

Thin Film Pressure Estimation of Argon and Water using LAMMPS

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Abstract

In this work, we investigate the pressure and density characteristics of water film when simulated using the emerging technique called many body dissipative particle dynamics method. This work also layout the methodology of estimating local pressure from LAMMPS simulation using Harasima scheme. Using the triangular shaped cloud interpolation function, pressure and density are estimated at local bins and compared with the experimental database. Our results show good agreement for the molecular dynamics results of the argon system, while the many body dissipative particle model fails to simulate the water properties at room temperature. In its current form, the many body dissipative particle method cannot be used for accurate liquid vapor interfacial simulations and heat transfer studies.

Keywords: Molecular Dynamics, MDPD, Dissipative Particle Dynamics, Local Pressure, Thin Films.

1. INTRODUCTION

In many applications to biological flow processes to heat transfer studies, despite of the continuous growth in the computational power during the last decades, it is still computationally impossible to simulate evaporation of a tiny water droplet using atomistic simulation. The main reason is that the time scale required to evaporate one molecule of water is reasonably high which makes it years of real computational time to simulate a droplet or thin film of water using molecular dynamics (MD) simulations [1]. In this scenario, coarse grain molecular dynamics (CGMD) [13] and dissipative particle dynamics (DPD) methods [7] catch attention. While CGMD models are still limited to problem specific selective clustering of multiple atoms into a group, DPD method is scalable and works based on the hydrodynamics theory [6, 8, 14, 21, 22]. DPD technique is a mesoscopic method which drastically reduces the fast degrees of freedom while maintaining the behavior of slow entities and provides insights into macro spatial and temporal scales.

In DPD method, a coarse grain bead represents multiple water molecules or can represent an entire cluster of molecules. Though the time integration and dynamics looks similar to MD, the soft pair interaction potential of DPD allows to have large time steps of integration. The DPD force field consists of combination of a repulsive conservative force, a dissipative force and a random force. The DPD governing equations can be derived from fluctuating Navier Stokes equation and can be considered as a particle-based Lagrangian representation of the continuity and momentum equations at the mesoscopic level. For the past two decades, DPD has caught attention in simulating fluid flow, biological systems [31][33] and transport phenomenon.

Despite of its attractive benefits, DPD technique has a serious drawback – it cannot simulate liquid-vapor interface. This is due to the presence of repulsive conservative force term, which prevents the use of DPD from problems like multiphase fluid systems, heat transfer processes [4, 26, 28, 30], biological diffusion reaction processes etc. To address this issue, there are many emerging variations [32] of DPD technique. One of the leading approaches is called many body

dissipative particle dynamics (MDPD) method [2, 23]. In this method, the conservative force term is modified with an attractive term and repulsive term with a local density dependent function. This enables us to simulate interfaces with multiple phases of liquid and vapor. Though there exist some studies related to the droplet mechanics, the possibility of heat transfer simulations, especially droplet and thin film evaporation is not well explored using this method. The main objective of this work is to simulate the liquid vapor co-existence of MDPD water and estimate pressure and density variation.

The estimation of the pressure, velocity and density at local spatial coordinates is of high importance in the field of thermal and fluid transport, especially at nano and micro scales. The accurate simulation of the pressure gradient is essential to study the wicking effects and Marangoni flows. In this work, we utilize LAMMPS software [18] to simulate a thin film of liquid water film suspended with vapor on both sides using MDPD method. At room temperature we studied the pressure and density variation along the normal direction of the film and found that it varies largely from the experiments. We report that this undesired variation of both density and pressure prohibits to use MDPD technique in heat transfer studies and interfacial phenomena.

