# Molecular Dynamics Simulation for the Atomization Process of a Nanojet

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**Abstract:** In this research, the atomization process of a nanojet is investigated by molecular dynamics simulation. Liquid argon nanojet made of 44000 Lennard-Jones molecules is examined under various simulation parameters to study their influence on the nanojet atomization process. Snapshots of the molecules, evolution of the density field, and evolution of the intermolecular force are analyzed. The present simulation results can provide insight into the fundamental mechanism of the atomization process and will be helpful for the design of nanojet devices such as nano-printer or nano-sprayer.

Keywords: Nanojet, Atomization Process, Molecular Dynamics Simulation

### Nomenclature

intermolecular force
Boltzmann constant
fundamental cell characteristic length
molecular mass
number of molecules
intermolecular distance
cut-off radius of Lennard-Jones potential function
temperature
time
time step
volume
velocity of molecule <i>i</i>
Cartesian coordinates

#### Greek

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ε	energy parameter of Lennard-Jone	es potential function
ρ	density	
σ	length parameter of Lennard-Jone	s potential function
$\phi$	Lennard-Jones potential function	

### **Subscripts**

L	liquid phase
V	vapor phase

### **Superscripts**

*	non-dimensionalized quantity
_	averaged quantity

## 1 Introduction

Evolution of a nanojet has received considerable attentions due to its unique characteristics and wide range of applications, e.g. ink-jet printing, fuel injection, bioengineering, etc. Previous theories and modeling techniques about jet injection have been developed focused on much larger thermodynamic systems with continuum assumptions. However, direct application of these theories to nano-scale systems is uncertain. Conventional liquid jet breakup and spray models require many assumptions and experimental correlations that are difficult to obtain in nanojet. Nanojet devices use an actuator to eject atoms or molecules through a nano-atomizer. However, the fabrication of the actuator and nano-atomizer is very complex. In addition, there exist major challenges for the nano-locating and nano-driving systems and assembly of these components. Therefore, to build a nanojet actually is still a complex task. On the other hand, molecular dynamics (MD) can offer novel insights into the underlying atomistic mechanisms and nanometer-scale behavior due to their high temporal and spatial resolution.

Recently, MD has become a popular numerical tool for understanding nanosized phenomena. MD is a simplified approach. The fast electron motions are excluded by the contribution of the Born–Oppenheimer approximation (1927) and the motion of molecules can be simplified as the motions of nuclei. The only input for MD is an interatomic or intermolecular potential. Owing to numerical simplicity, the effective pair potential which neglects higher-body terms is commonly used. However, in spite of these simplified approaches, MD could be an excellent tool for a wide

range of application fields where the quantum effect is negligible[Shin, Oschwald, Micci and Yoon (2005)]. Nair, Farkas, and Kriz (2008) studied the indentation response of Ni thin films of thicknesses in the nanoscale using molecular dynamics simulations with embedded atom method (EAM) interatomic potentials. The simulation results show that the contact stress necessary to emit the first dislocation under the indenter is nearly independent of film thickness and that in the elastic regime, the loading curves observed start deviating from the Hertzian predictions for indentation depths greater than 2.5% of the film thickness. Chen, Cheng and Hsu (2007) evaluated the fundamental mechanical properties of single/multi-walled carbon nanotubes (S/MWCNTs) using MD simulations. The force field between two carbon atoms is modeled with the Tersoff-Brenner (TB) potential while the inlayer/interlayer van der Waals (vdW) atomistic interactions are simulated with the Lennard-Jones (L-J) potential. The effectiveness of the MD simulations is demonstrated by comparing the computed results with the theoretical/experimental data available in literature. They found that the effect of the inlayer vdW atomistic interactions can not be neglected and should receive attention in the MD simulations of the mechanical properties of CNTs. Tang and Advani (2007) performed nonequilibrium MD simulations to investigate water flow around a single-walled carbon nanotube. It was shown that classical continuum mechanics does not hold when the drag forces on the nanotube are considered. Matsumoto, Nakagaki, Nakatani and Kitagawa (2005) studied the internal structure-changes around the crack tip and the pertinent crack growth behavior in an amorphous metal by MD simulation. The Finnis-Sinclair potential for  $\alpha$ -iron was used to describe the interatomic potential. Computed results show that nanoscale crystalline phase grows around the crack tip and that the distribution of deformation zones and deformation mechanism are significantly altered. Wei, Srivastava and Cho (2002) investigated the temperature dependence of the plastic collapse of single-wall carbon nanotubes under axial compression by classical MD simulations using Tersoff-Brenner potential for C-C interactions. The thermal fluctuations are shown to drive nanotubes to overcome the energy barriers leading to plastically collapsed structures which have significantly lower strain energy than fins-like structure.

