between distant molecules within the cell, the collision pairs were chosen according to the acceptance-rejection technique in space within the cell in a way such that close particles are more probable to form collision pair than distant ones.

Results and Discussion

The temperature profiles for different Knudsen numbers are plotted in figures (2) to (6) against the normalized distance (X/L) together with the analytical solution of the continuum model (Springer, 1971). The analytical solution takes the form:

$$T_{norm}^2 = 1 + \left[\left(\frac{T_H}{T_L} \right)^2 - 1 \right] \left(1 - \frac{X}{L} \right) \quad (5)$$

The results from the Monte Carlo method agrees with those of the continuum model for gas gap thickness

higher than 5λ , which correspond to Knudsen numbers lower than 0.2. As the distance between the two plates decreases Knudsen number increases, the non-continuum effects start to show up and deviations at the two plates start to appear. At a distance of one mean free path, the discrepancies are about 10% in temperatures of gap adjacent to hot and cold plates. The density distributions between the two plates are shown in figures (7) to (11). The Monte Carlo method succeeds in showing the wall jumps in density of gas adjacent to the wall for Knudsen number greater than 0.2, while the continuum solution fails to show the effect of temperature jumps on density profile. This effect is very clear when Knudsen number is equal to 1.0. The density jump is about 10% too.

Fig. (12) compares the results of the heat flux between the two plates normalized to the free molecule heat flux obtained using DSMC method with those obtained using the following methods:

- (i) Continuum method (Bird 1967)

$$\frac{q_c}{q_f} = \frac{25\pi}{64} \frac{[(T_H/T_L)^{3/2} - 1]}{(T_H/T_L)^{1/2} [(T_H/T_L)^{1/2} - 1]} \times Kn \quad (6)$$

where q_c is the continuum heat flux q_f is the free molecule heat flux given by:

$$q_f = -2^{3/2} \rho \pi^{-1/2} R^{3/2} T_H^{1/2} T_L^{1/2} (T_H^{1/2} - T_L^{1/2}) \quad (7)$$

- (ii) Ohwada method (Ohwada 1996)
- (iii) Four moment method (Ohwada 1996)
- (iv) Eight moment method (Ohwada 1996)

The sample problem has been chosen to be that given in Ohwada's work. For Knudsen numbers greater than 0.2, the DSMC results agree with the 4-moment solution and Ohwada method. For lower Knudsen numbers, DSMC deviate from 4-moment method and approach that of the continuum solution. The curve shows that the continuum solution is not adequate to represent the heat flux between the two plates for Knudsen number higher than 0.2. The 8-moment results lie in between the DSMC results and the continuum solution.

For Knudsen numbers lower than 0.2, both Ohwada and DSMC results approach the continuum solution. The DSMC results follow the continuum solution with a statistical deviation less than 15%. This deviation is due to statistical scattering of DSMC results around the exact value. The limitations on the considered number of molecules result in such statistical fluctuations.

The relation between the run time values (obtained by a Personnel Computer (PC) of version PIII with 550 MHz processor) and the number of molecules in simulation is shown in Fig. (13). It is obvious from the figure that the run time is approximately proportional to the square of the number of simulating molecules N^2 .