2. SIMULATION METHODOLOGY

To simulate the interfacial pressure and vapor-liquid density distribution, a system with thin liquid film suspended between vapor films is commonly used. In this work, we will use argon system to validate our pressure and density calculation method and non-dimensionalized many body dissipative particle system to simulate and investigate water. A liquid vapor co-existing system as shown in Fig. 1 is modeled using MATLAB software [16]. The liquid region is modeled in the middle and vapor on either side. Past studies [27][34][25] related to pressure estimation shows a minimum liquid film thickness of 3 nm and periodic width of 5 nm are required to simulate pressure accurately. For the argon molecular system, 5 nm \times 5 nm \times 5 nm liquid film is chosen with 5 nm thick vapor on either sides (Fig. 1b) and for the MDPD system 7.5 nm \times 7.5 nm \times 7.5 nm liquid film is chosen with 7.5 nm thick vapor on either sides.

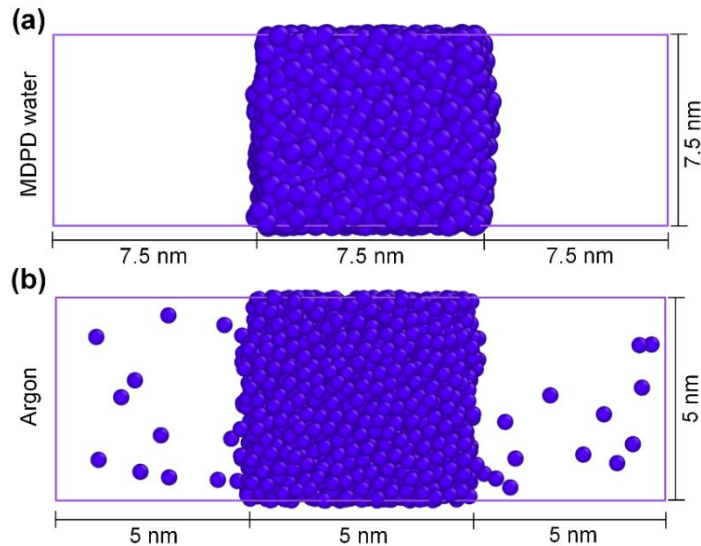


FIGURE 1: Computational models for (a) MDPD water and (b) Argon. The thin films are suspended between vapor regions on either side. The size of the system along the 3rd dimension (normal to the plane of figure) is same as the height of the system (5 nm for argon, 7.5 nm for MDPD).

The modeling and simulation details of the MDPD and argon systems are given in the next sub sections, followed by the local pressure estimation details.

2.1 MDPD System Methodology

In the many body dissipative particle dynamics formalism, the bead pair interaction force for N beads is given by,

$$F_i = \sum_{i \neq j}^N [F_{ij}^C + F_{ij}^D + F_{ij}^R] \quad (1)$$

The conservative force component is given by,

$$F_{ij}^C = A\omega_A(r_{ij})\mathbf{e}_{ij} + (\rho_i + \rho_j)B\omega_B(r_{ij})\mathbf{e}_{ij} \quad (2)$$

The first term represents an attractive interaction ($A < 0$) and second term is a local density dependent many body repulsive interaction ($B > 0$). The weight functions ω_A and ω_B are chosen as,

$$\omega_A(r) = 1 - r_{ij}/r_c, \text{ if } r_{ij} < r_c \quad (3)$$

$$\omega_B(r) = 1 - r_{ij}/r_d, \text{ if } r_{ij} < r_d \quad (4)$$

The dissipative force is given by,

$$F_{ij}^D = -\gamma\omega_D(r_{ij})(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij})\mathbf{e}_{ij} \quad (5)$$

$$\omega_D(r) = (1 - r_{ij}/r_c)^2, \text{ if } r_{ij} < r_c \quad (6)$$

The random force is given by,

$$F_{ij}^R = \frac{\delta\omega_R(r_{ij})\alpha}{\sqrt{\Delta t}}\mathbf{e}_{ij} \quad (7)$$

