

## Prediction of the Thermal Conductivity of Gas Mixtures Using Direct Simulation Monte Carlo Method

Mohamed M. Elafify, <sup>1</sup>Khalil M. Elawadly and <sup>2</sup>Sherif G. Elsharkawy  
Nuclear Engineering Department, <sup>1</sup>Mathematics and Engineering Physics Department,  
Faculty of Engineering, Alexandria University, Alexandria 21544, Egypt  
<sup>2</sup>College of Engineering and Technology, Arab Academy for Science and Technology,  
Alexandria, Egypt

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**Abstract:** The thermal conductivity of gas mixture filling the gap between two parallel plates was obtained and analyzed using Direct Simulation Monte Carlo technique (DSMC). The thermal conductivity of the gas mixture is not a simple linear relation between the conductivities of gas species in the mixture. The DSMC method provides the right technique for simulating molecules to determine the thermal conductivity of the mixture. The molecules are considered as hard sphere ones while the gas gap boundaries are diffusive surfaces. Two sets of values of temperatures had been used. The first set considers the hot and cold plate temperatures at 325.7 and 245.7 K, respectively. This set is used to examine the efficiency and credibility of the DSMC method when used for a gas mixture and to assure that the results show the expected temperature and pressure profiles similar to those obtained in the case of single gas molecules. The second set uses temperatures of 306 and 300 K to evaluate the thermal conductivity at the average temperature value of 303 K. The molar fractions with position had been checked to make sure that the DSMC simulates the collisions and motion of different gas molecules in the right way. The results were consistent and the relative difference between them is due to the normal statistical fluctuations arising due to the low number of simulating molecules than real ones. The DSMC technique is a well-established method to represent and calculate the macroscopic properties of a gas mixture especially when the gas is in the transition region between continuum and free molecular regimes.

**Key words:** Direct simulation monte carlo method, thermal conductivity, gas mixtures

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### INTRODUCTION

Thermal conductivity of gas mixtures is needed in many engineering applications. In gas gap of a nuclear reactor fuel element helium and gaseous fission products form an example of such applications. In Gas cooled reactors (GCR's), gas properties are important for establishment of temperature profiles in fuel. In many welding and contact applications the thermal conductivity of the gas is needed to calculate the contact heat transfer coefficient precisely. However, owing to experimental difficulties, few data are available for such a problem. A precise knowledge of the formula governing the composition dependence of the thermal conductivity of gas mixtures in terms of values of its pure components is hardly available. A number of expressions have been proposed which have met varying degrees of success. It is logical that, the thermal conductivity of these mixtures should be fully understood at a molecular level before trying to interpret the behavior of more complex systems.

A theory of thermal conductivity using dense hard sphere model was worked out by Thorne<sup>[1]</sup>, who extended the Enskog theory to dense hard sphere mixtures. Dipippo *et al.*<sup>[2]</sup> presented a method, based on the modified theory presented by Thorne, allows the computation of thermal conductivity of binary mixtures of mono-atomic gases. The method uses measurements of the thermal conductivity for the pure components up to the same density as for the mixtures together with the zero-density thermal conductivity at one composition for a given gas. Anathony *et al.*<sup>[3]</sup> measured the thermal conductivities of gaseous mixtures of helium with hydrogen or deuterium at 77.6 and 283.2 K. The results they obtained are shown to be accurately predictable on the basis of the Hirschfelder-Eucken equation<sup>[3]</sup> using a potential function for the interaction between a helium atom and a hydrogen molecule calculated quantum mechanically by Tsapline and Kutzelnigg<sup>[4]</sup>, Saxena and Jody<sup>[5]</sup> had computed the thermal conductivity for helium and neon in the temperature range 500-2500 K from heat transfer data that

is taken in the temperature-jump regime. They cleared that; the corrected conductivity values are pressure independent and are in good agreement with the values calculated from heat transfer data in the continuum regime. Francis *et al.*<sup>[6]</sup> had measured the thermal conductivity of helium at atmospheric pressure in the temperature range 800-2100 K using column method. Their results were compared with previous thermal conductivity measurements and showed good agreement. Elafify *et al.*<sup>[7]</sup> had calculated the thermal conductivity of pure noble gases using DSMC method; their work has showed a good agreement with the 8-moment method. The main advantage of DSMC method appears when dealt with high Knudsen number, where continuum model fails to represent interactions of gas molecules near free particles.

**Direct simulation monte carlo technique for gas mixtures**

**Through out this work the DSMC method is going to be used to predict the thermal conductivity for gas mixture:**

In a gas mixture consisting of a total of (s) separate species (p, q, etc), the Boltzmann equation becomes a set of simultaneous equations. The Boltzmann equation for species (p) of the mixture can be written in the form<sup>[8]</sup>:

$$\frac{\partial}{\partial t}(n_p f_p) + c_p \cdot \frac{\partial}{\partial r}(n_p f_p) = \sum_{q=1}^s \int_{-\infty}^{+\infty} \int_0^{4\pi} n_p n_q (f_p^* f_{1p}^* - f_p f_{1p}) c_{rpq} \sigma_{pq} d\Omega dc_{1q} \quad (1)$$

Where:

- $c_{pq}$  : is the relative speed between particles of species p and q respectively =  $|c_p - c_{1q}|$
- $f_p, f_{1q}$  : are the distribution functions of colliding particles before collision
- $f_p^*, f_{1q}^*$  : are the distribution functions of colliding particles after collision
- $n_p$  : is the molecular density for species p
- $n_q$  : is the molecular density for species q
- $\sigma_{pq}$  : is the collision cross section of the molecules of the two species p and q
- $\Omega$  : is the solid angle
- $c_p, c_{1q}$  : are the velocity vectors of the colliding partners
- $t$  : is the time and
- $r$  : is the position vector

Since this equation is an integro-differential equation, mathematical solution of such equation is complicated. Another technique of attacking such a problem is the use of Monte Carlo method. The Direct Simulation Monte Carlo method (DSMC) is a simulation method applied to

simulate the real gas flow through the field of propagation. The essential DSMC approximation is the uncoupling of the molecular motion and the intermolecular collisions over a small time interval or step  $\Delta t_m$ . All the molecules are moved (including the computation of the resulting boundary interactions) over a distance appropriate to this time step. This is followed by the calculation of a representative set of intermolecular collisions for sum of time intervals  $\Delta t_c$ 's that are appropriate for the time interval of the motion  $\Delta t_m$ . The time interval of any collision should satisfy the collision frequency appropriate for each species in the mixture. Using the expression<sup>[8]</sup>:

$$\Delta t_c = \frac{1}{N_p \sigma_{pq} n_q c_{rpq}} + \frac{1}{N_p \sigma_{pq} n_p c_{rpq}} \quad (2)$$

where:

