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Molecular dynamics studies of anomalous transport in rarefied gases

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rarefied gas flows, free path distribution, Lévy flights, mean free path, molecular dynamics

ABSTRACT

We investigate the thermodynamically non-equilibrium gas dynamics by measuring molecular free path distribution functions, inter-molecular collision rates and wall dependent mean free path (MFP) profiles using the molecular dynamics (MD) method. The simulations cover a wide range of fluid densities for single-wall case, parallel walls cases and a cube with all periodic walls. The simulations are validated by deducing the theoretical unconfined MFP values at standard pressure and temperature conditions. The free path MD measurements of individual molecules convey that conventional exponential distribution function is not valid under rarefied conditions and molecules follow Lévy type flights, irrespective of the presence of a wall. MFP profile measurements for confined planar surfaces in the transition flow regime show sharp gradients close to the wall, while theoretical models predict shallower gradients. As gas transport properties can be related to the MFP through kinetic theory, our MD data may help to modify the constitutive relationships, which may then be fed into the Navier-Stokes equations for better effective modeling of micro gas flows in the transition flow regime.

1. INTRODUCTION

Studies of flows in micro- and nanochannels have been motivated primarily by their extensive technological applications in engineering, medical and other scientific areas [1]. Many of these devices would involve gas flows, and investigations of these flows at microscales raise questions regarding the non-standard behaviour of the fluid, as noticed in numerous experiments. The key parameter indicating the degree of departure from continuum fluid mechanics, the Knudsen number Kn, is defined as the ratio of the gas molecular mean free path λ (MFP) to the characteristic system length scale L. A detailed understanding of the physical behaviour of gases over a wide range of Knudsen numbers is imperative for the design of miniature devices and for the manipulation of materials at the molecular scale.

There are great difficulties in investigating microscale/rarefied gas flows experimentally [1]. Conventionally bulk properties can be measured reliably, such as average mass flowrate through a channel. Interpretation of these integral flow parameters, however, is problematic because there can be multiple causes of deviation of these quantities from those expected from conventional macroscopic theory, assigning their relative contributions is difficult. In addition, fitting of macroscopic theories to experimental data with the aid of tuning parameters, may not be physically realistic. This is due to the fact that fluid dynamic effects occurring over disparate physical scales are intensely coupled with a number of significant thermodynamic criticalities.

In this situation, methods for simulating microflows have come to the forefront. Many of the unusual effects observed in rarefied gas flow systems arise from the gas not being in thermodynamic equilibrium. To test this, fundamental properties of the gas – the inter-molecular collision rate, the molecular velocity distribution and the distribution of free paths between inter-molecular collisions need to be measured over a range of

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rarefied conditions. These properties can be measured in molecular dynamics (MD) simulations of a moving gas in unconfined and confined spaces [2]. MD is an appropriate method, compared to other simulation methods such as direct simulation Monte Carlo (DSMC) [3], to estimate these fundamental properties as it is the only deterministic approach, allowing for realistic molecular behaviour, i.e. molecular attractions, repulsions, movements and scatterings. The spatial and temporal variation of these averaged collision properties can give an indication of the non-equilibrium processes occurring in rarefied gases. This information is very difficult to obtain experimentally, so MD can be used to to explore unresolved issues in anomalous transport in rarefied gases.

The major objective of this paper is to to assess the distribution of molecular free paths, collision rates and mean free path profiles of non-equilibrium gases by molecular dynamics. Our simulations comprise of a cube with six periodic boundary conditions and single planar wall and two parallel planar walls cases. The working gas is Neon and the interaction of molecules is simulated using the Lennard-Jones (LJ) intermolecular potential. Such numerical experiments in non-equilibrium gas dynamics are useful for assessing the range of validity of classical distribution functions and traditional kinetic theories. It is well-known that transport property coefficients of gases (i.e. viscosity and thermal conductivity) can be interpreted in terms of the collisions of gas molecules, and of the free paths of the molecules between collisions [4, 5]. Hence, the present atomistic simulations are an invaluable tool for hypothesizing modified constitutive relationships appropriate for thermodynamically non-equilibrium flows.

