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Numerical And Experimental Research Of Design Optimization Of Baths For The Production Of Nanofibers By The Electrospinning

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Abstract.
A study and analysis showed that the increase in production and the quantity of nanofibers obtained from electrospinning may be provided not only by increased potential gradient between the electrodes, but also by the suitable distribution of the intensity of the electrostatic field. Through numerical simulation using finite element method was found that the intensity distribution of the electrostatic field is influenced not only by a potential gradient, type and shape of the electrodes, polymer properties and its concentration, humidity, ambient temperature, but also by other parameters, such as relative permittivity of the material and shape of the construction geometry. Experiments have been done with the functional baths for polymer solution deposition with a different geometry and various relative permittivities. In experiment where polymer PVP with TiO_2 at 23.2 ± 3 °C and humidity of 14.4 ± 3 % and potential gradient 60 kV was determined that proposed changes in design and relative permittivity can be achieved the increasing of nanofiber production about 50 ± 3%.

Introduction

Increase of an efficiency, respectively increase of the amount of nanofibres spinned from rotating electrodes is complicated complex problem that has been subjected to an investigation of process dependencies on the current setting of electrode distance, the voltage value, properties of the polymer solution, ambient humidity and temperature, material parameters such as the relative permittivity of the material. The performed analyses have shown that the increase of production efficiency and the amount of the nanofibers produced by electrospinning can be achieved not only by increasing the potential gradient between the oppositely charged electrodes, but also by a suitable distribution of the intensity of electrostatic field [1]. The electrostatic field is influenced by the construction design of the reservoir, which serves as the holder of a rotating electrode and storage of the polymer solution during the electrostatic spinning from roller - the Nanospider principle. During development of this technology a number of procedures that allow changing the arrangement of the nanofibers in the layer were created. Thus the electrospinning process can be optimized [1-4].In [5], the authors describe a model simulation using finite element method (FEM), where spinning device with four different collectors for the preparation of the desired structure including desired fiber alignment are analyzed. These results can be used for the optimization of the nanofiber production efficiency through different collector design. In [6] the simulation using the FEM software COMSOL Multiphysics is shown. The shape of electrostatic field and the between the electrodes is solved using simulations were analyzed. FEM simulation is very practical tool during the study of complex phenomena, especially in the optimization, because it can also help to build the corresponding analytical models [4-8].

Materials and methods

Theory

The potential distribution and the electric field intensity at the electrospinning technology using principle of spinning from the roller is very difficult and practically immeasurable. A certain possibility is to create a simulation in the FEM environment. The FEM model can be typically arranged: the electrode - polymer solution - reservoir - the external environment - closed box, as was described in [1-2]. The electric field can be approximately defined as limiting force acting on unit charge by the equation (1).

$$\vec{E} = \lim_{q \to 0} \frac{\vec{F}}{q} \; . \tag{1}$$

where $\vec{E}$ is intensity of electric field, $\vec{F}$ is acting force, q is elementar charge.

The electric $\vec{E}$ field can be determined by the voltage between two positional vectors r1 and r2 defined by the equation (2)

$$U = \int_{r_1}^{r_2} \vec{E}dl = \varphi(r_1) - \varphi(r_2) \, . \tag{2}$$

where $\varphi(r_i)$ expresses the potential of the electric field.

In materials (the external environment) defines the vector of electric induction $\vec{D}$ described by the equation 3.

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P} \; . \tag{3}$$

where ε_0 is permittivity of vacuum ($\varepsilon_0 = 8{,}854187817 \cdot 10^{-12} F \cdot m^{-1}$), $\vec{P}$ is electrical polarization described by equation (4).

$$\vec{P} = \varepsilon_0 \chi \vec{E} \; . \tag{4}$$

where χ expresses the electric susceptibility of the material (for air it is $\chi = 0{,}00054$).

