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Velocity distribution and velocity correlation of mixture of gases in a nanochannel

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ABSTRACT

Molecular dynamics study of non-reacting and disparate mass binary gas mixture is conducted. To investigate the gas–surface interaction properties of the gas mixture, in non-continuum regime, the rarefied gas confined in a nanochannel is considered. While keeping the bulk number density a constant, the interaction properties of gas mixtures at different molar concentration of individual components are determined. The study discusses the calculation of accommodation coefficients and prediction of the reflected gas distribution using accommodation coefficients. The Maxwell-type model that use calculated values of accommodation coefficients accurately predicts the reflected tangential and normal distributions. The model is validated for different wall-fluid conditions. The velocity correlation of individual gases demonstrates that the individual components of gas mixture are accommodated in different proportion. The result from the study will be beneficial in the analysis and development of potential applications involving the flow of gas mixture in a nanochannel.

1. Introduction

Gas–surface interaction properties of confined fluids in micro and nanoscale systems are of great interest in the present time due to various emerging applications like thermal management of nanoscale systems, gas chromatography etc. [1]. The present study deals with the calculation and analysis of non-equilibrium gas–surface interaction properties of a binary gas-mixture in a nanochannel. The study of binary gas-mixture would be a basis for the study of multi component gas-mixtures that demand more comprehensive approach. The interaction properties of confined fluid in a nano-sized structure, as in a nanochannel, are different from bulk properties as the fluid–solid interaction and the fluid–fluid interaction are extremely significant at such smaller dimensions. The knowledge of momentum and energy accommodation to the surface of a channel wall is absolutely necessary for the improved design for various gas flow applications such as sorting, analysis, removal of a component etc. from a sample. It is well known that the accommodation properties are fundamental to any gas–surface interaction that are reacting or non-reacting.

The gas–surface interactions can be effectively analysed by molecular based numerical schemes [2–5]. Of these Molecular Dynamics (MD) method provides a deeper understanding of mechanism of gas–surface interaction, especially in the realm of nano-sized channels. The MD simulations have been used to study the separation properties of gas-mixtures through nanopores [6–8], diffusion of gases [9,10], interaction of single gas on gas-adsorbed solid surfaces [11,12] etc. A number of interesting phenomenon have been revealed by the MD analysis of internal rarefied gaseous flows for a single gas include accommodation properties, velocity profiles, and velocity correlation [13–17].

The experimental studies on the accommodation properties of single gas and gas mixture at moderately rarefied conditions report incomplete accommodation [18,19]. In addition, numerical study on gas mixture, which determine the value of accommodation indirectly, shows that values indicative of incomplete accommodation has to be chosen to match with the experimental observations [20]. The knowledge of accommodation properties of a gas-mixture is very important as they have widespread technological applications [21]. This suggests the importance of accurate assessment of accommodation properties in such systems. Prabha and Sathian have studied the accommodation properties of mixture of gases with molecular dynamics [22]. In the present study, our aim is to predict the velocity distributions of reflected atoms from

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the solid surface, by using the calculated values of accommodation coefficients (ACs), and study the velocity correlations for a disparate mass gas mixture.

The objective of the study is to analyse gas–surface interaction properties of the system, in which the gas mixture with no macroscopic movement is confined between infinite parallel walls, at moderately rarefied conditions. MD simulations are carried out to investigate the gas–surface interaction properties of a binary gas-mixture (argon and xenon) on the walls (platinum) of a nanochannel at non-equilibrium conditions. The interaction properties of the mixture at different molar concentration of individual components are determined, keeping the bulk number density a constant. The energy accommodation coefficient (EAC) and its partial components are obtained for a gas-mixture with equal molar proportion. The reflected distributions in different directions are predicted with Maxwell-type boundary conditions using the calculated values of partial energy accommodation coefficients. Apart from these, speed distribution, collision rate, and velocity correlation in the tangential and normal directions are also examined.

2. Details of simulation

In this study, the infinite parallel solid walls of the nanochannel are assumed to be flat, smooth and without any defects. The simulation conditions are the same as in our previous study [22]. However, certain aspects of the simulation are briefly explained here. The dimension of the simulation box is $10 \times 12 \times 10$ nm and periodic boundary conditions are used in all directions. Initially, the solid atoms are packed with FCC structure and the gas atoms are arranged randomly with a number density of 1.27 nm^{-3}, which is low enough to keep the system at moderately rarefied conditions. The spacing between the solid walls (L) is 10 nm. The kinetic theory model for hard sphere molecules is used to calculate the mean free path and the Knudsen number (Kn) is found to vary from 0.114 to 0.152, thereby placing the system in the transition regime [23].