2. MOLECULAR DYNAMICS METHODOLOGY

Molecular dynamics is a computer simulation technique where the time evolution of a set of interacting molecules is followed. This is done by numerically solving the equations of motion (Newton's laws) of classical multi body systems. Given the positions, masses, and velocities of all particles in the system, and the forces on the particles, the motion of all molecules can be followed in time by calculating the (deterministic) particle trajectories. To simulate rarefied gas flows, the open source software OpenFOAM (Open Field Operation and Manipulation) [6] is used with the molecular dynamics routines implemented by Macpherson et al. [7, 8]. A noble gas is considered in the present work as it has monoatomic molecules, which makes it relatively straightforward to interpret theoretically and to model using MD. We study Lennard-Jones (LJ) molecules for a range of fluid densities and combination of specular and diffusive implicit walls. The molecules are spatially distributed in the domain and given a random initial Gaussian velocity distribution, corresponding to the prescribed gas temperature. When two molecules separated by a distance r, realistic description of the molecular behaviour can be obtained using the short-range repulsive and long-range attractive smooth and continuous Lennard-Jones potential given by:

$$V_{LJ}(r) = 4\epsilon \left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6} \right], \tag{1}$$

where ϵ is related to the interaction strength of the molecules and σ is chosen to be equal to the hard-sphere diameter of gas molecules in order to relate the molecular dynamics MFP measurements to the theoretical mean free path values. Formally, in the Lennard-Jones potential all interactions between all nonbonded particles have to be calculated, but since this potential vanishes at larger r, only the interactions with molecules within a certain cutoff radius r_c need to be calculated. Cut off radius of $r_c = 2.5\sigma$ is here chosen to closely resemble the original Lennard-Jones potential. The equations of motion are integrated using a leapfrog scheme [8] with a step size of 0.005τ, where $\tau = (m\sigma^2/\epsilon)$ ($10^{-12}s$) and m is the atomic mass. The spatially resolved flow parameters are written at intervals of 20τ, and the total run time of simulations is at least 3000τ - in the extreme rarefied case, up to 50000τ. In all simulations we model Neon gas, with molar mass m, σ, ϵ and λ at STP conditions as 20.180 $[kg/kmol]$, $2.5830 \times 10^{-10}[m]$, $7.1957 \times 10^{-22}[J]$ [3] and $1.233 \times 10^{-7}[m]$ [5] respectively.

2.1 Definition of Collision

In order to be able to record the distribution of molecular free paths, collision rates and mean free path values, we need to declare how a collision is defined in MD. It has been stated [2] that free paths between collisions can only be defined when the molecules are represented by step intermolecular potentials, such as the hard sphere (rather than a more physically realistic potential, such as the LJ). While the instance of a collision is unambiguous with a step potential, the time step of simulation correspondingly needs to be very close to zero [2], which

makes the simulation computationally highly expensive. As we have implemented the continuous LJ potential here, we set a closeness parameter, r_{col}, and declare a collision to have occurred if two molecules are closer to each other than this distance. Molecules start to exchange momentum as soon as they are within the distance of the cut-off radius r_c, and they start to repel each other when they are closer than σ. Hence, r_{col} lies between σ and 2.5σ, its appropriate value is evaluated through simulations of the the theoretical unconfined mean free path value for Neon gas at standard conditions. Results for a closeness parameter of σ are within about 1% of the theoretical MFP value. If r_{col} is set to 2.5σ, the MD simulation result obtained is 15% less than the theoretical MFP value. So we decide to choose σ as the appropriate value for r_{col}, and all the simulations in this paper have been carried out using this value. Note that theoretical value of MFP is calculated through the gas dynamic viscosity and density [5]:

$$\lambda_{Ne} = \frac{\mu}{\rho} \sqrt{\frac{\pi}{2RT}}, \tag{2}$$

where μ is gas dynamic viscosity, ρ is gas density, R is specific gas constant and T is temperature.

The current collision handling algorithm allows the evaluation of multiple collisions (collision events which involve three or more molecules simultaneously), whereas the step potential approach can only handle binary collisions. This has direct implications for identifying the limit of the dilute gas approximation employed when deriving the Boltzmann equation.

Three new molecular attributes, t_{LC}, Sp_C and Col are implemented in the default MD solver existing in the OpenFOAM: t_{LC} is the time of the last occurring collision, and Sp_C is the current speed of the molecule. The attribute Col keeps track of whether a molecule is currently undergoing a collision in which case it is activated (set to 1), which happens if the molecule is closer to any other molecule than the distance of σ. Col is deactivated (set back to 0) if the molecule is at a distance greater than σ to any other molecule and if it is currently activated.

