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Development of Control System for Indigenous Electrospinning Machine

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Abstract: Electrospinning is one of the versatile and relatively new method of producing nanofibers in different forms with potential applications in diverse fields.Repair and regeneration of human tissues and organs using biomaterials, cells and growth factors is a great challenge for tissue engineers and surgeons. These fine nano fibres can be used for many applications, including the fabrication of scaffolds for tissue engineering, drug delivery, biosensors, artificial bone, skin or cartilage implants etc. A drawback of the electrospinning process however, is the unstable behaviour of the liquid jet. This causes the fibres to be collected randomly without proper allignment. Controlling this process is therefore desirable. Studying the dynamics of the jet becomes easier and faster if it can be modeled. The dynamics of the jet is studied by modeling the jet behavior using Matlab. Changing the parameters results in a difference in the dynamical behavior of the jet. Increasing the elastic modulus resulted in less unstable behaviour of the jet.

Key words:

INTRODUCTION

Electrospinning, a process patented by Formhals in 1934,for the fabrication of textile yarns. After Formhals patent, a lot of researchers Vonnegut, Newbauer, Drozin, Simons, have constantly enriched the potential of electrospinning by their novel works. Since 1980's till present, with the advent of nanotechnology and simplicity to fabricate ultrathin fibres or nanomats of different fibres and varying diameters in the submicron or nanometer scale, electrospinning process has gained wide popularity. Electrospinning is the one of the most conventional and versatile method of producing nanofibres in different forms with potential application in diverse field. Nanofibres, defined as fibres with diameter of <100 nm to <500 nm, are desirable enhancements for a number of promising applications including medical, filtration, energy, textile, protective, structural, electrical and optical.From the paper Rob Van Vught *et al*. [1], an existing mathematical model which describes the mechanical system of masses that are interconnected with viscoelastic elements, are used to build a Matlab script on. The simulation features to cope up with the introduction of new and removal of old elements from the system The increase in number of patents for different applications related to electrospinning and a large number of universities and research institutes worldwide that includes various aspects of electrospinning process giving an insight about the electrospinning process in the recent years. Darell Hyson Reneker *et al*., has come up with the new parameter values of elastic modulus and strain for the simulation of the jet.Jet initiation is the combination of introducing charges to the electrospinning solution and subjecting it to an electric field. When the potential difference is same regardless of whether the voltage is applied to the needle or collector, acquiring of charges by the solution is dependent on where the charges are applied. When high voltage is applied to the collector, the solution has very little charges and a much higher potential difference is required to stretch the solution. However when the charge is applied to the solution through the needle, the solution will acquire additional electric charges which will react strongly to increment in the electric field. Therefore aplying an opposite voltage to the collector should only be used for facilitating electrospinning extension and not for jet initiation.The modeling of jet initiation is required for the process because the jet initiated ejects out the liquid that is instable. The instability of the jet causes damages in the fibre formed and thus the resulting fibre morphology is affected. In this paper, the following sections include the description of the electrospinning process, mathematical modeling of the jet and the simulation results of each mathematical script of the jet.

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Section 1

Process Description: The electrospinning is mostly done in solvent solution or in melt form. The basic setup for electrospinning as shown in Figure 1, consists of a high voltage supply, a syringe with a pipette tip or a needle and a metallic collector. In electrospinning, a polymer solution is charged with a high DC voltage to produce a charged jet that ejects from the pipette by a syringe pump.

The jet travels towards a rotating mandrel collector where it is collected as aligned fibre over an aluminium foil. The solution jet evaporates or solidifies on the way to collector screen to produce thin sub-micron size polymeric fibres. A wide range of polymeric materials can be used for the fabrication of nanofibres. When the diameter of polymer fibre material is scaled down from micro to nano scale, several amazing and unique characteristics are observed.

