INCREASE OF THE EFFICIENCY OF THE PRODUCTION LINES FOR THE SPINNING OF INORGANIC NANOFIBERS BY THE ELECTROSTATIC FIELD INTENSITY OPTIMIZATION

Michal Petru[1], Ondrej Novak[2], Petr Lepsik[3]
[1]Technical University of Liberec, Institute for Nanomaterials Advanced Technologies and Inovation, Liberec, Czech Republic
[2]Technical University of Liberec, Faculty of Textile Engineering Department of nonwovens, Liberec, Czech Republic
[3] Technical University of Liberec, Faculty of Mechanical Engineering Department of Machine Elements and Mechanism Liberec, Czech Republic

e-mail: michal.petru@tul.cz, petr.lepsik@tul.cz, ondra.novak@tul.cz

Increase of the intensity of the electrostatic field may be carried out in different ways, for example by increasing the charge or changing the environment conductivity. Higher overall intensity does not necessarily lead to an increase of productivity of nanofibers, because it is influenced also by the distribution of the intensity of the electrostatic field. Optimization efforts for a productivity increase of currently designed lines producing inorganic nanofibers is a very complex problem that depends on the distance of electrodes, voltage value, characteristics and type of the polymer solution, humidity, ambient temperature and other parameters. These parameters affect the potential and electric field intensity. Electrostatic field distribution is influenced by the design of reservoir filled with polymer solution. Geometric design and used construction material obviously affect the final intensity. For the assessment of distribution of electrostatic field in the design of production lines FEM simulation models have been created. FEM simulations were done for various material relative permittivity and design of the reservoir. For the comparison of the simulations and the real behavior the functional model of the reservoir was constructed and tested in a production line working on the Nanospider principle. Increase of the intensity of electrostatic field can be achieved by utilization of the suitable material of the reservoir.

Keywords
electrostatic field, intensity, potential, nanofibers, FEM, relative permittivity

1. Introduction

Electrospinning is one of the production processes, which is able to manufacture nanofibers. Electrospinning is the process of spinning using electrostatic forces, which are generated between oppositely charged electrodes. Among them is spinnable substance (polymeric solution or melt) with appropriate parameters, which is after charging attracted to the opposite electrode. This substance creates a fibre that may be partially or completely drawn. Their diameter is usually between 50 and 800 nm. Productivity of electrospinning was too low until the discovery of Nanospider method, which brings a significant improvement. This method does not use needles or tips, therefore it is called needless electrospinning. In this method the Taylor cones are formed directly on the surface of the polymer solution. It is obvious that the productivity is crucial for the industrial use with mass production. The goal is to get the small diameter of fibers and also high area weight with uniform distribution and minimum number of defects. The major parameters of this process are materials used for the manufacture of reservoir for the polymeric solution, roller, electrodes, as well as their geometry and type of spinnable solution and its properties. All these parameters affect the quality of prepared layers, fiber diameter and especially productivity. Electrical forces that are responsible for the formation of nanofibers and their quality are influenced by the geometry and intensity of the electrical field. A prediction or calculation is quite difficult, but the knowledge of the optimal arrangement for quality production is required. As a possible solution would be to use an analytical mathematical model, however it is unsuitable for a complicated geometry. In this case, it is preferable to use simulation using numerical model, for example the finite element method. Selected works dealing with the simulation of electrostatic field are described below. FEM simulation of the field strength in the modified electro spinning process is described in [Huang 2011]. This modification consists in the use of two electric sources, where the first one is high voltage for creation of nanofibers and second one is low voltage for controlled deposition of nanofibers on a substrate through a mask with microholes. The results show field strength between electrodes with and without mask. The principle of the controlled deposition and the cause of the different density of collected nanofiber layer can be explained by this method. In [Angammana 2011] the electric field distribution depending on arrangement of needles in the process of needle electrospinning is investigated. The simulation was performed in commercial software Comsol Multiphysics. The dependence of an electric intensity field on a distance between two needles was simulated. From results of the simulation it was found that the lower electric field strength is in the case of two needles, due to repulsion of field lines, but the overall field distribution was similar. Also it was found that single-needle arrangement requires lower minimum voltage for electrospinning process compared to arrangement with two needles. In [Wang 2007] a dielectric strength of nanofiber based thermal interface material was simulated. This material is designed for microelectronic applications; therefore the parameter of dielectric strength is very important. The simulation was done in Ansys software. The model was established as two-dimensional cross-section of nanofiber layer with real dimensions and applied voltage. The value of dielectric strength and the mechanism of the breakdown were found out from the results. It was explained as creation of free path for electric charge. Shape of this path is formed by the shape of pore channels. In [Komarek 2010] authors describe the construction of electrodes for electrospinning process which uses polymeric melts for production of nanofiber layer. The intensity of the electrical field for different geometries is calculated by the numerical simulation performed in the Comsol Multiphysics. The results show that the maximum intensity of elliptical field is concentrated on tips and edges. The obtained results of simulations are in the good agreement with the experiments. Article [Liang 2010] describes simulation of so called bubble electrospinnig. This method consists in creation of air bubbles in spinning solution. The bubble is deformed by electrostatic forces to elliptical shape. The shape of bubble is important for process efficiency. Between two electrodes with certain potential the electric field arises. Intensity of the electrostatic field has a significant effect on the efficiency of the process of the nanofiber formation. In [Vejrych 2012] authors added a gas, which changes the intensity of the electrostatic field in the process of electrospinning. The gas flows against negatively charged electrode and forms fibers. On the basis of this modification authors obtained new 3D structure, that has better mechanical properties. The numerical simulation of this process was done in the Comsol Multiphysics software. FEM numerical simulations are significant help in the study, comparison and optimization of processes of production lines working with