In Fig.1, the fluid/air interface for atomizer flow by macroscopic analysis from one of the author's previous studies [Yeh (2005)] is shown. It can be seen that the liquid evolves into threads in motion after leaving the atomizer. In the researches by Kawano (1998), as well as by Koplik and Banavar (1993), the vaporization process of a nano-scale liquid thread was analyzed by MD. The formation of liquid threads, like nanojet, is one of the most fundamental and important phenomena during the atomization process. However, the above simulation models were limited to an initially quiescent liquid thread, which is not emanating but intrinsically rearranges



Figure 1: Fluid/air interface for atomizer flow by macroscopic analysis [Yeh (2005)]

itself into droplets or smaller liquid threads. In addition, the MD simulation results of a time-dependent liquid flow are sensitive to initial velocities. Therefore, the above results can not be generalized to nanojets.

Moseler and Landman (2000) reported MD simulation results for the formation and instability of liquid nanojet. They pointed out that the details of nanojet breakup behavior obtained by MD are significantly different from the Navier-Stokes result. Shin, Oschwald, Micci and Yoon (2005) simulated argon nanojet injection under vacuum conditions by MD. They found that different injector shapes does not cause significant change in the nanojet breakup behavior. On the other hand, the liquid temperature inside the injector was found to be a controlling factor for the subsequent breakup characteristics. A higher liquid temperature is preferred for a faster nanojet breakup with a shorter breakup length. Choi, Kim and Kim (2006) investigated the capillary instability of nanometer-sized surface-tension-driven flow by MD with Lennard-Jones fluid. They found that the thermal fluctuation, which is significant in a nano-scale system, is the most important factor for various breakup scenarios of a nanojet.

In this study, liquid argon nanojets made of 44000 Lennard-Jones molecules are investigated under various simulation parameters to examine their influence on the

nanojet atomization process. Snapshots of the molecules, evolution of the density field, and evolution of the intermolecular force are analyzed. This can provide insight into the fundamental mechanism of the atomization process and will be helpful for the design of nanojet devices such as nano-printer or nano-sprayer.

#### 2 Molecular Dynamics Simulation Method

In this study, the atomization process of a liquid argon nanojet discharged into vacuum is investigated by MD simulation. The inter-atomic potential is one of the most important parts of MD simulation. Many possible potential models exist, such as hard sphere, soft sphere, square well, etc [Haile (1992)]. In this research, the Lennard-Jones 12-6 potential model, which is widely used, is adopted for calculation. It is

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

where *r* denotes the distance between two molecules,  $\varepsilon$  and  $\sigma$  are the representative scales of energy and length, respectively. The Lennard-Jones fluid in this research is taken to be argon for its ease of physical understanding. The parameters for argon are as follows [Kawano (1998)] : the length parameter  $\sigma$ =0.354 nm, the energy parameter  $\varepsilon/k_B$ =93.3K, and the molecular weight *m*=6.64×10<sup>-26</sup> kg, where  $k_B$ =1.38×10<sup>-23</sup> J/K denotes the Boltzmann constant. The cut-off radius  $r_c$  beyond which the intermolecular interaction is neglected is 5.0 $\sigma$ .