- $N_p$ : is the simulated number density of species p
- $N_q$ : is the simulated number density of species q
- The rest of symbols have their previous definitions.
- The mean collision rate for a species p molecule with species q molecule is given by Bird<sup>[8]</sup>:

$$v_{pq} = 2\sqrt{\pi} d_{eff}^2 n_q \left\{ \frac{2KT(m_p + m_q)}{m_p m_q} \right\}^{\frac{1}{2}} \quad (3)$$

Where:

- $d_{eff}$ : is the effective collision diameter of the two molecules given by Bird<sup>[9]</sup>:

$$d_{eff} = \frac{d_p + d_q}{2.0} \quad (4)$$

The mean collision rate for species p molecules is given by Bird<sup>[9]</sup>:

$$v_p = \sum_{q=1}^s v_{pq} \quad (5)$$

and the mean collision rate per molecule for the mixture is given by Bird<sup>[9]</sup>:

$$v = \sum_{p=1}^s \left\{ \left( \frac{n_p}{n} \right) v_p \right\} \quad (6)$$

The equilibrium mean free path for species p molecules is given by Bird<sup>[9]</sup>:

$$\lambda_o = \sum_{p=1}^s \left( \frac{n_p}{n} \left[ \sum_{q=1}^s \left\{ \pi d^2 n_q \left( 1 + \frac{m_p}{m_q} \right)^{\frac{1}{2}} \right\} \right]^{-1} \right) \quad (7)$$

The time step should be small in comparison with the mean collision time.

The hard sphere model is used to represent collision cross-section between molecules in the mixture. The

collision partners are chosen according to the collision probability of molecules. The collision probability of molecules increases with increasing the quantity:

$$\frac{\sigma_{pq} c_{rpq}}{(\sigma_{pq} c_r)_{max}}$$

The hard sphere cross-section is given by the following relation<sup>[10]</sup>:

$$\sigma_{pq} = \pi d_{ef}^2 \quad (8)$$

An acceptance rejection technique has been adopted to choose the collision partners based on  $\sigma_{pq} c_{rpq}$ . In the mean time, an acceptance –rejection technique based on position in the cell is adopted to choose partners for collisions. Despite of the fact that collisions do not depend on the position of molecules inside the cell, the probability of collision increases as the partners are closer to each other. The cell network is required only in physical space. This space network is used to facilitate the choice of the collision partners and for sampling of the macroscopic flow properties. The collisions are always treated as three-dimensional phenomena. The procedures for the establishment of the correct collision rate are based on the cells. After the collision takes place for the time interval  $\Delta t_c$ . The pre-collision velocity components are replaced with the post-collision values. For gas mixtures, it is favorable to consider the molecular masses of different species; this is because the collision frequency of heavy-heavy collisions would be small compared with that for light-light ones. Moreover, the cross collisions between light and heavy molecules would have little effect on the heavy gas. These will set the value of  $(\sigma_T c_r)_{max}$ , the acceptance rate for the heavy molecules will be low and the overall selection will be insufficient. So, for a collision between species (p) and (q) the acceptance condition is given by Bird<sup>[9]</sup>:

$$\frac{\sigma_{pq} c_r}{(\sigma_{pq} c_r)_{max}}$$

When reaching to the steady state heat flow, the properties in each cell are sampled and the output macroscopic properties like temperature, pressure, heat flux and thermal conductivity are calculated at this moment.

**Test problems:** For the sake of comparison with previous theoretical and experimental results, the following test problems had been set:

The position, velocity components, molecular masses, molecular diameters and initial temperatures for a

gas mixture consisting of two species (Neon and Argon) that are uniformly distributed in physical space are stored in the computer memory. The two species of molecules of inert gases are used to simulate the real gas molecules that are filling the field between the two parallel plates of the simulated region in our problem.

At start up of simulation all molecules are picked out from the maxwellian distribution at the temperature of the cold plate. Different ratios for the chosen species are used as have been done by Kisten *et al.*<sup>[10]</sup>. The ratio of each species is taken as the ratio of the partial pressure for each one according to the relation:

$$p_i = n_i K T \quad (9)$$

Where;

$p_i$ : is the partial pressure.

$n_i$ : is the number density of molecules of species I.

K: Boltzmann constant.

T: Absolute temperature.

Appropriate precautions are taken to ensure that the used data would satisfy the dilute gas conditions. These precautions consider the relation between the characteristic length (L) between the two parallel plates, the mean free path between molecules and the value of the mean molecular spacing between molecules. The dilute gas requires that the Knudsen number Kn should be small compared with unity. The corresponding value of the characteristic length (L) is at least ten times as large as the side of a cubic element containing 1000 molecules. The number of molecules per species in each cell should not be lower than 10 so that the fluctuations are minimum. The number of molecules in each cell is taken as 50 molecules per cell. The simulated molecules are arranged in one-dimensional array in the field between the two plates. At this moment, the molecular motion is initiated for all molecules and their mean free paths are calculated for each type of the two species. Minimum mean free path is chosen and applied to calculate the total number of cells through out the characteristic length (L). All molecules are moved through a distance appropriate to a time interval  $\Delta t_m$ . After that, all molecules are enforced to experience the principle of acceptance-rejection techniques based on both  $(\sigma_{pq} c_r)$  and position to choose the most probable molecules that are best neighbors to undergo a collision. Under this principle, all molecules of the two species are collided with one another regardless of their types. As the time counter increases by a time increment  $\Delta t_c$  according to the collision partners till the cumulated time of collisions finally reaches a value appropriate to the time of motion  $\Delta t_m$ . When the time of simulation  $\Delta t_s$  reaches a value at which the medium

between the two parallel plates reaches the equilibrium state, the steady flow condition is achieved. Then, all macroscopic properties such as temperature, pressure and density profile can be represented. Finally, the heat flux and thermal conductivity of the gas mixtures are to be calculated.

Two sets of values of temperatures had been used. The first set considers the hot and cold plate temperatures at 325.7 and 245.7 K, respectively. This set is used to examine the efficiency and credibility of the DSMC method and to assure that the results show the expected temperature and pressure profiles similar to single gas molecules. The second set uses temperatures of 306 and 300 K to evaluate the thermal conductivity at the average temperature of 303 K. This value has been picked up to compare our results with the experimental data given by Dipippo *et al.*<sup>[2]</sup>.

