COMPUTER MODELLING OF THE LYOCELL FIBRE SPINNING PROCESS

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Abstract

The cellulose Lyocell fibre spinning process can be divided into two processes, a dry spinning process in the air gap, and a wet spinning process in the coagulation bath. In order to simulate the process in the air gap, the heat capacity Cp, the density ρ, and the elongational viscosity η were measured by experiments carried out as a function of temperature and concentration of cellulose. The calculated diameters and temperature profiles along the spinning path were compared with the experimental results. The concentration of N-methyl-morpholine-N-oxide (NMMO) in the fibre (in the coagulation bath) was also measured during the experiments, and the diffusion coefficient was then calculated. Using the data obtained, the time during which the NMMO content in the fibre reaches the equilibrium state in the coagulation bath can be predicted.

Key words: *spinning process, modelling, simulation, cellulose fibres, Lyocell fibres, dry spinning, wet spinning*

1. Introduction

The Lyocell fibre spinning process is a dry-wet spinning process, and the process of fibre formation can be studied separately in the air gap and in the coagulation bath. The spinning dope, i.e. the cellulose N-methyl-morpholine-N-oxide monohydrate (NMMO-MH) solution, can be melted and solidified repeatedly without any change in its composition. The mass transfer between filament and the environment in the air gap can be neglected. That is why the spinning process in the air gap can be considered as melt spinning. The simulation of the melt spinning process is well known.

Any chemical reaction occurs in the coagulation bath, and cellulose is transformed to the solid state by diffusion of the solvent from the filament formed to the coagulation bath and water or diluted NMMO/water from the coagulation bath to the fibre. Therefore, the Lyocell spinning process in the coagulation bath can be considered as a wet spinning process without any chemical reaction.

However, the dependencies between the particular parameters of the spinning process are complex, and experiments aiming at obtaining optimal conditions are long-lasting and expensive. The disposition of a theoretical model and appropriate software would improve the optimisation process. This work is an approach to the elaboration of such a model.

2. Basis of the analysis

The spinning process of Lyocell fibres in the air gap can be considered as a melt spinning process. For a steady-state process of melt spinning, the following equations are well known [1, 2] but should be recalled as the basis for performing the measurements and calculations discussed below:
Mass continuity equation

$$\rho v \frac{\pi d^2(x)}{4} = W = \text{constant} \tag{1}$$

Moment a balance equation

$$\frac{\mathrm{d}F}{\mathrm{d}x} = \frac{\pi d(x)}{2}\rho_{\mathrm{a}} v_{\mathrm{a}}^2 C_{\mathrm{f}} + \frac{F\rho v}{\eta_{\mathrm{e}}} - \frac{Wg}{v} \tag{2}$$

Energy balance equation

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{4\alpha^*(T - T_s)}{\rho C_{\mathrm{p}} v d} \tag{3}$$

Rheological constitutive equation

$$\frac{\mathrm{d}v}{\mathrm{d}x} = \frac{F\rho v}{W\eta_{\mathrm{e}}} \tag{4}$$

where v, d, and T are the velocity, diameter and temperature of the running filament respectively (they are functions of the distance x from the spinneret along the spinning path); F is the tensile force acting on the filament at the given distance x; ρ, C_p, and η_e are the density, heat capacity, and apparent elongation viscosity of the cellulose NMMO-MH solutions respectively (all are functions of temperature and concentration of cellulose in the dope). If the concentration is fixed, ρ, C_p, and η_e are functions of temperature.

The data of density, heat capacity and elongational viscosityare unknown for cellulose solutions in NMMO-MH. Thus the density was measured by dilatometry, the heat capacity by the DSC method, and the elongational viscosity by using the non-isothermal spinning method for obtaining the parameters necessary to calculate the elongational viscosity values of the dope for different temperatures.

3. Results and discussion

Density and heat capacity measurements

Figures 1 and 2 present some results of measuring density and heat capacity in relation to temperature. Figure 1 (a and b) shows the relation between density and temperature for cellulose solutions in NMMO of different cellulose concentration. The different shapes of the curves for the heating and the cooling process are characteristic.

