Numerical simulation of the fiber spinning with the viscoelastic Giesekus constitutive model

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Abstract. The numerical simulation of the first stage of fiber-spinning process was performed. The single-mode Giesekus model was used for polymer fiber stress calculations. Fiber profiles, longitudinal velocity, tensile stress and apparent elongational viscosity were analyzed depending on the stretch speed and the degree of anisotropy of the polymer.

1. Introduction

High strength polymer fibers are the result of multi-stage processes [1–3]. To create a fiber with the desired properties, a deep understanding of each stage of the spinning process is required. Depending on polymer chemical composition, either the melt-spinning or solution-spinning methods are used. If polymer melting temperature is higher than the pyrolysis temperature, the melt-spinning is not suitable for fiber formation. In case of the solution-spinning, the solvent has to be removed. This can be achieved by its evaporation in the stream of the hot inert gas (dry spinning [4, 5]) or by using with a precipitation bath (wet spinning [6]). The most efficient solution-spinning method is the dry-wet spinning [7,8], with an air gap where the filament is pre-stretched and oriented. The dry-wet spinning method allows producing the high-performance fibers such as poly-p-phenylene terephthalamide (PPTA) [9], polybenzoxazole (PBO) [10], and the precursor of carbon fiber as polyacrylonitrile (PAN) [11].

For a more detail study of flow and stretching of polymer filament in the air gap, the numerical simulations were applied. In particular, the power law viscosity model for the polymer solution was considered [12, 13]. However, the more complex nonlinear viscoelastic equations [14, 15] made it possible to achieve a better agreement with experimental data allowing to obtain set of fundamental results. These models should take into account the nonlinear effects (normal stress differences, dependence of shear and elongation viscosity on deformation rate, etc), which have a significant impact on the fiber formation. The Giesekus model is one of the simplest and efficient viscoelastic models describing these effects. This model was used successfully to simulate the melt-spinning processes [16, 17].

In this paper, the Giesekus model is used to simulate the first stage of the dry-wet spinning procedure. The impact of the nonlinear viscoelastic effects on the dynamics of fiber formation in a wide range of the draw ratio is investigated.
Figure 1. Schematic representation of the fiber spinning process.

2. Model

The first stage of the dry-wet spinning process was investigated numerically by the example of a single fiber. The spinning solution enters to the cylindrical channel (die) and extrudes into the air-gap (the stretching domain) as shown in figure 1. The fiber is then drawing by a take-up roll. Due to the cylindrical symmetry of the fiber precursor, a two-dimensional axisymmetric computational domain was considered. The problem was solved in dimensionless variables, where the channel radius $R$ was considered as a characteristic length scale. The lengths of the channel and the air-gap are equal to $35R$ and $100R$, respectively. The numerical simulation domain has a width of $3R$, which is large enough not to affect the flow dynamics.

A constant velocities $U_{in}$ and $U_{out}$ are applied as the inlet and outlet boundary conditions at the die entry and exit from the air-gap domain, respectively, so that, the fiber is captured at a roll with a constant speed. The ratio $Dr = U_{out}/U_{in}$ is called as the draw ratio, which is varied from 0 to 30 in our calculations. The no-slip boundary condition is applied at the channel walls.

The hydrodynamics of the incompressible fluids is described by the following momentum and mass conservation equations:

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot \tau,$$

$$\nabla \cdot u = 0,$$

where $u = (u, v, w)$, $p$ and $\tau$ are velocity vector, pressure and stress tensor, respectively; $t$ is time; $\rho$ is the density. The air phase was considered as a Newtonian liquid, where the stress tensor was defined as $\tau_{air} = \eta_{air}(\nabla u + \nabla u^T)$. The stress tensor $\tau_f$ in a fiber phase consists of two contributions $\tau_f = \tau_s + \tau_p$ (the so called elastic viscous split stress scheme [18]). The
first term $\tau_s = \eta_f (\nabla \mathbf{u} + \nabla (\mathbf{u}^T))$ is due to the Newtonian solvent, while the second term $\tau_p$ is depend of polymer rheological properties. To calculate $\tau_p$ the single-mode Giesekus constitutive model [19, 20] was used:

$$\tau_p + \lambda \frac{\partial \mathbf{u}}{\partial t} + \frac{\alpha \lambda}{\eta_p} \mathbf{u} \cdot \nabla \mathbf{u} = -\phi \eta_p \left( \nabla \mathbf{u} + \nabla (\mathbf{u}^T) \right),$$

(3)

where $\eta_p$ is polymer viscosity, $\lambda$ is the relaxation time, $0 \leq \alpha \leq 0.5$ is the dimensionless mobility parameter quantifying the anisotropy degree and

$$\nabla \tau \equiv \frac{\partial \tau}{\partial t} + \mathbf{u} \cdot \nabla \tau - (\tau \cdot \nabla \mathbf{u}^T + \nabla \mathbf{u} \cdot \tau)$$

(4)

is the upper-convected time-derivative keeping the models frame-invariant. Variables with $\eta_p$, $\rho_p$ and $U_{in}$ where used as characteristic scales for viscosity, density and velocity, respectively.

At $\alpha > 0$, the Giesekus model predicts shear thinning and a limited increase in tensile stress. Moreover, it fits qualitatively well the rheometric measurements of the unbranched polymer melts and concentrated solutions both in shear and uniaxial extensional experiments [21]. For $\alpha \neq 0$ the Giesekus model provides the shear-thinning behavior both for the steady shear values of viscosity and first normal stress difference coefficient for a simple shear flow.