Table 1: Nano-atomizer dimensions, temperatures, number of molecules and simulation results

Case	$L_2^*$	$L_3^*$	$L_4^*$	$L_5^*$	<i>D</i> */2	$T_D^*$	N	$\overline{f_{\rho}}$
1	5.73	5.73	5.73	76.7	8.81	0.75	43970	1.34
2	5.73	5.73	5.73	76.7	8.81	1.5	43970	1.08
3	5.73	5.73	5.73	76.7	8.81	2.0	43970	0.94
4	5.73	5.73	5.73	76.7	8.81	3.0	43970	0.74
5	5.73	5.73	5.73	76.7	8.81	4.5	43970	0.59
6	8.66	5.73	2.79	76.7	8.81	2.0	43989	0.95
7	2.79	5.73	8.66	76.7	8.81	2.0	43949	0.92
8	5.73	8.67	5.73	76.7	5.87	2.0	43934	1.27
9	8.66	5.73	2.79	76.7	8.81	3.0	43989	0.75
10	2.79	5.73	8.66	76.7	8.81	3.0	43949	0.72
11	5.73	8.67	5.73	76.7	5.87	3.0	43934	1.10



Figure 2: Illustration of the nano-atomizer configuration and dimensions

The nano-atomizer is schematically shown in Fig.2. The simulation domain comprises a cubical box of side length 3600, with periodic boundary conditions applied in all three directions. The nano-atomizer is placed at the center of the box. Simulation parameters are listed in Table 1, which include nano-atomizer dimensions, temperatures, number of molecules and simulation results. The time integration of motion is performed by Gear's fifth predictor-corrector method [Haile (1992)] with a time step of  $t^*=0.0001$  (i.e. 0.25 fs). The initial number density of the liquid argon within the nano-atomizer is  $\rho_L^*=0.819$ . Note that all quantities with an asterisk in this paper, such as  $L^*$ ,  $D^*$ ,  $\rho^*$ ,  $t^*$ ,  $T^*$ , etc., are non-dimensionalized in terms of  $\sigma$ ,  $\varepsilon$ , and *m*, i.e.,  $L^* = L/\sigma$ ,  $D^* = D/\sigma$ ,  $\rho^* = N\sigma^3/V$ ,  $t^* = t(\varepsilon/m)^{1/2}/\sigma$ ,  $T^* = k_B T/\varepsilon$ . The argon molecules inside the nano-atomizer are liquid and the nano-atomizer is made of rigid argon molecules. A push panel composed of 600 argon molecules is constructed with a downward velocity of 120m/s. In this study, the interactions among liquid argon molecules, nano-atomizer and push panel are taken into account.

The procedure for MD simulation includes three stages : initialization, equilibration and production. Initially, equilibration is performed for liquid molecules in a rectangular parallelepiped with length and width equal to the initial diameter of the liquid argon molecules  $(2L_3^* + D^*)$  and with height equal to the initial length of the liquid argon molecules  $(L_5^*)$ . The initial velocities of molecules are decided by the use of normal random numbers. Velocity rescaling is performed at each time step by Eq.(2) to make sure that the molecules are at the desired temperature  $T^*$ :

$$v_i^{new} = v_i^{old} \sqrt{\frac{T_D}{T_A}} \tag{2}$$

where  $v_i^{new}$  and  $v_i^{old}$  are the velocities of molecule *i* after and before correction, respectively; and  $T_D$  and  $T_A$  are the desired and the actual molecular temperatures, respectively. The liquid molecules are equilibrated for  $10^6$  time steps at the desired temperature  $T^*$ . The achievement of the equilibrium state is confirmed by obtaining the radial distribution function. After equilibrium is achieved, the rectangular parallelepiped for the liquid molecules is truncated to the desired cylindrical liquid molecules, the nano-atomizer molecules, and the push panel molecules are put together into the computational domain and the production stage proceeds thereafter. A minimum image method and the Verlet neighbor list scheme [Haile (1992)] to keep track of which molecules are actually interacting at a given time interval of 0.005 are used in the equilibration and production stages.

