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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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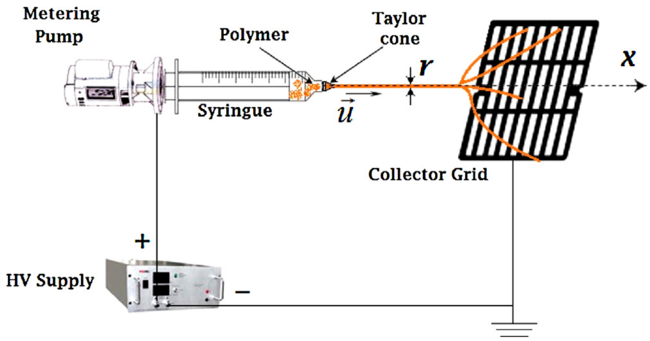

Fig. 1. Electrospinning process setup.

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

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

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:

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

So, the following stationary conditions are obtained:

$$\begin{cases} \dfrac{\partial^2\lambda(\zeta,s)}{\partial s^2} - \dfrac{\partial}{\partial s}\left[\lambda(\zeta,s)\dfrac{h'(s)}{h(s)}\right] = 0 \\ 1+\lambda(\zeta,\zeta)\dfrac{h'(\zeta)}{h(\zeta)} - \left.\dfrac{\partial\lambda(\zeta,s)}{\partial s}\right|_{s=\zeta} \\ \lambda(\zeta,\zeta)=0 \end{cases} \tag{19}$$

At this stage, the Lagrange multiplier can be identified:

$$\lambda(\zeta,s) = h(s)\left(\int\frac{ds}{h(s)} - \int\frac{d\zeta}{h(\zeta)}\right) \tag{20}$$

Finally, the iteration formula can be obtained as:

$$u_{n+1}(\zeta) = u_n(\zeta) + \int_0^\zeta \lambda(\zeta,s)\left(u_n''(s) + \frac{h'(s)}{h(s)}u_n'(s) + f(s,u_n(s)) - g(s)\right)ds \tag{21}$$

This algorithm is applied to the Bratu equation:

$$\begin{cases} \dfrac{\partial^2 y}{\partial \zeta^2} - \lambda e^y = 0; \quad \zeta\in[-1,1] \\ \text{with}: \ y(0)=0; \quad y'(0)=0; \quad \lambda=2 \end{cases} \tag{23}$$

Since here $h(\zeta) = cst$ and $h'(\zeta) = 0$, and according to Eqs. (18)–(20), we have:

$$\lambda(\zeta,s) = s-\zeta \tag{24}$$

Consequently, the iteration formula can be obtained as:

$$u_{n+1}(\zeta) = u_n(\zeta) + \int_0^\zeta [(s-\zeta)(u_n''(s) - 2e^{u_n(s)})]\,ds \tag{25}$$

Finally, starting with the initial approximation $u_0(\zeta) = 0$, we obtain the successive approximations:

$$\begin{cases} u_0(\zeta)=0 \\ u_1(\zeta)=\zeta^2 \\ u_2(\zeta)=\zeta^2+\dfrac{\zeta^4}{6}+\dfrac{\zeta^6}{30}+\dfrac{\zeta^8}{168}+\cdots \\ u_3(\zeta)=\zeta^2+\dfrac{\zeta^4}{6}+\dfrac{2\zeta^6}{45}+\dfrac{11\zeta^8}{840}+\cdots \\ u_4(\zeta)=\zeta^2+\dfrac{\zeta^4}{6}+\dfrac{2\zeta^6}{45}+\dfrac{17\zeta^8}{1260}+\cdots \\ \quad\vdots \end{cases} \tag{26}$$

with the final solution to Eq. (13): $y(\zeta) = \lim_{n\to\infty} u_n(\zeta)$

4. Solution using The Boubaker Polynomials Expansion Scheme *BPES*

4.1. Presentation

The Boubaker Polynomials Expansion Scheme BPES (Agida & Kumar, 2010; Awojoyogbe & Boubaker, 2009; Barry & Hennessy, 2010; Belhadj, Onyango, & Rozibaeva, 2009; Belhadj, Bessrour, Bouhafs, & Barrallier, 2009; Fridjine & Amlouk, 2009; Ghanouchi, Labiadh, & Boubaker, 2008; Kumar, 2010; Milgram, 2011; Slama, Bouhafs, & Ben Mahmoud, 2008; Slama, Bessrour, Bouhafs, & Ben Mahmoud, 2009; Tabatabaei, Zhao, Awojoyogbe, & Moses, 2009; Yildirim, Mohyud-Din, & Zhang, 2010) is a resolution protocol which has been successfully applied to several applied-physics and mathematics problems. The BPES protocol ensures the validity of the related boundary conditions regardless main equation features. The BPES is mainly based on Boubaker polynomials first derivatives properties:

