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Electro-spun organic nanofibers elaboration process investigations using comparative analytical solutions

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ABSTRACT

In this paper Enhanced Variational Iteration Method, EVIM is proposed, along with the *BPES*, for solving Bratu equation which appears in the particular elecotrospun nanofibers fabrication process framework. Elecotrospun organic nanofibers, with diameters less than 1/4 microns have been used in non-wovens and filtration industries for a broad range of filtration applications in the last decade. Electro-spinning process has been associated to Bratu equation through thermo-electro-hydrodynamics balance equations. Analytical solutions have been proposed, discussed and compared.

1. Introduction

Electrospinning is a process for elaborating nanofibers with diameters about 20 nm by forcing a fluidified polymer through a spinneret by an electric field (Fig. 1). This process has been proposed and patented early by Formhals (Formhals, 1934) in 1934, but its description through thorough thermal and electrical hydrodynamics was studied in detail only in the recent years (Doshi & Reneker, 1995; Fong & Reneker, 2001; Gibson, Schreuder-Gibson, & Rivin, 1999; Gibson, Schreuder-Gibson, & Rivin, 2001; Huang, Zhang, Kotaki, & Ramakrishna, 2003; Kenawy et al., 2002; Khil, Cha, Kim, Lim, & Bhattarai, 2003; Lannutti, Reneker, Ma, Tomasko, & Farson, 2007; Lee et al., 2006; Otsu, 1979; Petrou & Bosdogianni, 1999; Pinto et al., 2003; Schreuder-Gibson, 1998; Taylor, 1954). Under the influence of the electrostatic field, a pendant droplet of the polymer solution at the capillary tip, at the outer edge of a controlled syringue, is deformed into a conical shape (Taylor cone) (Taylor, 1954). If the voltage surpasses a threshold value, electrostatic forces overcome the surface tension, and a charged fine jet is ejected (Doshi & Reneker, 1995; Fong & Reneker, 2001; Gibson et al., 1999). This jet moves toward a collector grid. The main controlling parameters of the process are hydrostatic pressure in the capillary tube and external electric field, material viscosity, conductivity, dielectric permeability, surface tension, and temperature gradient.

In this paper, the electrospinning process is studied in terms of fluid velocity at the level of the outer edge of the syringue. It has been demonstrated that the problem can be expressed through second-order nonlinear ordinary differential Bratu equation (Aregbesola, 2003; Barray et al., 2000; Boyd, 1985, 1986; Bratu, 1914; He, 1997, 2001, 2003):

$$u''(\zeta) + \lambda e^{u(\zeta)} = 0; \quad -1 < \zeta < 1 \tag{1}$$

subjected to boundary conditions; $u(0) = b_0 = 0$ and $u'(0) = b_1 = 0$ where the prime denotes differentiation with respect to x, and a, b_0 and b_1 are constants.

Solutions to this equation have been performed using the Enhanced Variational Iteration Method (EVIM) and the Boubaker Polynomials Expansion Scheme (BPES).

2. Process theoretical formalization

The main equations which govern the electrospinning process (Spivak & Dzenis, 1998; Spivak, Dzenis, & Reneker, 2000) are mass balance, linear momentum balance and electric charge balance equations respectively:

$$\nabla.\vec{u} = 0 \tag{2}$$

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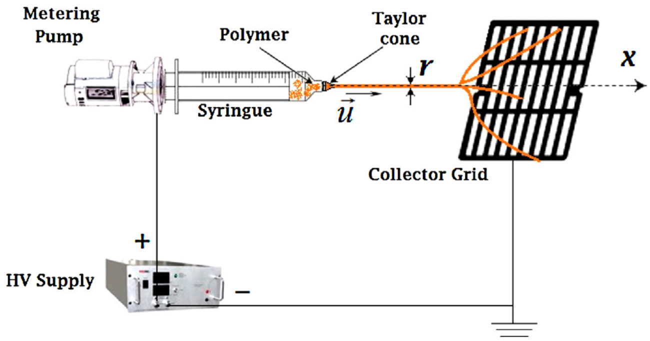

Fig. 1. Electrospinning process setup.

$$\rho(\vec{u}.\nabla)\vec{u} = \nabla F^m + \nabla F^e \tag{3}$$

$$\nabla.\vec{J} = 0 \tag{4}$$

where $\vec{u}$ is the axial velocity, $\vec{J}$ is the electrical current density, ρ is material density, F^m and F^e are terms which represent viscous and electric forces, respectively.

In the case of steady state jet ignoring the thermal effort, the electrically generated force is dominant, the monodimensional momentum equation is hence:

$$u\frac{\partial u}{\partial x} = \frac{2\sigma E}{\rho r} \tag{5}$$

where u is the modulus of the axial velocity, r is the radius of the jet at axial coordinate x (Fig. 1), σ is the surface charge density, and E is electric field in the axial direction.