2.2 Recording the Free Path

For recording the free paths of individual molecules, it is not convenient to directly measure the travelled distance of the molecule as a difference between the current position of the molecule and the position of its last collision when periodic boundaries conditions are implemented, which are typical in MD simulations. Instead the molecular free path, l, is obtained by:

$$l = (t_C - t_{LC}) \times Sp_C, \tag{3}$$

where t_C is the current simulated time, which is easily accessible to the default solver. The attribute t_{LC} is set to the current simulation time when a collision occurs. The present method records the molecular free paths in every time step, unlike the conventional method of measuring the molecules' travelled distance between two successive collisions, which only can be recorded at certain times once collisions occur. The major advantage of the present method is that we can calculate the probability that molecules travell a distance with out experiencing a collision, i.e. the free path distribution function. The average of these free paths of all simulated molecules is expected to recover the mean free path value. It should be noted that this recording of collisions and free paths does not affect the original way the MD solver predicts the dynamics of the gas.

3. SIMULATION RESULTS AND DISCUSSION

Figure 1 is a schematic illustration of the various MD measurements we perform on Neon gas. Collision rate probabilities, distribution of free path lengths, and steady state mean free path values at different rarefied conditions are measured in an unconfined cube. Mean free path profiles as a function of wall distance are recorded for planar one-wall and parallel-wall cases, and the walls are modelled as specularly reflecting surfaces.

3.1 Unconfined Box

To validate our MD method we chose to test for the unconfined value of the mean free path and the exponential distribution of free paths of Neon gas at standard conditions. We have simulated a cube shaped geometry with periodic boundary conditions, i.e. the system is simulated as if it is surrounded by infinite copies of it self.
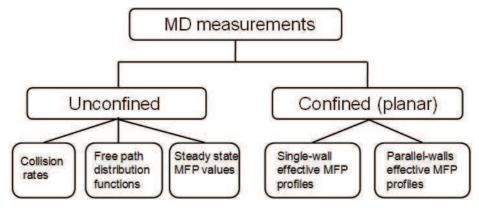
Figure 1: Schematic representation of the gas molecules fundamental properties measurements using molecular dynamics.

In practical terms, this means that when molecule leaves one side of the domain, it is wrapped-round and reintroduced on the other side, retaining the same velocity. The side-length of the simulated cube is chosen to be the MFP of Neon at STP conditions ($\lambda_{Ne} = 1.233 \times 10^{-7}[m]$ [5]) and the box is filled with 51505 molecules at a density (ρ) of 0.9011 [kg/m^3]. A mesh consisting of 16^3 cells is applied so that there are more than 12 molecules on average per cell, while at the same time the cells are sufficiently small in order to decrease the computational time cost [8].

Figure 2 shows the recorded mean free paths for Neon gas as a function of simulation time. The first case, Fig. 2(a), at the standard density value of 0.9011 [kg/m^3] is simulated for 3×10^{-9} [s] and the MD measurements reach MFP value of 1.221×10^{-7} [m] differing from the theoretical value of MFP (λ_{Ne}) within about 0.96%. We also counted the binary collisions separately by discarding a molecule as undergoing a collision if its counterpart molecule is already undergoing a collision, i.e. a molecule with $Col = 0$ cannot collide with a molecule with $Col = 1$. At standard density, among the total number of collisions, binary collisions are recorded to be around 96.92%, and the rest are multiple part collisions. If we only record binary collisions, the mean free path measurements by MD predict a MFP of 1.262×10^{-7} [m]. This value is close to the kinetic value of the mean free path (λ_k) given by [4]:

$$\lambda_k = \frac{m/N_{Av}}{\pi \rho \sigma^2 \sqrt{2}}, \tag{4}$$

where N_{Av} is Avogadro's number, 6.0221415×10^{23} and the above equation yields a MFP value of 1.255×10^{-7} [m]. This indicates that the kinetic theory description of mean free path is accurate if collisions are purely binary and also gas is under equilibrium. Fig 2(a) demonstrates that the dilute gas assumption may not be valid at higher densities cases, although the gas is under equilibrium.