The source of the flow of electrical charge is induction more precisely electric field. The Gauss theorem of electrostatics is applied (3. Maxwell equation) describing that the flow (divergence) of electric vector induction through closed surface which surrounds the charge is proportional to the amount of charge q and does not depend on the shape of the surface S which describes the Einstein summation convention (5).

$$div\vec{D} = \lim_{\Delta V \to 0} \frac{\int_S \vec{D} d\vec{S}}{\Delta V} \equiv \partial_i D_i \text{ and } \oint_S \vec{D} dS = q \, . \tag{5}$$

where V the volume of the electric field.

In the electrostatic field the work done by the charge q on close loop is independent on the path. It is described by a closed integral according to equation (6).

$$rot\vec{E} = \left(rot\vec{E}\right)_i = \lim_{\Delta S_i \to 0} \frac{\oint \vec{E} d\vec{l}}{\Delta S_i} = \varepsilon_{ijk} \partial_j E_k = 0 \, . \tag{6}$$

where ε_{ijk} is Levi – Civita permutation symbol.

From equation 6 and 7 follows that the intensity of the electric field $\vec{E}$ can be seen as potential gradient ϕ describable by the Laplace - Poisson equation as follows in equation7.

$$grad\,\phi = -\frac{\rho_{\vec{D}}}{\varepsilon_0}. \tag{7}$$

where ρ_D is the density of electric induction.

Numerical analysis

Numerical model was created in the COMSOL Multiphysics FEM software, which allows the modeling of electric fields, flow in piezomaterials, compression of isotropic and anisotropic materials and other physical phenomenon. This software contains a wide variety of tools for simulation of the various problems, which are described by partial differential equations. This allows the modeling of the vector distribution of momentum of strained nanostructures on the basis of the previous equations. COMSOL uses for the calculation the implicit algorithm, where individual states of the analyzed compression are updated gradually in time t to time t+dt according to Equation (8). Physical parameters of the FEM model are seen in Table 1.

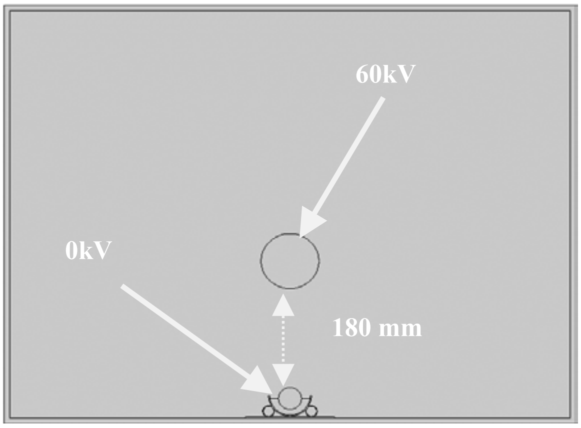
$$\delta u_{i+1} = u_{i+1}^{t+\Delta t} - u_i^{t+\Delta t}. \tag{8}$$

where $u_i^{t+\Delta t}$ is vector of nodal displacements for ith iteration in the time $t+\Delta t$.

It allows modeling of the vector distribution of electrostatic potential and to determine the approximate stress intensity based on the equations (1 – 7). Using the corresponding boundary and initial conditions can be studied and then compared the design of the reservoir for polymer solution in the production line. The potential distribution and electric field intensity can be studied in iso-surfaces, therefore a 2D model with the geometric dimensions of the real line, reservoir and electrodes was made with input voltage at the positive electrode 60 kV and a negative electrode 0 kV (Fig.1). The model was proposed with adaptive networking with the accent on local densification of elements (Fig.2).