### 3 Results and Discussions

In the following discussion, a liquid argon nanojet of length  $L_5^*$  and diameter  $2L_3^* + D^*$  is pushed by a panel into vacuum through a nano-nozzle of orifice diameter  $D^*$ , as illustrated in Fig.2. Simulation conditions are listed in Table 1.

### 3.1 Nanojet Atomization Process

Figure 3 shows the atomization process for a nanojet of  $L_2^* = L_3^* = L_4^* = 5.73$ ,  $L_5^* = 76.7$ ,  $D^*/2=8.81$  and  $T^*=0.75$ , which corresponds to a nanojet of length 26.2 nm and diameter 10 nm, and a nano-nozzle of orifice length 2nm, diameter 6 nm, as well as an actual temperature of 70 K. The dot in Fig.3 indicates the center of the molecule. From the figure it is found that the nanojet does not break up. Owing to the low temperature, the molecular kinetic energies are so low that the molecules congregate near the orifice exit. Very few liquid molecules evaporate at this low temperature. At a higher temperature  $T^*=1.5$  (140 K), as depicted in Fig.4, the molecules leave the orifice exit earlier than at  $T^*=0.75$ , due to their higher molecular kinetic energies. More liquid molecules evaporate at this higher temperature is further increased to  $T^*=2.0$  (187 K), as shown in Fig.5, evident evaporation is observed. Many evaporated molecules are produced and the non-evaporated liquid molecules concentrate within the central region. Figure 6 depicts the snapshots for temperature  $T^*=3.0$  (278 K). It is observed that breakup of the nanojet occurs and its spray

angle is larger than at  $T^*=2.0$ . The spurted molecules from the nano-atomizer are more evenly distributed at this temperature. If the temperature is further increased to  $T^*=4.5$  (420 K), as shown in Fig.7, the spray angle is even larger than at  $T^*=3.0$ and the spurted molecules from the nano-atomizer are much more uniformly distributed as compared to the lower temperature cases. Comparison of Figs.3, 4, 5, 6 and 7 reveals that the liquid nanojet evaporates quicker at higher temperatures. This will be further illustrated in later sections discussing the density distribution and the intermolecular force.



Figure 3: Atomization process for case 1 in Table 1

To investigate the influence of nozzle geometry on the nanojet atomization, comparison of the snapshots at  $t^*=80$  for four different nozzle geometries and  $T^*=2.0$ or 3.0 is shown in Figs.8 and 9. Note that Figs.8(a), (b), (c) and (d) correspond to cases 6, 3, 7 and 8, respectively, in Table 1; while Figs.9(a), (b), (c) and (d) correspond to cases 9, 4, 10 and 11, respectively, in Table 1. In Figs.8(a), (b), (c) and 9(a), (b), (c), the nozzle orifice diameters are equal (6 nm)but the nozzle ori-



Figure 4: Atomization process for case 2 in Table 1



Figure 5: Atomization process for case 3 in Table 1



Figure 6: Atomization process for case 4 in Table 1



Figure 7: Atomization process for case 5 in Table 1



Figure 8: Comparison of the snapshots at  $t^* = 80$  and  $T^* = 2.0$  for four different nozzle geometries

fice lengths are varied; while in Figs.8(d) and 9(d), the nozzle orifice length is the same as for Figs.8(b) and 9(b) (2 nm)but the nozzle orifice diameter is smaller (4 nm). By a careful comparison of Figs.8(a), (b) and (c), it can be observed that, on the basis of identical nozzle orifice diameter, a nanojet from a nozzle with a shorter orifice length ( $L_2$ )moves farther. On the other hand, from Figs.8(b) and (d), on the basis of identical nozzle orifice length, a nanojet from a nozzle with a larger orifice diameter moves farther. Figure 9 reveals similar tendency. Note that



Figure 9: Comparison of the snapshots at  $t^* = 80$  and  $T^* = 3.0$  for four different nozzle geometries

the nano-atomizer in this research is basically a plain-orifice atomizer. As pointed out by Lefebvre (1989), in a practical plain-orifice atomizer, resistance increases with nozzle orifice length/diameter ratio. Therefore, a nanojet from a nozzle with a smaller orifice length/diameter ratio moves farther due to its smaller resistance. This will be further illustrated in later sections discussing the density distribution and the intermolecular force.