Figures 2(b) and 2(c) show the MFP measurements at density values of 0.4837 [kg/m^3] and 0.1055 [kg/m^3] respectively. These two simulations are carried out at relatively rarefied conditions and the corresponding side-lengths of the cube are chosen to be $1.25 \times \lambda_{Ne}$ and $2.5 \times \lambda_{Ne}$ respectively. Both these rarefied cases are simulated up to $4 \times 10^{-9}[s]$ and $10 \times 10^{-9}[s]$, respectively, as intermolecular collisions are reduced and the steady-state MFP values are reached more slowly compared to the standard density case. Multiple-particle collisions are reduced with decrease in gas density, and fluctuations in MFP values relatively increase. MD predicts MFP values of $2.275 \times 10^{-7}[m]$ for case (b) and $10.289 \times 10^{-7}[m]$ for case (c), and the results differ from the theoretical values within about 1.07% and 2.31% respectively. The MD data for case (c) underpredicts the theoretical value, which may be due to the rarefaction effects. Although the binary collisions assumption is appropriate in this rarefied case, the MD data underpredicts also the kinetic value of mean free path given by Eq. (4), which assumes the gas is in equilibrium.

3.1.1 Distribution of Free Paths

Besides the value of mean free path, the distribution of individual molecular free paths is also of interest [4]. For a group of similar gas molecules moving at a speed $\bar{v}$ with a collision rate of $\dot{\theta}_v$, the molecular mean
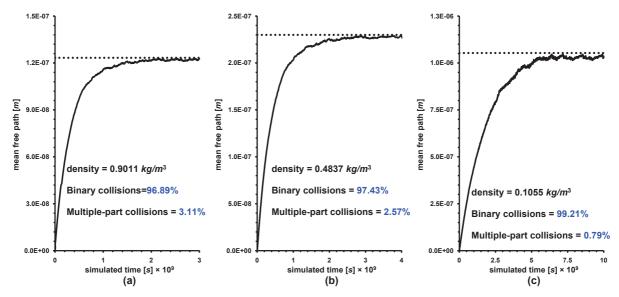
Figure 2: Steady-state relaxation profiles of the mean free path measurements as a function of simulation time for density values of (a) 0.9011 $[kg/m^3]$, (b) 0.4837 $[kg/m^3]$ and (c) 0.1055 $[kg/m^3]$. The theoretical values of the mean free paths [5] are illustrated by the straight dotted lines.

free path $\lambda = \overline{v}/\dot{\theta}_v$. If the gas molecules are in thermodynamic equilibrium, then the distribution of free path lengths, $\psi(r)$, can be derived as [4]:

$$\psi(r) = \lambda^{-1}p(r) \text{ and } p(r) = \exp\,(-r/\lambda), \qquad (5)$$

where $p(r)$ describes the probability of a molecule traveling distance r without experiencing any collision with other moving molecules in the group. If the gas is not bounded, the MFP of the gas molecule ensemble is simply $\int_0^\infty r\psi(r)dr = \lambda$. By *thermodynamic equilibrium* we mean that the probability of a certain microscopic state, averaged over the details of the interactions, does not change in time or space [9]. So, Eq. (5) is only valid under equilibrium conditions, i.e. if $\dot{\theta}_v$ is constant or fluctuations in $\dot{\theta}_v$ are negligible.

Figure 3 shows the variation of collision rate per unit number density as a function of MD simulation time for densities of 0.9011 $[kg/m^3]$ and 0.1055 $[kg/m^3]$. At standard density conditions Fig 3a, the mean and standard deviation of collision rate are 4.1×10^{-11} and 9.49×10^{-12}, respectively and thus the temporal fluctuations are low. For the rarefied case Fig 3b, the fluctuations are significantly higher and the ratio of standard deviation to mean of collision rate is around 0.77. One can infer from Fig. 3b that the assumption of collision rate to be constant in time may not be valid under rarefied conditions, so the probability distribution of free paths is not necessarily exponential in form.

Although, it is certainly difficult to evaluate the actual probability distribution function $\psi(r)$, introducing non-equilibrium by means of physical arguments could allow us to propose a distribution function that may be more appropriate for non-equilibrium conditions than the exponential one [9]. Non-equilibrium gas transport is often better described using Levy/power-law type of distribution functions [10, 11]. Montroll and Scher [11] pointed out that a finite moment of the probability distribution function implies an exponential character of the randomness. A distribution function with diverging higher-order moments, such as the standard deviation, is essential to non-equilibrium transport.