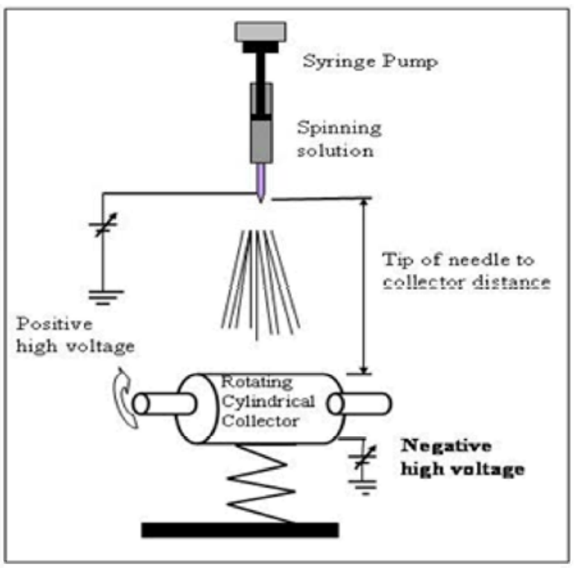

Fig. 1: Block diagram Electrospinning process

The unique characteristics of electrospun nanofibres make them suitable candidate for many applications, such as tissue engineering scaffolds, skin or bone or cartilage implants, biosensors, wound dressing, protective clothing, filtration, electronics, absorbing media and energy storage. Several other methods have been used to fabricate nanoscale polymeric fibres, such as meltblowing, bicomponent spinning, forcespinning and flash spinning. In most cases, a high positive DC voltage of several tens of kV is applied to the polymer solution and the collector is grounded. A syringe pump is mostly used to flow the polymer solution out of the syringe at constant flow rate. When the electric field is applied to the polymer solution in the syringe, charge is induced at the tip of the needle where the liquid is held together by surface tension. Electrostatic repulsion counteracts the surface tension of the liquid. When the increase of intensity of electrical field, the shape of the liquid at the tip of the needle changes from hemispherical shape to a more elongated conical shape known as Taylor cone. Further increase of electrical field intensity takes the repulsive force to a critical threshold level where it exceeds the surface tension of the liquid and a jet ejects from the tip of the Taylor cone. Charge repulsion inside the jet and the interaction between external electrical field and the jet causes it to experience a bending instability. The unstable jet starts to loop and stretch thinner with each loop until it reaches the collector. The solvent evaporates and leaves dry fier on the collector. Hundreds of different polymers have been electrospun into nanofibres for various potential applications. Features of the jet in electrical field are matter of great interest. There are experimental validations supporting the conical shape projection of liquid jet. A mathematical equation of critical voltage was developed by Taylor which is given below:

$$V_c^2 = 4 * \left(\frac{H^2}{L^2}\right) * \left\{\ln\left(\frac{2L}{R}\right) - 1.5\right\} * (0.117 * \pi * R * \gamma)$$

Where V_c is critical voltage, H is the distance between tip and collector, L is the length of capillary tube, R is radius of the tube, γ is the surface tension of the liquid.In order to study the dynamic behavior of the jet its important to derive the mathematical model of the motion of jet caused by the acting on it. Section 2 includes the script of the mathematical model for different parameter values and including perturbations in each script.

Section 2

Mathematical Model: The mathematical modeling is done using the equation sof viscoelastic force, Coloumb force, electric force and surface tension force. A forces applied on single bead *i* is calculated. Since all the different forces are define the equations of motions are derived using Newton's second law of motion. The position vector $r_i = ix_i + jy_i + kz_i$ of bead i then be calculated as

$$\frac{d^2 r_i}{dt^2} = \sum_{j=1, j=i} Q/\overline{l}^2 (Lr_i - Lr_j) + V_k - F_v \varepsilon \frac{\overline{\sigma}_{ui}}{l_{ui} L}(L_{r_{i+1}} - Lr_i) + \frac{F_v \varepsilon \overline{\sigma}_{bi}}{l_{bi} L}(Lr_i - Lr_{i-1}\ )$$
$$+A\ 1/\sqrt{x_i^2 + y_i^2}\ [ix_i + jy_i]$$

These are the dimensionless equations of motion, since it gives better relations between the lateral displacements and the vertical jet.