#### 3.2 Density Distribution

It is important that the system be in equilibrium state before statistical values of the local properties can be taken. However, owing to the computational capacity limitations, the MD simulation can not proceed to a macroscopically long period. Nevertheless, the purpose of this paper is not to discuss statistical values of the local properties but to investigate the atomization process of a nanojet, which is important and conducive to the understanding of the fundamental mechanism of the atomization process. Criteria have to be made to quantify the discussion regarding the nanojet atomization process. Unfortunately, such criteria are still arbitrary in the literature. Because the system temperature in this study is kept at the desired temperature, a constant temperature criterion is not suitable for the discussion of the atomization process. In this research, a nanojet is considered to vaporize faster if the distribution of molecules reaches a uniform state quicker during the atomization process. This criterion essentially concerns with the evolution of the density distribution. The density at a specified point in the fundamental cell can be defined as

$$\rho = \lim_{\delta V \to 0} \frac{\delta N}{\delta V} \tag{3}$$

where  $\delta V$  is a small volume surrounding the point considered and  $\delta N$  is the number of molecules inside the volume  $\delta V$ . The density defined by Eq.(3) is actually an averaged density of a small volume surrounding the point considered. The value will approach the density at a specified point if the volume  $\delta V$  shrinks to that point. However, for a meaningful density field, the volume  $\delta V$  can not be too small because when  $\delta V$  becomes too small, it is difficult to obtain a definite value for  $\delta N/\delta V$ . In this study, the volume  $\delta V$  is taken to be a sphere with non-dimensionalized radius  $R^*=2$  and with its center located at the point considered. This is an optimal choice after numerical test.

Figure 10 shows the evolution of density uniformity factor for nanojets at different temperatures and the conditions of  $L_2^* = L_3^* = L_4^* = 5.73$ ,  $L_5^* = 76.7$ ,  $D^*/2 = 8.81$  (cases  $1 \sim 5$  in Table 1). The density uniformity factor is defined as

$$f_{\rho} = \frac{\sum_{N} \left(\rho^{*} - \rho_{eq}^{*}\right)_{t^{*}} \Delta V}{\sum_{N} \left(\rho^{*} - \rho_{eq}^{*}\right)_{t^{*} = 0} \Delta V}$$
(4)

where *N* is the initial number of liquid molecules in the fundamental cell,  $\rho^*$  and  $\Delta V$  are the density and volume of molecule *i*, respectively, as defined by Eq.(3), and  $\rho_{eq}^*$  is the density value when the molecules are uniformly distributed, i.e.,  $\rho_{eq}^* \equiv N/$  Vol, where Vol is the volume of the fundamental cell. The density uniformity factor  $f_{\rho}$  as defined by Eq.(4) represents the deviation from uniform state. From Fig.10 it is observed that a higher temperature nanojet evaporates faster than a lower temperature one and this corroborates the results of Figs.3~7 as discussed in section 3.1. The time averaged value of the density uniformity factor,  $\overline{f_{\rho}}$ , in a time



Figure 10: Evolution of the density uniformity factor for different temperatures (cases 1-5 in Table 1)



Figure 11: Evolution of the density uniformity factor for different orifice lengths at  $T^*=2.0$  (cases 3, 6 and 7 in Table 1)



Figure 12: Evolution of the density uniformity factor for different orifice lengths at  $T^*=3.0$  (cases 4, 9 and 10 in Table 1)

interval of  $t^*=0$  to 80, as listed in Table 1, also reveals this observation. In Fig.10, it is noted that at lower temperatures ( $T^*=0.75$  and 1.5), the density uniformity factor increases first and then decreases. For a lower temperature nanojet, the momenta of the liquid molecules away from the push panel in the nano-atomizer are low while the molecules near the push panel have relatively higher momenta due to the action of the push panel. This results in a compression effect that leads to the increase of the density uniformity factor at the earlier stage of the atomization process; while





Figure 13: Evolution of the density uniformity factor for different orifice radii at  $T^*=2.0$  (cases 3 and 8 in Table 1)

Figure 14: Evolution of the density uniformity factor for different orifice radii at  $T^*=3.0$  (cases 4 and 11 in Table 1)

at a later stage, the density uniformity factor drops because of the ejection of the molecules.

