A RACHFORD-RICE LIKE EQUATION FOR SOLVENT EVAPORATION IN THE BUBBLE ELECTROSPINNING

by

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A Rachford-Rice like equation is established to describe rapid solvent evaporation in the bubble electrospinning or the bubbfil spinning. The model can be used to control fiber morphology, especially nanoporous fibers.

Key words: *nanofiber, nanoporous materials, bubble electrospinning, flash evaporation, Rachford-Rice equation*

Introduction

The bubble electrospinning [1-3] is to replace a Taylor cone in classic electrospinning by a polymer bubble. The electrostatic force is to overcome the surface tension of the bubble, which will be broken into pieces when the electrostatic force is large enough, and each fragment has a high ejecting velocity of about 300 m/s, and it can be further accelerated by the electrostatic force. The electrostatic force is replaced by other external forces, such as centrifugal force, flowing air, various mechanical forces in the bubbfil spinning process [4, 5]. A rapid solvent evaporation occurs due to a sudden drop of air pressure at the nozzles when a polymer bubble is broken at nozzles, and flash evaporation is also widely adopted for fabrication of nanoporous fibers [6, 7], controlling the solution concentration and pressure drop and temperature are important to adjust its porosity and size of the fiber. In the spinning process, multiple solvents are used to control the spinning process and the fiber morphology as well. For a multi-solvent solution, it is important to calculate the amounts of flashed solvents.

Solvent evaporation

During the spinning process, the mass conversation equation can be expressed [8]:

$$\pi r^2 \rho u = Q \tag{1}$$

where u is the velocity of the jet, ρ – the density of the jet, Q – the flow rate, and r – the fiber radius. The density can be calculated by the form:

$$\rho = \sum_{i=1}^{n} \rho_i z_i + \rho_s z_s + \rho_a z_a \tag{2}$$

where subscribes *i, s,* and *a* imply solvent, solute, and additive; z is concentration.

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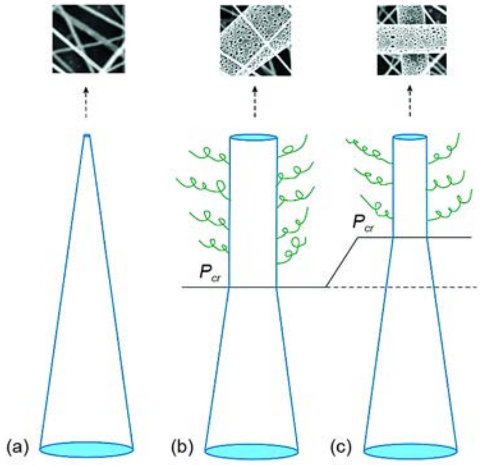

Figure 1. Solvent evaporation in the bubble electrospinning; (a) slow evaporation; (b) flash evaporation due to sudden pressure drop; (c) late flash evaporation

$$\sum_{i=1}^{n} z_i + z_s + z_a = 1 \tag{3}$$

In case for no additives and a fixed spinning condition, the fiber diameter and porosity in the fiber mainly depends upon solvent evaporation. A fast pressure drop results in a rapid flash evaporation, and the solution jet is solidfied immediately with nanoscale porosity as illustrated in fig. 1.

Slow evaporation of solvent will result in smooth fibers and its diameter mainly depends upon the velocity of the jets ejecting from a broken bubble. We use Laval nozzle to give a sudden pressure drop at the nozzle exist.

According to Bernoulli equation, the moving jet satisfies the following relationship:

$$\frac{P}{\rho} + \frac{1}{2}u^2 = B \tag{4}$$

where P is the fluid pressure. A higher velocity of the jet results in a smaller pressure. The nozzle is pinched at the middle, where the maximal velocity is obtained, and the distance between the pinched point to the exit of the nozzle can be used to control the pressure drop in the spinning process. A sudden pressure drop at the exist of the nozzle will results in porosity in fiber's surface, the higher pressure drop, the larger fiber size, and more nanoscale porosity, see fig. 2.