Table 1. Physical parameters of the material in FEM simulation

Material	Relative permittivity
Reservoir (PP)	2,3
Reservoir (steel)	1
Reservoir (wood)	4
Reservoir (glass)	7
Polymeric solution	81,6
Box - cover	3,5
External environment - air	1,00054



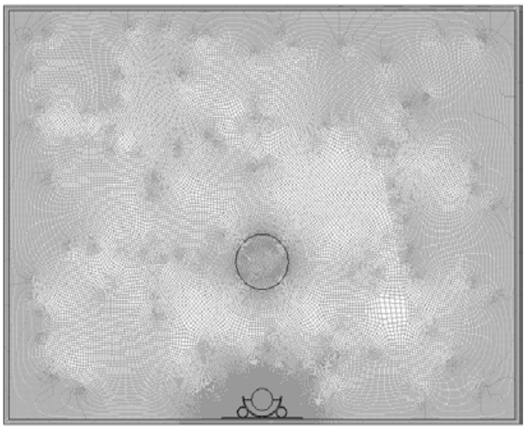


Fig. 1 Finite element model

Fig. 2 Adaptive meshing of the elements

Experimental analysis

Experiments and measurements were carried out with a total voltage 60 ± 0.5 kV. The same conditions were applied for the model simulations. The information about the spinning process effectiveness can be obtained from the experiment. The simulation is suitable for the determination of the intensity and distribution of the electric field. In each case a quantity of the nanofiber layer g.10min-1 formed at the negative electrode (collecting brush) was measured. The nanofibrous layer on the brush was removed and weighed after each experiment. Four positions of the reservoir were tested. In total, 16 measurements (four measurements at one position) were done to evaluate how significantly the relative permittivity of the material of reservoir influences spinning process. The distance between the spinning electrode and the brush collector was constant in all experiments, 180 mm. The polymer polyvinylpyrrolidone with titanium oxide was used - PVP (TiO2) for spinning. Conditions in the box were kept at the constant values during all measurements. Temperature was 23.2 ± 2 ° C and humidity 14.4 ± 3%. These conditions are suitable for the viscosity and chemical composition of the solution. During the experiment, the static brush collector rotated at 1 revolution per 10 min and the spinning electrode rotated at 5 rpm. Experimental device and detail of the electrode position is in Figure 3 - 4.