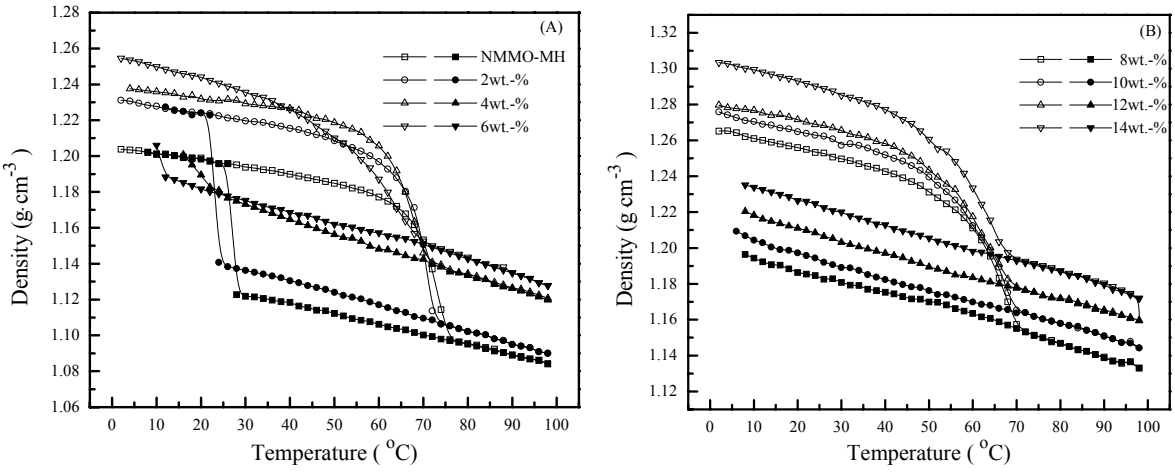

Figure 1. Density of NMMO-MH and cellulose solutions of different cellulose concentration as a function of temperature during the heating and the cooling process; open symbols: heating process, solid symbols: cooling process

Figure 2 shows the heat capacity of the cellulose solutions in NMMO of different concentrations as a function of temperature. It should be remembered that the temperature measurements were performed in ^{0}C as marked in Figures 1 and 2, whereas the temperature in equation 3 is in ^{0}K.

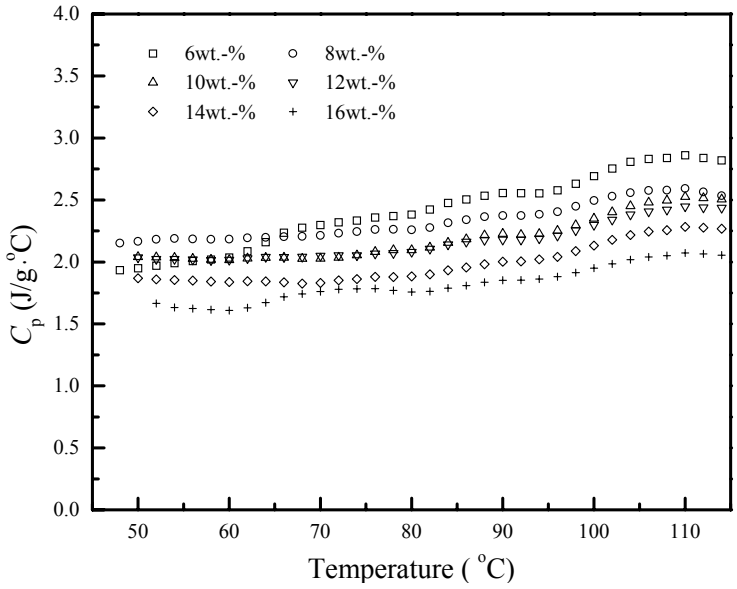

Figure 2. Heat capacity of cellulose solutions in NMMO-MH as a function of temperature for different cellulose concentration