We hypothesize a Power-law form for the probability distribution function for non-equilibrium MFP, with diverging higher-order moments, instead of the classical exponential form of distribution function. Here we propose for investigation the following molecular free path distribution function [15]:

$$\psi(r) = C(a + r)^{-n}, \qquad (6)$$

where a and C are constants with positive values determined through the zero and first moments. The range of values for the exponent n can be obtained by making one of the higher-order moments divergent. Zero and first
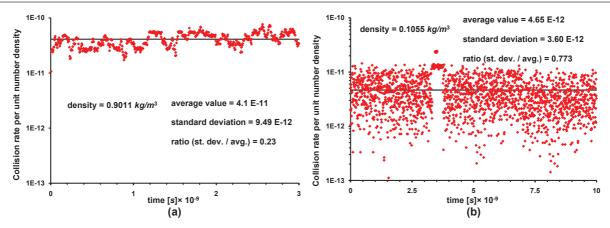
Figure 3: Collision rate per unit number density as a function of simulation time, for density values of (a) 0.9011 $[kg/m^3]$ and (b) 0.1055 $[kg/m^3]$. Mean values of all samples are illustrated by the straight lines.

moments are given as follows:

$$1 = \int_0^\infty C(a+r)^{-n} dr, \tag{7}$$

$$\lambda = \int_0^\infty C r (a+r)^{-n} dr. \tag{8}$$

Equation (7) requires the probability to range only from zero to one. Equation (8) defines the unconfined, conventional MFP value, λ. It then follows that $C = (n-1)a^{n-1}$ and $a = \lambda(n-2)$. If $n > 2$, $a > 0$, otherwise the distribution function is negative. The standard deviation (second moment) of the distribution function given by Eq. (6) diverges only for $n \leq 3$; so $2 < n \leq 3$. If one wishes to make the ith moment diverging, then $\max(n) = i + 1$. As $n \to \infty$, the distribution function will have finite moments, which is the condition required of an equilibrium distribution function. For a finite n, the distribution function describes a system deviating from equilibrium. Thus, n acts as a decisive parameter to define the extent of deviation from equilibrium.   Figure 4 depicts the variations of the probability a molecule travells a distance without

experiencing a collision, as a function of normalized distance (r/λ), at atmospheric and rarefied conditions (here λ refers to the theoretical MFP values at corresponding densities). At atmospheric density conditions, both MD measurements and the power-law model agree well with the classical exponential distribution functions. In this case $n = 16$ is used in the power-law model to fit the MD data, and this larger value of n conveys that the system is not far from equilibrium. Minor deviations from the exponential distribution are noticed, and this is probably due to the consideration of multiple particle collisions. At low density conditions, the deviations between the MD measurements and the classical distribution function are significant and the discrepancies are relatively high at longer free paths (see inset of Fig. 4(b)). The power-law model with an exponent n value of 9 has good agreement with the MD data, and this decrease in n illustrates that the system is moving towards non-equilibrium with decrease in density. Another major disagreement is that both the MD data and the power-law predict a long tail to the distribution function, while the classical function shows a much faster decay of free paths. This faster decay of free paths conveys that the system does not have many longer flights of molecules, and follows the Brownian motion described by Einstein [13]. However, this is only valid for times much larger than a characteristic time that, in turn, is much larger than the times characterising molecular collisions, and this condition may not be fulfilled under rarefied conditions. The MD data and power-law results show longer Levy-type free flights of molecules in Fig. 4(b), and this long tail of the distribution function implies higher-order moments are diverging.