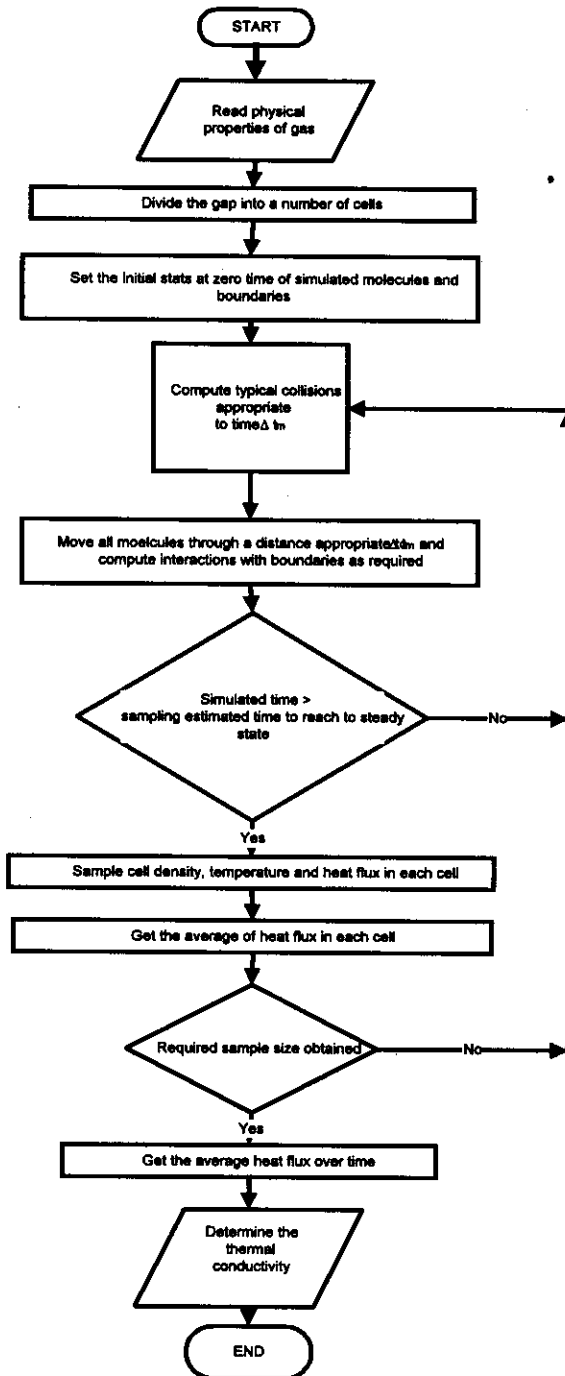


Fig 1: Flow Chart for the Methodology

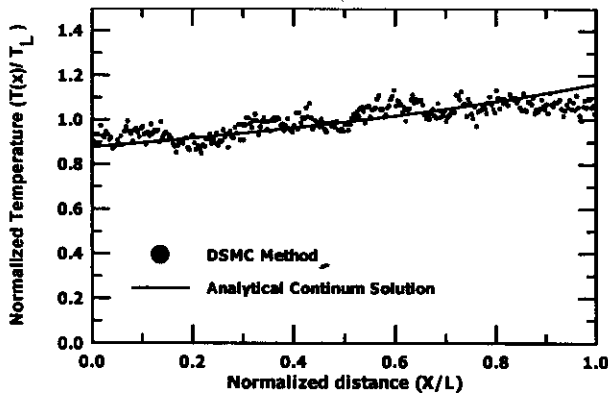


Fig. 2. Temperature profile between the two plates for distance equals 15 mean free path.

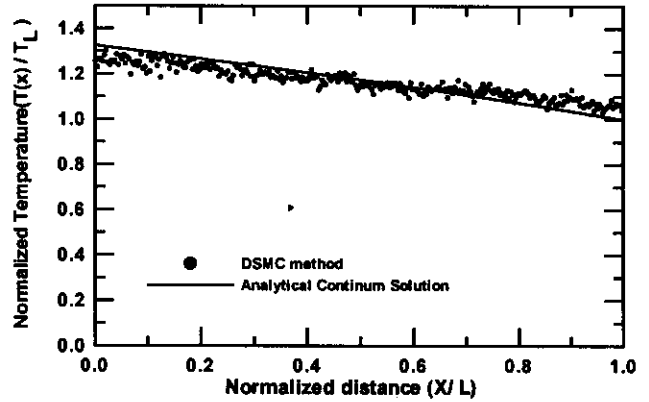


Fig. 5: Temperature profile between the two plates for distance 3 mean free path.

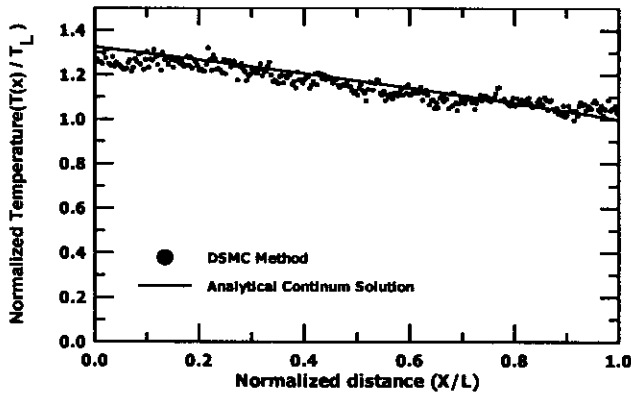


Fig. 3. Temperature profile between the two plates for distance equals 7 mean free path.