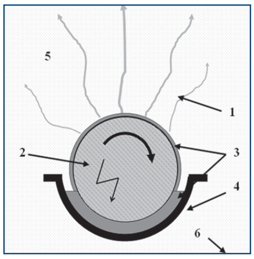

Figure 1. *Principle of Nanospider technology*

high voltage electrostatic field [Tsai 2011]. The corresponding FEM model allows to monitor, evaluate and compare processes which are very difficult to measure [Dekys 2012, Petru 2010, Petru, 2012] and to optimize existing equipment or production process according to the simulation.

2. Material and methods

2.1 Theory

The description of the potential distribution and the electric field intensity in the electrospinning technology using principle of spinning from the roller is very difficult and practically immeasurable. A certain possibility is to establish a model simulation in FEM environment. The FEM model can be typically arranged: the electrode – polymer solution – reservoir – the external environment – closed box, which is shown in Figure 1.

2.1.1 Mathematics and physics description

The electric field can be approximately defined as limiting force acting on unit charge by the equation 1.

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

where *E* expresses the electric field, *F* is acting force, *q* is unit charge. The energy of electrostatic field W_E can be subsequently defined by the work done by moving a point charge *q'* from ∞ to the distance *r* from point charge *q* by the equation 2. This formulation is based on the Gauss theorem of electrostatics by the equation 3. By subsequent derivation of the volume *V* can be expressed as the volumetric energy density of electrostatic field (Eq. 4).

$$W_E = -\frac{1}{2}\sum_j \phi_j q_j = \frac{1}{2}\sum_i \sum_j \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} \quad \text{for a single charge} \quad W_E = \frac{1}{2}\frac{qq'}{4\pi\varepsilon_0 r} \tag{2}$$

$$W_E = \frac{1}{2}\int_V div(\phi D)dV - \frac{1}{2}\int_V D(grad\,\phi)dV \tag{3}$$

$$\frac{dW_E}{dV} = \frac{1}{2}DE \approx \frac{1}{2}\varepsilon_r \varepsilon_0 E^2 \tag{4}$$

where ε_0 is the permittivity of vacuum (ε_0 = 8,854187817 . 10^{-12} F . m^{-1}), ε_r is the permittivity of the material, ϕ is the electrostatic potential gradient, *D* is electrical induction.

The resulting electrostatic potential φ_j at the place of j^{th} charge can be expressed the energy of the electrostatic field described by the equation 5.

$$\varphi_j = \sum_j \frac{q_i}{4\pi\varepsilon_0 r_{ij}} \quad \text{or for a single charge} \quad \varphi = \frac{q}{4\pi\varepsilon_0 r} \tag{5}$$

The resultant intensity of electrostatic field as negative gradient of potential between electrodes according to the relation (6) can be determined from value of electrostatic potential on positive and negative electrode.

$$E(r) = -grad\,\varphi(r) \tag{6}$$

2.2 FEM model describing the intensity and distribution of electric field

The model was created in Comsol Multiphysics in module AC / DC Electrostatics, which is focused on modeling of the electric fields and elastic fields in piezoelectric materials. This software contains a wide range of tools for a solving various problems described by partial differential equations by finite element method (in isotropic and anisotropic environments). It allows modeling of the vector distribution of electrostatic potential and to determine the approximate stress intensity based on the equations 1 – 6. Evaluation of the effect of various initial and boundary conditions can be utilized in the optimization of the construction design of the polymer reservoir 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. 2). The model was proposed with adaptive networking with the accent on local densification of elements (Fig. 3). The finite element mesh was created from 2D cubic axisymetric elements (12-node elements). For sufficiently accurate solution in geometrically complicated areas (radius, corners) and areas with assumed highest intensity of electrical field minimal size of elements 0,03 mm was created.