$$\omega_R(r) = (1 - r_{ij}/r_c), \text{ if } r_{ij} < r_c \quad (8)$$

The average local density at the position of the i^{th} bead is given by,

$$\rho_i = \sum_{j \neq i} 15/2\pi r_c^3 (1 - r_{ij}/r_c)^2 \quad (9)$$

Which is normalized so that, $\int_0^\infty 15/2\pi r_c^3 \left(1 - \frac{r_{ij}}{r_c}\right)^2 \mathbf{d}^3r = 1$. Here, r_{ij} is the distance between the beads, ω_A , ω_B , ω_D and ω_R are the interpolation functions, r_c and r_d are the cutoff radii, γ is a dissipative parameter, α is a Gaussian random number with zero mean and unit variance, Δt is the time step of integration and r_{ij} and v_{ij} are the relative displacement and velocities of the two beads. To satisfy Fluctuation-Dissipation theorem, $\delta^2 = 2\gamma k_B T$ has to be satisfied.

The DPD and MDPD simulations are usually carried out in dimensionless units and the Table 1 summarizes the unit conversion details. Based on the common values of the MDPD parameters found in the literature [3][24] we have adopted $r_c = 1$, $r_d = 0.75$, $A = -40$ and $B = 25$, $\gamma = 4.5$, $\Delta t = 0.005$. Utilizing the mass conservation relationship of DPD and molecular dynamics (MD) simulations, it is shown that: $\rho_{MD}r_c^3 = N_m\rho_{DPD}$. Here, $N_m = 5$ (number of water molecules per MDPD bead), $\rho_{DPD} = 6$ (number of MDPD beads within the cutoff sphere), $\rho_{MD} = 33.369/nm^3$ (number of water molecules per unit volume). This leads to: $r_c = 0.965 \text{ nm}$ and for the given MDPD film system as shown in the Fig. 1a, with a liquid region density of 1000 g/L , 2816 beads are required.

Parameter	Symbol	Conversion	value
Distance	σ	$r^* = r/\sigma$	0.965 nm
Time	$\tau = \sqrt{((m\sigma^2)/\epsilon)}$	$t^* = t\sqrt{(\epsilon/(m\sigma^2))}$	$5.8e^{-12} s$
Force	F	$F^* = F\sigma/\epsilon$	N/A
Energy	E	$E^* = E/\epsilon$	$\epsilon = k_B T$
Pressure	P	$P^* = P\sigma^3/\epsilon$	N/A
Velocity	v	$v^* = v\tau/\sigma$	N/A

TABLE 1: MDPD Conversion Factors.

The time step of MDPD simulations are taken as 0.005 (28.9 fs in real units). All simulations are performed by minimizing the system using conjugate gradient method [5] for 1000 steps, followed by 100,000 steps of equilibration, and followed by 100,000 steps of production run. The integration scheme used was velocity verlet [15] and thermostat was Nose Hoover [17]. The simulations are carried out at 300 K. The results including pressure and position information is written to a file at every 25 steps interval.

2.2 Argon System Parameters

The argon system is simulated using the standard 12/6 Lennard Jones (LJ) potential [9]. The force field is given as below.

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]; \text{ for } r < r_c \quad (10)$$

Here, $\epsilon = 0.2404 \text{ kcal/mol}$, $\sigma = 0.34 \text{ nm}$ and cutoff radius as $r_c = 1.8 \text{ nm}$. The time step of integration is 5 fs . The integration scheme used was velocity verlet and thermostat was Nose Hoover. The simulations are carried out at 90 K, equilibration for 50,000 steps and production runs for half a million steps. The results including pressure and position information is written to a file at every 50 steps interval.

