Molecular Dynamic Simulation of an Electrohydrodynamic Liquid Jet

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Abstract

The dynamic behavior of a conducting liquid jet issuing from an electrified nozzle is well known as a whipping type motion in the DC electric field (lateral instability), and as a controllable harmonic sausage type motion in the AC-DC electric field (varicose instability). These types of instability are simulated using molecular dynamics (MD) technique in 3-D. The Simulation results give valuable insight into the field coupling mechanisms of force and charge relaxation on the surface of the jet, and the disintegration process of the jet associated with the physical properties of the liquids. The whipping motion that results from the relaxation of surface stress with the increase in tangential pressure tensor, which is produced by the interaction of charge molecules with the field. The harmonic sausage motion results from the synchronization of local concentration of charged molecules with the applied AC frequency under the influence of AC superimposed DC field. The charged molecules produce strong pressure stress, which induces a reduction in surface tension and results in a characteristic electrohydrodynamic (EHD) motion.

1. Introduction

Electrohydrodynamic (EHD) atomization has been investigated experimentally for many industrial processes; fine powder production, painting, ink-jet printing, spray drying, fuel spraying, etc [1-5]. In addition, the behavior of instability and disintegration of EHD jets have been studied by some researchers [6-14]. They obtained analytical solutions based on the Navier-Stokes and the Maxwell equations. However, their solutions offer inadequate information on the contribution of electric charge on the disintegration of the jet. The understanding of the charge relaxation to the surface of a liquid jet and the contribution of the liquid molecules to the disintegration process are very important.

Molecular dynamics (MD) simulation is a powerful technique utilized to investigate the fundamental mechanisms of jet break-up phenomenon, that is mainly used in the fields of chemical and material sciences. This technique can provide insight into the important mechanisms such as the ensemble averaging of molecular micro-property. The properties such as dynamics or thermodynamics of local space are investigated by following each molecule trajectory [15]. Some researchers have studied the surface tension of many fluids and obtained good agreement with the experimental results and theory [16,17]. The disintegration process of liquid jet has been studied using MD technique; e.g. non-electrified model [18], and the EHD instability such as lateral and varicose types [19,20].

In this paper we report useful information on the fundamental disintegration mechanisms of an electrified liquid jet and give the important elements associated with the unstable EHD phenomenon based on MD simulation.

2. Calculation Procedure

Theoretical analysis of spatial and temporal behavior of an electrified liquid jet is a complex process. It is because the unstable EHD motion caused by all interactive forces results in different modes of atomization; (Taylor cone, lateral instability, and varicose instability). Therefore, to simplify the model, it is required to control the EHD instability in this simulation. The present study only considers the effect of charged molecules in a liquid jet under a vapor environment. In this study, the water molecules of the liquid jet are assumed as solid molecules, which are distributed to form FCC (Face Cubic Center Lattice) arrangement in a retangular box of periodic boundary conditions in three directions. The molecular numbers of both liquid and vapor phases are gained from the experimental liquid-vapor coexistence curve at room temperature. The smooth boundary between the liquid

and the vapor phases is built by performing pre-calculation with a quarter of simulation time step. The periodic boundary condition and calculation procedure are the same as those reported in [20,21]. The Lennard-Jones potential is assumed as the interaction between molecules. The time step is 0.002τ, where τ (=$(m\sigma^2/w)^{1/2}$), m (=0.2993×10^{-25} kg), σ (=0.342 nm) and w (=293 K/k_B) are reduced parameter of weight, length and potential, respectively. The dimension of the jet is taken as 37.6nm in length and 3.4nm in diameter, in which the number of molecules were 5583, and the length of fundamental simulation cell (L) is about 18.8nm (Table 1). These dimension were used to minimize computational time (which took a few days using Alpha 800 CPU).

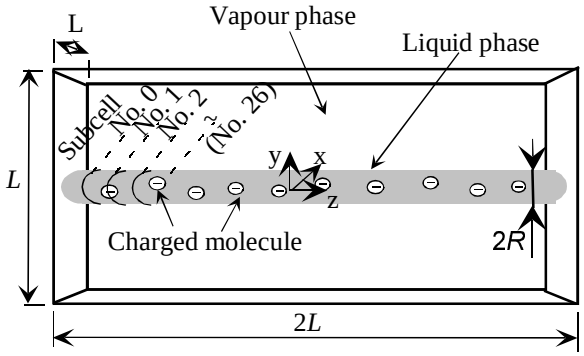


Figure 1. Schematic of simulation cell

Cell size; L [m]	18.8×10^{-9}
Liquid jet radius; R [m]	1.7×10^{-9}
Liquid density; ρ_l [kg/m^3]	1142.45
Vapour density; ρ_g [kg/m^3]	1.76
Temperature; T [K]	293.0
Pressure; P [kPa]	101.3

