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Numerical study on polymer nanofibers with electrically charged jet of viscoelastic fluid in electrospinning process

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Abstract: Electrospinning is a useful and efficient technique to produce polymeric nanofibers. Nanofibers of polymers are electrospun by creating an electrically charged jet of polymer solution. Numerical study on non-Newtonian and viscoelastic jets of polymer nanofibers in electrospinning process is presented in this work. In particular, the effect of non-Newtonian rheology on the jet profile during the electrospinning process is examined. The governing equations of the problem are solved numerically using the Keller-Box method. The effects of yield stress and power-law index on the elongation, velocity, stress and total force are presented and discussed in detail. The results show that by increasing the values of yield stress, the fluid elongation is reduced significantly.

Key words: nanofibers; electrospinning; electrically charged jet; viscoelastic fluid; synthetic polymers

1 Introduction

Electrospinning presents a new level of versatility and a wide range of materials into the micro/nanofiber range. An old technology has been improved into nontextile applications in recent years, electrospinning is unique among nanofiber fabrication techniques regarding to process control and materials combinations. This has led to it being recognized as a basic technology that will yield products for a wide range of uses including electronics, drug delivery, chemical sensors, filtration, and solid-state lighting applications [1–3].

In the electrospinning process, a polymer liquid is held by its surface tension at the end of a vessel tube in which an electric field is applied. Mutual charge repulsion causes a force directly opposite to the surface tension. When the strength of the electric field is intensified, the hemispherical surface of the solution at the tip of the vessel tube extends to form a conical shape known as the Taylor cone [4–6]. The main objective of electrospinning experiments is to reduce the radius of the collected fibers. According to the mass conservation, this object is equal to enlarging the jet length by the time it arrives the collecting plane. Also the bending instability is a worthwhile object that can be under control. So it is important to make minimum the length of the initial stable jet region. Evaluating this stable region is consistent for comparing with the results of electrospinning experiments [7]. In review of importance of the nanotechnology, electrospinning has become an interesting object of recent studies. CARROL and JOO [8] investigated the effect of electrical conductivity and viscoelasticity on the jet profile during the initial stage of electrospinning. THERON et al [9] studied the experimental investigation and modeling of multiple jets during the electrospinning of polymer solutions. Their results show that how the external electric fields and mutual electric interaction of multiple charged jets affect their path and evolution during electrospinning. CARROLL et al [10] examined modeling and experiments of three electrospinning systems which are axisymmetric instabilities in electrospinning of different polymeric solutions, non-isothermal modeling of polymer melt electrospinning, and control of nanoparticle distribution and location during electrospinning. The physical properties of R600a with nanoparticles and without nanoparticles were studied experimentally [11, 12]. ZOLFAGHARIAN et al [13] presented a comprehensive review of the existing 3D printed actuators. Two groups of models have been extended for electrospinning: the first model relates to the jet fiber as following the continuum mechanics equations [14, 15]. The second model is the jet considered as a series of discrete elements following the Newtonian mechanics equations [16]. Both models consider Newtonian with a linear strain–stress constitutive relation.

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In the present work, the performance of non-Newtonian rheology on the jet dynamics is examined. The prime goal is to find whether a non-Newtonian rheology can reduce the elongation dynamics, thereby reducing the stable jet length.

2 Mathematical modeling

Mathematical modeling is a vantage point to reach a solution in an engineering problem, so the accurate modelling of nonlinear engineering problems is an important step to obtain accuratre solutions [17–21]. Most technical problems in fluid mechanics and heat transfer problems are inherently nonlinear. These problems and phenomena can be modeled by ordinary or partial nonlinear differential equations to find their behavior in the environment. Therefore, some different methods have been introduced to solve these equations, such as the variational iteration method (VIM) [22], adomian decomposition method (ADM) [23], homotopy perturbation method (HPM) [24, 25], differential transformation method (DTM) [26, 27], Keller-box method (KBM) [28–30], modified homotopy perturbation method (MHPM) [31], differential quadrature method (DQM) [32, 33], least square method (LSM) [34–36], Galerkin method (GM) [37], collocation method (CM) [38, 39], parameterized perturbation method (PPM) [40], optimal homotopy asymptotic method (OHAM) [41, 42] and exp-function method [43].