On-line filament diameter measurements

Figure 3 shows the diameter development of Lyocell fibres in the air gap and in the coagulation bath. It can be seen that the deformation of the spinning solution stream forming the fibre mainly takes place near the spinneret and changes only slightly in the rest of the air gap. The diameter also decreases much more quickly with the increasing take-up velocity, because the tensile stress in the spun filament (in the spinning solution stream) increases with the increase in the take-up velocity and deformed the stream (filament) more comprehensively. The diameter of the filament while immersed in the coagulation bath is kept almost at the same level, as can be clearly seen in Figure 3b. This is because two kinds of diffusion take place in the coagulation bath: the solvent included in the filament diffuses into the coagulation bath, and the coagulant of the coagulation bath diffuses into the filament. These conditions cause the mass transformation to be maintained in an almost balanced state, and the total amount of the filament mass almost does not change on its path through the coagulation bath.

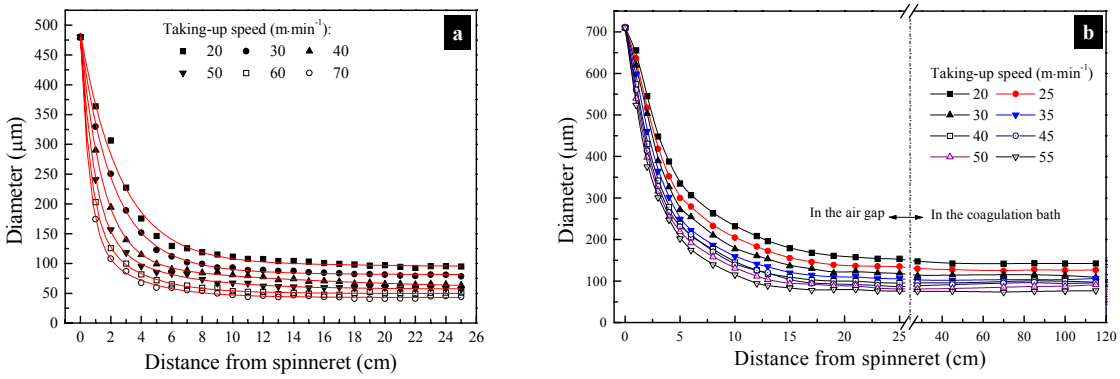

Figure 3. Diameter of the filament formed as function of the distance from the spinneret;
a) cellulose concentration 10%, mass throughput 0.1246 g/min
b) cellulose concentration 8%, mass throughput 0.26 g/min

On-line filament surface temperature measurements in the air gap

Figure 4 shows the changes in the surface temperature of spun Lyocell fibres in the air gap. It is visible that the surface temperature of the filament decreases along the spinning path, and that the decrease is faster with the increase in the take-up velocity. Such behaviour can be observed because the efficient heat transfer coefficient of the filament is related to its cross-section area in an inverse ratio. With increasing take-up velocity, the filament diameter decreases more quickly and thus the cross-section area of the filament also decreases more quickly. Therefore, the efficient heat transfer coefficient of the filament increases rapidly, which makes the heat transfer between the filament and the environment much more intensive; also, the surface temperature decreases sharply with increasing take-up velocity.