3.2 Confined Planar Surfaces

Equations (5) and (7) show that the mean free path of the gas molecule ensemble reduces to the theoretical value of MFP only if the gas is not bounded. If a solid bounding surface is included in the system, however, some molecules will hit the surface and their free flight paths will be terminated. The MFP of all the gas molecules in the system will therefore be smaller than λ, due to this boundary limiting effect. Stops [14] derived this geometry dependent MFP based on the exponential distribution function and Dongari et al. [15] developed
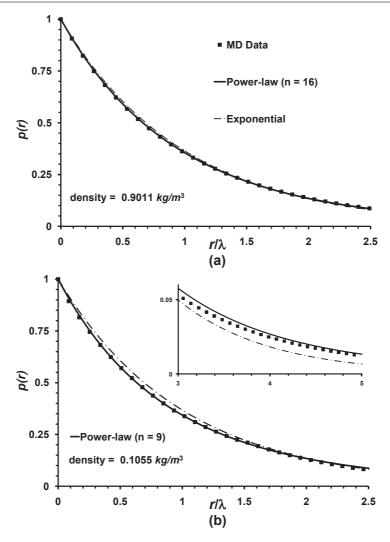
Figure 4: Probability of distance travelled by molecules without experiencing a collision, presented as a function of normalized distance, for gas density values of (a) 0.9011 [kg/m^3] and (b) 0.1055 [kg/m^3]. Molecular dynamics measurements are compared with the exponential and power-law distribution functions. Power-law exponent n values are taken as 16 and 9 in (a) and (b) cases, respectively.

it using the power-law form of distribution. The power-law exponent n value is considered to be 3, for both single- and parallel-wall comparisons below.

Here we conduct MD measurements of the MFP of gas molecules when bounding planar surfaces are introduced into the system, and compare the simulations with theoretical geometry dependent MFP solutions [14, 15]. A gas molecule's collision with a wall should terminate the free path in the same way as an inter-molecular collision, and so the MFP value should be shortened in the near-wall region. We carry out the simulations in a six sided configuration using two reflective bounding surfaces, together with two pairs of periodic boundaries, which replicates a parallel plate with infinite width and length. The reflective surfaces are chosen to yield only specular reflections, where the molecular tangential velocity is maintained and the molecular normal velocity just changes sign. In determining the wall effects on the free paths we will once again use the formulation for the travelled distance of a molecule since it experienced its last collision, given by Eq. (3). Molecular reflections on planar surfaces are simulated by setting t_{LC} to current simulated time, as done before for gas inter-molecular collisions. We examine the two cases consisting of the mean free path profile affected by a single- and parallel planar walls.

For simulating the mean free path profile for the single-wall case, we use domain side lengths of $1 \times \lambda_{Ne}$ in the periodic boundaries directions, and $2 \times \lambda_{Ne}$ in the bounding surface directions. The configuration uses 16 $\times$ 16 cells in the periodic boundaries directions, and 40 cells in the bounding surface directions. The simulated
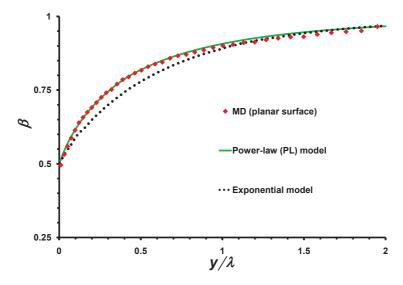
Figure 5: Variation of normalized mean free path, β, with normalized distance from a surface for planar single-wall case. Comparison of molecular dynamics simulation data with power-law (PL) [15] and exponential [14] effective MFP models.

gas is represented by 102950 molecules and the sampling of the effective/geometry-dependent MFP (λ_{eff}) profile is made over 2 nano seconds, taken after 3 nano seconds settlement, in terms of the simulation time. One reflective wall surface is used to simulate the bulk of the flow, so that only one-wall effects are taken into account; this is done by setting all reflected molecules at one wall to have experienced a collisionless travel of one mean free path by setting t_{LC} equal to the current simulated time minus λ_{Ne}/Sp_C.

Figure 5 shows the variation of normalized effective MFP profiles (i.e. $\beta = \lambda_{eff}/\lambda$) with normalized wall distance, y/λ. MD simulations are in close agreement with the power-law predictions, although minor deviations are noticed in the bulk region. Both the measurements and the power-law model have a sharp gradient close to the wall, while the exponential model has shallower gradients and underpredict the MFP values in the wall vicinity. All three solutions converge to the unconfined MFP value in the bulk region, as expected.