In this work, consider a rectilinear electrified liquid jet in an electric field parallel to its axis. All variables are assumed to be constant over the radial axis of the jet and change over the Z axis, only. So the flow is considered one-dimensional model. The fiber is represented by tow charged dimer. Each of dimer possesses a charge e and mass m (see Fig. 1). l is the filament length, h the distance of the collector plate from the injection point, and V_0 the applied voltage.

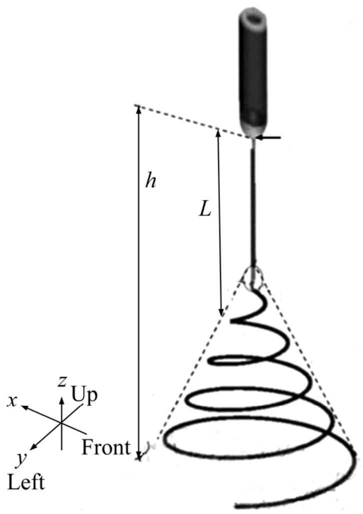

Fig. 1 Schematic drawing of electrospinning process

Let the position of one of the dimer be fixed by non-Coulomb forces. The other dimer is acted by the Coulomb repulsive force $-e^2/l^2$. Also, the force applied to the external field is $-eV_0/h$.

The momentum balance is as follows [44]:

$$m\frac{\mathrm{d}v}{\mathrm{d}t}=-\frac{e^2}{l^2}+\frac{eV_0}{h}+\pi a^2\sigma \tag{1}$$

where a is the cross-section radius of the bead and v is the velocity of bead which satisfies the kinematics equation:

$$\frac{\mathrm{d}l}{\mathrm{d}t}=-v \tag{2}$$

The stress σ for a viscoelastic fluid is as follows:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}t}=-\frac{1}{\tau}(\sigma-\sigma_{\mathrm{HB}}) \tag{3}$$

where σ_{HB} and τ are the Herschel–Bulkley stress and time relaxation constant, respectively [45] and σ_{HB} is defined as follows:

$$\sigma_{\mathrm{HB}}=\sigma_{\mathrm{Y}}+\left(\frac{\mathrm{d}l}{l\mathrm{d}t}\right)^n \tag{4}$$

where σ_{Y} is the yield stress, n is the power-law index and μ_0 is the effective viscosity.

In the Eq. (4), the case of n=1 and σ_{Y}=0 reclaims the Maxwellian fluid model. In Eqs. (3) and (4), the Maxwell, the power-law and the Herschel–Bulkley models are combined.

Also, the Bingham fluid (σ_{Y}>0), shear-thinning fluid (n<1), and shear-thickening fluid (n>1) are utilized for a wide range of polymeric and industrial fluids, recently [46].

Introducing the dimensionless parameters, the length scale is defined as:

$$L=\left(\frac{e^2}{\pi a_0{}^2 G}\right)^{0.5},\quad G=\frac{\mu_0}{\tau} \tag{5}$$

where a_0 is the initial radius at t=0. The other dimensionless groups are given by:

$$Q=\frac{e^2\mu_0{}^2}{L^3 mG^2} \tag{6}$$

$$F=\frac{\pi a_0{}^2\mu_0{}^2}{LmG} \tag{7}$$

$$V=\frac{eV_0\mu_0{}^2}{L^3 mG^2} \tag{8}$$

where Q, V and F are related to the relative strength of Coulomb, viscoelastic and electrical forces, respectively.

Equations (1)–(4) are obtained in the following dimensionless form:

$$\frac{\mathrm{d}l}{\mathrm{d}t}=W \tag{9}$$

$$\frac{\mathrm{d}W}{\mathrm{d}t}=V+\frac{Q}{l^2}-\frac{F\sigma}{l} \tag{10}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}t}=\sigma_{\mathrm{Y}}+\left(\frac{W}{l}\right)^n-\sigma \tag{11}$$

And the initial conditions are as follows:

$$l(0)=1,\ W(0)=0,\ \sigma(0)=1 \tag{12}$$

3 Numerical method

In this work, Keller-box method has been employed as an efficient numerical method for solving the above problem using Maple 15.0 software. The Keller Box scheme is a face-based method for solving partial differential equations that has numerous attractive mathematical and physical properties. The scheme discretizes partial derivatives exactly and only makes approximations in the algebraic constitutive relations appearing in the partial differential equation (PDE). The exact Discrete Calculus associated with the Keller-box scheme has been found to be fundamentally different from all other mimetic (physics capturing) numerical methods. Actually, Keller box is a variation of the finite volume approach in which unknowns are stored at control volume faces rather than at the more traditional cell centers. Its name alludes to the fact that in space-time, the unknowns sit at the corners of the space-time control volume which is a box in one space dimension on a stationary mesh. The original development of the method [47] dealt with parabolic initial value problems such as the unsteady heat equation. The method was made better by BRADSHAW et al [48] as a method for the solution of the boundary layer equations.

