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The effect of characteristic length on mean free path for confined gases

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HIGHLIGHTS

- The work gives insight into the influence of characteristic length on the MFP.
- The effect of characteristic length on MFP is significant at low fluid densities.
- The variation of MFP with characteristic length is non-linear for a solid wall.

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ABSTRACT

Molecular Dynamics simulations are performed to investigate the influence of system boundaries and characteristic length (L) of the system on the mean free path (MFP) of rarefied gas confined to the walls of a nano-channel. Isothermal Lennard-Jones fluid confined between Reflective walls and platinum walls at different number densities (0.31 atoms/nm^3 and 1.61 atoms/nm^3) are independently considered. The MFP is calculated by the Lagrangian approach of tracking the trajectory of each atom and averaging the distance between successive collisions. The percentage of fluid–wall collisions is observed to predominate over fluid–fluid collisions at high levels of rarefaction. The influence of L (varying from 6 nm to 16 nm) on MFP is examined in this regime. At lower Knudsen number (Kn), it is observed that the effect of L on MFP is minimal. However, at higher rarefaction the characteristic dimension influences the MFP significantly for various wall configurations.

1. Introduction

Nano-scale fluid flow has drawn a great deal of attention because of its significance in the micro/nano mechanical systems. The behaviour of gases in the nano-conduits of micro-pumps, micro-turbines, micro-heat exchangers, etc., is affected by the level of rarefaction of gases and also by the wall–gas interaction parameters at the interface [1]. Knudsen number (Kn), the ratio of mean free path (MFP) to characteristic length (L) of the system, which is a direct measure of the level of rarefaction has a significant effect on the boundary conditions in the transition regimes [2]. In slip regime also the Knudsen number has a significant effect on the flow parameters in the micro-channels [3].

Many experimental as well as numerical studies have been successful to extend the validity of Navier–Stokes equations beyond the continuum regime, i.e. to these size affected domains [4]. Various numerical techniques are employed by

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researchers to model physical systems in molecular simulations of rarefied gases [5]. Navier–Stokes equations can be applied to slip flow regime with boundary conditions modified so as to incorporate the changes observed in this regime [6]. Prabha and Sathian successfully extended the applicability of Navier–Stokes equations for early transition flow in a nano-channel by employing second order boundary conditions [7]. Confined gas flow studies at different length scales prove that as the rarefaction levels increase, the fluid exhibits a gradual transformation from continuum regime to transition flow regime. This demands for alternate theoretical approaches for modelling the fluid flow in the respective flow regimes.

Computation of MFP of gases in nano-channels is crucial for the prediction of the properties of the system [8]. Flow properties are generally calculated from theoretical expressions with MFP obtained from empirical relations [9]. In general, these empirical relations provide little information regarding the influence of channel size on MFP. However, works of Stops [10] and Dongari et al. [11] reported a power law variation of MFP along characteristic dimension for gases confined between reflective wall boundaries. For moderately dilute gases confined between solid walls, corresponding to the transition regime, Prabha et al. [12] have reported that the reduction in MFP near the walls is significantly higher than that for the reflective wall boundary.

The MFP of an ideal mono-atomic gas with diameter d as given by the kinetic theory equation, depends on number density alone. It is given by

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 N_v} \tag{1}$$

where N_v is the number density.

The kinetic theory of gases conveys that the origin of thermo-physical transport coefficients like viscosity and thermal conductivity can be related to the collisions of constituent atoms [13]. In rarefied gas flows bounded by planar walls, the slip occurring close to the wall–gas interface is quantified using Maxwell's first order slip model or second order slip model and the system mean free path appears in both the relations. Prabha et al. calculated the thermo-physical properties of Poiseuille flow in nano-channels by approximating the value of MFP as given in Kinetic theory expression (Eq. (1)) to employ in slip models [9].

For particles with extended potentials MFP (λ_v) can be defined in terms of viscosity, and is given by the expression,

$$\lambda_v = \frac{\eta}{\rho}\sqrt{\frac{\pi m}{2 K_B T}} \tag{2}$$

where η is the dynamic viscosity, ρ is the fluid density, m is the particle mass, K_B is the Boltzmann constant and T is the temperature [14]. Accordingly for an isothermal wall bounded gas, if the dynamic viscosity is maintained constant, MFP is inversely proportional to density. The characteristic length does not come into picture in these theoretical models. However, the property variations in slip and transition regimes as a function of channel dimension has been a topic of investigation for many years.

In the present paper we study the dependence of MFP on the characteristic length of the domain. Argon, a mono-atomic ideal gas at a constant temperature (300 K) is used as the gaseous medium in two different cases of confinements viz. reflective wall and platinum wall. The characteristic dimension is varied while maintaining the average gas atomic number density a constant. This ensures that all the parameters used in the calculation of MFP from kinetic theory relations are kept constant. Molecular dynamics (MD) simulations have been used to simulate the system [15]. The variation of average MFP and the local MFP in constitutive sub-domains (bins) are calculated for both the confinements. The variation in relative percentage of fluid–wall collisions to total collisions substantiates the conclusions made. It is interesting to note that MFP of confined gases is modified by changing the characteristic length of the domain. All simulations are performed using LAMMPS [16]. The results of the study are applicable to stagnant gaseous systems confined to the walls of a nanochannel. The information derived from the study can be used to improve the accuracy of boundary conditions and the calculated values of thermo-physical properties, where mean free path has a major role to play.

2. Methodology

2.1. Simulation model

A three dimensional system containing argon gas confined between two infinite parallel walls constitutes the simulation domain. The Lennard-Jones (LJ) potential with a cut-off distance equal to three times the diameter of molecule is used to model the interactions [17]. The Ar–Ar interaction strength is taken to be 0.996 kJ/mol and that of Xe–Xe interaction as 1.834 kJ/mol [18]. For Argon atoms, σ is chosen to be 0.340 nm, where σ is the characteristic length parameter in LJ potential. The strength for Pt–Pt interaction is taken to be 31.36 kJ/mol and that of Pt–Ar interaction as 0.658 kJ/mol at a characteristic length of 0.294 nm [18]. The thickness of the wall is 1 nm and the wall atoms (18 928 atoms) are arranged in FCC crystal structure (Fig. 1). The thickness of the wall considered is larger than the 3σ distance for the interaction between wall particles and fluid atoms.

Periodic boundary conditions (PBC) are employed in the x and z directions. This ensures infinite parallel wall assumption in those directions. The simulation domain is filled with argon gas with a constant number density and the characteristic