Development of Matlab Script and Simulations: The Matlab script is developed for the simulations of the jet with the specific parameters and initial conditions. Initial condition are needed for the ode 45 integration. The basic initial condition vector for one bead is given as

$$u_o = [x_o, \dot{x}_o, y_o, \dot{y}_o, z_o, \dot{z}_o, \sigma_{uio}, \sigma_{bio}]^T$$

Straight Jet: The first simulation that is made, is to check how the system reacts to its initial conditions. The Coulomb forces in the mathematical model are thought to cause the instability of the jet. these Coulomb forces push the beads away from their equilibria after being perturbed. This means that in the ideal case where the beads are not perturbed, the jet will not show unstable behaviour. To check this, the initial positions x, y and corresponding velocities x', y' of the beads is set to 0. The initial condition vector for the jet at the moment the integration starts, then becomes

$$u_o = [0,0,0,0,\frac{h}{N}.i,0,0,0]^T$$

where h is the distance between drop and the collector. In all simulations h is set to 20 cm, N is the total amount of beads that together form the fluid jet and i is the number of a specific bead in the system. The initial positions x, y and corresponding

velocities x', y' of the beads is set to 0

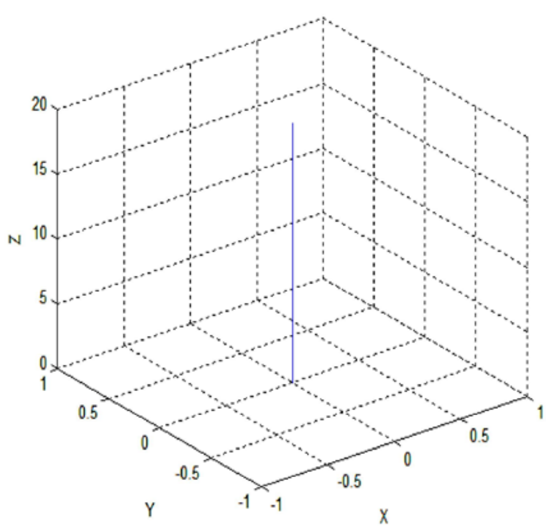

Fig. 2(a): Simulation of straight jet in 3D

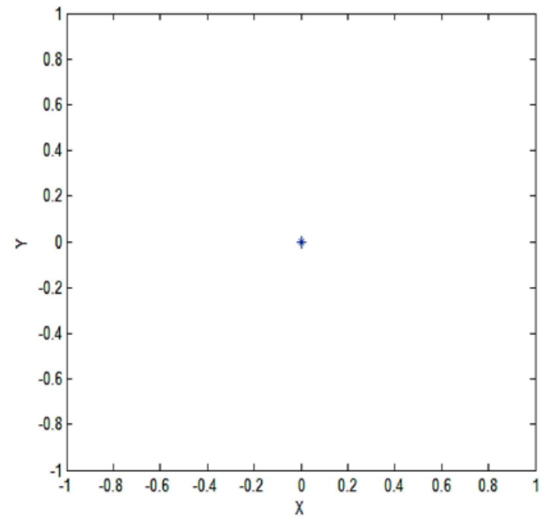

Fig. 2(b): View on the collector plane

First Version of the Script: The first version of scripts includes disturbances of forces unlike the straight jet. In the first simulation there was no perturbation involved.The perturbation of jet is introduced to simulate the unstable behavior of jet. First the state of jet is visualized before the integration starts, i,e. it is the visualization of the initial conditions of the jet before the simulation starts. The initial conditions are

$$u_o = [10^{-3}Lsin\left(\frac{2\pi i}{20}\right), 0, 10^{-3}Lsin\left(\frac{2\pi i}{20}\right), 0, \frac{h}{N}.i, 0,0,0]^T$$

Dimensionless quantities are used to get accuate value in the fluid jet.The dimensionless length scale equations used here is

$$L = \sqrt{e^2/\pi a_0^2 G}$$

$$e = 8.48$$

$$a_0^2 = 150 \times 10^{-4}$$

$$G = 1 \times 10^{-6} = 100000$$

$$L = \sqrt{\frac{8.48^2}{3.14} \times 0.150^2 \times 1000000}$$

$$L = 3.1352$$

For different values of T ranging from 1 to 10 is substituted in the initial conditions of the script. The Coloumb force is given as

$$f_i = \frac{e^2}{R_{ij}^2}[I\times x_i - \frac{x_j}{R_{ij}} + j\times y_i - \frac{y_j}{R_{ij}} + k\times z_i - z_j/R_{ij}]$$

k=1/R
therefore from the fig, $R_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$
for i =1….N.

Table 1: Values of the position vector for different value of N

N	R_{ij}
1	0.0849
2	0.1679
3	0.2545
4	0.3393
5	0.4241
6	0.5089
7	0.5937
8	0.6785
9	0.7633
10	0.8481

The perturbation of the jet are shown in the figure 3(a) and (b).

