

# Dynamics Simulation of Electrospun Ribbon Instability Section

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**Abstract:** In recent years, there are more and more researches on electrospinning, but some problems are still difficult to solve, such as the difficulty of controlling the structural size of the product fiber. Therefore, we need to explore basic theories, perform dynamic analysis on the jet behavior, so that the quality of the produced fiber is good and the output is large.

In this paper, mechanical analysis of the unstable segment of electrospun charged jet is carried out and the dynamic model of the jet is established. The trajectory of the jet in the unstable segment is calculated using Matlab software. Basing on the Maxwell viscoelastic model, establish a dynamic model of the jet. Taking a single jet in a single-needle electrospinning device as the research object. The jet is discrete into multiple charged particles, and the movement trajectory of the charged particles is simulated using Matlab software. The results show that the influence of voltage on jet trajectory distribution is obvious.

**Keywords:** Electrospinning; Viscoelastic Model; Mechanical Analysis; Simulation

## 1. Introduction

In the electrospinning process, the polymer solution forms a jet under the action of high-voltage static electricity, and the jet is composed of an infinite number of fluid particles. This paper mainly performs numerical calculations on the trajectory of the jet. A dynamic model is set to simulate the unstable section of the jet to analyze the force of the particles.

## 2. Calculation method

The method of using Matlab simulation is the slope method: first, the interval is discretized, and the upper and lower limits of the x-axis, y-axis, and z-axis are input. The value range of the x-axis and y-axis is  $[-6, 6]$ , and the value of the z-axis is  $[26, 30]$ , which is divided 50 equal parts, and then perform the following calculation. In the process of two-dimension simulation drawing, each trajectory is divided into x-axis component and y-axis component according to the data, that is, the force received by particle  $i$  can be decomposed into x-axis and y-axis components. As it is very short that the particle separation distance can be taken as a straight line. The particle trajectory can be gotten by solving the x-axis and y-axis coordinates of particle  $i$  and the deflection angle of the xoy plan<sup>[2]</sup>. In the process of three-dimensional dynamic simulation of jet particles, the movement trajectory of each micro-element segment in space is decomposed into x-axis component, y-axis component and z-axis component. As the distance between adjacent particles is very small, each trajectory can be approximated as straight line, and only solve the coordinates of the particle  $i$  and the deflection angle of the xoy plane. The deflection angle of the z axis to simulate the three-dimension trajectory of the jet in the unstable section. The premise is that you need to input parameters such as voltage, calculate the surface tension, viscoelastic force, Coulomb force, and electric field force that particle  $i$  is subjected to to obtain the size and direction of the particle's total force<sup>[3]</sup>. The entire particle coordinates obtained by calculation, the deflection angle of the xoy plane and the deflection angle of the z-axis are brought into programming to simulate the movement trajectory from particle 1 to particle  $i$  (including 2D and 3D trajectory diagrams).

## 3. Establishment of a model of jet dynamics

According to the Newton's second law the resultant force acting on the particle  $i$  in the unstable section of the jet is<sup>[1,2]</sup> □

$$m_i \frac{d^2 r_i}{dt^2} = m_i \frac{dv_i}{dt} = f \quad (1)$$
$$\vec{r}_i = \vec{i}x_i + \vec{j}y_i + \vec{k}z_i$$