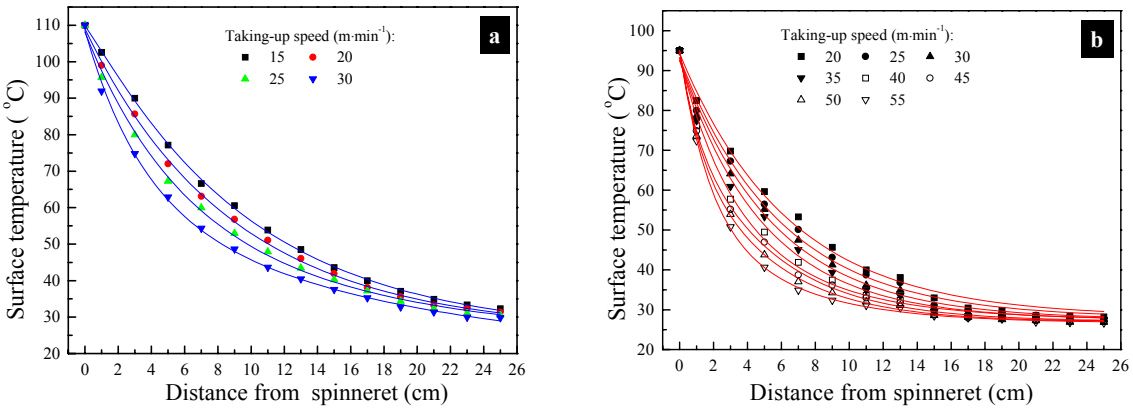

Figure 4. Filament surface temperature changes in the air gap; a) cellulose concentration 10%, mass throughput 0.1246 g/min; b) cellulose concentration 8%, mass throughput 0.26 g/min

On-line tensile force measurements

Figure 5 demonstrates the tensile force applied on the filament which is formed at the end of the air gap and in the coagulation bath, at different distances from its beginning for different take-up velocities. It can be seen that the tensile force at the end of the air gap increases linearly with the increasing take-up velocity (Figure 5.a). The linear increase is caused by the increase in friction between the running filament and the surrounding air, and the increase in the rheological force with the increasing velocity of the running filament. The tensile force also increases linearly with the increasing take-up velocity for the filament in the coagulation bath and with the increase in the coagulation bath length (Figure 5.b). In this case, the friction between filament surface and the coagulant mainly contributes to the increase in tensile force applied to the spun filament.

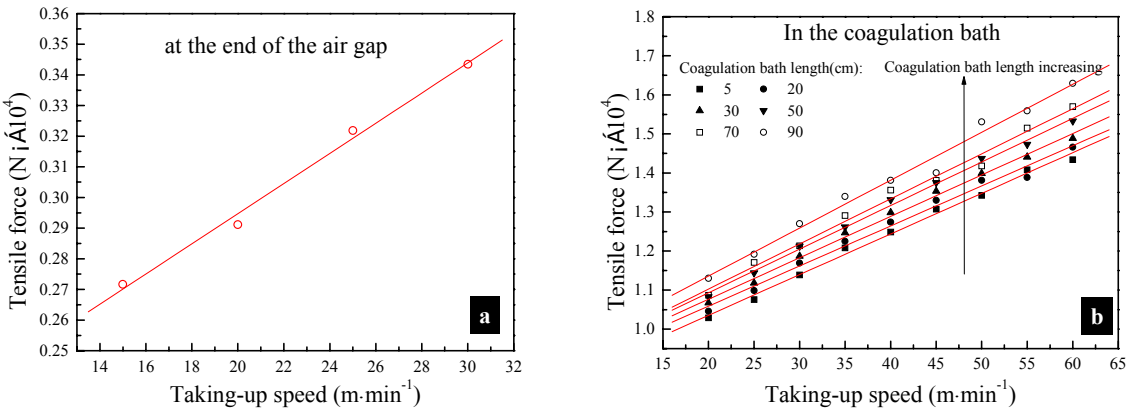

Figure 5. Tensile force applied on the filament at different take-up velocities: a) at the end of the air gap, cellulose concentration 10%, mass throughput 0.1246 g/min; b) in the coagulation bath, cellulose concentration 8%, mass throughput 0.26 g/min

All the dependencies presented in this article up to now have been examples of the measurement results obtained. As can be seen from the figures, regression equations for the particular curves can be achieved for further calculations. However, to make the article more readable they are not presented here.

Calculation of the elongational viscosity of cellulose NMMO-MH solutions

The experimental data presented above allows us to calculate the elongational viscosity for the different conditions existing during the spinning of cellulose Lyocell fibres. The relation between elongational viscosity and the temperature at different elongation rates for two values of cellulose concentrations are shown in Figure 6 (a and b).

