

A MULTI-PHASE FLOW MODEL FOR ELECTROSPINNING PROCESS

by

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An electrospinning process is a multi-phase and multi-physical process with flow, electric and magnetic fields coupled together. This paper deals with establishing a multi-phase model for numerical study and explains how to prepare for nanofibers and nanoporous materials. The model provides with a powerful tool to controlling over electrospinning parameters such as voltage, flow rate, and others.

Keywords: *electrospinning, multi-phase model, nanofibers, nanoporous materials*

Introduction

Because of ultra-high specific surface, nanofibers are potentially of great technological interest for the development of electronic, catalytic, and hydrogen-storage systems, invisibility device and others. Electrospinning has evinced more interest and attention in recent years due to its versatility and potential for applications in diverse fields [1]. It introduces a new level of versatility and broader range of materials into the micro/nanofiber range.

During the electrospinning process, the charged jet pulled from a capillary orifice is accelerated toward the target by a constant external electric field, and rapidly thins and dries as a result of elongation and solvent evaporation. The shape and surface morphology of charged jet can be tunable by adjusting electrospinning parameters such as voltage, flow rate, and others. Its mechanical mechanism has been received much attention in recent years. Some numerical analysis and experiment verifications have been carried out to research mechanical mechanism of charged jet arising in the electrospinning process [2-10].

Electrospinning is a multi-phase and multi-physics process involving electrohydrodynamics, mass and heat diffusion and transfer, evaporation, *etc.* Many studies have been conducted to understand the process and a number of mathematical models have been developed [6-10]. However, almost all these models are single-phase models, and can't offer in-depth insight into physical understanding of many complex phenomena which cannot be fully explained experimentally.

In this paper, a multi-phase model is presented to explain how to prepare nanofibers and nanoporous materials by electrospinning. The multi-phase flow model takes into account

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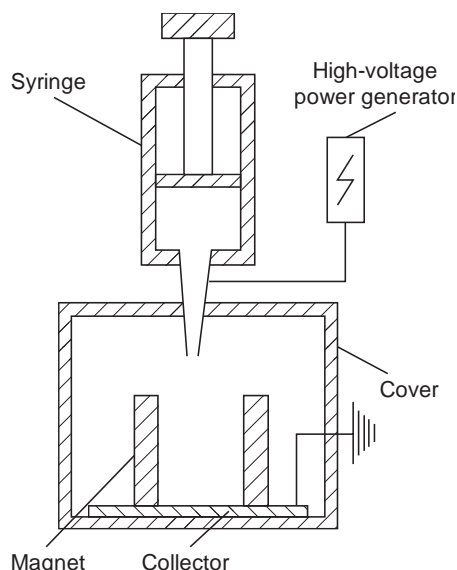


Figure 1. Electrospinning-dilation

solvent evaporation and dispersion of additive particles, which play pivotal roles in determining the internal fiber morphology of the electrified jet to be described here. In future, based on the model, the effects of various electrospinning parameters, such as voltage, flow rate and solvent evaporation rate, on quality of product, will be systematically carried out, finally the model will be further ameliorated according to the experimental data. The model can be used to optimize and control the electrospinning parameters.

During the electrospinning process, the charged jet pulled from a capillary orifice is accelerated by a constant external electric field, and the liquid jet is injected in the air (fig. 1). The state of the charged jet can be calculated by solving the modified Navier-Stokes equations under the influence of electric field and magnetic field and the interface between the two fluids has been determined by using the volume of fluids method.