Table 1. Simulation parameters

In the present simulation, the contribution of surface tension and pressure tensor of liquid jet, which are important parameters for atomization process, were addressed in the jet propagation direction. The parameter values were obtained from statistical averaging using Equation (1) in each subcell. The liquid jet is divided into 27 subcells in jet direction as shown in Figure 1. This is because if the total number of molecules contained within a subcell is small, the properties which we want to investigate will be swamped by the thermodynamic fluctuation. Therefore, to investigate the local parameters of simulation (such as thermodynamic and dynamic properties), enough molecules are needed (basically about 100 molecules at least [15]). In this simulation 200 molecules were used. The equation for statistical averaging used in this study is:

$$\langle A \rangle = \frac{1}{N}\sum_{n=1}^{N} A(\tau) \ , \tag{1}$$

where < > represents the statistical averaging and A is thermodynamic or dynamic properties such as pressure or surface tension. N is the molecule number contained in each sub-cell,

The instant pressure tensor is calculated by Equation (2-1) [21].

$$P = <\rho> k_B T + W/V \ , \tag{2-1}$$

$$W(r_{ij}) = -\frac{1}{3}\sum_{i}\sum_{j>i} \mathbf{r}_{ij}\cdot\nabla_r w_{ij} \ , \tag{2-2}$$

where ρ is the molecular density of subcell and is given by N/V , V is the volume of subcell, k_B is the Boltzmann constant (=1.38×10^{-23}), and W is the Virial function which is the term considering the effect of molecular interaction into pressure. Other parameters in Equation (2-2), $\mathbf{r}$ and w are distance between centers of two molecules, and molecular potential, respectively. All the interactions of molecules are calculated when the distance is smaller than the cutoff length (r=2.5σ). The instant surface tension is calculated from Equation (3) as the pressure difference between the tangential and radial components [16].

$$\gamma(k) = \frac{L_z}{N_s}\left\{p_t(k) - p_r(k)\right\}$$

$$= \frac{1}{L_x L_y}\left\langle \sum_{(i,j)}^{(k)} \frac{1/2(\mathbf{x}_{ij}^2 + \mathbf{y}_{ij}^2) - \mathbf{z}_{ij}^2}{\mathbf{r}_{ij}} \cdot \mathbf{f}(r_{ij}) \right\rangle \quad , \tag{3}$$

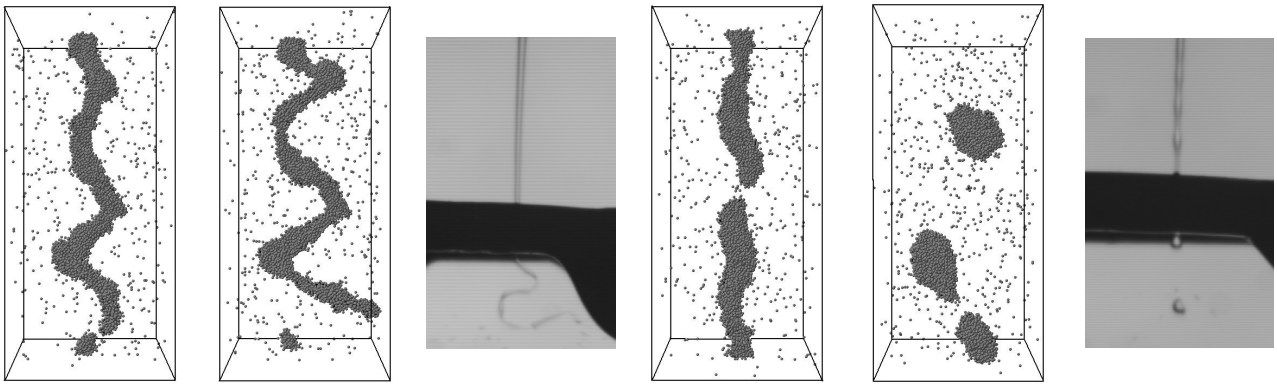
where $L_{x,y,z}$ is the length of subcell in each Cartesian coordinate.

3. Results and Discussion

3-1. Disintegration process of electrified jet

The 3D graphical-snapshot of the present study under the DC electric fields are shown in Figure 2(a). The interfacial disturbance occurs on the surface of the jet after starting the calculation, and develops into the "whipping" (lateral instability) of the jet from side to side, at 60ps.