$$\begin{cases} \left.\sum_{q=1}^{N} B_{4q}(x)\right|_{x=0} = -2N \neq 0; \\ \left.\sum_{q=1}^{N} B_{4q}(x)\right|_{x=r_q} = 0; \end{cases} \tag{27}$$

and:

$$\begin{cases} \left.\sum_{q=1}^{N} \dfrac{dB_{4q}(x)}{dx}\right|_{x=0} = 0 \\ \left.\sum_{q=1}^{N} \dfrac{dB_{4q}(x)}{dx}\right|_{x=r_q} = \sum_{q=1}^{N} H_q \\ \text{with}: \ H_n = B'_{4n}(r_n) = \left(\dfrac{4r_n[2-r_n^2]\times\sum_{q=1}^{n}B_{4q}^2(r_n)}{B_{4(n+1)}(r_n)} + 4r_n^3\right) \end{cases} \tag{28}$$

Several solution have been proposed through the BPES in many fields such as numerical analysis (Belhadj, Onyango, et al., 2009; Belhadj, Bessrour, et al., 2009; Kumar, 2010), theoretical physics (Agida & Kumar, 2010; Barry & Hennessy, 2010), mathematical algorithms (Yildirim et al., 2010), heat transfer (Ghanouchi et al., 2008), homodynamic (Awojoyogbe & Boubaker, 2009; Slama et al., 2009), material characterization (Slama et al., 2008), fuzzy systems modeling (Tabatabaei et al., 2009) and biology (Fridjine & Amlouk, 2009; Milgram, 2011).

4.2. Application

The Boubaker Polynomials Expansion Scheme BPES is applied to the system (1) through setting the expression:

$$y(\zeta) = \frac{1}{2N_0}\sum_{k=1}^{N_0}\lambda_k \times B_{4k}(\zeta r_k) \tag{29}$$

where B_{4k} are the 4k-order Boubaker polynomials, $\zeta\in[-1,1]$ is the normalized variable, r_k are B_{4k} minimal positive roots, N_0 is a prefixed integer and $\lambda_k|_{k=1\ldots N_0}$ are unknown pondering real coefficients.

Thanks to the properties expressed by Eqs. (27) and (28), boundary conditions are trivially verified in advance to resolution process. The system (13) is hence reduced to:

$$\left\{ \frac{1}{2N_0}\sum_{k=1}^{N_0}\lambda_k \times \frac{d^2B_{4k}(\zeta r_k)}{dx^2} = 2\,exp\left(\frac{1}{N_0}\sum_{k=1}^{N_0}\lambda_k\times B_{4k}(\zeta r_k)\right)\right. \tag{30}$$

The BPES solution is obtained by determining the non-null set of coefficients $\tilde{\lambda}_k|_{k=1\ldots N_0}$ that minimizes the absolute difference Δ_{N_0}:

$$\begin{cases} \Delta_{N_0} = \left|\left(\dfrac{1}{2N_0}\sum_{k=1}^{N_0}\tilde{\lambda}_k\times\Lambda_k\right) - \left(\dfrac{1}{2N_0}\sum_{k=1}^{N_0}\tilde{\lambda}_k\times\Lambda'_k\right)\right| \\ \text{with}: \\ \Lambda_k = r_k^2\displaystyle\int_0^1 \dfrac{d^2B_{4k}}{dx^2}(\zeta\times r_k)dx \\ \Lambda'_k = \displaystyle\int_0^1 (B_{4k}(\zeta\times r_k))\,dx \end{cases} \tag{31}$$

Table 1
Solutions of Bratu equation along with error data.