4 Results and discussion

To solve the governing equations numerically, we have used the Keller-box method. In order to validate the present solution of the problem and find the accuracy, the comparison between Keller-Box method and numerical results is done [49]. A good agreement between the present method and the numerical results of PONTRELLI et al [49] is observed in Table 1, which confirms the validity of the proposed solution. It can be concluded from this table that the accuracy and reliability of this method are excellent.

In the present study, the Maxwell fluid is considered as a reference case in which n=1 and σ_{Y}=0, and the non-dimensional group is assumed as Q=F=12 and V=2 which is related to the experimental case of L=0.3 cm and τ=10^{-2} s. The interest of the present study is to show how the properties of the fluid material affect the dynamics of electrified jets.

Table 1 Compared results for stress term (σ) with those by PONTRELLI et al [49]

t	Present study	Ref. [49]	Error/%
0	0	0	0
0.5	0.619493	0.617	0.458324
1	0.832576	0.833	0.09088
1.5	0.802704	0.800	0.338
2	0.720041	0.717	0.470837
2.5	0.637856	0.633	0.714105
3	0.568249	0.567	0.279235
3.5	0.511485	0.508	0.62
4	0.465085	0.467	0.33893
4.5	0.426516	0.425	0.356706
5	0.393812	0.392	0.547745

The time elevation of the elongation $l(t)$, the velocity $W(t)$, the stress $\sigma(t)$ and total force F_{tot} for the various values of n (0.2<n<1.8) are shown in Fig. 2. In fact, in this figure the effect of the shear-thinning and shear-thickening is investigated. It is observed that the effect of changing the values of n on the dimer elongation is very slight which is due to the fact that that the stress term made by $1/l$ can be neglected compared to the external field. As seen, in the early stage of progression, W/l>1, so for the case n>1, the stress contribution is increased in comparison with Maxwellian fluid (n=1). Also, it is seen that for the case n=1.8, at the temporary time 1<t<2, the viscoelastic drag causes a slightly decreasing velocity $W(t)$. For the case n=0.2, the stress remains firm and it is rational because at t>1, W/l<<1.

Figure 3 shows the effects of yield stress (σ_{Y}) on the elongation $l(t)$, the velocity $W(t)$, the stress $\sigma(t)$ and total force F_{tot}. It is seen that by increasing the values of yield stress, the fluid elongation ($l(t)$) is reduced significantly. Also it is shown that for the all values of σ_{Y} (σ_{Y}=0.2, 0.5, 0.8), the velocity $W(t)$ is decreased in the temporary time 1<t<2.

Eventually, the aim of the work is to investigate the effective force applied on the dimer as a function of its elongation. The effective force is defined as follows which expresses the sum of Coulomb repulsion and viscoleastic drag.

$$F_{\mathrm{eff}}(l)=Q\left(\frac{1}{l^2}-\frac{\sigma(l)}{l}\right) \tag{13}$$

Figure 4 indicates the effect of exponent n and yield stress σ_{Y} on the effective force. It is seen that the manner of the effective force versus the elongation is the same as