For evaluating the error bars in each composition, batches of runs with different sets of random numbers are performed. The average values of such runs with the error bars are presented in a figure. At least four batches are done for each composition. More batches are done for compositions of low partial pressure of any of the two components. It had been found that, when partial pressure of any of the components is low, the error in calculations is higher if the same number of batches were used. This is interpreted by the low number of simulating molecules of such type when the total number of molecules per cell is fixed.

## RESULTS AND DISCUSSION

Figures (1a, b and c) show the temperature, density and pressure profiles for the test problem with the first set of temperature values (245.7 and 325.7 K). They are similar to the figures obtained for a single gas<sup>[7]</sup>. These Figures are presented to show that DSMC method has succeeded

to simulate the gas mixtures behavior as well as in the case of single gas. This set of temperatures had been used to compare with previous work.

For evaluating thermal conductivity at 303 K, the second set of data for temperatures 300 and 306 K had been used. It is obvious that, the gradients are not clear in Figs. (2a, b and c) since the difference in temperature between hot and cold plates is low.

Figures (3a, b and c) and Figs. (4a, b and c) show the same behavior. Also, the effect of variation of mole fraction is not clear in the temperature profiles.

Figures (5a, b, c and d) show the distribution of the partial mole fraction for each species between the two parallel plates during steady state at the end of run. The mole fraction fluctuates around its average value in each cell. The curves show that, there is no accumulation of any of the two species of the gas mixture at any position, which assures the uniform distribution of the mixture and right representation of the collision and motion of simulated molecules. In spite of the variation in number density in each cell, the molar fractions are invariant. Figs. (6a, b, c and d) show sample the outputs of the heat flux against time. The value fluctuates around an average value of heat flux for different composition of the gas mixtures, which means that, the steady state equilibrium has been achieved. A time average is used to determine the average value of heat flux within the gas.

Figure (7) shows the thermal conductivity of gas mixture at different values of compositions compared with the experimental data taken from Garrabos (McElhannon and McLaughlin, 1975). The curve uses a plot of best-fit polynomial to show the results. Error bars are used to represent the error percentage in these when the DSMC method is used. It is obvious from the figure that the DSMC results are in good agreement with the Garrabos data.

Despite of the high error in some of the results, the DSMC method is the most reliable technique when

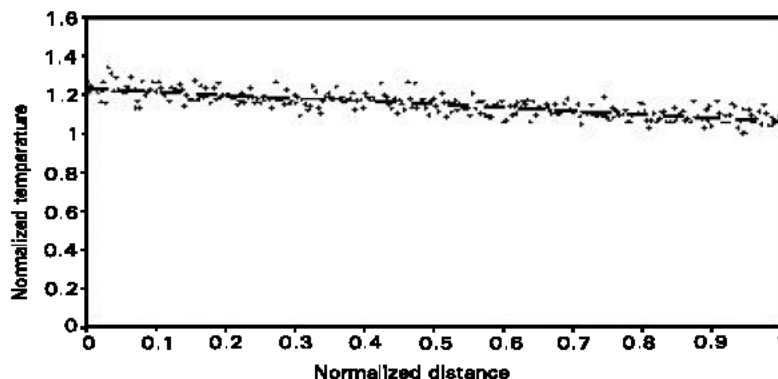


Fig. 1a: Normalized temperature profile for a gas mixture combination of 0.61 Neon and 0.39 Argon mole fractions at pressure 1.01 bar at temperature 325.7 and 245.7 K

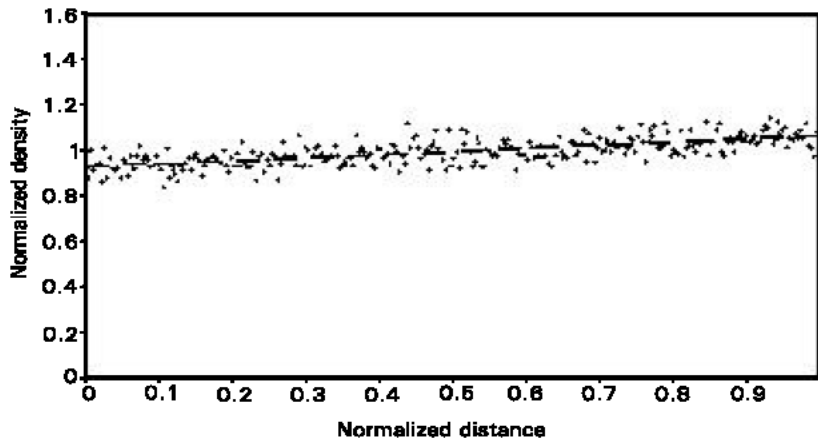


Fig. 1b: Normalized density profile for gas mixture combination of 0.61 Neon and 0.39 Argon mole fractions at pressure 0.01 bar and temperatures 325.7 and 245.7 K

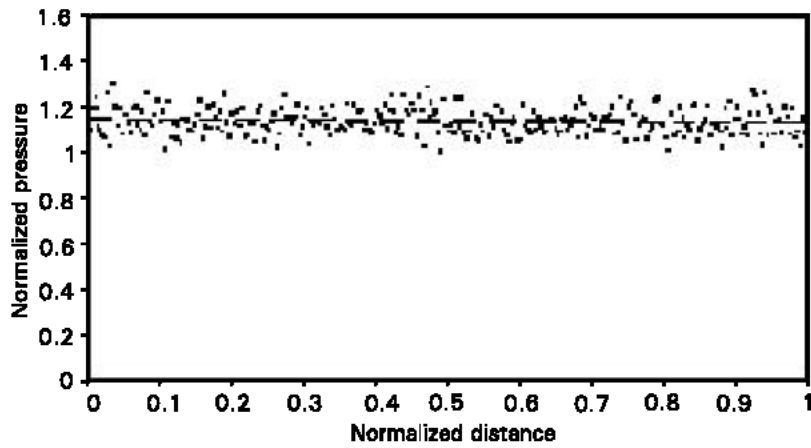


Fig. 1c: Normalized pressure profile for a gas mixture combination of 0.61 Neon and 0.39 Argon mole fractions at pressure 0.01 bar and temperatures 325.7 and 245.7 K