Second Version of the Script: The second version of the script was adapted to cope with the shortcomings of the first version. Dimensionless equations are adopted as in customary to fluid mechanics. The dimensionless equation for the equation of motion is given as follows

$$\frac{md^2r_i}{dt^2} = \sum_{j=1}^{N}\frac{e^2}{R_{ij}^2(r_i - r_j)} - \frac{eV_0}{h}k + \pi(\overline{\sigma_{ui}} + \frac{Gln(l_{ui})}{l_{ui}} + (r_{i+1} - r_j) - \pi a_{bi}^2(\overline{\sigma_{bi}} + \frac{Gln(l_{bi})}{l_{bi}(r_i - r_j - 1)}$$
$$- \alpha\pi a_{0v}^2 k_i/\sqrt{x_i^2 + y_i^2[ix_i + jy_i]}$$

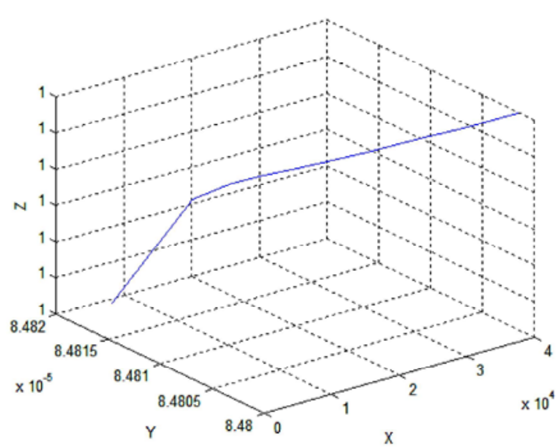

Fig. 3(a): Simulation of the first version of the script, N = 10, V0 = 10 kV, axis units are in cm.

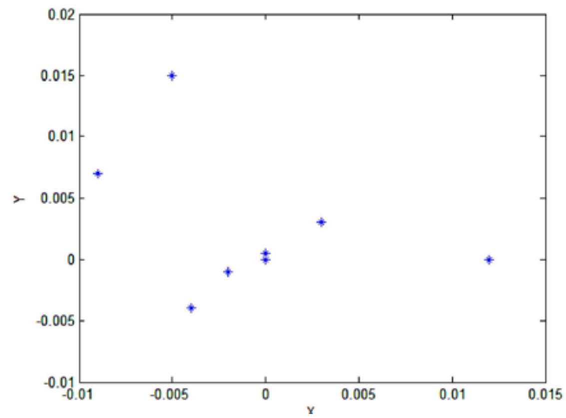

Fig. 3(b): 2D view on the collector plane.

To use the equation of motion a coordinate transformation of the system is obtained, since the coordinates u=($u_1 \ldots u_8$) need to be used for all the beads in the system. For minimal simulationsthe number of beads should be at least three. Therefore, the state of each bead is determined by eight differential equations. The matlab script is constructed in such a way that state vector grows, as more number of beads are introduced in the system.This set of differential equations only applies for one bead, say bead i. But also the coordinates of its neighbours, bead i - 1 and i + 1, are required to solve these equations. This is no problem as long as bead i has 2 neighbour beads.

However, when in the simulation the first bead starts to travel downward, it obviously does not have a predecessor, i.e. there is no bead i - 1. Therefore all the coordinates in the system that belong to bead i - 1 are given an alternative value, i.e., in this case they get the same value as the coordinates of bead i itself. This is because there is no element between bead i and i - 1, since bead i is the first bead in the system. It is necessary to set some of the terms in the differential equations for bead i equal to zero, to prevent singularities in the equations.

Something similar happens when a new bead has just been introduced in the system. For this bead, the successor, bead i + 1, does not yet exist. This means that coordinates in this case will get the values that belong to starting position of a new bead. To use all these coordinates in the Matlab simulation, a coordinate transformations takes place, where all coordinates together form a vector u, with u_1 the x coordinate of bead i, u_2 the time derivative of this x coordinate, u_3 the y coordinate and so on.Some of the transformed coordinates are

$$x_i = u(8 * i - 1)$$

$$x_i = u(\dot{8} * i - 6)$$

$$x_i = u(8 * i - 5)$$

$$\dot{y}_i = u(8 * i - 4)$$

$$x_i = u(8 * i - 3)$$

$$\dot{z}_i = u(8 * i - 2)$$

$$x_{i+1} = u(8 * (i + 1) - 7)$$

$$\dot{x}_{i+1} = u(8 * (i + 1) - 5)$$

The second version of the script was adapted to cope with the shortcomings of the first version which were mentioned in the previous section. Performing the same simulation with the new script yields the results shown in Figure 4(a) and (b). In this figure again a view is shown on the collector plate, showing the incoming beads. The area covered by the beads hitting the collector plate is approximately the same as was in the simulations performed in the previous section. However, adapting the script to remember the bead position as was described in the previous section, is thought to be a useful addition to the script.