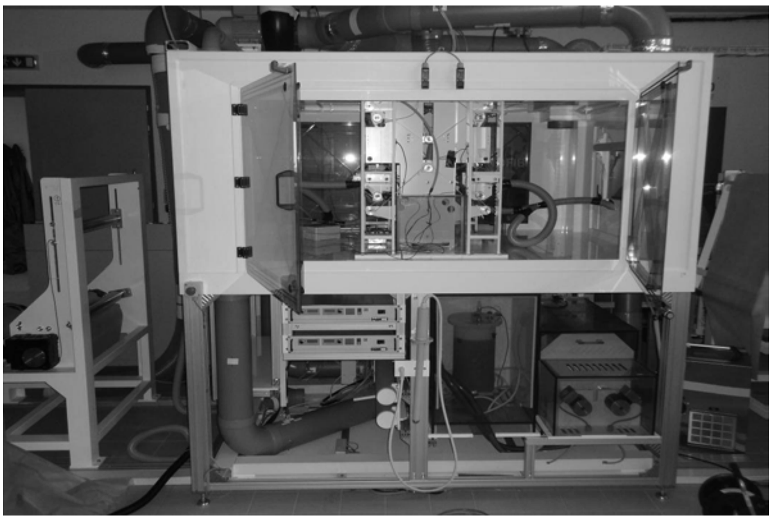


Figure 3 Experimental measurements in box of producing device

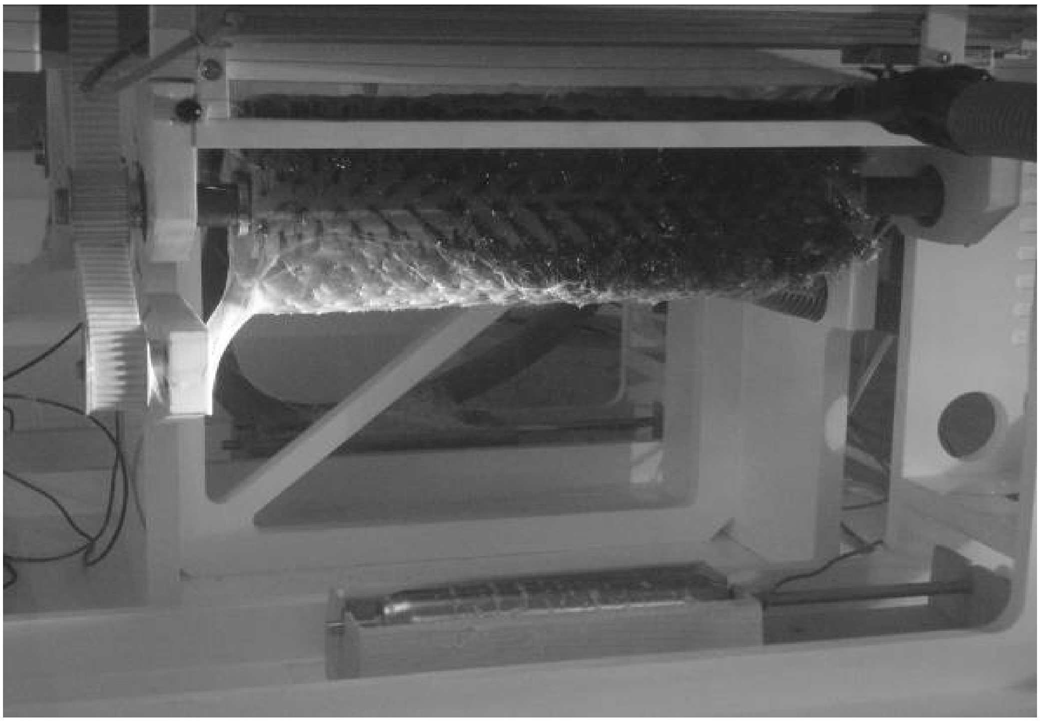


Figure 4 Detail: Position of the rotating electrode in bath reservoir and collecting electrode (brushe) inside of the box

Results and discussion

All the analyzed inorganic nanofiber structures obtained from spinning solution PVP (TiO2) from metal, plastic, wood and glass baths were analyzed using a microscope Nova NanoSEM (Fig. 4). The results of the numerical simulations (Fig. 5) showed that a maximum of intensity of electric field has the glass bath reservoir 526.23 statvolt / cm. Compared with the current bath from polypropylene material (PP) the intensity is about 64% higher. Experimental results showed that the highest weight of the spinned layer and thus the efficiency of the spinning process has a glass bath (2.19 ± 12 g) which is about 50 ± 3% higher when compared to PP. All results are given in Table 2.

Table 2 Results of numeric and experimental analysis

Time of process / Potential (10 min) (0/60kV)	Maximal intensity (statvolt/cm) [1)]	Average mass of real structure (g)			
Type of reservoir	FEM model	Position 1	2	3	4
PP	320,22	1,18±06	0,72±14	1,44±01	1,48±29
Steel	296,84	1,01±11	0,75±01	1,59±12	0,51±06
Wood	329,78	1,35±19	1,45±05	0,89±07	1,47±22
Glass	526,23	1,58±3	2,08±07	2,39±12	1,82±14

