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# MOLECULAR PLANE POISEUILLE FLOW FOR THE TIP4P AND LENNARD-JONES POTENTIALS

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## ABSTRACT

A modified Verlet algorithm in the field of non-equilibrium molecular dynamics with the Lennard-Jones and TIP4P potentials are proposed to predict the velocity profiles in the plane Poiseuille flow problems. Three kinds of Knudsen number ( $Kn$ ) and the varied wall boundary types ( $f$ ) are employed. It is worth mentioning that the realistic values of the repulsive core, the energy parameter of potential, and the molecular mass in water are adopted in these problems. It means that the proposed simulation is more practical than those of previous researches.

When  $Kn \leq 0.0068$ , the numerical result shows that Navier-Stokes theory is fail due to the deviation of the velocity profiles from the classical velocity profiles of the classical approach. These cases demonstrate that the velocity gradient increases with  $Kn$ , and decreases with the increases of  $f$  for both of the two potentials. Furthermore, the phenomena at the wall-fluid interface do not agree with Maxwell's hypothesis because the tangent velocity of the molecules does not vanish at wall boundary.

## NOMENCLATURE

$a$	= molecular acceleration
$\bar{a}_D$	= a uniform induced acceleration
$f$	= wall boundary conditions
$F_{ij}^*$	= dimensionless force on molecule $i$ due to $j$
$2h$	= the characteristic width of the channel
$k_B$	= Boltzmann's constant
$Kn$	= Knudsen number
$m$	= mass
$N$	= number of molecules
$q$	= charge
$r_{ij}$	= position of molecule $i$ relative to $j$
$t$	= time
$T$	= temperature
$T_a^*$	= the temperature after collision process
$T_s^*$	= the initial temperature of the system
$u$	= $x$ -component of the molecular velocity
$v$	= velocity
$V_i^*$	= the molecular velocity after collision process
$V_i^{*,new}$	= the correlated molecular velocity
$\varepsilon$	= energy parameter in potential
$\varepsilon_0$	= permittivity of vacuum
$\zeta$	= random number
$\lambda$	= the mean free path
$\xi$	= random number in range $(0,1)$

$\rho$	= the fluid number density
$\sigma$	= the size of the repulsive core between two water molecules (i.e., the molecular diameter)
$\tau$	= dimensionless time
$\phi$	= potential
superscripts and subscripts	
*	= denotes dimensionless unit
$LJ$	= denotes using Lennard-Jones potential
$TIP4P$	= denotes using TIP4P potential
$x$	= denotes $x$ -component of the variable
$y$	= denotes $y$ -component of the variable

## INTRODUCTION

Non-equilibrium molecular dynamics is a method to solve the classical equations of motion (Newton's equations) when the problem is focus on the interactions among the molecules in the system to obtain the transient dynamic properties of the molecular system. It has been applied to predict the thermal conductivity of the solid thin-film [1], the thermal conductivity of the bulk silicon and the nanowires [2], the thermal conductivity of the superlattices [3], heat propagation [4], interphase properties and inter-phase transport [5], etc.

The first research in the field of molecular dynamics is proposed by Alder and Wainwright [6]. Alder and Wainwright study the dynamic behavior of the particles for a hard-sphere potential when the particles move at constant velocity and the elastic collision among the particles is perfect. The first research included Lennard-Jones potential in the field of molecular