The resultant particle should satisfied as<sup>[1,2]</sup>

$$\begin{aligned}
f &= f_{vei} + f_{si} + f_{ei} + f_{Ci} \\
f_{vei} &= \pi a_{ni}^2 \sigma_{ni} \left[ \frac{x_{i+1} - x_i}{l_{ni}} \vec{i} + \frac{y_{i+1} - y_i}{l_{ni}} \vec{j} + \frac{z_{i+1} - z_i}{l_{ni}} \vec{k} \right] \\
&\quad - \pi a_{di}^2 \sigma_{di} \left[ \frac{x_{i+1} - x_i}{l_{di}} \vec{i} + \frac{y_{i+1} - y_i}{l_{di}} \vec{j} + \frac{z_{i+1} - z_i}{l_{di}} \vec{k} \right] \\
f_s &= - \frac{\alpha \pi a_{av}^2 k_i}{\sqrt{x_i^2 + y_i^2}} \left[ |x_i| \text{sign}(x_i) \vec{i} + |y_i| \text{sign}(y_i) \vec{j} \right] \\
f_e &= -e \frac{V}{a_0 \ln[2(h/a_0)^{1/2}]} \vec{k} \\
F_{Ci} &= \frac{1}{4\pi\epsilon_0} \sum_{\substack{j=1 \\ j \neq i}}^N \frac{e^2}{R_{ij}} \left[ \vec{i} \frac{x_i - x_j}{R_{ij}} + \vec{j} \frac{y_i - y_j}{R_{ij}} + \vec{k} \frac{z_i - z_j}{R_{ij}} \right]
\end{aligned} \tag{2}$$

In the formula,  $\vec{i}, \vec{j}, \vec{k}$  are respectively representing the Cartesian coordinate system three direction unit vectors,  $m, f$  is quality and force of the  $i$ th particle respectively,  $\epsilon_0$  is dielectric constant and  $N$  is total number of particles. In the formula,  $q_1, q_2$  denotes two charge quantities respectively,  $l$  is the distance between the charges,  $k_e = 1/\epsilon_0$  is the Coulomb force constant,  $\epsilon_0$  is the vacuum capacitance,  $\epsilon_0 = 8.854 \times 10^{-12}$  F/m.

## 4. Simulation of experiment program

### 4.1 Initial model values and simulation parameters

Set the simulation parameters as follows: particles charged is  $e = 2.84 \times 10^{-9}$  C, particle mass is  $m = 2.84 \times 10^{-9}$  kg, elastic modulus is  $\eta = 10^4$  kg/(m·s), the viscosity coefficient is 10MPa, the solution surface tension coefficient is  $\alpha = 0.07$  N/m, the needle diameter is  $a_0 = 2 \times 10^{-3}$  m, the initial length of the elastic element in the viscoelastic model is  $L = \sqrt{e^2 / \pi a_0^2 E}$ .

Only when the distance between the tip particle and the needle is greater than the initial length  $L$  of the viscoelastic element, the simulation will start.

The initial values of the parameters defined in the model are:

Define  $t = 0$  as the initial moment of charged particles;

At the beginning of the simulation, the number of jet particles is  $N = 2$ , and the longitudinal distance from the needle is  $L$  and  $2L$  respectively, and the initial velocity of both particles is zero.

At the initial moment, the viscoelastic stress of the particles and the chain length between the connected particles are also zero, that is  $\sigma_{d1} = 0$ ;  $l_{d1} = 0$ ;  $\sigma_{nN} = 0$ ;  $l_{nN} = 0$ .

The specific steps of the numerical calculation of the electro-jet kinematics model of the electrospinning ribbon:

- (1) Initial time  $t = 0$ , initial position of charged particles, initial velocity.
- (2) Calculate the viscoelastic force, surface tension, Coulomb force and electric field force acting on the particles at time  $t$ .
- (3) According to formula (2), calculate the position of the particle now.
- (4) Repeat steps (2)-(3) for each particle.

## 5. Numerical simulation of trajectory of single jet

Taking the single needle electrospinning device as an example. According to the kinematic model of the unstable section of the electrospinning jet described, a voltage of 14 KV is applied to the needle using the Matlab simulation method, the distance from the needle to the receiving plate is  $h = 30$  cm, and the receiving plate does not move relative to the polymer jet, keeping the receiving plate stationary. Then

input parameters, carry out simulation, reach the bottom, simulation stop. In this simulation, the z-axis distance range is set to [26, 30], the set voltage is 14KV, and the receiving distance is set to 30 cm.