The velocity $\mathbf{u}$ and pressure $p$ fields of a two-phase liquid were calculated numerically using the finite-volume-based code and the open-source rheoTools toolbox [22, 23] of the OpenFOAM (open source field operation and manipulation) [24] calculation platform. To track the interface between phases the VOF (volume of fluid) method was used [25]. The local density at each point $x$ of the computational domain were represented as continuous function $\rho(\phi) = \rho_f \phi + \rho_{air}(1-\phi)$ of the fraction $\phi(x,t)$, where $\rho_f$ and $\rho_{air}$ are densities of the fiber and air phases, respectively. This fraction $\phi(x,t)$ is equal to 1 in the region occupied by the fiber, $\phi = 0$ in the air phase, and $0 < \phi < 1$ in the narrow interfacial zone $\Omega$. The momentum equation (1) was integrated simultaneously with the mass conservative equation(2), Giesekus constitutive equation (3) and transport equation for the fraction $\phi$:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = 0.$$

(5)

The local stress tensor was calculated as $\tau(\phi) = \tau_f \phi + \tau_{air}(1-\phi)$. The influence of the surface tension and gravitational force were not considered in our calculations. To overcome the high Wissenberg problem [26] the log-conformation procedure was used [27, 28]. The separation of velocity and pressure fields was carried out by means of PISO (-pressure-implicit with splitting of operators) algorithm. The MULES (multidimensional universal limiter with explicit solution) method, accounting the compressive flux at the interface between the phases was used to minimize diffusion effects [29]. The numerical simulation was performed on the non-uniform Cartesian mesh with 47 300 cells, the maximum values of the mesh spacing in the horizontal and vertical directions were taken as $\delta x = \delta y = 0.05$.

3. Results

The constant values of the throughput average velocity $U_{in} = 0.333$ and retardation parameter $\beta = 1/9$ were considered. The calculations were carried out until the stationary state. Figure 2(a) shows effect of the take-up speed on the fiber radius $R_f$ along the spinning line $x = 0$ for $\alpha = 0.05$. At the die exit, $R_f$ increases by 1.75 times due to the swelling induced by the normal stresses, representing viscoelastic behavior of a polymer. The grows of take-up speed or draw ratio Dr from 0 (which corresponds to the free-surface flow) to 30 leads to a decrease in fiber transversal dimension up to the output radius value $R_f^{out}$. According to the volume rate consistency, the radius $R_f^{out}$ depends on the draw ratio equal to $R_f^{out} = Dr^{-0.5}$, figure 2(b).
Figure 2. The dependence of the fiber radius $R_f$ along the spinning line (a) and the output fiber radius $R_f^{\text{out}}$ (b) on the draw ratio $Dr$ for $\alpha = 0.05$.

Figure 3. Evolution of the fiber radius $R_f$ along the spinning line for different values of the mobility parameter $\alpha = 0.01$ (solid line), 0.05 (dashed line), 0.5 (dotted line) for $Dr = 10$.

The swelling degree at the die exit depends upon the mobility parameter $\alpha$. Decrease in $\alpha$ leads increase in swelling degree. Evolution of the fiber radius $R_f$ along the spinning line for $\alpha = 0.01$, 0.05, 0.5 is shown in figure 3.

The axial flow velocity $u$ of the fiber decreases at the die exit and then increases along the fiber. The increase in the longitudinal velocity at the end of the fiber becomes sharper with increasing in $Dr$, figure 4(a). The stretch rate increases non-uniformly along the fiber. This can be seen from the derivative of the longitudinal velocity $\partial u / \partial x$ along the tensile axis shown...
Figure 4. Longitudinal velocity $u$ (a) and derivative $\partial u/\partial x$ (b, c) along the fiber axis for various draw ratio $Dr$, $\alpha = 0.05$.

in figure 4(b). Figure 4(c) indicates the increase in the longitudinal velocity derivative $\partial u/\partial x$ along the tensile axis. It follows from figures 4 that the fiber undergoes the abrupt stretching near the die exit. Then there is a slight decrease in fiber tension which is followed by increase in stretching till the outer boundary.

The tensile stress profiles, representing by the first normal stress difference $N_1 = \tau_{xx} - \tau_{yy}$ along the fiber axis are shown in figure 5. Swelling at the exit of the die leads to negative values of $N_1$. At some distance from the die exit, the tensile stress increases slowly keeping about zero value and then increases significantly closer to the outlet boundary. The tensile stress increases with increase in draw ratio $Dr$ and decrease in $\alpha$ parameter.
Figure 5. Effect of draw ratio Dr on the tensile stress $N_1$ along the fiber axis for $\alpha = 0.01$ (dotted line), 0.05 (dashed line), 0.5 (solid line).

Figure 6. The apparent elongational viscosity $\eta_e$ behavior along the fiber axis for Dr = 10 (solid line), 20 (dashed line), 30 (dotted line) at $\alpha = 0.05$.

Figure 6 shows evolution of the apparent elongational viscosity $\eta_e = N_1/(\partial u/\partial x)$ along the fiber axis on the draw ratio. Its value increases dramatically close to the outlet boundary. This
means that the tensile stress increases faster than the stretching rate. Increase in the draw ratio also results in viscosity growth. However, the difference is becoming less noticeable for Dr = 20 and 30 which indicates a proportional growth in tensile stress and strain rate. This increase in the elongational viscosity indicates the fiber hardening with strain growth closer to the outlet boundary.

4. Conclusions

The numerical simulation has shown that the final fiber radius $R_f$ decreases with increasing draw ratio Dr and does not depend on the mobility parameter $\alpha$ of the Giesekus constitutive equation. The mass conservation condition results in the sharp increase of the longitudinal velocity, strain rate and tensile stress along of the fiber-spinning axis closer to the outlet boundary. Moreover, the growth degree is higher for larger draw ratio Dr and smaller the parameter $\alpha$. The fiber hardening was observed near the outlet.

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