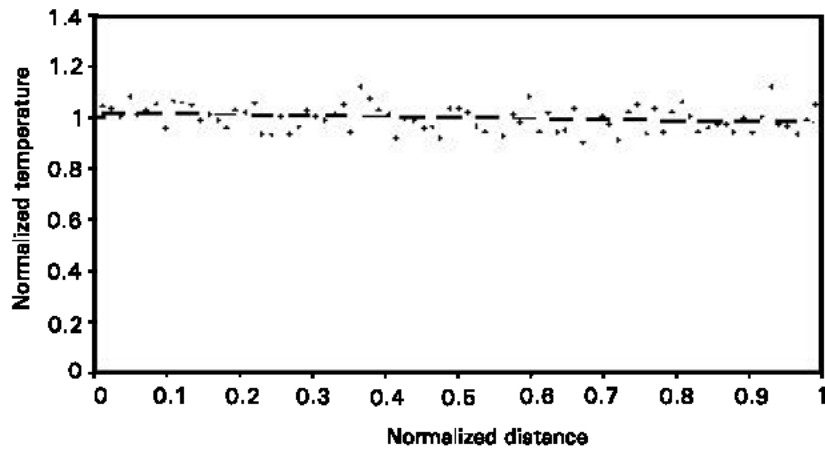


Fig. 2a: Normalized temperature profile for gas mixture combination of 0.205 Neon and 0.795 Argon mole fractions and temperatures 300 and 306 K

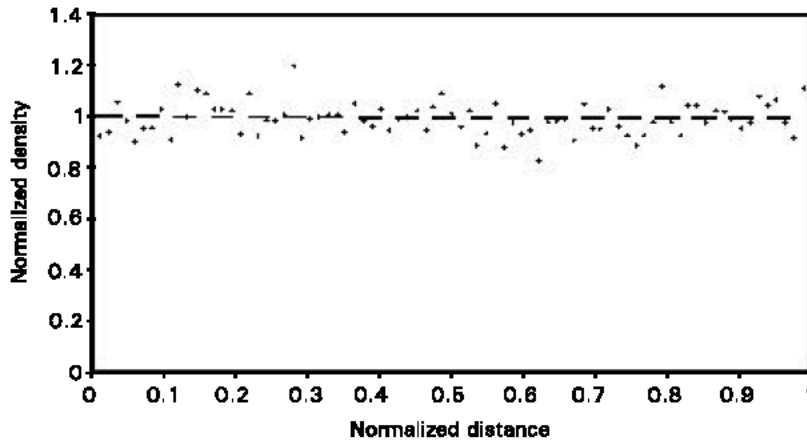


Fig. 2b: Normalized density profile for gas mixture combination of 0.205 Neon and 0.795 Argon mole fractions at pressure 1.01 bar and temperatures 300 and 306 K

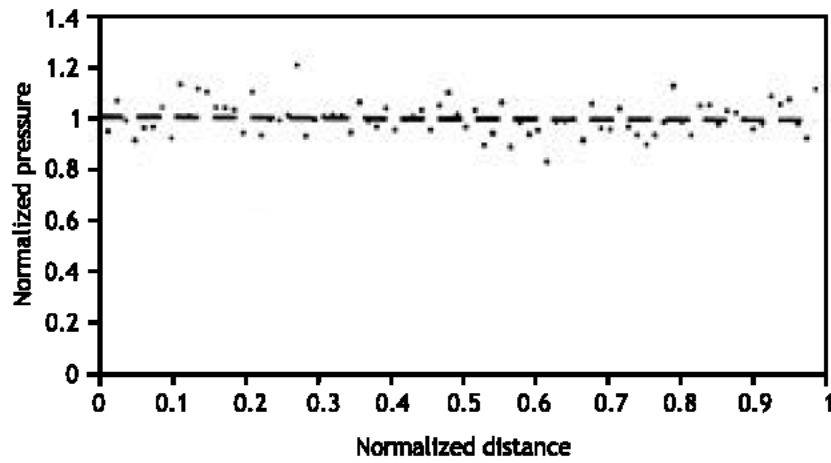


Fig. 2c: Normalized pressure profile for a gas mixture combination of 0.205 Neon and 0.795 Argon mole fraction at pressure 1.01 bar and temperature 300 and 306 K

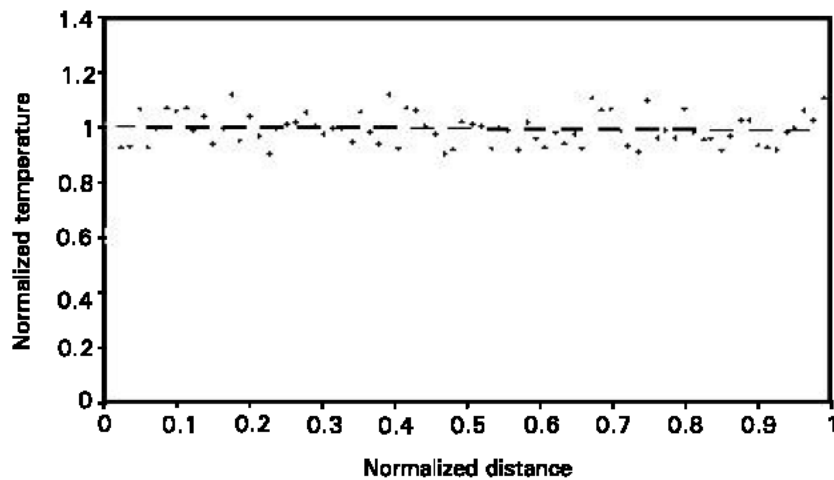


Fig. 3a: Normalized temperature profile for a gas mixture combination of 0.61 Neon and 0.39 Argon mole fractions at pressure of 1.01 bar and temperatures 300 and 306 K

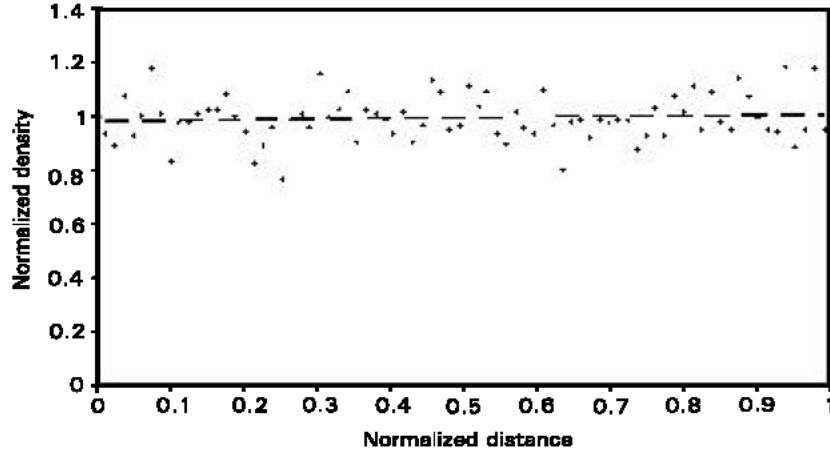


Fig. 3b: Normalized density profile for a gas mixture combination of 0.61 Neon and 0.39 Argon mole fractions at pressure of 1.01 bar and temperatures 300 and 306 K

