Numerical modeling and experimental study of solution-blown nonwovens formed on a rotating drum

Arkaprovo Ghosal [a], Sumit Sinha-Ray [a], Suman Sinha-Ray [a, b, c], Alexander L. Yarin [a, *], Behnam Pourdeyhimi [d]

[a] Department of Mechanical and Industrial Engineering, University of Illinois at Chicago, Chicago, IL 60607-7022, USA
[b] Corporate Innovation Center, United States Gypsum, 700 US 45 N, Libertyville, IL 60048, USA
[c] Department of Materials Science and Engineering, Indian Institute of Technology, Indore, Madhya Pradesh 452017, India
[d] 3427 The Nonwovens Institute, Box 8301, North Carolina State University, Raleigh, NC 27695-8301, USA

ARTICLE INFO

ABSTRACT

In this work the three-dimensional architecture and properties of solution-blown laydown formed on a rotating drum are studied using the system of quasi-one-dimensional equations of the dynamics of free liquid polymer viscoelastic jets moving, evaporating and solidifying, while being driven by a surrounding high-speed air jet. Solution blowing of multiple polymer jets simultaneously issued from a nosepiece and collected on a rotating drum is modelled numerically. The numerical results on the volumetric porosity of nonwoven laydown are compared with the experimental data of the present work. The numerical predictions are in good agreement with the experimental data and elucidate the effect of the angular drum velocity on the mass and angular fiber distribution, as well as the volumetric porosity and permeability of the solution-blown nonwovens. It was found that instead of doing any upstream modification of the solution blowing process, the easiest way to control the laydown structure (the mass and angular fiber distribution, as well as the volumetric porosity and permeability) is to vary the angular velocity of the collecting drum.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

In the previous works of this group a comprehensive theory of solution blowing was developed with a goal to predict properties of nonwoven laydowns formed by this method [1]. Solution blowing is an attractive novel method of formation of polymer micro-fibers and nanofibers from polymer solutions, while nanofibers belong to a wide class of nano-scaled or micro- and nano-textured materials expected to be delivered by nanotechnology. Over the last two decades nanotechnology has become a household name. According to a recent survey by The National Science Foundation (NSF) and The National Nanotechnology Coordination Office (NNCO) the global market size of nanotechnology in 2013 was of the order of $1 trillion [2], with micro- and nanofibers becoming an integral part of the nanotechnology deliverables. According to the recent Market Research Reports, the market size of nanofibers in 2009 was $80.7 M, which is forecasted to grow to a staggering $2.2B by 2020

[3]. Micro- and nanofibers have already revealed a multitude of applications in micro- and nano-fluidics [4–6], controlled drug delivery [7–10], agriculture and food science [11], microelectronics cooling [12–14], etc. (see the recent comprehensive monograph [15], as well as several preceding reviews in Refs. [16,17]). A significant widening of micro- and nanofiber applications in general, and of solution-blown micro- and nanofibers, in particular, requires a thorough understanding of the physical foundations of the process, its optimization and scaling up to the industrial level.

One of the most popular methods of forming nanofibers is electrospinning [15–24]. However, electrospinning suffers from two significant drawbacks: (i) because of the poor scalability, electrospinning is a slow process and electrospun fiber production en masse is time consuming and relatively expensive; (ii) high voltage required for electrospinning makes it rather incompatible for utilization in a large-scale industrial facility. In recent years solution blowing of polymer micro- and nanofibers has been developed to overcome some of these difficulties [25–27]. In solution blowing process polymer solution is issued into a coaxial high-speed air jet which stretches the polymer jet directly, and

triggers additional stretching due to the onset of bending instability [1,15]. Solution blowing results in formation of polymer micro- and nanofibers and the fiber production rate is atleast an order of magnitude higher than in the case of electrospinning. When the air jet is supersonic, solution blowing is capable of producing nano-fibers in the 20—50 nm range [28]. A few layers of such tiny nanofibers deposited on a commercial filter have already been used as very effective van der Waals collectors of ~100 nm nanoparticles from dilute aqueous suspensions practically without affecting pressure head [29]. Recently, solution blowing was scaled up and implemented using an industrial nosepiece [30].

It should be emphasized that solution blowing is an offshoot of meltblowing process, where a molten polymer jet is issued into a high-speed air jet resulting in microscopic polymer fibers [31—40]. Therefore, both processes involve three-dimensional stretching and bending of viscoelastic polymer jets entrained by the surrounding high-speed air jet. The difference between the two processes stems from the fact that in meltblowing polymer jet is cooled down by the surrounding air and thus, solidifies, whereas in solution blowing solvent evaporates and polymer in the jet precipitates and forms a solid polymer micro- or nanofiber.

Accordingly, the numerical model of polymer solution jet dynamics in solution blowing in Ref. [1] significantly benefited from the previously developed numerical models of polymer jets in meltblowing [38—40]. However, in distinction from the numerical models of meltblowing, numerical reconstruction of the detailed three-dimensional architecture of solution-blown laydown and its dependence on the governing parameters of the process has never been attempted, as to our knowledge. Numerical efforts on modeling of solution blowing are also significantly hindered by the lack of the experimental data on solution-blown nonwovens with sufficient information on the values of the governing parameters in the experiment. Therefore, the motivation of the present work is in concerted modeling of solution blowing and its experimental investigation under controlled conditions. The numerical code employed in the present work stems from our previously developed code [1], albeit extends it to accommodate fiber collection on a rotating vacuumized drum, as well as provides it with post-processing tools, which allow one to restore the three-dimensional structure of collected fibrous laydown, its fiber size and mass distributions, as well as the corresponding porosity and permeability.