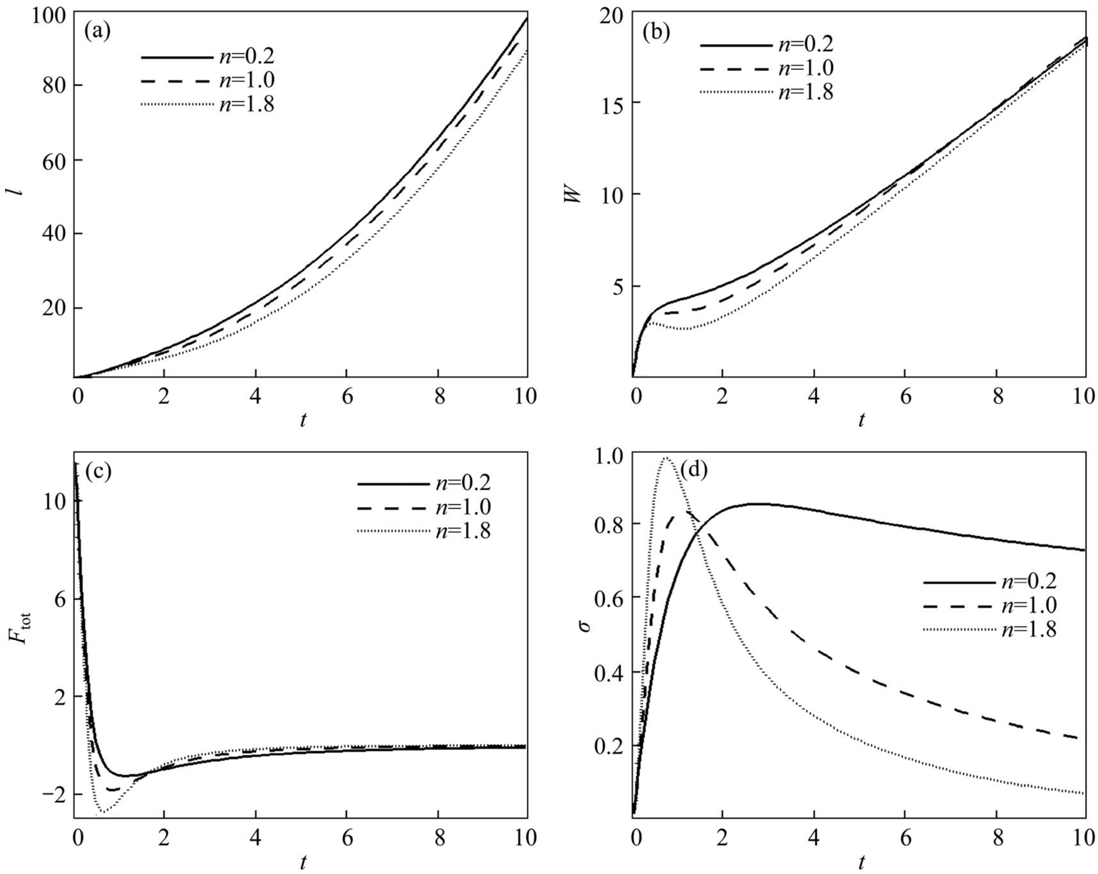

Fig. 2 Elongation (a), velocity (b), total force (c) and stress (d) as a function of time for different values of n when σ_Y=0