Governing equations

The modified Navier-Stokes equations governing heat and a jet under the influence of electric field and magnetic field are [10]:

– Maxwell's equations

$$\frac{\partial q_e}{\partial t} + \nabla \cdot \mathbf{J} = 0 \quad (1)$$

$$\nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0 \quad (2)$$

$$\nabla \times \mathbf{H} - \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} = \frac{1}{c} \mathbf{J} \quad (3)$$

where q_e is the electric charge, \mathbf{E} – the electric field, \mathbf{J} – the current, \mathbf{B} – the magnetic induction, \mathbf{H} – the magnetic field, \mathbf{D} – the atomic displacement vector, and c – the velocity of light in a vacuum ($c = 2.998925 \pm 0.0006 \cdot 10^8$ m/s),

– continue equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (4)$$

where ρ is the density of the jet, and \mathbf{u} – the velocity of the jet,

– momentum equation

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \mathbf{t} + \rho \mathbf{f} + q_e \mathbf{E} + (\nabla \cdot \mathbf{E}) \mathbf{P} + \mathbf{F}_m \quad (5)$$

where \mathbf{t} is the stress tensor, \mathbf{f} – the body force, \mathbf{P} – the polarization, and \mathbf{F}_m – the magnetic force,

$$\mathbf{F}_m = q_e \frac{1}{c} \mathbf{u} \times \mathbf{B} + \frac{1}{c} \mathbf{J} \times \mathbf{B} + (\nabla \mathbf{B}) \mathbf{M} + \frac{1}{c} [(\mathbf{P} \times \mathbf{B}) \mathbf{u}] + \frac{1}{c} \frac{\partial}{\partial t} (\mathbf{P} \times \mathbf{B}) \quad (6)$$

where \mathbf{M} is the magnetization,
– energy equation

$$\rho c_p \frac{DT}{Dt} = Q_h + \nabla \mathbf{q} + (\mathbf{J} - q_e \mathbf{u}) \left(\mathbf{E} + \frac{1}{c} \mathbf{u} \times \mathbf{B} \right) - \left(\mathbf{E} + \frac{1}{c} \mathbf{u} \times \mathbf{B} \right) \frac{D\mathbf{P}}{Dt} - \left(\mathbf{M} + \frac{1}{c} \mathbf{u} \times \mathbf{P} \right) \frac{D\mathbf{B}}{Dt} + Q_f \quad (7)$$

where \mathbf{q} is the heat, Q_h – the source term, and Q_f – the energy loss caused by the air drag.

This set of conservation laws can constitute a closed system when it is supplemented by appropriate constitutive equations for the field variables such as polarization. The most general theory of constitutive equations determining the polarization, electric conduction current, heat flux, and Cauchy stress tensor has been developed by Eringen and Maugin [11, 12].

Modeling of turbulent flow

The k - ε turbulent model is applied to deal with turbulent flows in strong electric fields. The Reynolds time-mean equations for continuity and momentum are of the same form as governing equations if transient quantities are replaced by time-mean quantities. But the stress tensor in turbulence includes an extra contribution from eddy viscosity besides the part due to molecular viscosity [13].

Interface tracking of the jet surface

Tracking the exact interface location is therefore of predominant importance in the numerical model. The volume of fluid (VOF) [14] model, which attempts to track the interface based on the mass conservation, has been widely adopted. In the VOF model theory, the volume fraction of q^{th} fluid in the cell is denoted as α_a , and then the following three conditions are possible:

$\alpha_a = 0$ if the cell is empty of the q^{th} fluid,

$\alpha_a = 1$ if the cell is full of the q^{th} fluid, and

$0 < \alpha_a < 1$ if the cell contains the interface between the q^{th} fluid and one or more other fluids.

The interface(s) between the phases is tracked by the solution of a continuity equation for the volume fraction of one or more of the phases, for the q^{th} phase, the equation has the form of eq. (1):

$$\frac{\partial(\alpha_q \rho_q)}{\partial t} + \nabla(\alpha_q \rho_q \mathbf{u}_q) = \sum_{p=1}^n (\dot{m}_{pq} - \dot{m}_{qp}) \quad (8)$$

where \mathbf{u}_a and α_a are the velocity vector and volume fraction of the q^{th} phase, p and q are the phase index, and \dot{m}_{pq} (\dot{m}_{qp}) is the mass transfer from phase $q(p)$ to phase $p(q)$.