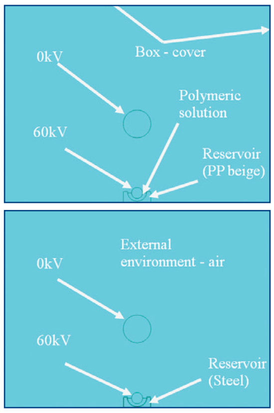

Figure 2. *FEM model*

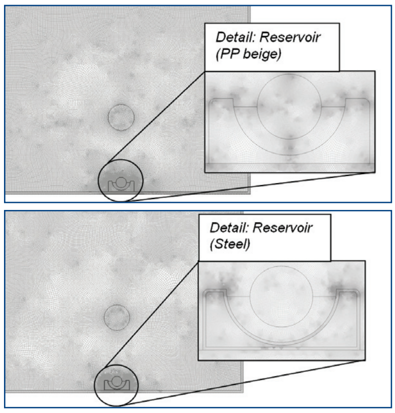

Figure 3. *Adaptive meshing of the elements*

Material properties of particular construction and technology elements of the line with Nanospider technology were taken from material sheets of manufacturer. For the analysis of the electrostatic field is required only one material property – relative permittivity. Values applied in the model simulations are shown in Table 1.

Material	Relative permittivity [-]
Reservoir (PP beige)	2,3
Reservoir (Steel)	1
Polymeric solution	81,6
Box – cover	3,5
External environment – air	1,00054

Table 1. *Physical parameters of the material in FEM simulation*

2.3 Experiment

For the assessment of the production efficiency of nanofibers two designs of reservoirs were compared. Namely the existing reservoir from polypropylene (PP beige) which mechanical properties are characterized by high stiffness, good tensile strength and especially resistance to acids, alkalis and solvents with a relatively low density ~ 0.900±6 g.cm^{-3} and the function model of the reservoir from thin wall austenitic stainless steel (CSN EN 10 027–1: X5CrNi 18–10), which is resistant to acids and solvents. The construction design of both reservoirs is shown in Fig. 4.

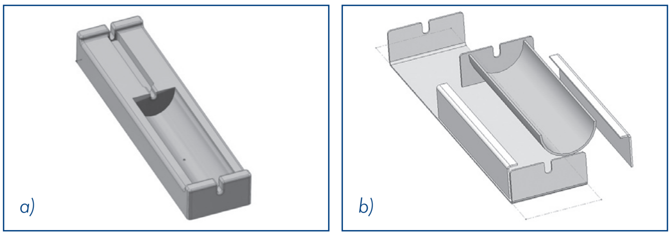

Figure 4. *a) Reservoir (PP beige), b) Reservoir (Steel)*

The experiment for an assessment of the spinning process was carried out on the real line of Elmarco Company (Fig. 4).

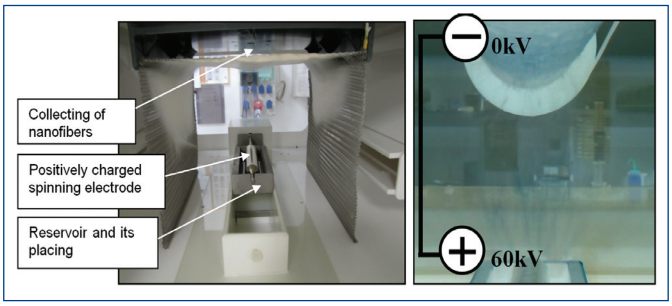

Figure 5. *Production of nanofibers by the Nanospider methode*

3. Results

The potential distribution (Fig. 6 to 7) is very similar for both constructions, so it can be assumed that the proposed construction of metal reservoir will be functional in the process of spinning. The results of the intensity distribution are shown in Figure 8 and 9. The intensity was expressed in units statvolt/cm (1statvolt = 299,793 volt). The maximum value of electric field intensity is in the case of the current structure of PP beige. The simulation results shoved ~ 321 statvolt/cm for PP and the value of ~297 statvolt / cm for the metal reservoir. The difference is 21.5 statvolt / cm. Thus the current version has about 7% higher value of the maximum intensity of electrostatic field. The relative permittivity of the environment is a constant describing the proportion of the material permittivity and the permittivity of vacuum. The value of the relative permittivity in the spinning chamber is directly influenced by the type of the polymeric solution, air humidity, and the type of electrode. [Komarek 2010, Angammana 2011]. Experiment for comparison of preceeding and new design of bath reservoir was performed, but it couldn´t determine the intensity of electrostatic field. In both cases the productivity was comparable. In the presented paper the homogeneity of the production is compared. The model analysis was performed with current and optimized design of the reservoir in the range of relative permittivity from the value of 0.1 to 3.5 (plastic materials have a relative permittivity in the range 1,8-4 and metallic materials is 1 ± 0.3) to define the effect of the applied material relative permittivity. This gradually stepwise changing value of the relative permittivity showed different trends (Fig. 10).