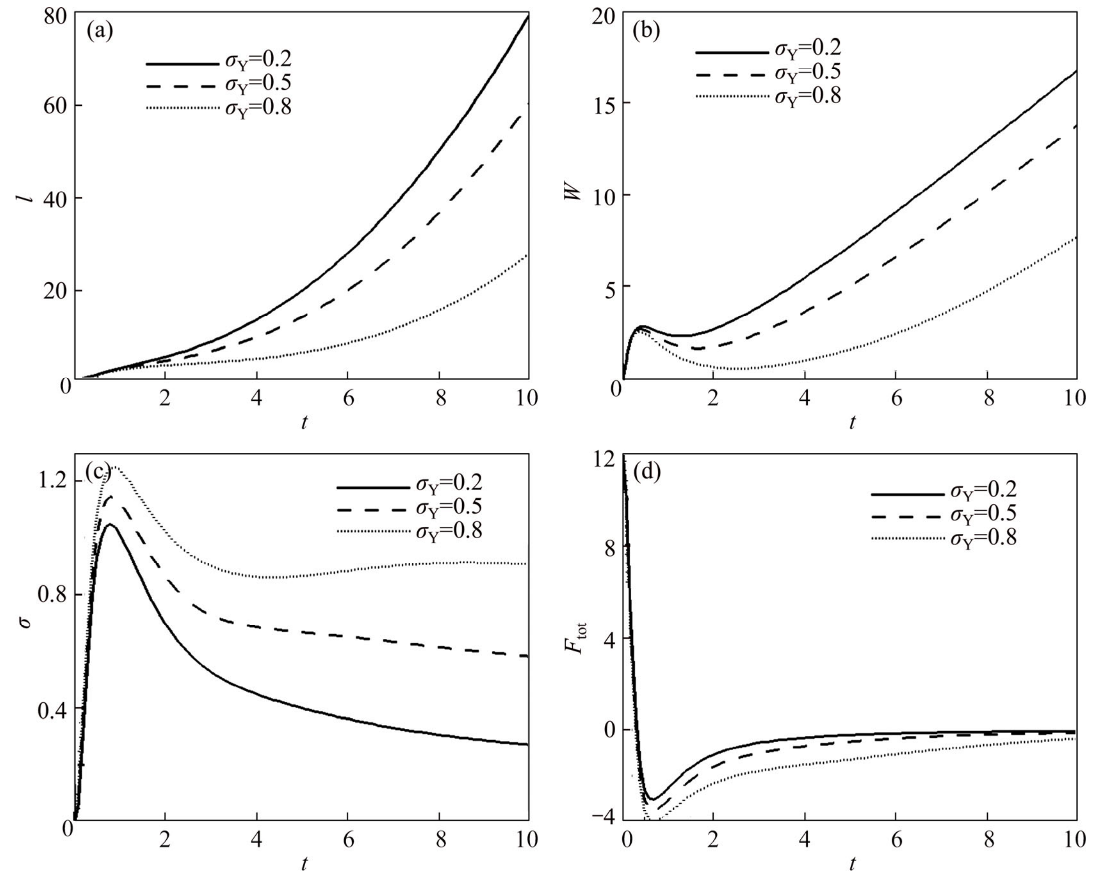

Fig. 3 Elongation (a), velocity (b), stress (c) and total force (d) as a function of time for different values of σ_Y when n=1.8

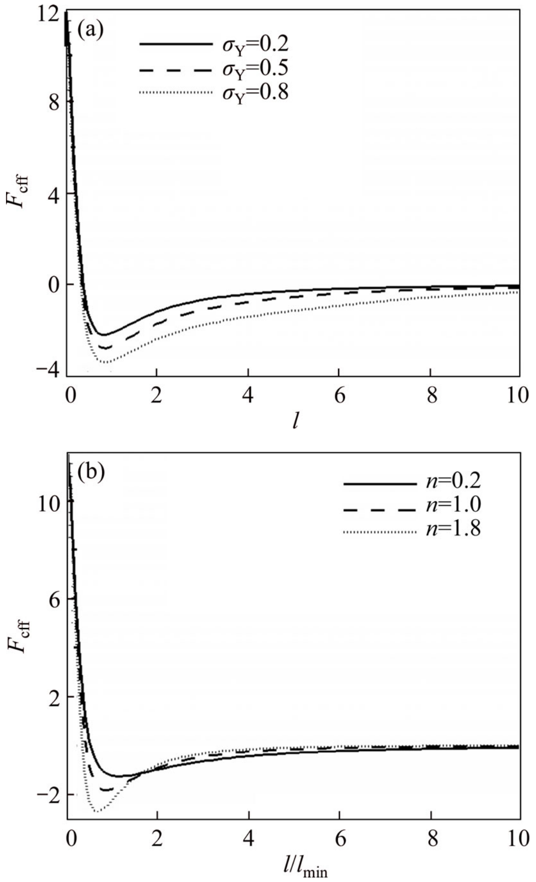

Fig. 4 Effective forces as a function of elongation=l for different values of n=1 (a) and σ_Y=0 (b)

its behavior with the time. The minimum peak which occurs in the figure is related to the crossover length (l_X) at which Coulomb repulsion and viscoelastic drag come to an exact balance as follows:

$$l_X \sigma(l_X) = 1 \quad (14)$$

For the case $l<l_X$, the Coulomb repulsion component is significant and for the case $l>l_X$, the viscoelastic drag is commanding, in order that $F_{\rm eff}(l)<0$, until a minimum is obtained. For $l>l_{\rm min}$, the effective force increases again to reach zero value at $l\to\infty$.

5 Conclusions

The flow of electrically charged jet with viscoelastic fluid is considered to examine the effect of non-linear rheology on electrospinning process. The numerical technique applied to solve the present problem is the Keller-Box method. The present results are in excellent agreement with the numerical ones in reference [49] and it affirms that the accuracy and reliability of this method is excellent. The results show that when σ_Y=0, for shear-thickening fluid (n>1), the dimer undergoes a shorter elongation and velocity, and for shear-thinning fluid (n<1), it corresponds to a larger stress than n=1. Also, the main conclusion is that the stable jet length is significantly reduced for the yield stress fluids in electrospinning process.

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