The eq. (8) is not solved for the primary phase. The primary-phase volume fraction is computed based on the equation:

$$\sum_{q=1}^n \alpha_q = 1 \quad (9)$$

In this study, two immiscible fluids are considered as one effective fluid throughout the calculation domain, the physical properties of which are calculated as weighted averages based on the distribution of the liquid volume fraction, thus being equal to the properties of each fluid in their corresponding occupied regions and varying only across the interface [9], for example:

$$\rho = \rho_l \alpha_q + \rho_a (1 - \alpha_q) \quad (10)$$

where l and a are densities of liquid and air, respectively.

The model makes use of the two-fluid Eulerian model for a two-phase incompressible flow, where phase fraction equations are solved separately for each individual phase; hence, the equations for the phase fractions can be expressed as [15]:

$$\frac{\partial \alpha_q}{\partial t} + \nabla(\alpha_q \mathbf{u}) + \nabla[\alpha_q \mathbf{u}_r (1 - \alpha_q)] = 0 \quad (11)$$

where $\mathbf{u}_r = \mathbf{u}_l - \mathbf{u}_a$ is the vector of relative velocity.

Material properties equations

Based on the local value of α_q , the appropriate properties used in the momentum equations are determined by the volume-fraction-averaged equation:

$$\varphi = \sum \alpha_q \varphi_q \quad (12)$$

where φ is the volume-fraction-averaged properties such as density and viscosity used in the momentum equations and α_a and φ_a are the volume fraction and the properties for the q^{th} fluid.

Discrete phase modeling study for particle motion

The multi-phase flow model should take into account dispersion of additive particles, which are insoluble in solution and play an important role in determining the internal fiber morphology of the electrified jet to be described here. To mathematically model the electrospinning process, the discrete phase method (DPM) is now being used in this study.

The trajectory of a discrete phase particle by integrating the force balance on the particle is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle, and can be written as:

$$\frac{d\mathbf{u}_p}{dt} = \mathbf{F}_D(\mathbf{u} - \mathbf{u}_p) + \frac{\mathbf{g}(\rho_p - \rho)}{\rho_p} + \mathbf{F} \quad (13)$$

where \mathbf{u} is the fluid phase velocity, \mathbf{u}_p – the particle velocity, ρ – the fluid density, ρ_p – the particle density, \mathbf{F} – an additional acceleration (force/unit particle mass) term which can be important under special circumstances, $\mathbf{F}_D(\mathbf{u} - \mathbf{u}_p)$ – the drag force per unit particle mass, and:

$$\mathbf{F}_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \text{Re}}{24} \quad (14)$$

where μ is the molecular viscosity of the fluid, d_p – the particle diameter, C_D – the drag coefficient which have been given by Morsi and Alexander [16], and Re – the relative Reynolds number, which is defined as:

$$\text{Re} = \frac{\rho d_p}{\mu} |\mathbf{u}_p - \mathbf{u}| \quad (15)$$

The additional force term, \mathbf{F} , in eq. (13) can include forces on particles that arise due to the pressure gradient in the fluid, the temperature gradient, rotation of the reference frame, and so on.

According to the multi-phase flow model presented, a standard finite-different interpolation schemes and the explicit approach are used to the volume fraction equation. The face values of the q^{th} volume fraction are interpolated by using geometric reconstruction scheme. A realizable k - ε model is used to model the turbulent viscosity. The flow of particles will be modeled by FLUENT using the discrete phase model. This model predicts the trajectories of individual particles. Heat, momentum, and mass transfer between the particles and the solution will be included by alternately computing the discrete phase trajectories and the solution phase continuum equations.

Conclusions

In this paper, a multiphase flow model will be established considering solvent evaporation and dispersion of additive particles for the electrospinning process under coupled multi-field (*e. g.*, electric field, magnetic field, and fluid field). Based on the model, numerical simulation and experiment verification will be carried out to research mechanical mechanism of multiphase jet arising in the electrospinning process in future. And we will apply FLUENT to simulate the multiphase jet numerically for gaining significant insight into understanding of its mechanical mechanism. Finally the model will be further ameliorated according to the experimental data. The model can be used to optimize and control the electrospinning parameters.

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