[1)] 1statvolt=299,793 volt

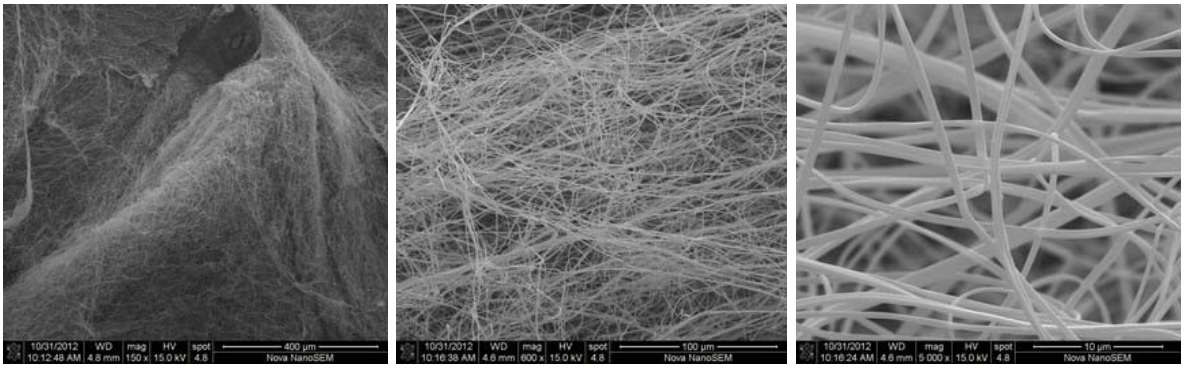


Figure 4 SEM pictures of fibrous nanostructure – magnification 150, 600 and 5000x