2. Numerical model

As in Ref. [1], modeling of solution-blown polymer jets employs the quasi-one-dimensional equations of the dynamics of thin liquid jets in the momentless approximation (cf. the details in Refs. [15,41]). Namely, the model implies the existence of an about 1 mm-long straight section of polymer jet near the die exit, where its bending stiffness is too high to let it bend, and a much longer bending part of the jet up to the collector (cf. Fig. 1a). In solution blowing the cross-sectional diameter of polymer jets diminishes from about 1.2 mm to about 12 μm over the straight part due to the jet stretching by the surrounding high-speed air and solvent evaporation [1]. At the end of the straight part polymer jets possess a very low bending stiffness (diminishing with the cross-sectional jet radius a as a^4), and begin to experience a vigorous bending driven by the aerodynamic distributed lift forces. The polymer jets are also subjected to the aerodynamic drag force, turbulent pulsations, as well as solvent evaporation (cf. Fig. 1b). All the above-mentioned processes are described using the following quasi-one-dimensional mass and momentum balance equations [15,41,42].

$$\frac{\partial \lambda f}{\partial t} + \frac{\partial fW}{\partial s} = -D_a b \pi \lambda \qquad (1)$$

$$\frac{\partial \lambda f \mathbf{V}}{\partial t} + \frac{\partial fW\mathbf{V}}{\partial s} = \frac{1}{\rho}\frac{\partial P\boldsymbol{\tau}}{\partial s} + \lambda f\mathbf{g} + \frac{\lambda}{\rho}\mathbf{q}_{total} \qquad (2)$$

In Eqs. (1) and (2) t is time, s is an arbitrary coordinate reckoned along the jet axis, $f(s,t) = \pi a^2$ is the cross-sectional area (the cross-section is assumed to stay circular even in bending jets, which is a plausible approximation according to [41]), W is the velocity of polymer solution along the jet relative to a cross-section with a certain value of s, the stretching factor $\lambda = |\partial R/\partial s|$, with $\mathbf{R}(s,t)$ being the position vector of the jet axis, $\mathbf{V}(s,t)$ is the absolute velocity of polymer solution in the jet, ρ is the polymer solution density, $P(s,t)$ the magnitude of the longitudinal internal viscoelastic force in the jet cross-section, $\boldsymbol{\tau}$ is the unit tangent vector of the jet axis, $\mathbf{g}$ gravity acceleration, and $\mathbf{q}_{total}$ is the overall aerodynamic force applied by the surrounding gas to a unit jet length.

The projections of the momentum balance equation onto the accompanying trihedron of the jet axis, namely, the unit tangent vector $\boldsymbol{\tau}$, the unit principal normal vector $\mathbf{n}$, and the unit binormal vector $\mathbf{b}$, are kindred to the hyperbolic wave equation, as described in detail in our previous works [38,40,43]. Accordingly, they are solved numerically using the implicit numerical scheme of the generalized Crank-Nicolson type with the central difference spatial discretization at three time levels used in Refs. [38,40,43] and described in detail in Ref. [44]. Our previous works [38,40] also discuss in full detail the implementation of the initial and boundary conditions, whereas our previous work [39] specifies the post-processing procedure which allows one to reconstruct the three-dimensional architecture of the predicted laydown using the predicted touch-down times of the individual jet elements, their locations on the collecting screen and the cross-sectional radii of the as-deposited filaments.

The term on the right-hand side in the continuity equation (1) describes solvent evaporation. The factor b involved in this term reads [42]

$$b = 0.495\mathrm{Re}_a^{1/3}Sc^{1/2}\left[C_{s,eq}(T) - C_{s,\infty}\right] \qquad (3)$$

where D_a is the vapor diffusion coefficient in air, Re_a is corresponding Reynolds number, Sc is the Schmidt number and C_s is solvent concentration. Subscript eq corresponds to the equilibrium vapor concentration over the polymer solution surface determined by temperature T, while subscript ∞ corresponds to the vapor content far away from the jet surface in the surrounding air. Equations (1) and (3) show that solvent evaporation rate is dependent on temperature T through the dependence of the equilibrium solvent concentration over the polymer jet surface on temperature $C_{s,eq}(T)$. This dependence is typically derived from the Antoine equation, or similar equations available for different solvents [45—47]. Since solution blowing is an isothermal process, temperature T is known as a room temperature. This temperature is typically above the theta-temperature, and thus the solvents are initially good. However, when the solvent concentration in the polymer jet decreases and, accordingly, polymer concentration C_p increases, the strongly nonlinear dependences of the zero-shear viscosity and the relaxation time on C_p given by Eq. (4) below practically arrest the polymer solution deformation, and effectively mean polymer precipitation due to a high concentration when the polymer-polymer self-interactions prevail.

In the notation used the boldfaced characters denote vectors. Also, the longitudinal force in the jet cross-section $P(s,t) = f(\tau_{\tau\tau}$-