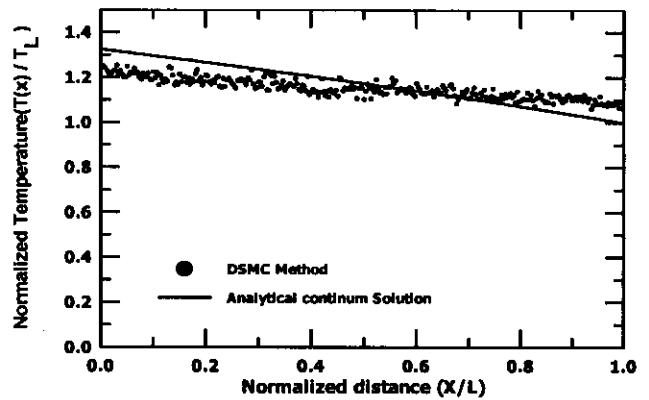


Fig. 6. Temperature profile between the two plates for distance equals one mean free path.

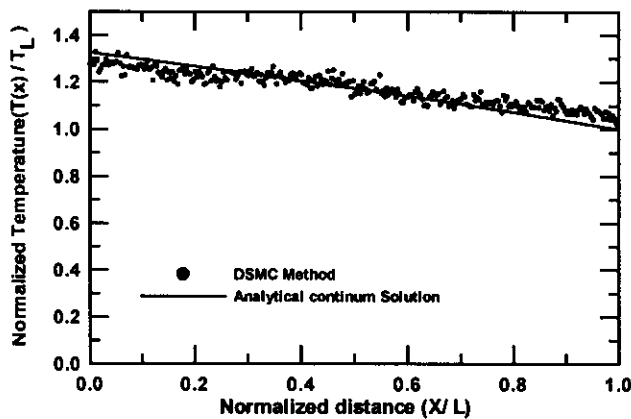


Fig. 4: Temperature profile between the two plates for distance 5 mean free path.

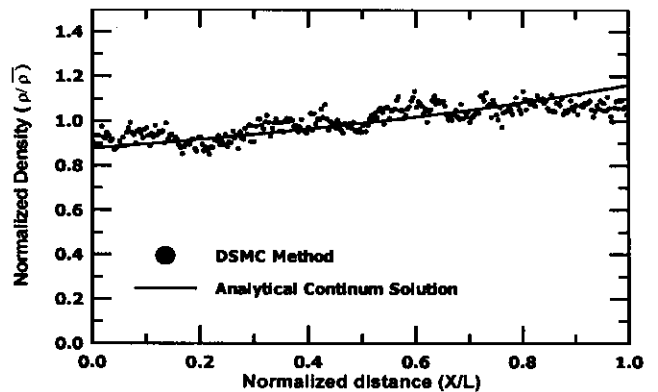


Fig. 7. Density distribution between the two plates for distance equals 15 mean free path.

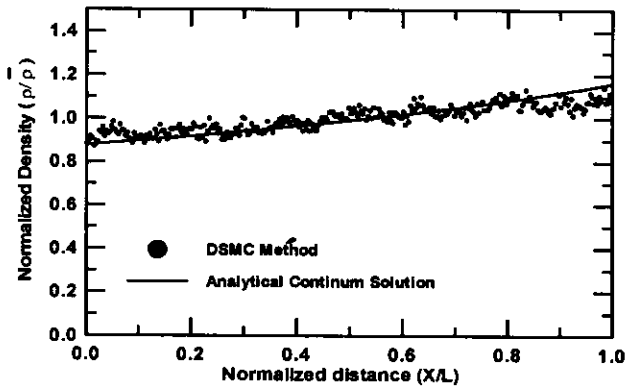


Fig. 8. Density distribution between the two plates for distance equals 7 mean free path.

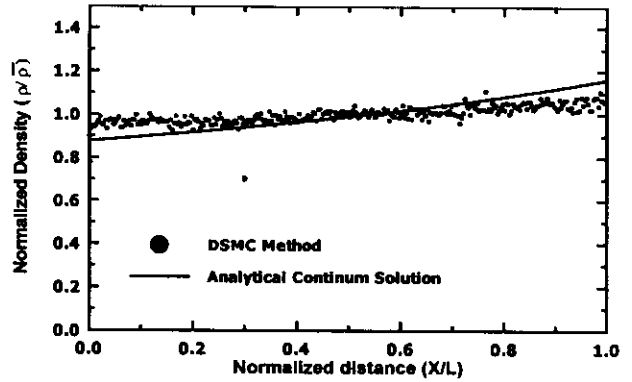


Fig. 11. Density distribution between the two plates for distance equals one mean free path.