The 3D graphical-snapshot of the present study under an AC superimposed onto a DC electric fields are shown in Figure 2(b). The effect of an AC frequency on the electric field is expressed by three cycles of charged molecules distribution in the axial direction. The rapid break-up and the three droplets creation occurs because of the concentration of charged molecules at the break-up points of the jet. The experimental sequence in Figure 2(b) is exhibiting the influence of the applied AC frequency (2.25 kHz) on the disintegration process, which results into sausage instability, at a flow rate of 3.5ml/min [22]. Both simulation results of the present study are the same as those reported in [20].

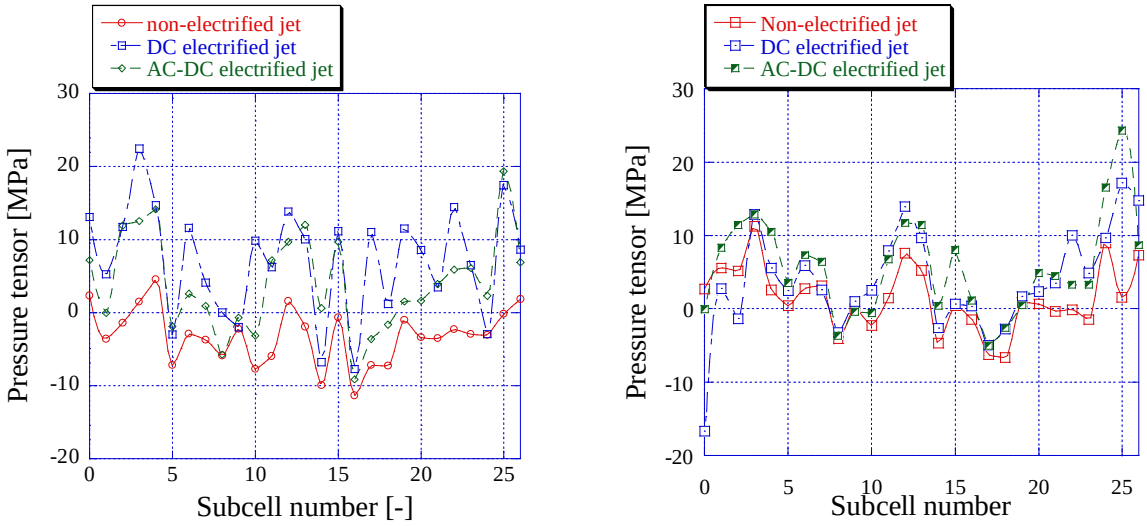


(a) DC electrified jet motion. (b) AC-DC electrified jet motion.

Figure 2. Comparing the disintegration processes of electrified water jet between MD simulation and experimental result under the temperature 293K and pressure 101.1kPa

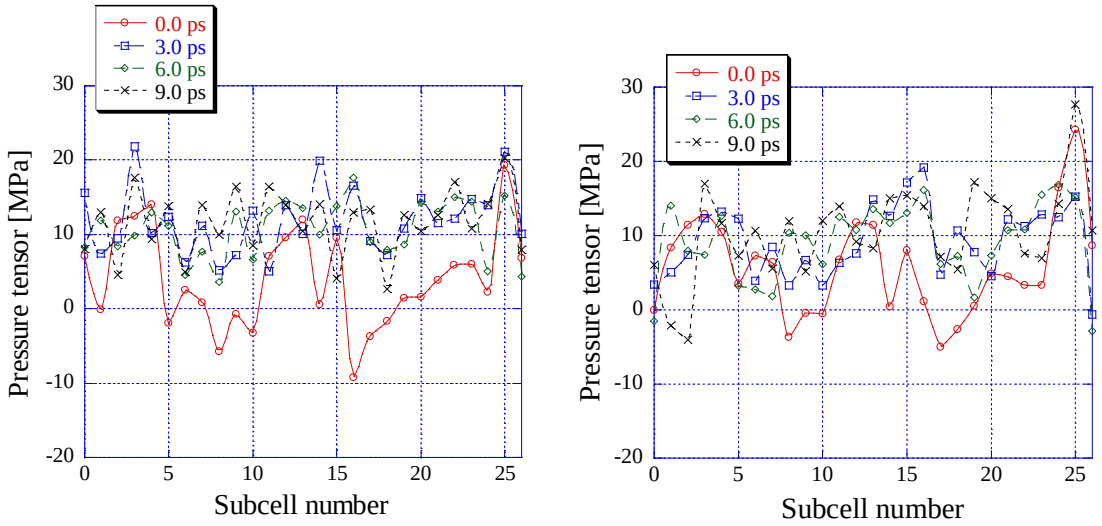
3-2. Analyzing the instability dynamics of EHD jet

The pressure distributions of tangential and radial components in a liquid jet, which are calculated from ensemble averaging in each subcell using Equation (1), are shown in Figure 3 for the three types of jet conditions; non-electrified, DC electrified, and AC-DC electrified liquid jets at 0.0ps. The cause of unstable distribution (non-uniform) in both graphs may be that the thermal fluctuation that exists or the time averaging was not considered. The present simulation scale is not sufficiently large; therefore, the process of disintegration occurs quickly.