The resulting electric field intensity for the value of the relative permittivity of 0.6 is in the case of (PP beige) shows ~ 290 statvolt/cm and in the case of the metal the maximal intensity is ~ 321 statvolt/cm. Thus the difference is ~ 31 statvolt/cm. The optimized design shows 11 % higher intensity.

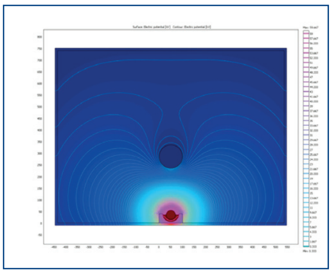

Figure 6.
FEM design (PP beige): Potential

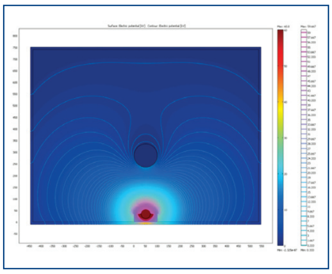

Figure 7.
FEM design (Steel): Potential

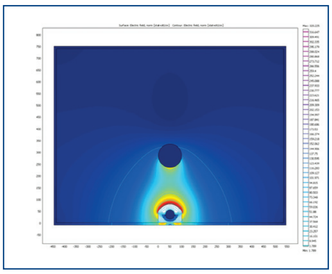

Figure 8.
FEM design (PP beige): Intensity

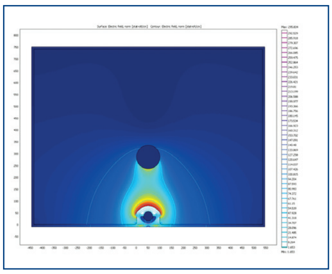

Figure 9.
FEM design (Steel): Intensity

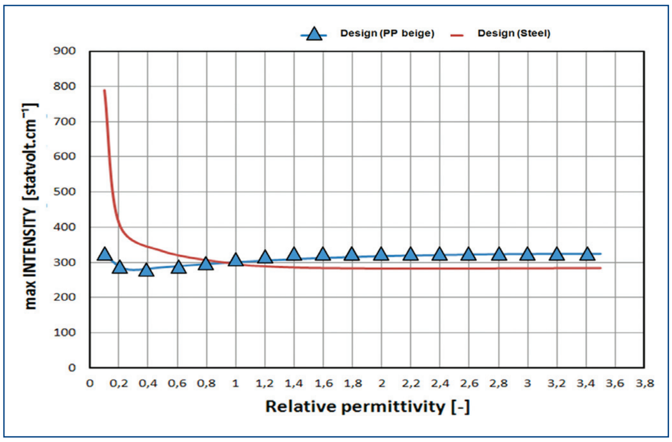

Figure 10. *The maximum electric field intensity depending on the design of reservoirs with different relative permittivity*

4. Conclusions

This article deals with the optimization of the electrostatic field distribution in the construction of the line producing inorganic nanofibers. One possibility is the modification of the current design of the reservoir from polypropylene (PP beige), which serves as a carrier of the electrode and especially as a storage of the polymeric solution for electrospinning "from the roller" – which is known as the Nanospider technology. For this purpose, the simulations of the potential and electric field intensity distribution in the process of spinning in the environment of the finite element method were performed. The resulting analysis showed that the intensity of electrostatic field is significantly influenced by the relative permittivity of the material and also by the design of the reservoir geometry. From obtained results it can be concluded that for lower values of the relative permittivity of the reservoir material (0.2 to 0.5) would be advantageous to increase the intensity of the electrostatic field by the use of thin wall construction. Similarly for the higher values of permittivity (2 – 3.5) would be beneficial to use a thicker construction of the reservoir. Currently, the functional model is tested in Elmarco company, and other functional models from various materials with different values of the relative permittivity are prepared.

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Contacts

Ing. Michal Petru, Ph.D.
Technical University of Liberec
Institute for Nanomaterials
Advanced Technologies and Inovation
Studentska 1402/2, Liberec, 461 17, Czech Republic
tel.: +420 777 996 636, +420 485 353 313
michal.petru@tul.cz