2.3 Local Pressure Estimation

The reasoning behind local pressure estimation from MD simulation is still a topic of debate. One of the credible method of estimating local pressure from MD is Irving Kirkwood formulation [11]. According to this method, the pressure tensor consists of two components, a) kinetic energy component and b) virial component. The pressure tensor at any special coordinate (r_p) is given by,

$$P(r_p) = \sum_{i=1}^N m_i v_i \otimes v_i \delta(r_i - r_p) + \sum_{i=1}^{N-1} \sum_{j=i+1}^N r_{ij} \otimes F_{ij} \delta(r_i - r_j) \delta(r_i - r_p) \quad (11)$$

Here P is the pressure, m is mass of i^{th} atom, v is velocity, r_i and r_j are the position vectors of i^{th} and j^{th} atoms respectively, N is number of atoms, r_p is the position vector of p^{th} grid point, $r_{ij} = r_i - r_j$, F_{ij} is the force, and δ is the Dirac delta function.

However, this formulation needs estimation of the pressure from the pair interaction forces during the integration and to be allocated at runtime. Most of the freely available open source MD codes like LAMMPS [18] doesn't have this feature. One reason is the increased computational overhead during the run time and another reason is the requirement of re-running the entire simulation if we chose to change the local grid spacing or weight functions for pressure estimation.

To circumvent these issues, in this paper we propose to follow Harasima method [19], which assigns the pressure contribution of i^{th} and j^{th} atoms to the nearest local bins or grids. In LAMMPS using the stress/atom compute module [18] we can obtain the stress per atom given by the following equation.

$$S_{\alpha\beta} = - \left[m v_{\alpha} v_{\beta} + \frac{1}{2} \sum_{i=1}^{N_p} (r_{1\alpha} F_{1\beta} + r_{2\alpha} F_{2\beta}) \right] \quad (12)$$

Here, α and β are indices for x, y, z components, m is mass, v is velocity, N_p is the number of pair interactions, r is the position coordinate and F is the force component. The resulting quantity ($S_{\alpha\beta}$) have the units of pressure*volume and has to be divided with appropriate volume to get the meaningful stress/pressure.

For systems like thin film suspended on vapor, the problem can be treated as a 1 dimensional and the local pressure will be pressure defined at local bins along z-axis (axis normal to the liquid vapor interface in Fig. 1). To get a smooth distribution of the pressure we will choose an interpolation function. There exists a wide range of options to choose for interpolation function, however here we limit our studies with triangular shape cloud function (TSC) proposed by Hockney and Eastwood [10].

$$W(x) = \begin{cases} \frac{3}{4} - \left(\frac{x}{H}\right)^2 & \text{when } |x| \leq \frac{H}{2} \\ \frac{1}{2} \left(\frac{3}{2} - \frac{|x|}{H}\right)^2 & \text{when } \frac{H}{2} \leq |x| \leq \frac{3H}{2} \\ 0 & \text{otherwise} \end{cases} \quad (13)$$

Here, $x = z_i - z_p$ is the difference between position of i^{th} atom and p^{th} grid point, H is the grid spacing. This function will distribute the pressure values to the nearest 3 grid points appropriately. For our MD simulation results, we have used a grid spacing of 0.1 nm. The same TSC function can be used to estimate the local density variation. The pressure components are given by

$$P_{\alpha\beta}(z_p) = -S_{\alpha\beta} W(z_i - z_p) / 3V_{slab} \quad (14)$$

Here, V_{slab} is the slab volume, and denominator has a factor of 3 due to the fact that the TSC function smears the pressure over 3 slabs. A computer code written in C++ language is developed to read the files from LAMMPS output and estimate the pressure and density profile of the thin film systems.

3. RESULTS AND DISCUSSION

The computational simulations of both argon and water are conducted using MD simulations and MDPD simulations respectively. LAMMPS is used for all MD and MDPD simulations, MATLAB [16] is used for modeling the systems, OVITO software [20] is used to visualize the data, and a C++ code written by the author is used to estimate the local pressure and density.

3.1 Argon system

The 5 nm × 5 nm × 15 nm argon system is simulated using LAMMPS at 90 K and results are printed out at every 50 time steps. The density profile along the z-axis is estimated using the TSC function and plotted in Fig. 2. The ensemble average density value near to the center of the liquid region shows 1375 kg/m³. This is close to the density value found in experiments (1378 kg/m³) tabulated in NIST webbook of chemistry thermo-physical properties [12].