Figure 11 shows the evolution of density uniformity factor for different orifice lengths on the basis of identical nozzle orifice diameter (6 nm)and the conditions of  $L_3^*=5.73$ ,  $L_5^*=76.7$ ,  $T^*=2.0$  (cases 3, 6 and 7 in Table 1). It is observed that a nanojet with a shorter orifice length evaporates quicker. The time averaged value of the density uniformity factor,  $\overline{f_{\rho}}$ , in a time interval of  $t^*=0$  to 80, as listed in Table 1, also reveals this observation. This corroborates the results of Figs.8(a), (b) and (c) as discussed in section 3.1. In addition, it is also observed that, as time elapsed, the influence of the orifice length mitigates. This is because as time elapsed, more and more molecules spurt from the atomizer and hence the interaction between the liquid molecules and the rigid atomizer molecules mitigates due to the decrease of number of molecules inside the atomizer. Figure 12 also reveals this tendency. However, as can be observed from Fig.12, the influence of the orifice length becomes less pronounced at a higher temperature because of the higher molecular kinetic energy to overcome the resistance caused by the orifice. Figure 13 shows the evolution of density uniformity factor for different orifice diameters on the basis of identical nozzle orifice length (2 nm)and the conditions of  $L_4^*=5.73$ ,  $L_5^*=76.7$ ,  $T^*=2.0$  (cases 3 and 8 in Table 1). It is observed that a nanojet with a larger orifice diameter evaporates quicker. The time averaged value of the density uniformity factor,  $\overline{f_{\rho}}$ , in a time interval of  $t^*=0$  to 80, as listed in Table 1, also reveals this observation. This corroborates the results of Figs.8(a) and (d) and also reveals previous observation that a nanojet from a nozzle with a smaller orifice length/diameter ratio evaporates quicker. Similar tendency is obtained from Fig.14 for a higher temperature nanojet.



Figure 15: Evolution of the averaged non-dimensionalized intermolecular force for different temperatures (cases 1–5 in Table 1)



Figure 16: Evolution of the averaged non-dimensionalized intermolecular force for different orifice lengths at  $T^*=2.0$  (cases 3, 6 and 7 in Table 1)



Figure 17: Evolution of the averaged non-dimensionalized intermolecular force for different orifice lengths at  $T^*=3.0$  (cases 4, 9 and 10 in Table 1)



Figure 18: Evolution of the averaged non-dimensionalized intermolecular force for different orifice radii at  $T^*=2.0$  (cases 3 and 8 in Table 1)



Figure 19: Evolution of the averaged non-dimensionalized intermolecular force for different orifice radii at  $T^*=3.0$  (cases 4 and 11 in Table 1)

#### 3.3 Intermolecular Force

The intermolecular force is an indication of the surface tension experienced by the liquid particles and has a great effect upon the atomization process. Lefebvre (1989), Chigier (1999)and Hiroyasu (2000) pointed out that surface tension and interfacial force are the major controlling mechanisms for atomization. Owing to the vacuum environment, the aerodynamic effect on the atomization process is negligible in this study. Thus, the surface tension becomes the major controlling mechanism for the atomization process. Figure 15 shows the evolution of averaged non-dimensionalized intermolecular force for nanojets with different temperatures and the conditions of  $L_2^* = L_3^* = L_4^*=5.73$ ,  $L_5^*=76.7$ ,  $D^*/2=8.81$  (cases 1~5 in Table 1). The averaged non-dimensionalized intermolecular force at time  $t^*$  is defined as

$$\overline{F_{t^*}^*} = \frac{\sum_{i=1}^{N} F_{i,t^*}^*}{N}$$
(5)