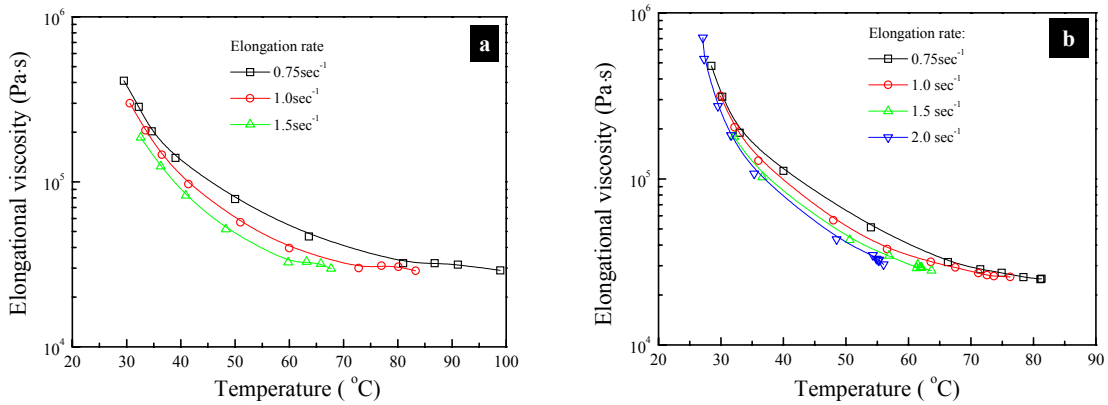

Figure 6. Elongational viscosity of cellulose NMM-MH solutions as a function of temperature; cellulose concentration: a) 10 wt.%, b) 8 wt,%

Simulation of parameters of the filament formed

With all the presented data obtained, the differential equations demonstrated in chapter 1 can now be solved numerically, and the calculation results can be compared with data obtained by measurements.

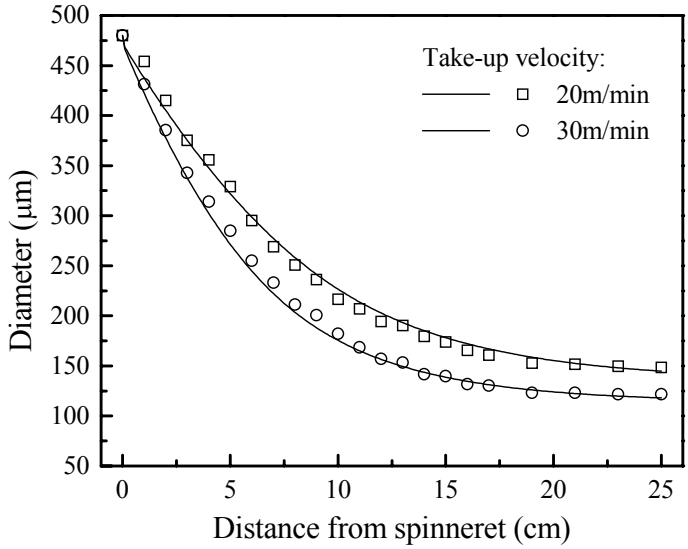

Figure 7. Comparison of calculated (lines) and experimental (symbols) data of the Lyocell fibres diameter development in the air gap as a function of the distance from the spinneret for two take-up velocities: 20 m/min, and 30 m/min; cellulose concentration: 10 wt.%, mass throughput: 0.386 g/min, spinning temperature: 118^{0}C, cooling temperature: 18^{0}C, spinneret diameter: 480 μm