ζ	Exact	BPES	EVIM	Quadratic error vs. exact	
				BPES	EVIM
−1.00000	1.23125	1.21882	1.20639	1.545E-4	6.18E-4
−0.93103	1.03166	1.02125	1.01084	1.084E-4	4.335E-4
−0.86207	0.8589	0.85023	0.84156	7.517E-5	3.007E-4
−0.79315	0.70868	0.70153	0.69438	5.112E-5	2.045E-4
−0.72414	0.57784	0.57202	0.5662	3.387E-5	1.355E-4
−0.65517	0.46401	0.45934	0.45467	2.181E-5	8.724E-5
−0.58621	0.36534	0.36166	0.35798	1.354E-5	5.417E-5
−0.51724	0.28039	0.27758	0.27477	7.896E-6	3.158E-5
−0.44828	0.20807	0.20598	0.20389	4.368E-6	1.747E-5
−0.37931	0.14746	0.14598	0.1445	2.19E-6	8.762E-6
−0.31034	0.0979	0.09692	0.09594	9.604E-7	3.842E-6
−0.24138	0.05884	0.05825	0.05766	3.481E-7	1.392E-6
−0.17241	0.02987	0.02958	0.02929	8.41E-8	3.364E-7
−0.10345	0.01072	0.01061	0.0105	1.21E-8	4.84E-8
−0.03448	0.00119	0.00118	0.00117	1.0E-10	4.0E-10
0.03448	0.00119	0.00118	0.00117	1.0E-10	4.0E-10
0.10345	0.01072	0.01061	0.0105	1.21E-8	4.84E-8
0.17241	0.02987	0.02958	0.02929	8.41E-8	3.364E-7
0.24138	0.05884	0.05825	0.05766	3.481E-7	1.392E-6
0.31034	0.09792	0.09692	0.09592	1.0E-6	4.0E-6
0.37931	0.14746	0.14689	0.14632	3.249E-7	1.3E-6
0.44828	0.20807	0.20599	0.20391	4.326E-6	1.731E-5
0.51724	0.28039	0.27761	0.27483	7.728E-6	3.091E-5
0.58621	0.36534	0.36178	0.35822	1.267E-5	5.069E-5
0.65517	0.46401	0.45943	0.45485	2.098E-5	8.391E-5
0.72414	0.57784	0.57211	0.56638	3.283E-5	1.313E-4
0.79313	0.70868	0.70165	0.69462	4.942E-5	1.977E-4
0.86207	0.8589	0.85038	0.84186	7.259E-5	2.904E-4
0.93103	1.03166	1.02144	1.01122	1.044E-4	4.178E-4
1.00000	1.23125	1.21906	1.20687	1.486E-4	5.944E-4

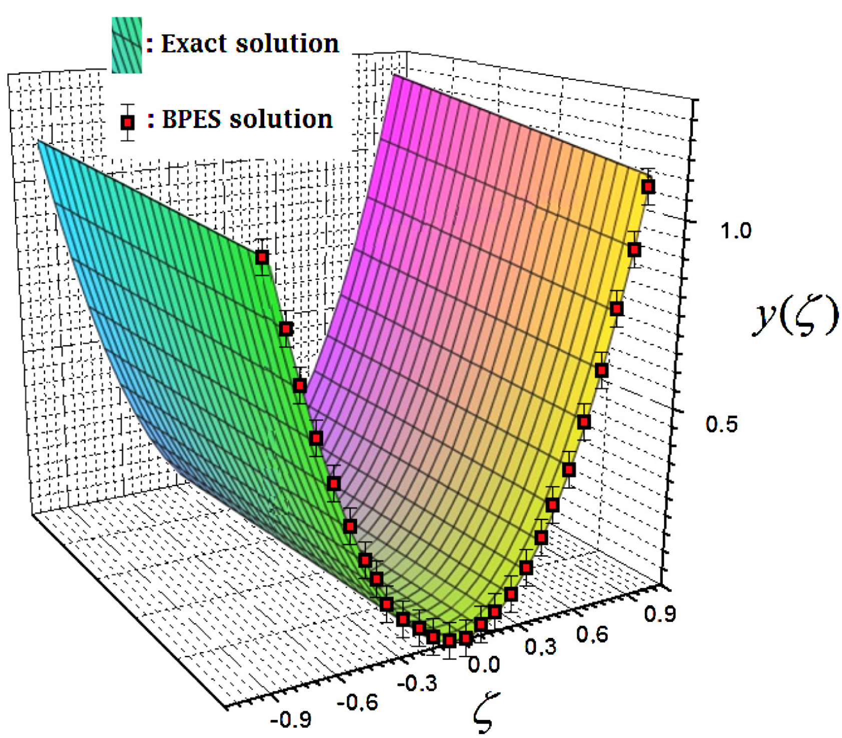

Fig. 2. Solution plots.