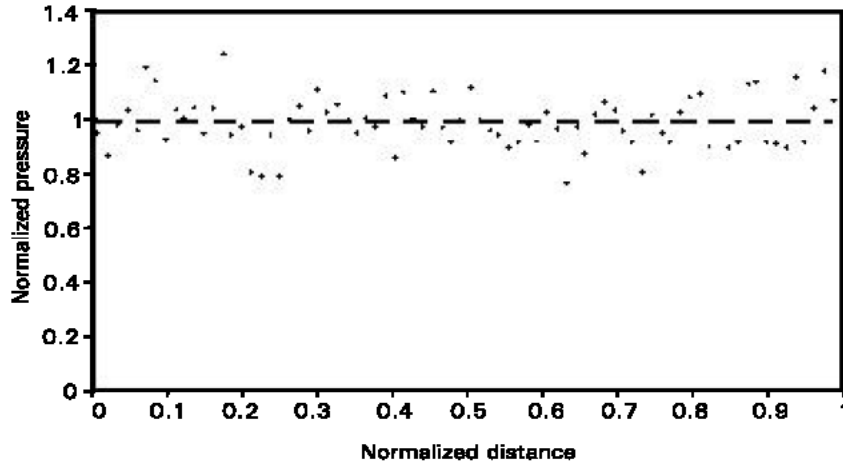


Fig. 3c: Normalized pressure profile for a gas mixture combination of 0.61 Neon and 0.39 Argon mole fractions at pressure of 1.01 bar and temperatures 300 and 306 K

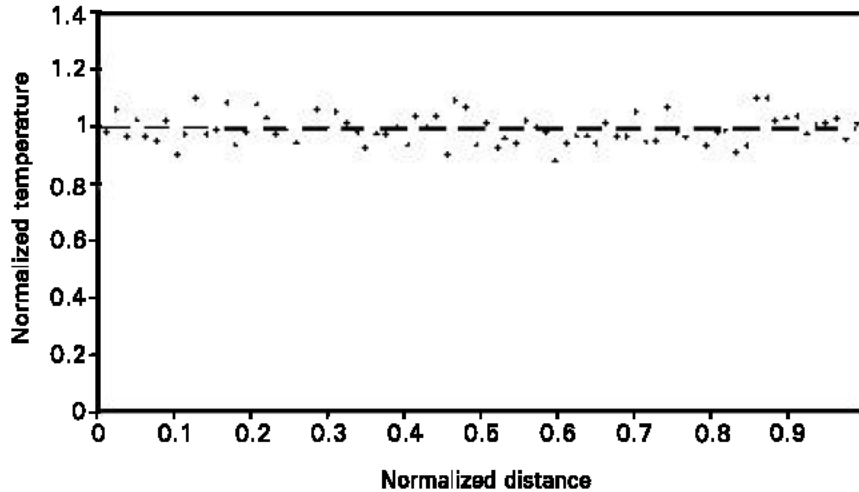


Fig. 4a: Normalized temperature profile for a gas mixture combination of 0.79 Neon and 0.21 Argon mole fractions at pressure of 1.01 bar and temperatures 300 and 306 K

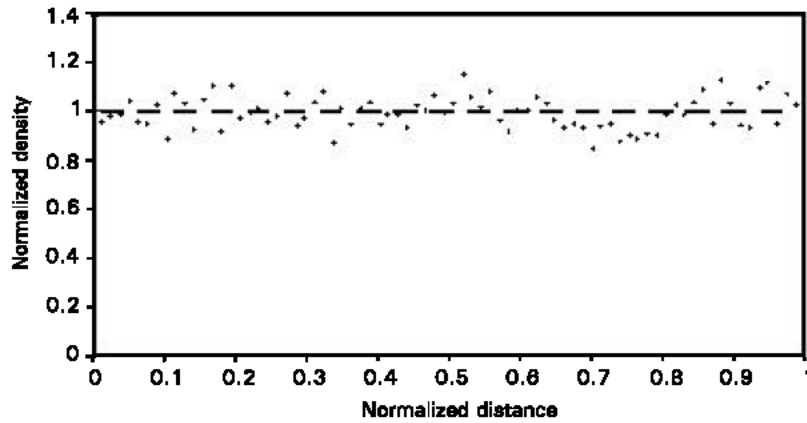


Fig. 4b: Normalized density profile for a gas mixture combination of 0.79 Neon and 0.21 Argon mole fractions at pressure of 1.01 bar and temperatures 300 and 306 K

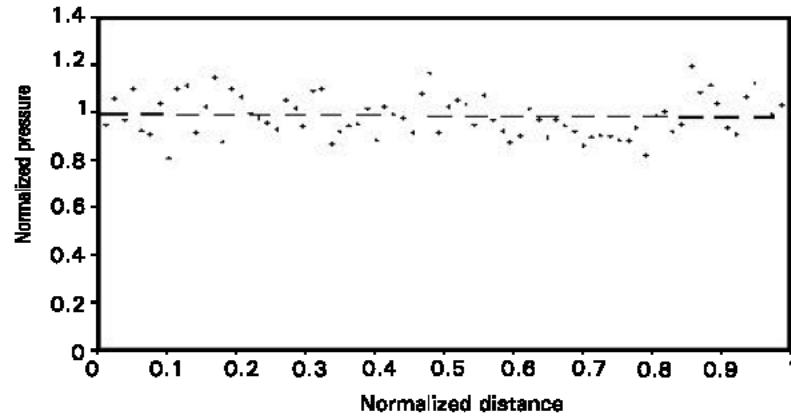


Fig. 4c: Normalized pressure profile for a gas mixture combination of 0.79 Neon and 0.21 Argon mole fractions at pressure of 1.01 bar and temperatures 300 and 306 K