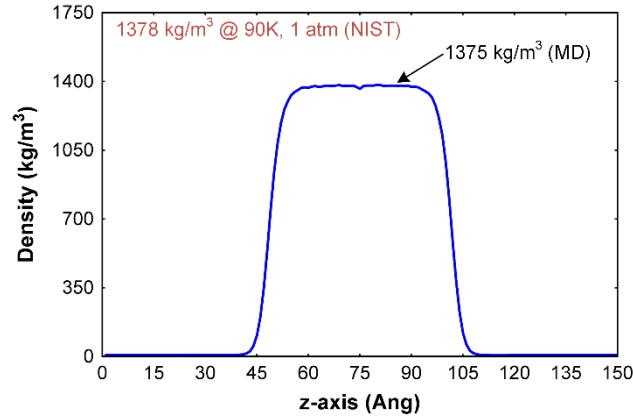


FIGURE 2: Density variation of argon film using LJ potential. The simulated density values matches with the experimentally observed values of density from NIST [12].

The C++ code is used again to estimate the average total pressure along the z-axis and the difference between normal and tangential pressure components of the system. The total pressure of the system is given by $P = \text{Trace}(P_{\alpha\beta})/3$, normal pressure component is given by $P_N = P_{zz}$ and the tangential component of the pressure is given by $P_T = (P_{xx} + P_{yy})/2$.

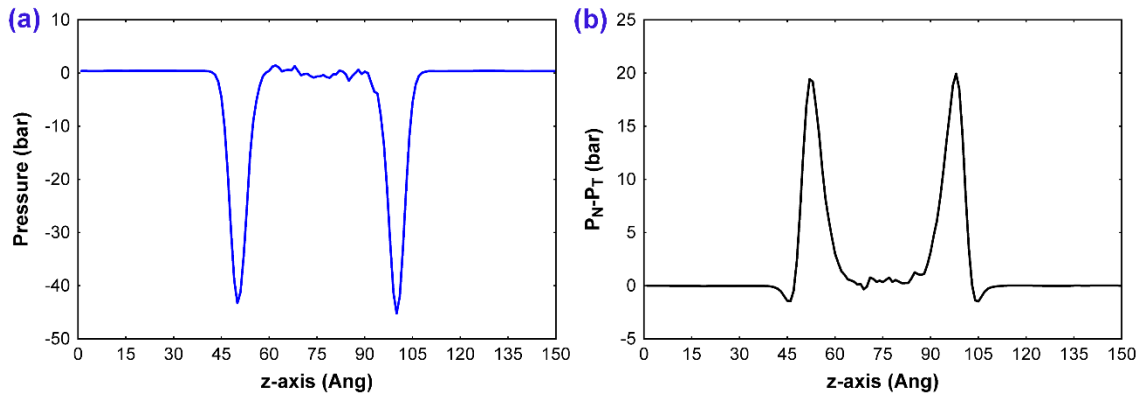


FIGURE 3: Pressure variation along the system. (a) Distribution of average pressure of the system along z-axis, (b) Variation of difference between normal and tangential pressure components along z-axis.

The average pressure results (Fig. 3a) of argon system shows good agreement with the previously reported pressure profiles [25, 27, 29, 34]. The average pressure is 1 atm at both liquid and vapor regions, and an expected negative pressure peaks are observed at the interfaces due to the interfacial surface tension. The difference between the normal and tangential component is crucial for the estimation of surface tension and our results (Fig.3b) show the same trend as reported earlier in the literature [25, 27, 34].