(a) Tangential component (b) Radial component

Figure 3. Local pressure tensor on the jet at initial state (0.0ps)



(a) Tangential component (b) Radial component

Figure 4. Investigation of the pressure tensor on the time development of AC-DC electric jet

The tangential component of pressure tensor increases when the charged molecules are distributed in the liquid jet. The increment of tangential component may indicate localization of charged molecules. Therefore, the distribution of tangential pressure component has three cycles oscillation under the condition of an AC-DC electrified jet. The difference in radial component of pressure tensor is not so conspicuous, even though the charged molecules are distributed in the liquid jet.

Figure 4 shows time difference of pressure tensor after starting the simulation. The tendency of both tangential and radial pressure component does not differ too much. It is presumed for EHD disintegration process that the strong tangential pressure component in the liquid jet is kept until it breaks up continuously. Thus, if the bending of liquid jet happens under the condition of compressing pressure force, the tangential pressure component becomes three types of pressure component; circumferential, axial and radial component. Each pressure component accelerates the bending of the liquid jet, and results in a whipping motion.

Consideration of the surface tension is very important for investigating the jet instability. Change of surface tension of the liquid under the influence of the electric field occurs because charged molecules in a liquid jet increase the tangential component of the pressure tensor (Figure 3). Under the condition of DC electric field, the reduction in surface tension is large at every subcell. However, when an AC-DC electric field is applied, the charged molecules are concentrated at the breakup points. (see Figure 5)

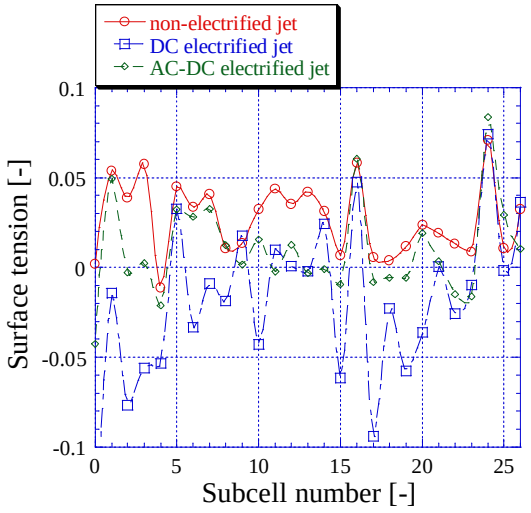


Figure 5. Local surface tension of each electric condition

It becomes obvious from these results that the whipping motion of the DC electrified liquid jet is caused by the increasing pressure strength of tangential component under the instability condition with decreasing of surface tension. This phenomenon starts from the event of jet-bending at first in this simulation. This is because the charged molecules inside the liquid jet typically influence the increase of the pressure tensor in the tangential direction (Figure 3(a)). After that, strong tangential pressure divides into three types of pressure components (circumferential, axial and radial component). Each pressure components induces accelerative bend motion, and results in a whipping motion. The charged molecules produce strong pressure field, which is typically in the tangential direction of the liquid jet. Therefore, when the AC superimposed DC electric field is applied to the liquid jet, controllable uniform droplet sizes are created in harmonic frequency between AC electric field and the pressure tensors.

4. Conclusion

The present study has shown that the dominant parameter of the unstable EHD jet motion can be qualitatively analyzed by estimating the tangential component of pressure tensor, from the micro molecular property of the test liquid, using MD simulation. The varicose jet phenomenon, which generates small droplets in the radial direction, at first starts from the bend motion by the strong tangential pressure field. This strong pressure field continues until the droplets are produced. Those characteristic phenomena of EHD takes place under the unstable relaxed surface tension condition.

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Nomenclature

i :	molecule index	x,y,z :	cartesial coordinate
k_B :	Bolzman constant [J/K]	ρ :	density [kg/m^3]
L :	cell size [m]	σ :	considerable molecular diameter [m]
m :	molecular weight [kg]	τ :	time step [s]
N :	molecular number contained in subcell	γ:	surface tension [N/m]
P :	pressure [Pa]		
R :	liquid radius [m]	**Subscription**	
r :	distance between molecules	l :	liquid
T :	temperature [K]	g :	vapor
w :	potential depth [J]		
W:	virial function		

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