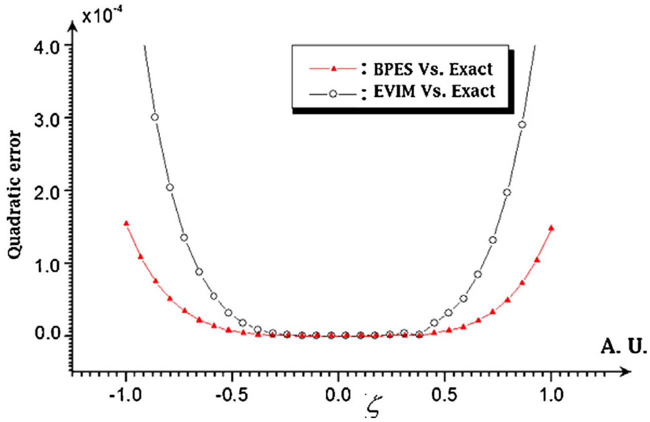

Fig. 3. Quadratic error plots.

The final solution is hence:

$$y(\zeta) = \frac{1}{2N_0}\sum_{k=1}^{N_0}\tilde{\lambda}_k \times B_{4k}(\zeta r_k) \tag{32}$$

5. Results, plots and discussion

Numerical solutions obtained by the two methods are gathered in Table 1.

Plots of the BPES solution are presented in Fig. 2, along with exact solution.

It is known that jet acceleration process, in electrospinning is characterized by a sharp increase in maximum velocity once jet is released from syringe exit (Kenawy et al., 2002; Khil et al., 2003; Lannutti et al., 2007; Lee et al., 2006; Otsu, 1979). Such an increase is attributed to the electric field effects. Meanwhile, material inertia causes a slow transition from a fluid state column to a diffused jet. In a small region just around the edge of 'Tailor cone' (Fig. 1), high-pressure and electrical field effects accelerate the material flow toward downstream so that velocity increase occurs at a meaningful distance from the origin ($x=0$).

Fig. 2 displays a velocity profile which matches perfectly the two condition $y(0)=0$ and $y'(0)=0$, in concordance with the results of Aregbesola (2003), Wazwaz (2005) and Khuri (2004). This finding indicates that if the jet inertia does not keep itself under a compact state along a short path, no persisting electrospinning exists. Such a motion is simply important and necessary transient phenomenon resulting in a better fiber quality because mechanical/chemical processes cannot provide sufficient energy to overcome material compactness at the level of jet initial formation loci. The obtained velocity profile was also in good agreement with the results which were monitored by Xueyan et al. (2012), Charernsriwilaiwat, Opanasopit, Rojanarata, Ngawhirunpat, and Pitt Supaphol (2010), Neamnark, Rujiravanit, and Supaphol (2006) and Lingyan and Ziegler (2013).

This study also explores the velocity dependency at the end of the process (collection stage).

For accuracy purposes, error analysis has been carried out for the two performed method. Examining the quadratic error plots (Fig. 3) shows that the amplitudes of the error are more exaggerated for the EVIM method, particularly in the vicinity of domain edges ($\left|\zeta\right| > 0.9$). The behaviors of both solutions at the central zone ($\left|\zeta\right| \approx 0$) confirm the success of a conjoint forcing of the two condition $y(0)=b_0=0$ and $y'(0)=b_1=0$.

Moreover, Fig. 2 monitors an exponential profile in the range $\left|\zeta\right| < 0.9$ with a quadrature error which does not exceed 5.0×10^{-4} on the whole range (Table 1 and Fig. 3). The obtained profile is in good agreement with the conditions evoked by Fong and Reneker (2001) and Gibson et al. (1999, 2001).

6. Conclusion

In this study, analytical and numerical solutions to Bratu equation have been performed using the Enhanced Variational Iteration Method EVIM, along with the BPES, as guides to understanding velocity profiles in electro-spinning mountings. Electro-spinning process has been appropriately associated to Bratu equation through thermo-electro-hydrodynamics balance equations. Solutions have been proposed, discussed and favorably compared to some results in the related literature. The challenges of fully quantitative modeling of the electrospinning process should be feasible, including both stable and unstable operating regimes, starting from the existing equations of electrodynamic theory, velocity control and productivity improvement of the electrospinning process. These items are also essential features and merit more future studies.

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