3.2 MDPD system

The MDPD simulation results with the standard parameters ($A = -40$ and $B = 25$) did not yield a liquid vapor interface, instead the entire system was at a single-phase density around 300 kg/m^3 . The expected density was 1000 kg/m^3 and hence we conducted additional simulations by varying the strength of the attraction parameter from -40 to -90 . We saw a gradual increase in density until A reached a value of -90 . Beyond which the density remained almost constant until $A = -93$ and then shown a drastic deviation and abnormal behavior at $A = -94$. Beyond $A = -94$, the system was trying to implode and the simulation became unstable.

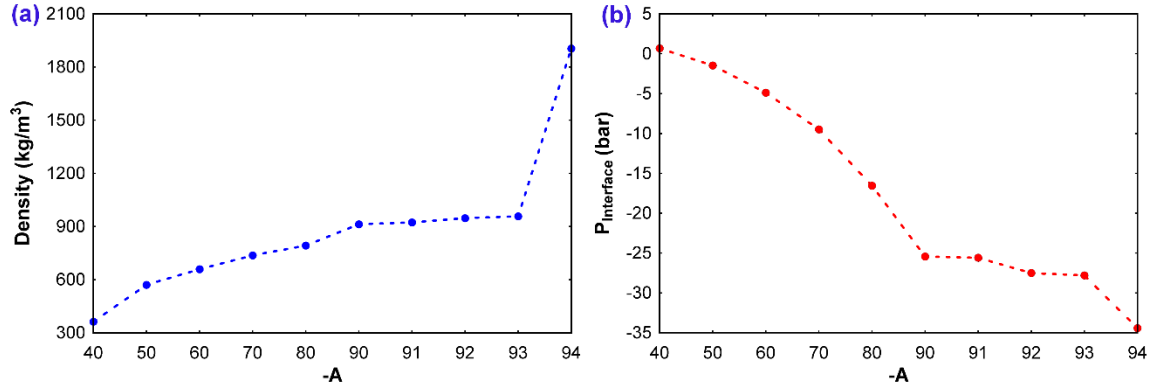


FIGURE 4: Trend of the variation of (a) density and (b) interfacial pressure of the MDPD film for varying parameter of A (ranges from -90 to -94).

The density variation of the MDPD system with varying A is shown in the Fig. 4a. At $A = -94$, the density became 1900. Similarly, the interfacial maximum pressure is estimated and plotted in Fig. 4b. There was no interface when $A = -40$, and it shown the same trend as the density variation. To understand more about the profile variation we have plotted the density profile with respect to varying A from -90 to -94 in Fig. 5. The black dome shaped profile corresponding to the $A = -94$ shows the extreme packing of particles towards the center.

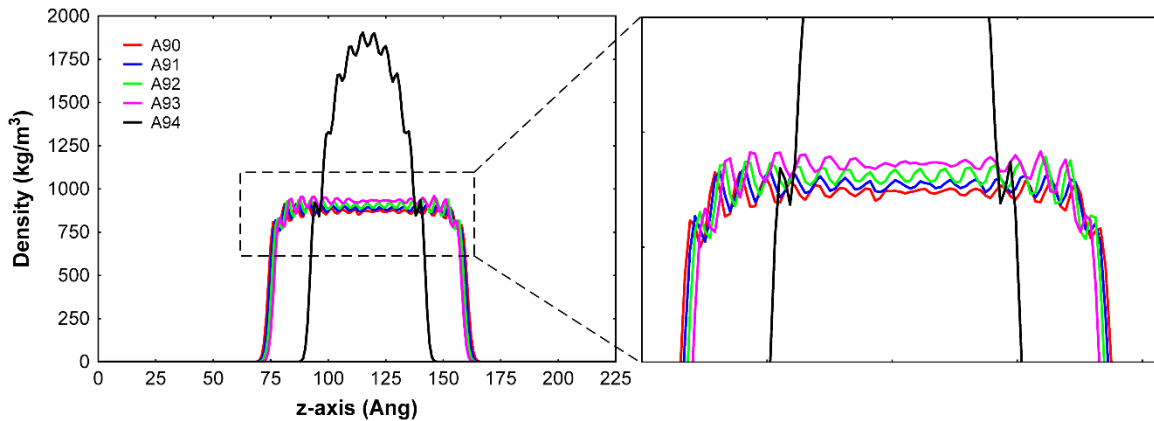


FIGURE 5: Density variation in MDPD water system for different values of A. The value of attraction parameter A ranges from -90 to -94 and corresponding density variation is shown with a close-up into the liquid region on the right.