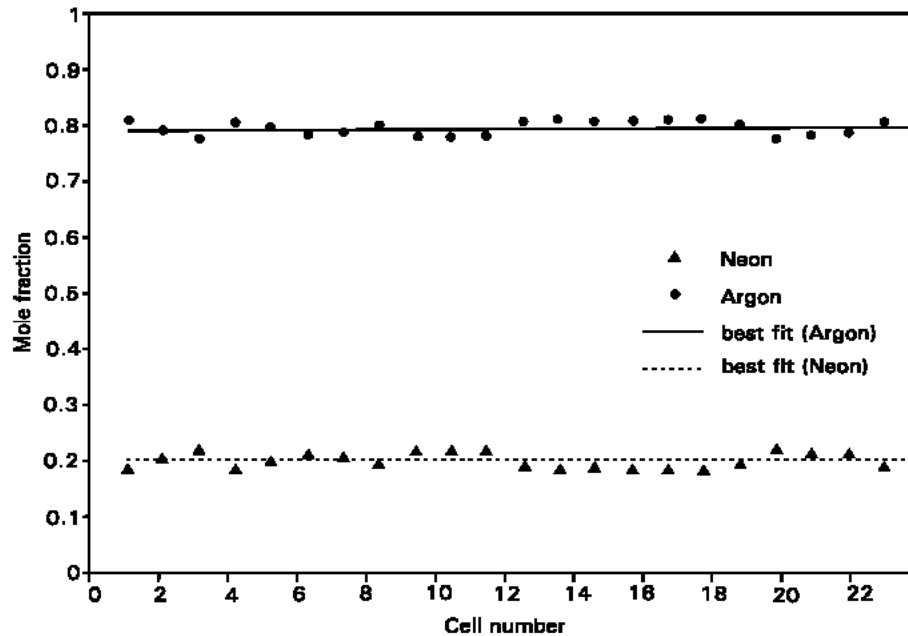


Fig. 5a: The distribution of the Molar fractions for the gas mixture ratios of Neon (0.205) and Argon (0.795) along the normalized distance between the two parallel plates at steady state



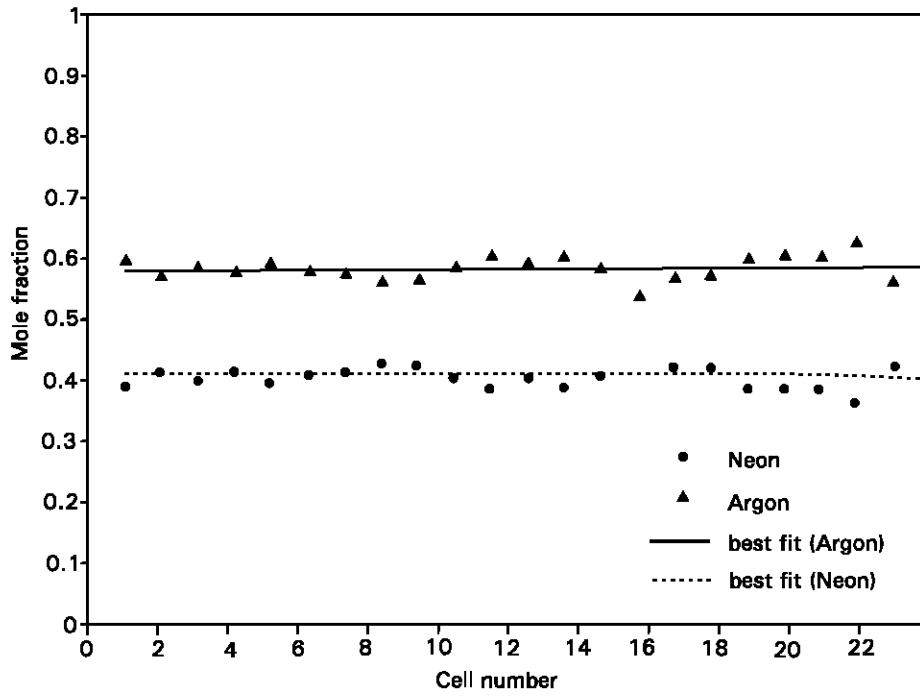


Fig. 5b: The distribution of the Molar fractions for the gas mixture ratios of Neon (0.41) and Argon (0.59) along the normalized distance between the two parallel plates at steady state

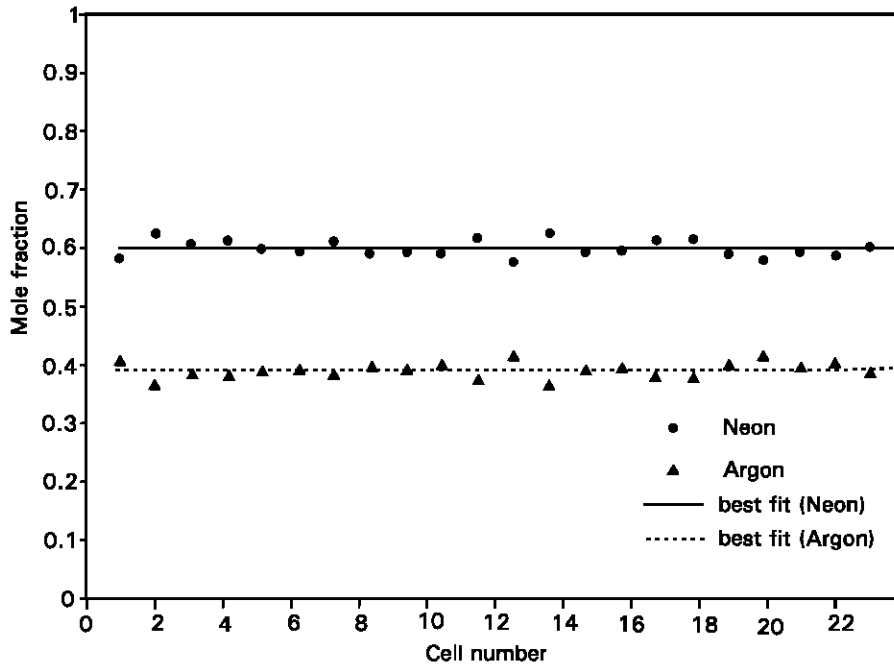


Fig. 5c: The distribution of the Molar fractions for the gas mixture ratios of Neon (0.61) and Argon (0.39) along the normalized distance between the two parallel plates at steady