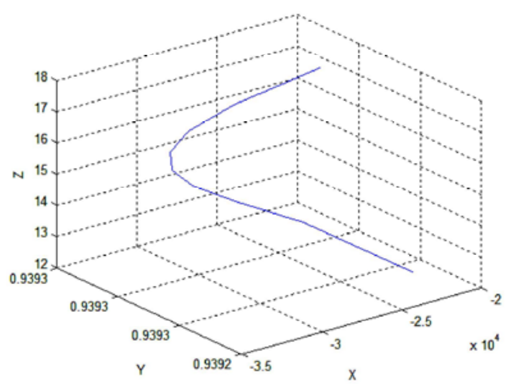

Fig. 4(a): Simulation of the second version of script.

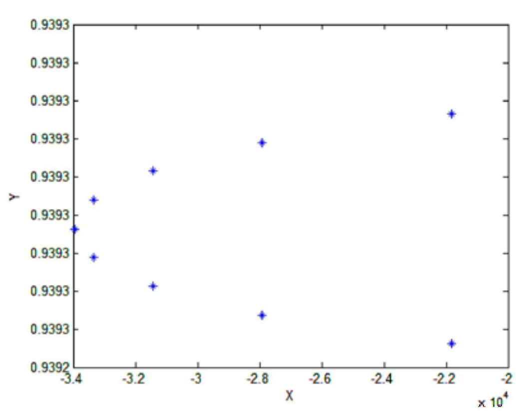

Fig. 4(b): View on the collector plane in 2D.

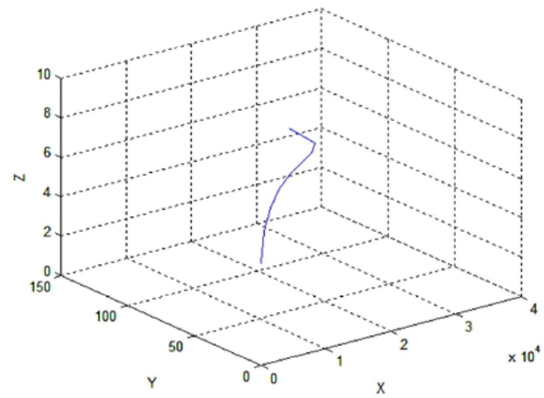

Fig. 5: Snapshot of the established jet at a certain moment during the simulation, axis units are in cm.

CONCLUSION

The purpose of the chapter is to create a model that can simulate the electrospinning process and study the instability of the fluid jet. The different versions of matlab scripts that were used for these simulations seemed to have shortcomings. It was adpted several times to cope up with these shortcomings, yielding better results. The electrospinning process is dependent on a lot of different parameters. Changing these parameters will lead to changes in the process. The influence of the viscosity, the surface tension, the elastic modulus, the initial jet radius and the applied voltage was studied. Simulations that were performed with a different capillary height, do not show noticeable behaviour, as was the case when changing the viscosity. Changing the surface tension coefficient did not show noticeable differences in the dynamical behaviour. Increasing the elastic modulus did have some influence on this behaviour, something which can be explained since increasing this modulus causes the jet to be 'stiffer'. The initial jet radius seems to have a large effect on the dynamics of the jet. Increasing the radius leads to more unstable behaviour, decreasing the radius yields the opposite. The relation between the initial jet radius and the dynamical behaviour of the jet might be an interesting subject for further study, since this should be a parameter that can be changed relatively easily. Increasing the applied voltage also leads to more unstable behaviour, decreasing it does not have much influence on the dynamics. This all means that by changing some system parameters, the dynamical behaviour can be influenced, at least slightly. If attempts are being made to control the electrospinning process, it is important to know which parameters have a large influence on the systems dynamical behaviour and, in which order they can be changed.

REFERENCES

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