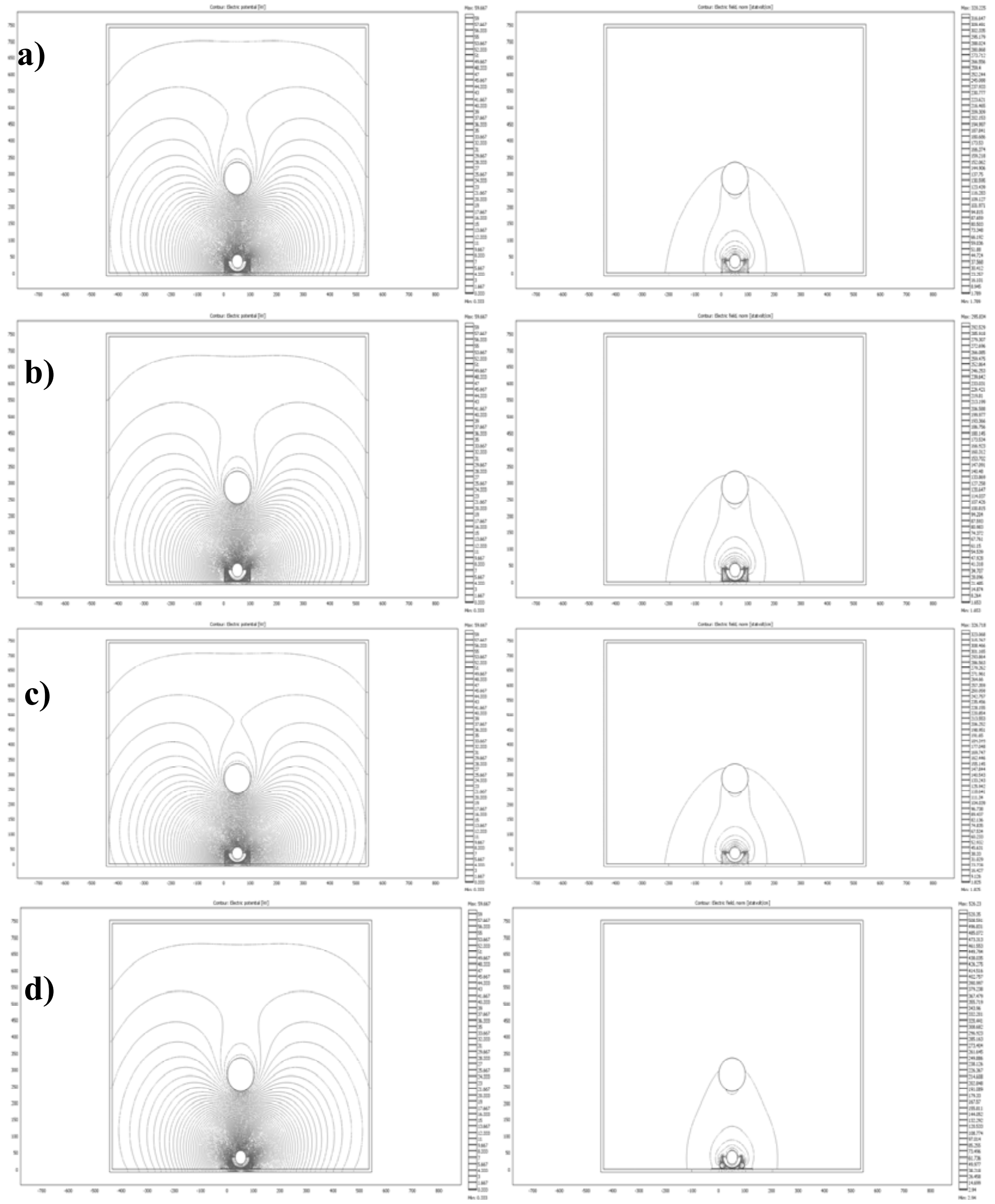


Figure 5 FEM model of intensity and potential distribution – a) PP, b) steel, c) wood, d) glass

Conclusions

Numerical simulation is modern and fast tool for the optimization of different properties of materials, devices and their parts. In this article FEM model was utilized for the evaluation of different materials used for construction of reservoir of the polymeric solution in the process of electrospinning. The article describes how the electrostatic field can be influenced by the different permittivity of materials from point of view of intensity distribution. Results of the FEM model compared with experiment show, that this method is very suitable for the optimization of electrospinning process.

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References

[1] M. Petru, O. Novak, P. Lepsik, “Increase of the efficiency of the production lines for the spinning of inorganic nanofibers by the electrostatic field intensity optimization,” MM Science Journal, December, 2012, pp. 382-385.

[2] J. H. Yu, S. V. Fridrikh, G. C. Rutledge, “Production of submicrometer diameter fibers by two-fluid electrospinning”, Advanced Materials, Vol. 16, No.17, 2004, pp. 1562–1566.

[3] L. Dong, Y. Liu, R. Wang, W.M. Kang, B.W. Cheng, “Mathematical Model of Electric field distribution at a critical state in bubble electrospinning, ” Journal of Fiber Bioengineering and Informatics, Vol. 3, No. 2, Textile Bioengineering and Informatics Society, pp. 117-120.

[4] M. Petru, O. Novak, D. Vejrych, P. Lepsik, FEM study of the strain kinematics in the 3D nanofibrous structure prepared by the electrospinning process, Applied Mathematics, Vol. 111, No. 4, 2013, pp. 412-421.

[5] Y. Wang, et al., "Modeling and fabrication of electrospun polymer nanofibers with tailored architectures for tissue engineering scaffold applications," Computational Intelligence for Measurement Systems and Applications, CIMSA '09, IEEE International Conference on , 11-13 May 2009, pp.226-229, doi: 10.1109/CIMSA.2009.5069954

[6] X. Wang, H. Niu, X. Wang, T. Lin, “Needleless Electrospinning of Uniform Nanofibers Using Spiral Coil Spinnerets,”Journal of Nanomaterials, Volume 2012, Article ID 785920, pp.1-9, 2012, doi:10.1155/2012/785920

[7] M. Petru, O. Novak, D. Herak, S. Simanjuntak, “Finite element method model of the mechanical behavior of Jatropha curcas L. seed under compression loading,” Biosystems Engineering, Vol. 111, No. 4, 2012, pp. 412-421. doi:10.1016/j.biosystemseng.2012.01.008

[8] M. Dekys, O. Broncek, “Measuring strain of the lattice towers,” Communications – Scientific Letters of the University of Zilina, Vol. 14, No. 3, 2012, pp. 39-42.