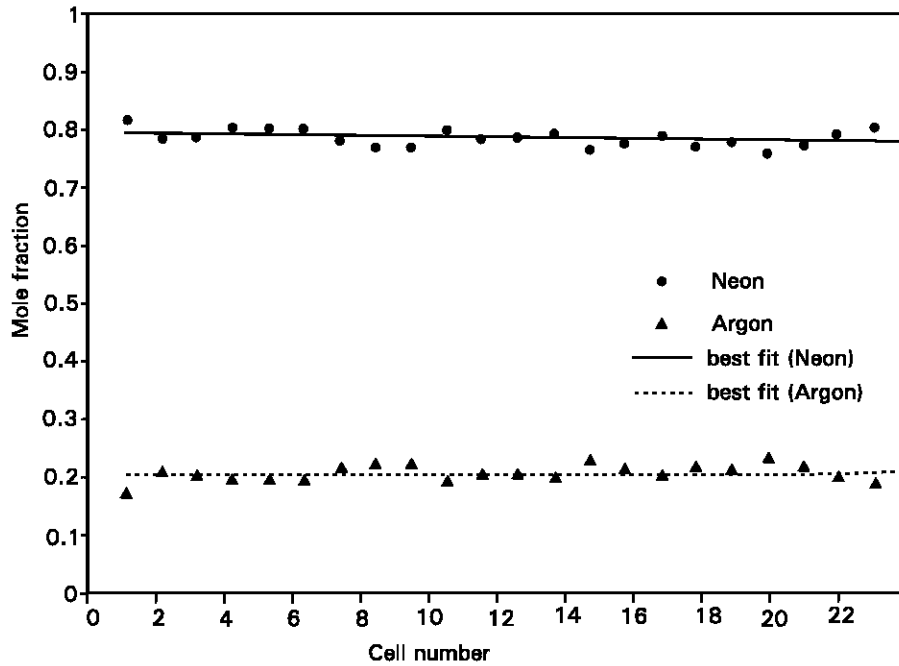


Fig. 5d: The distribution of the Molar fractions for the gas mixture ratios of Neon (0.79) and Argon (0.21) along the normalized distance between the two parallel plates at steady state

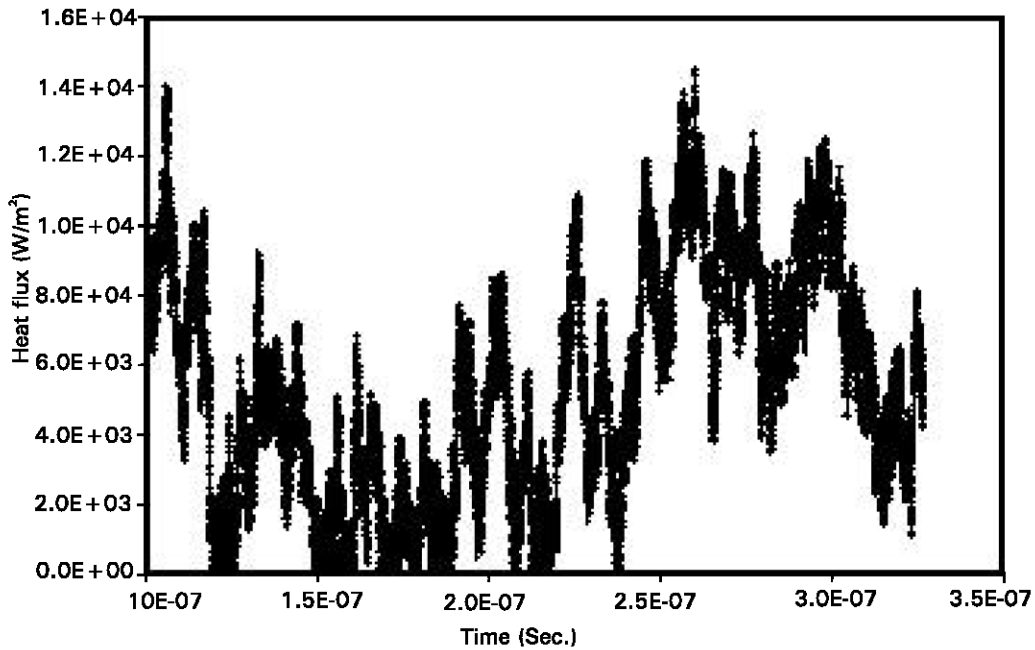


Fig. 6a: Heat flux pattern between the two parallel plates having temperature difference for Neon concentration of 0.35

approaching the free molecules level where Knudsen number greater than 0.1 since it has no approximations and it doesn't assume the continuum model.

The thermal conductivity of gas mixture consisting of two different species of monoatomic gas at pressure of

1.01 bar and 303 K have been examined using DSMC method. The values of thermal conductivity of the mixture has been determined at different mole fractions and compared with experimental results. Different batches of runs have been executed to calculate the statistical error

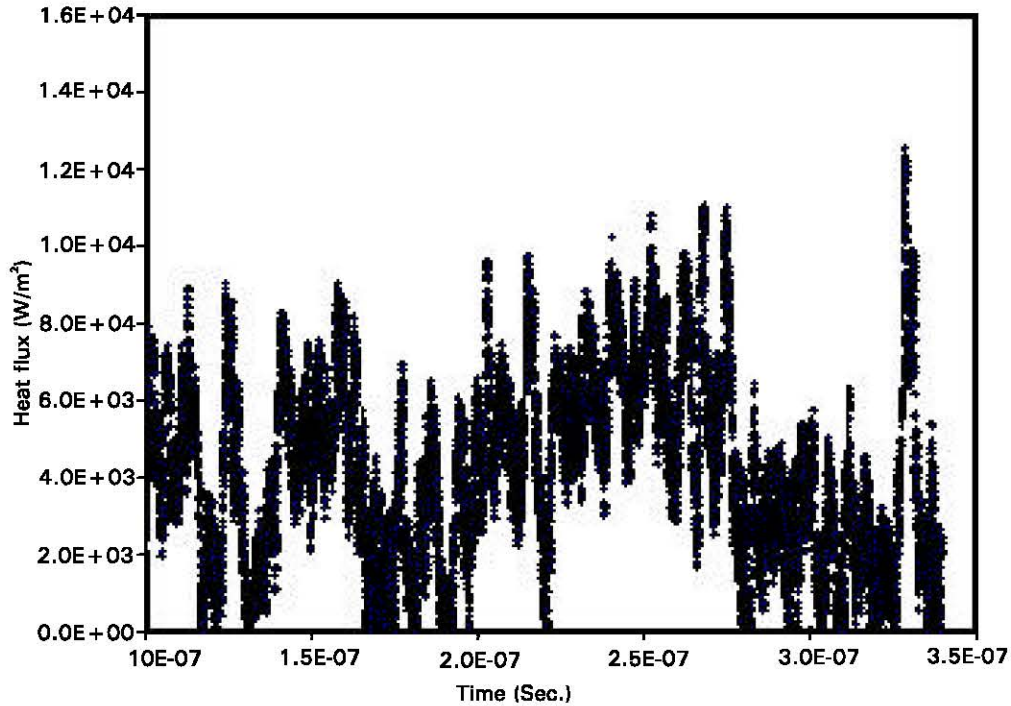


Fig. 6b: Heat flux pattern between the two parallel plates having temperature difference for Neon concentration of 0.45