For simulating the parallel-wall case, a similar geometry is used and the Knudsen number is tuned by changing the gas density value. At low-density/high-Kn cases, as the total number of molecules are less, the number of cells in the periodic boundaries directions are accordingly decreased, so that there are at least 10 molecules on average per cell. Results for the normalized MFP between two parallel surfaces are presented in Figure 6. The total simulation time varied from 5 to 20 nano seconds, based on the degree of rarefaction. MD simulation results for planar smooth surfaces are compared with both PL and exponential distribution function-based MFP models for various Kn in the transition regime. At $Kn = 0.2$, which is just beyond the slip-flow regime, the PL model is in fair agreement with the MD data in the near-wall region but deviates slightly in the bulk region. The exponential model underpredict the MD data in the near-wall Knudsen layer and shows fair agreement in the bulk flow. As the value of Kn increases, and the flow becomes increasingly transition-continuum, the classical model fails to predict the effective MFP in the wall region, as well as in the bulk. Effective MFP values predicted by the PL model compare very well to the MD data for both $Kn = 0.5$ and 1, although it overpredicts for $Kn = 1$ in the bulk. By $Kn = 2$, when both the wall Knudsen layers completely overlap each other, the PL model shows significant deviations from the simulation data and overpredicts in the near-wall region, although there is fair agreement in the bulk region. The MD data shows a relatively sharp gradient of effective MFP in the near-wall region, compared to the theoretical predictions.

4. CONCLUSIONS

A molecular dynamics simulation tool has been used to assess the gas fundamental properties: inter-molecular collision rates, molecular free path probability distribution, and mean free path values in unconfined and confined planar spaces. We simulated Neon gas molecules using the simple Lennard-Jones interaction potential
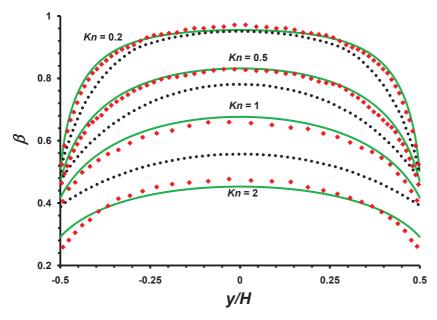
Figure 6: Variation of normalized mean free path, β, with normalized distance from a surface for the planar parallel-surfaces case. Comparison of molecular dynamics simulation data with power-law (PL) [15] and exponential [14] effective MFP models for Knudsen numbers ranging from the slip to the transition flow regimes. Symbols and lines are as in Fig. 4.

function. Theoretical mean free path values are deduced for different values of gas density by simulating an unconfined gas domain in space with periodic boundary conditions. As the rarefaction increases, multiple particle collisions become negligible in comparison with binary collisions and the dilute gas assumption is held to be valid under these conditions. These simplified assumptions employed in kinetic theory may introduce noticeable errors at typical atmospheric conditions [1].

Inter-molecular collision rate measurements show fewer fluctuations at standard density conditions, while the standard deviation is significantly high for a low density case, which illustrates the non-equilibrium nature of the rarefied gas. Correspondingly, molecular free path measurements predict a long tail, the classical exponential distribution function only being accurate under equilibrium conditions. The MD data follow a Levy flights behaviour, and compare well with the power-law distribution function.

Molecular free paths are terminated when gas molecules hit a bounding wall surface, so wall-dependent MFP measurements have been carried out for planar single- and parallel-walls cases. MD data is compared with the exponential and power-law based effective MFP solutions. The exponential solution underpredict the measurements in the near-wall region for both single- and parallel-wall cases, and shows shallower gradients close to the wall. Both the MD data and the power-law model predict sharper gradients in the near-wall region, with the power-law model having good agreement with the measurements up to $Kn \sim 1$. Deviations start to increase with further increase in Kn due to the overlap of Knudsen layers from both wall surfaces. The present MD results support the argument that anomalous behaviour of rarefied gases is better described with Levy/power-law type of distribution functions, as compared to the classical exponential function.

Wall-scaling modelling of constitutive relationships [16, 17] has been shown to usefully extend the applicability of Navier-Stokes-Fourier equations into the transition regime rarefied gas flows. However, these models are purely empirical, employing with some tuning parameters, and may not offer deeper physical understanding into the complex dynamics of rarefied gases. One may appropriately derive modified constitutive relationships and slip/jump boundary conditions based on Levy/power-law types of free path distribution functions, as gas transport properties are related to MFP through kinetic theory.

MD simulations in the present work only involve simple geometries with planar surfaces and isothermal gases with no external flow. It is important to validate the power-law model for distribution functions with MD data for complex geometries, employed with the combination of specular-diffusive and explicit walls, and for

non-isothermal/isothermal fluid flows.

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