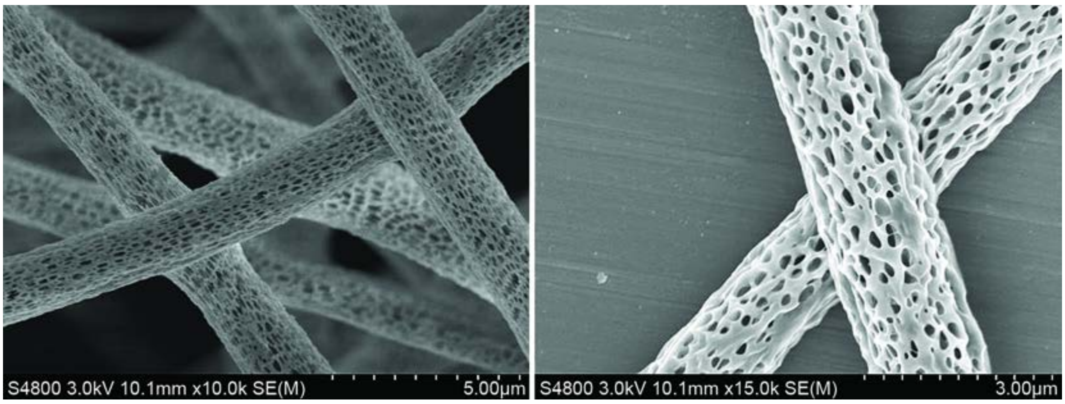

Figure 2. Flash evaporation for fabrication nanoscale porous fibers using chloroform as a main solvent

Rachford-Rice like equation

Flash calculation is essential for the design of many important equilibrium-staged separation processes including distillation, and Rachford-Rice equation is used for this purpose.

For a polymer bubble with multiple components including solvents and additives, we have the following equations.

Mass conservation

$$Q = V + F \tag{5}$$

where V and F are vaporized part and left flow, respectively.

Component mass conservation

$$Qz_i = Vy_i + Fx_i \tag{6}$$

where z_i, y_i, and x_i are the fraction of component i in the ejecting jet, fraction of solvents, and fraction of liquid, respectively.

Evaporation relation

$$y_i = k_i x_i + \mu_i \nabla p_i \tag{7}$$

where k_i is the equilibrium constant, ∇p_i – the pressure difference between the flowing jet and the environmental air pressure, and μ_i – a constant. When $\mu_i = 0$, eq. (7) turns out to the basic assumption in Rachford-Rice equation.

According to eq. (4), we have:

$$y_i = k_i x_i + \frac{1}{2}\mu_i \rho_i u^2 = k_i x_i + \eta_i \rho_i \tag{8}$$

where $\eta_i = \mu_i u^2/2$.

Submitting eq. (8) into eq. (6) and solving x_i, we have:

$$x_i = \frac{Qz_i - V\eta_i\rho_i}{Vk_i + F} = \frac{z_i - \varphi\eta_i\rho_i}{\varphi(k_i - 1) + 1} \tag{9}$$

By eq. (8), we have:

$$y_i = k_i \frac{z_i - \varphi\eta_i\rho_i}{\varphi(k_i - 1) + 1} + \eta_i\rho_i = \frac{k_i z_i + \eta_i\rho_i(1-\varphi)}{\varphi(k_i - 1) + 1} \tag{10}$$

Using the following relation:

$$\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} x_i \tag{11}$$

we obtain a Rachford-Rice like equation, which is:

$$\sum_{i=1}^{n}\left\{\frac{k_i z_i + \eta_i\rho_i(1-\varphi)}{\varphi(k_i - 1) + 1} - \frac{z_i - \varphi\eta_i\rho_i}{\varphi(k_i - 1) + 1}\right\} = 0 \tag{12}$$

or

$$\sum_{i=1}^{n}\left\{\frac{(k_i-1)z_i+\eta_i\rho_i}{\varphi(k_i-1)+1}\right\}=0 \tag{13}$$

When $\eta_i = 0$ or $\mu_i = 0$, eq. (13) becomes Rachford-Rice equation [9-12]. To solve eq. (13), we can use the variational iteration method, the homotopy perturbation method, or even the ancient Chinese mathematics [13-17].

Conclusion

This paper gives a self-contained theoretical model for solvent calculation of multi-component jets in the bubble electrospinninng. The model is of critical importance for controlling fiber morphology, especially nanoporous fibers. This model considers the effect of high velocity of the moving jets. Though the model seems to be rigorous, we still need experimental verification, which is under way and the results will be reported in a separate paper.

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