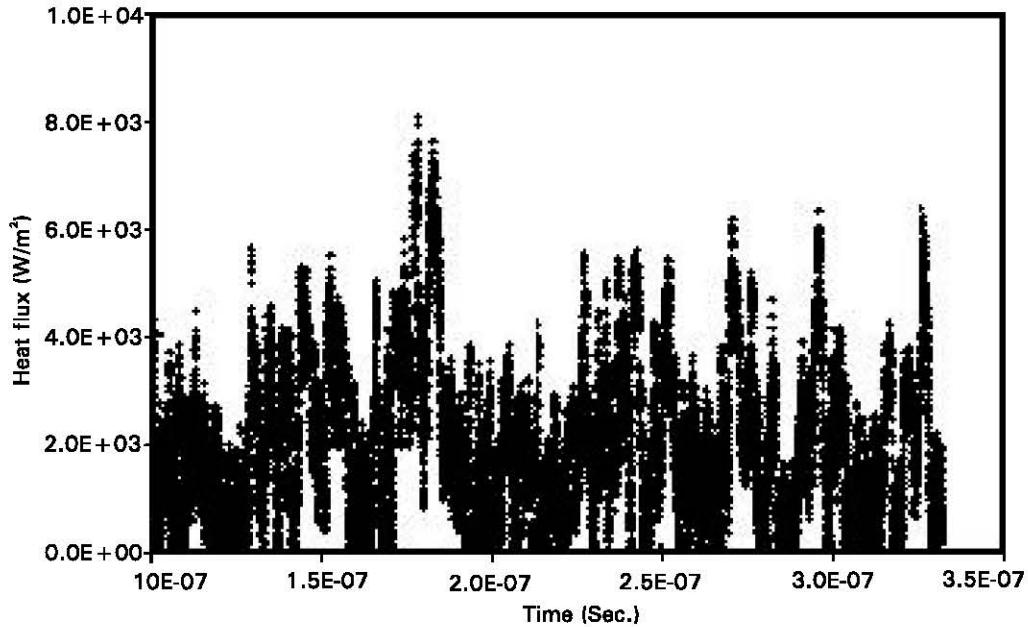


Fig. 6c: Heat flux pattern between the two parallel plates having temperature difference for Neon concentration of 0.55

in the determined values. The error was less than 15% in all cases. It has been found that the thermal conductivity of the gas mixture is not a simple linear relation depending on the thermal conductivities and molar fractions of the species. The error bars show that the statistical error increases as one of the species concentration is lower than the other. That is clear in Fig. (7) since error bars

amplitude increase around the 50% molar fraction. For pure gases this error is at minimum since all simulating molecules are of the same type. The results are consistent and the relative differences between the experimental and Monte Carlo results are within the statistical fluctuations of the method arising due to low number of simulating molecules than real ones. The DSMC method is a well-

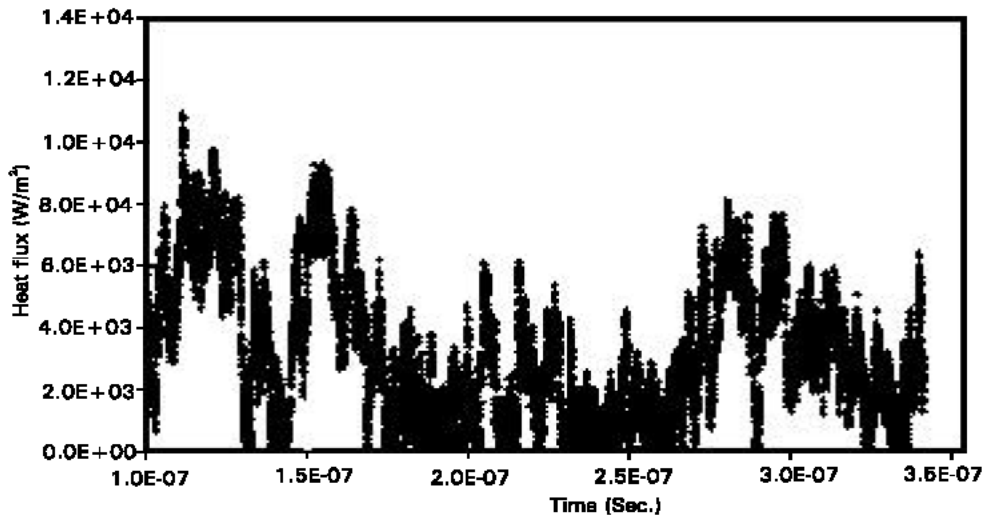


Fig. 6d: Heat flux pattern between the two parallel plates having temperature difference for Neon concentration of 0.65

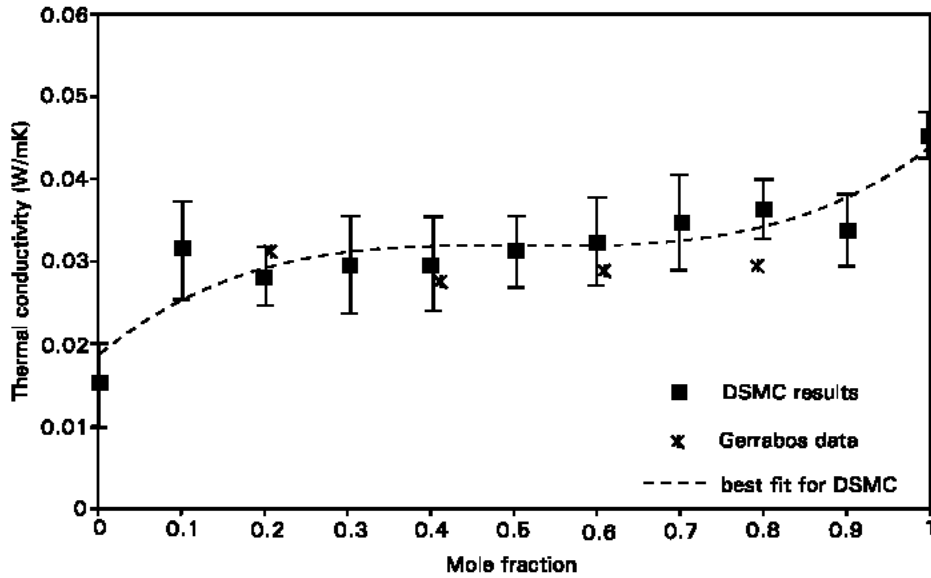


Fig. 7: Comparison between the thermal conductivity results obtained from DSMC method and the experimental data obtained from garrabos for different combination of gas mixtures Neon and Argon

established method for representing and calculating the macroscopic properties of a gas mixture especially when the gas is in the transition region between continuum and free molecular regimes. One of the main advantages of DSMC method is its uniqueness in representing the gas molecules for various Knudsen numbers.

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