The inset of the Fig. 5 shows the layered density variation of water at any value of A . Also, the vapor density is zero and average density of the liquid in the middle ranges from 870 kg/m^3 to 930 kg/m^3 while A was changing from -90 to -93 . The experimentally observed [12] density is 996.56 kg/m^3 at 300 K and atmospheric pressure which is 7% higher than the MDPD simulation results.

The pressure variation of the MDPD system at different values of A is given in Fig. 6. Figure 6a show the average pressure variation along the z-axis and Fig. 6b shows the difference between normal and tangential components. After estimating surface tension using $\gamma = \int_0^{15nm} (P_N - P_T) dz$, we found that it ranges from $7.29 \times 10^{-7} \text{ mN/m}$ to $8.12 \times 10^{-7} \text{ mN/m}$ depending on the value of A .

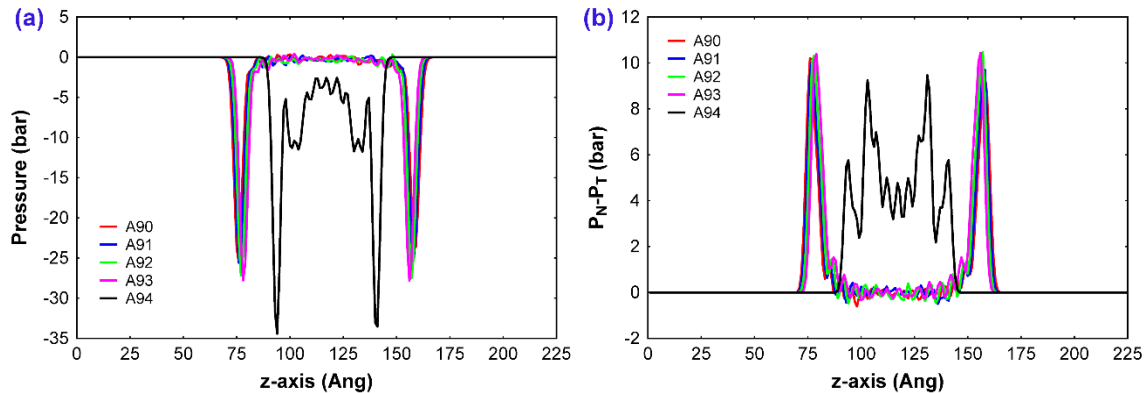


FIGURE 6: Pressure profile variation in an MDPD water system. (a) The average pressure profile variation along z-axis for different values of parameter A (ranges from -90 to -94.) (b) $P_N - P_T$ pressure profile variation along z-axis for different values of parameter A (ranges from -90 to -94).

These differences in prediction of density and pressure are highly undesired if we are interested in studying the accurate interfacial properties of water using MDPD.

4. CONCLUSION

We have investigated the local pressure and density characteristics of water film using many body dissipative particle dynamics method. We also laid out a method to estimate the local pressure from the stress/compute module of LAMMPS software. Using Harasima pressure calculation scheme and the triangular shaped cloud interpolation function, pressure and density are estimated at local bins and compared with the experimental database. The results show very good agreement for the molecular dynamics simulation of the argon system. But the many body dissipative particle model fails to simulate the water properties at room temperature. We conclude that in its current form, the many body dissipative particle method cannot be used for accurate liquid vapor interfacial simulations and heat transfer studies.

5. ACKNOWLEDGEMENT

The author would like to express his gratitude towards University of Jamestown for providing high performance computational resources and the support towards this project.

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