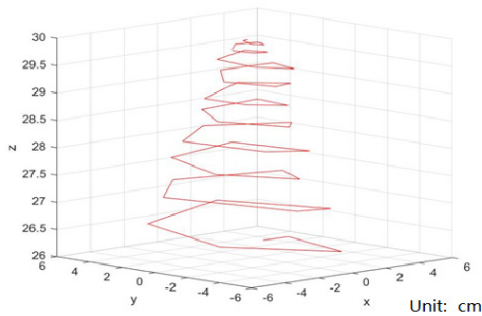


Figure 1 Simulation of the motion trajectory of a single jet

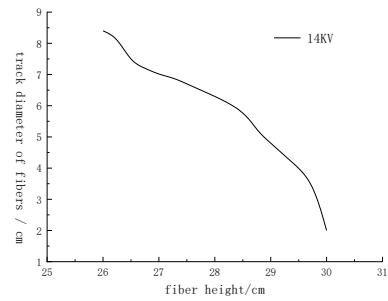


Figure 2 Relationship between diameter and heightand

Figure 1 is the simulation results of the electrospinning motion trajectory. The electrospay ribbon electro-jet has a spiral shape as a whole, gradually diffusing outward, and the closer it is to the receiving plate, the larger the trajectory diameter that is, the greater the rotation amplitude. Figure 2 shows the relationship between the trajectory diameter of the jet and the height of the jet. We can see that the diameter of the trajectory of the jet increases gradually with the direction away from the needle. It can be seen from the comparison between Figure 1 and Figure 3 that the trajectory obtained from the model is basically consistent with the real trajectory of the electrospinning jet.

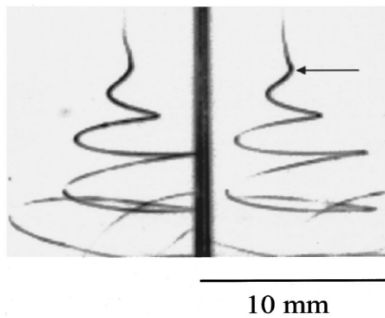


Figure 3 Curve of unstable section of electrospay ribbon electrojet

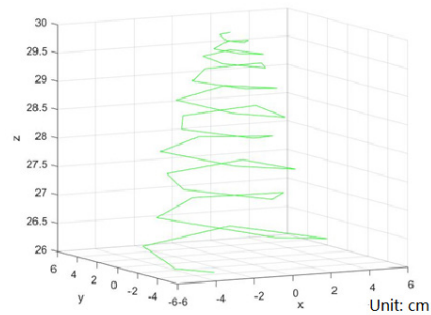


Figure 4 Simulation of the trajectory of a single jet

Next, set the second set of simulation voltage to 16 KV. The other parameters remain the same as the first set of parameters. Figure 4 is a three-dimension diagram of the simulation of the trajectory of a single jet.

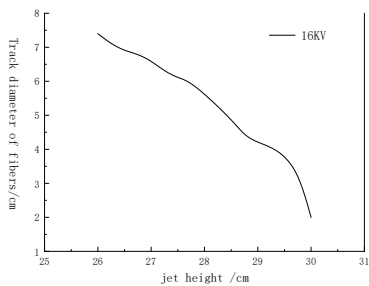


Figure 5 Relationship between diameter and height

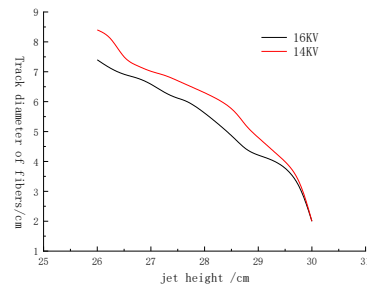


Figure 6 Relationship between diameter and input voltages

Figure5 shows the change of the diameter of the jet trajectory when  $h = 30$  cm and  $V = 16$  KV. Figure6 shows the relationship between the trajectory mode diameter of a single jet and different voltage values at 14 KV and 16 KV, respectively. As can be seen from Figure6, the increase in voltage “constrains” the track diameter of electrospinning from becoming larger.

## 6. Summary

Based on the established jet motion equations Matlab is used to numerically calculate the trajectory of a single jet in this paper. The calculation method and flow chart of jet trajectory simulation are involved. The relationship among the height of the jet and the diameter of the fiber trajectory and the different voltage conditions is analyzed. The influence on the diameter of the jet trajectory, and the actual experimental result.

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