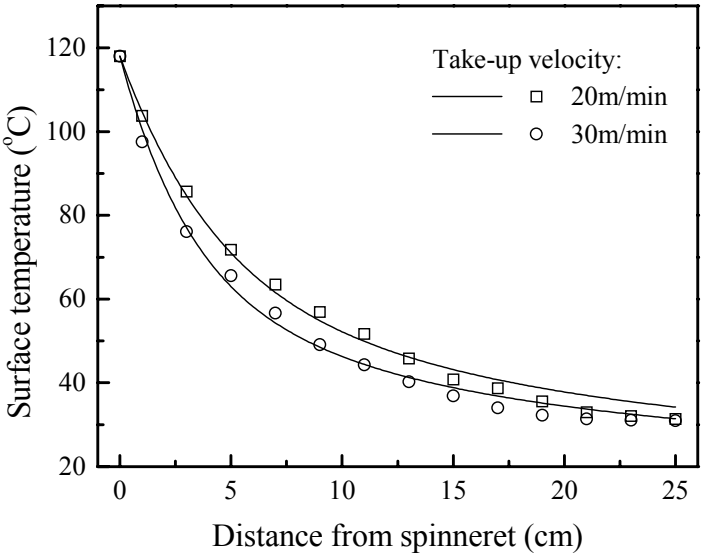

Figure 8. Comparison of calculated (lines) and experimental (symbols) data of the Lyocell fibres surface temperature in the air gap as a function of the distance from the spinneret for two take-up velocities: 20 m/min, and 30 m/min; cellulose concentration: 10 wt.%, mass throughput: 0.386 g/min, spinning temperature: 118^{0}C, cooling temperature: 18^{0}C, spinneret diameter: 480 μm

Figures 7 and 8 show two examples of such a simulation. As can be seen, data of the diameter of the filament formed and its surface temperature can be calculated for different spinning conditions (in Figures 7 and 8 these are cellulose concentration, mass throughput, spinning temperature, cooling air temperature, spinneret diameter, and two take-up velocities) beginning at distance = zero from the spinneret along the spinning path up to the coagulation bath. As can be seen, the experimental data fits the calculated data very well considering the practical application.

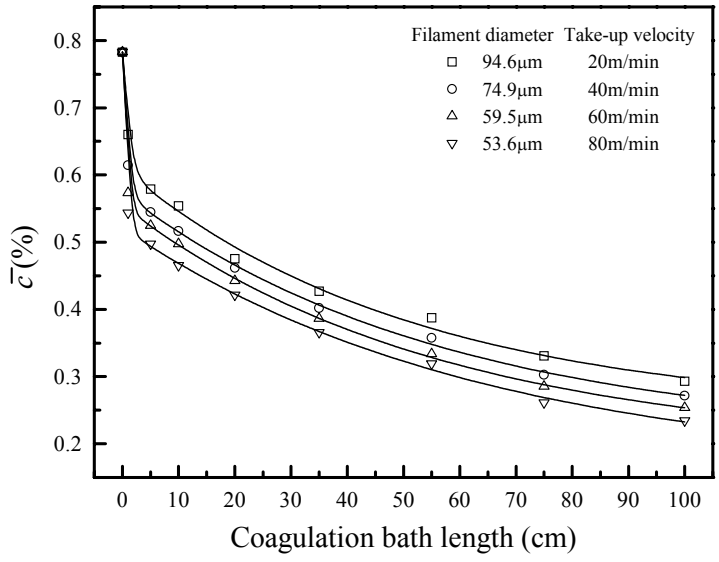

Figure 9. Average concentration of NMMO in Lyocell filaments along the coagulation bath; coagulation bath: water, temperature of the coagulation bath: 20^{0}C

On the other hand, the mechanism of the wet spinning part is much simpler; it is a diffusion-controlled process. Experiments on the spinning process were carried out to determine the diffusion rate of the solvent (NMMO monohydrate) and non-solvent (water or NMMO diluted aqueous solutions) during the coagulation process. The NMMO concentration in the moving filament was calculated using the off-line method. The development of NMMO concentration in the freshly formed filaments was determined

with the increase in the time that the filament is immersed in the coagulation bath, and by which the diffusion rate of NMMO and water during coagulation (and the coagulation behaviour of the Lyocell fibres in the coagulation bath) could be studied. Furthermore, the influence of NMMO concentration in the coagulation bath and the diameter of the filament during the coagulation process could be discussed. Figure 9 shows some experimental results of the dependence of average concentration of NMMO in Lyocell fibres on the length of the coagulation bath (the displacement distance of the filament in the coagulation bath).

Conclusions

With all the data presented, the average diffusion coefficient of NNMO in the Lyocell fibre spinning process can be calculated and combined with Fick's second law; also, the time during which the NMMO content attained its equilibrium state in the coagulation bath can be predicted. This information helps optimisation of the spinning conditions for a given fibre spinning problem.

Acknowledgement

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References

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