The interactions are modelled using Lennard–Jones (LJ) potential [24]. The potential is defined as

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad (1)$$

wherein σ and ϵ represents the characteristic length and energy parameters respectively. The LJ model is used for all interactions and the parameters used in the simulation are listed in Table 1 [13,14]. The cut-off distance (2.5σ) is selected by considering the factors such as the force field strength, rarefaction levels etc. [22]. The interaction parameters for Ar–Xe interaction are computed by Lorentz-Berthelot mixing rules [24]. The trajectories of the atoms are calculated using Velocity-Verlet algorithm. The temperature is controlled using Berendsen thermostat and the temperature of both the walls are maintained at 300 K [25]. The total simulation is divided into two parts; one part is the equilibration phase and the other part is production run from which the data for calculations are obtained. The atoms impending collision with the solid wall are tracked in the collision tracking plane. The location of the collision tracking plane is decided to be at the wall–gas interaction cut-off distance which is at 0.8 nm from the solid wall. It is 2.5 times the characteristic diameter (σ) for the largest of the two gas atoms (xenon). Parallel algorithms for classical molecular dynamics are used for implementing MD simulations with short range forces [26].

Table 1
The values of LJ parameters and mass are given. The units are given in the brackets.

Interaction	σ (nm)	ϵ (J)
Ar–Ar	0.340	1.654×10^{-21}
Xe–Xe	0.393	3.045×10^{-21}
Pt–Pt	0.247	5.207×10^{-20}
Pt–Xe	0.320	1.700×10^{-21}
Pt–Ar	0.294	1.093×10^{-21}

3. Results and discussion

Unless specified otherwise, the results reported are for gas at 400 K and the mixture at equal molar concentrations. The temperature of the gas is controlled in the region between collision tracking planes, so as not to influence the accommodation mechanism [16,22].

3.1. Speed distribution

When a gas-mixture is maintained at constant temperature, the individual components of the gas-mixture, streaming towards a direction, will be having the same energy distribution as that of bulk gas [22]. Alternatively, for a disparate mass gas-mixture, the velocity/speed distribution of individual components will be having dissimilar distributions whereby, the notion of collision rate is obtained. The probability distribution describing the scatter of molecular speeds approaching the solid surface is given in Fig. 1. The collision data are used for the illustration of speed distribution. As seen from the figure, it is a skewed distribution with the most probable speed is below the average speed. The distributions of individual constituents can also be observed from the figure. The heavier gas has a higher peak indicating less averaged speed whereas the lighter gas has a lower peak. The speed distribution of mixture of gas is close to the lighter gas constituent showing that the lighter gas chiefly contributes to the gas mixture distribution.

At every point, the distribution for the mixture is located between the individual gas distributions. It has been observed that the incident distribution can be expressed as a linear combination of distributions of its constituents. It is given as

$$f_v = f_1 f_{v1} + f_2 f_{v2} \quad (2)$$

where f_1 and f_2 are the fractions of collisions as constants for the linear combination. The collision rates of individual components

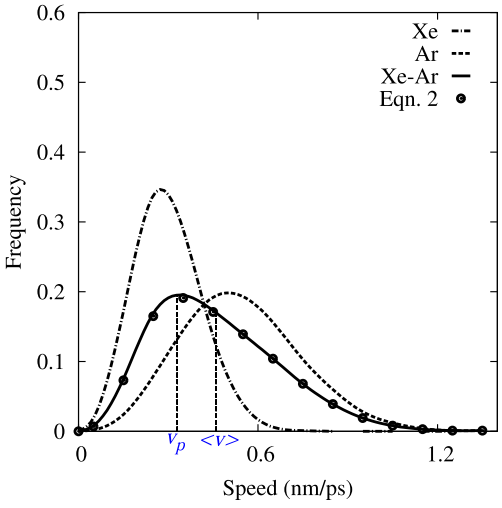

Fig. 1. The incident speed distribution for the gas mixture, and for each component gas of the mixture.