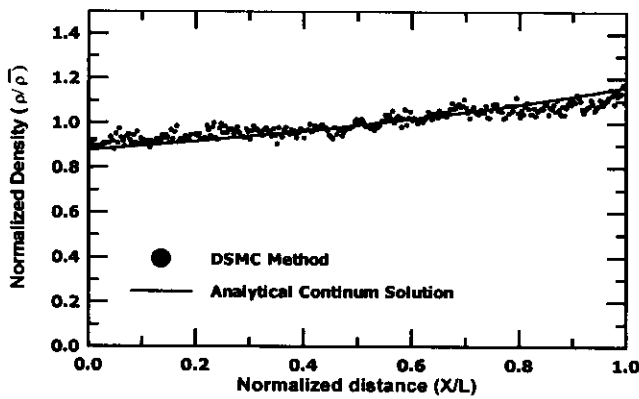


Fig. 9. Density distribution between the two plates for distance equals 5 mean free path.

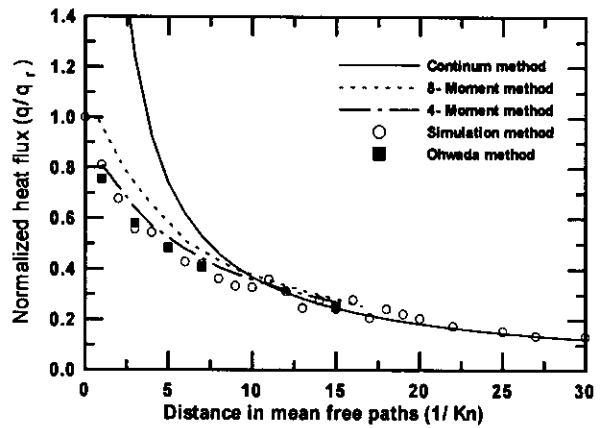


Fig. 12: Comparison of heat flux between the two plates for different Knudsen numbers using various method of solutions.

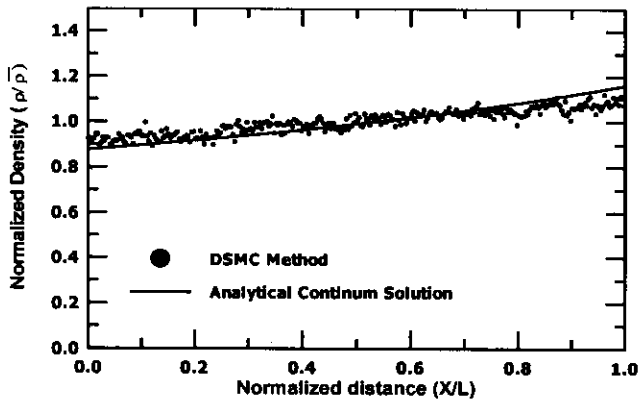


Fig. 10. Density distribution between the two plates for distance equals 3 mean free path.

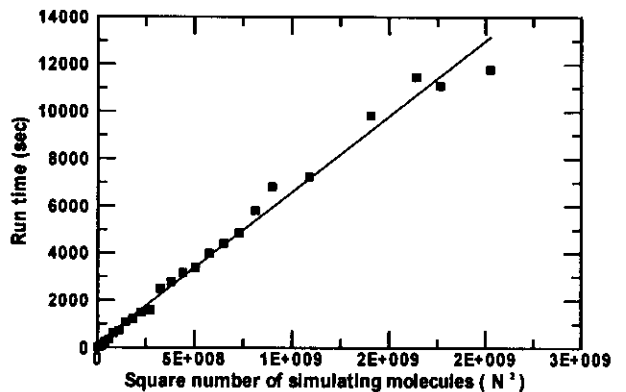


Fig. 13: relation between the squared number of simulating molecules and the run time taken by the computer to calculate the heat flux.

Conclusion

The heat transfer problem of a rarefied gas between two parallel plates has been discussed using DSMC method for hard sphere molecules and diffusive boundary conditions. Comparisons have been made with available theoretical and numerical results. The DSMC method gives good results for the low Knudsen number gas gap heat flux. The difference between continuum model and DSMC results was lower than 15%. This difference is mainly due to the effect of statistical fluctuations for low Knudsen number gas gap. The difference decreases as number of simulating molecules increases. A high number of molecules are required for representing the actual behavior of molecules in continuum conditions. The thermal conductivity of the gas gap is better determined using Monte Carlo Simulation.

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