By introducing the charge balance equation:

$$2r\sigma E + r^2 kE = I \tag{6}$$

where I is the electrical current intensity and k is a constant which depend only on temperature in the case of an incompressible polymer, it gives:

$$u\frac{\partial u}{\partial x} = \frac{E(I - r^2 kE)}{\rho r^2} \tag{7}$$

Then, by introducing the variable:

$$y = -6Ln(u) \tag{8}$$

it gives:

$$\frac{\partial y}{\partial x} = -\frac{6E(I - r^2 kE)}{\rho r^2} e^{y/2} \tag{9}$$

By differentiating the last equation, along with assuming weak r-dependence (Spivak et al., 2000) of the variable x, we have:

$$\frac{\partial^2 y}{\partial x^2} + \frac{3E(I - r^2 kE)}{\rho r^2} e^{y/2}\frac{\partial y}{\partial x} = 0. \tag{10}$$

Finally, by combining both the equations, it gives:

$$\begin{cases} \dfrac{\partial^2 y}{\partial x^2} - \lambda e^y = 0 \\ \text{with}: \lambda = \dfrac{18E^2 (I - r^2 kE)^2}{\rho^2 r^4} \end{cases} \tag{11}$$

which is the monodimensional Bratu equation.

3. Enhanced Variational Iteration Method (EVIM)

3.1. Presentation

The aim of this section is to extend the existing VIM to the Enhanced Variational Iteration Method EVIM in order to solve Bratu-like second order nonlinear ODE with variable coefficients:

$$\left\{ u''(\zeta) + \frac{h'(t)}{h(t)}u'(\zeta) + f(\zeta, u(\zeta)) = g(\zeta)u(0) = k_1, \quad u'(0) = k_2 \right. \tag{12}$$

where $f(\zeta, u(\zeta))$ and $g(\zeta)$ are continuous real valued functions, k_1 and k_2 are given constants, $h(\zeta)$ is a continuous and differentiable function with $h(\zeta) \neq 0$. Approximate solutions to the above problem were presented in (Kıymaz & Mirasyedioglu, 2005) by applying the Adomian decomposition method.

In this paper, we use the EVIM method to solve numerically the following Bratu problem:

$$\begin{cases} \left.\dfrac{\partial^2 y}{\partial \zeta^2} - \lambda e^y\right|_{\lambda=2} = 0; \quad -1 < \zeta < 1 \\ \text{with}: \ y(0) = 0; \quad y'(0) = 0 \end{cases} \tag{13}$$

3.2. EVIM method fundaments

In order to illustrate the basic concept of the method, we consider the following general nonlinear differential equation given in the form:

$$Lu(\zeta) + Nu(\zeta) = g(\zeta) \tag{14}$$

where L is a linear operator, N is a nonlinear operator and $g(\zeta)$ is a known analytical function. We can construct a correction functional according to the variational method as:

$$u_{n+1}(\zeta) = u_n(\zeta) + \int_0^\zeta \lambda(\zeta, s)(Lu_n(s) + N\tilde{u}_n(s) - g(s))\,ds; \quad n \geq 0 \tag{15}$$

where λ is a general Lagrange multiplier, u_n is the nth approximate solution and $\tilde{u}_n$ denotes a restricted variation (which means $\delta\tilde{u}_n = 0$). Successive approximations u_{n+1} are obtained by applying the Lagrange multiplier along with an adequately chosen initial term $u_0(\zeta)$.

The final solution is hence given by:

$$u = \lim_{n\to\infty} u_n \tag{16}$$

3.3. Resolution algorithm

We now derive the algorithm for solving (13). To do this, we construct the correction functional as follows:

$$u_{n+1}(\zeta) = u_n(\zeta) + \int_0^\zeta \lambda(\zeta, s)\left(u_n''(s) + \frac{h'(s)}{h(s)}u_n'(s) + \tilde{f}(s, u_n(s)) - g(s)\right)\,ds \tag{17}$$

Making the correction functional (Eq. (17)) stationary with respect to u_n, noticing that $\delta u_n(0) = 0$, yields:

$$\begin{aligned} \delta u_{n+1}(\zeta) &= \delta u_n(\zeta) + \delta\int_0^\zeta \lambda(\zeta, s)\left(u_n''(s) + \frac{h'(s)}{h(s)}u_n'(s) + \tilde{f}(s, u_n(s)) - g(s)\right)\,ds = \delta u_n(\zeta) \\ &+ \left.\left(\lambda(\zeta, s)\frac{h'(s)}{h(s)}\delta u_n(s) + \lambda(\zeta, s)\delta u_n'(s) - \frac{\partial\lambda(\zeta, s)}{\partial s}\delta u_n(s)\right)\right|_{s=\zeta} \\ &+ \int_0^\zeta \left[\left(\frac{\partial^2\lambda(\zeta, s)}{\partial s^2} - \frac{\partial}{\partial s}\left[\lambda(\zeta, s)\frac{h'(s)}{h(s)}\right]\right)\delta u_n(s)\right]\,ds = 0 \end{aligned} \tag{18}$$