where *N* is the total number of molecules in the fundamental cell and  $F_{i,t^*}^*$  is the resultant force of the non-dimensionalized intermolecular force vector acting on molecule *i* at time  $t^*$ , i.e.  $F_{i,t^*}^* = (F_{x,i,t^*}^{*2} + F_{y,i,t^*}^{*2} + F_{z,i,t^*}^{*2})^{1/2}$ , where  $F_{x,i,t^*}^*$ ,  $F_{y,i,t^*}^*$  and  $F_{z,i,t^*}^*$  are the components of the intermolecular force vector at the *x*, *y* and *z* directions, respectively, acting on molecule *i* at time  $t^*$ . Note that in the above definition of  $\overline{F_{t^*}^*}$ , *N* is the total number of molecules in the fundamental cell, which includes liquid, vapor and solid molecules (atomizer and push panel); while in

the definition of density uniformity factor, Eq.(4), N is only the initial number of liquid molecules in the fundamental cell, i.e. the solid molecules are excluded. The intermolecular force diminishes with time because of the increase of distances between molecules as the nanojet vaporizes. From Fig.15, it is observed that a higher temperature nanojet evaporates faster than a lower temperature one. This corroborates the results of Figs.3~7 discussed in section 3.1 and Fig.10 in section 3.2. In Fig.15, it is also noted that although a higher temperature nanojet has a larger intermolecular force at the earlier stage of the atomization process due to its higher momentum, it evaporates faster and therefore the intermolecular force decays quicker. Figure 16 shows the time averaged value of the averaged nondimensionalized intermolecular force for different orifice lengths on the basis of identical nozzle orifice diameter (6 nm)and the conditions of  $L_3^*=5.73$ ,  $L_5^*=76.7$ ,  $T^*=2.0$  (cases 3, 6 and 7 in Table 1). It is observed that a nanojet with a shorter orifice length evaporates quicker. This corroborates the results of Figs.8(a), (b) and (c) as discussed in section 3.1 and Fig.11 as discussed in section 3.2. In addition, it is also observed that, as time elapsed, the influence of the orifice length mitigates. As explained in section 3.2, more and more molecules spurt from the atomizer as time elapsed. This causes the interaction between the liquid molecules and the rigid atomizer molecules to mitigate due to the decrease of number of molecules inside the atomizer. Figure 17 also reveals this tendency. However, as can be observed from Fig.17, the influence of the orifice length becomes less pronounced at a higher temperature because of the higher molecular kinetic energy to overcome the resistance caused by the orifice. Figure 18 shows the evolution of averaged nondimensionalized intermolecular force for different orifice diameters on the basis of identical nozzle orifice length (2 nm)and the conditions of  $L_4^*$ =5.73,  $L_5^*$ =76.7,  $T^*=2.0$  (cases 3 and 8 in Table 1). It is observed that a nanojet with a larger orifice diameter evaporates quicker. This corroborates the results of Figs.8(a) and (d) as discussed in section 3.1 and Fig.13 as discussed in section 3.2 and also reveals that a nanojet from a nozzle with a smaller orifice length/diameter ratio evaporates quicker. Similar tendency can be observed from Fig.19 for a higher temperature nanojet.

#### 4 Conclusions

In this study, the atomization process of a nanojet is investigated by molecular dynamics simulation. It is found that a liquid nanojet evaporates faster at a higher temperature. On the basis of identical nozzle orifice diameter, a nanojet from a nozzle with a shorter orifice length evaporates quicker. However, the influence of the orifice length mitigates as time elapsed. In addition, the influence of the orifice length becomes less pronounced at a higher temperature. On the other hand, on the basis of identical nozzle orifice length, a nanojet from a nozzle with a larger orifice diameter evaporates quicker. The present simulation results reveal that a nozzle with a smaller orifice length/diameter ratio produces better atomization. This corroborates the results from conventional macroscopic analysis.

**Acknowledgement:** The author gratefully acknowledges the grant support from the National Science Council, R.O.C., under the contract NSC97-2221-E-150-029.

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