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OBSERVATIONS ON LYOCELL FIBRE FORMATION

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Abstract

A computer simulation of the lyocell air-gap spinning process has been developed. By combining this with empirical observations and results of fundamental studies, major advances in understanding have been achieved. These have been applied to deliver significant efficiency improvements in commercial Tencel production.
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Abstract

In order to develop a commercially viable lyocell production process, it is essential to maximise spinning stability. This requires a good understanding of the fundamental factors that influence fibre formation. In this paper, the results of studies of those factors will be reviewed. In particular, development of a computer simulation of the interactions within the lyocell air-gap is described. Model predictions are compared with practical measurements. Key findings that have been implemented to improve commercial lyocell production are highlighted.

INTRODUCTION

The basic principles for ‘air-gap’ spinning of lyocell fibres are well-known. Laboratory scale production (up to a few hundred filaments) is, from a practical standpoint, relatively straightforward. However, the process equipment required is expensive so maximising productivity of the fibre formation step is essential for viable commercial manufacture of Lyocell. For staple fiber, there are typically several million individual filaments per spinning line.

The major industrial players have intensively studied lyocell fibre formation and proposed various design solutions. In this paper, we present a history of spinning productivity development within Tencel. In particular, we will highlight the role played by computer simulations of fibre formation within the air-gap.

Overview

There are obvious trade-offs to consider when optimising a fibre production process, such as:

- Polymer content & flow properties of spinning solution
- Production speed
- ‘Unit productivity’ (e.g. jet size, filament packing)
- Design simplification (e.g. minimise costs, maintenance)
- Process ‘robustness’ (ease of operation, resistance to problems/fluctuations)

To enable an optimum solution to be arrived at, a key technical question to answer is:

‘Why do filaments break?’

The question is simple, for lyocell the answer is very complex. There are complex interactions between the various parameters during fibre formation. A good fundamental understanding of these is a pre-requisite for successful commercial implementation. In commercial lyocell operation, the air-gap process is particularly intolerant of individual filament breakages. There are many factors that influence filament breakage, some practical/operational, some technical. This paper will focus on developing understanding of the technical factors, examples of which are shown in figure 1. For example, discovery of the significance of a cooling cross-draught was critical to successful scale-up. Understanding the mechanism to enable design optimisation has been a high priority.

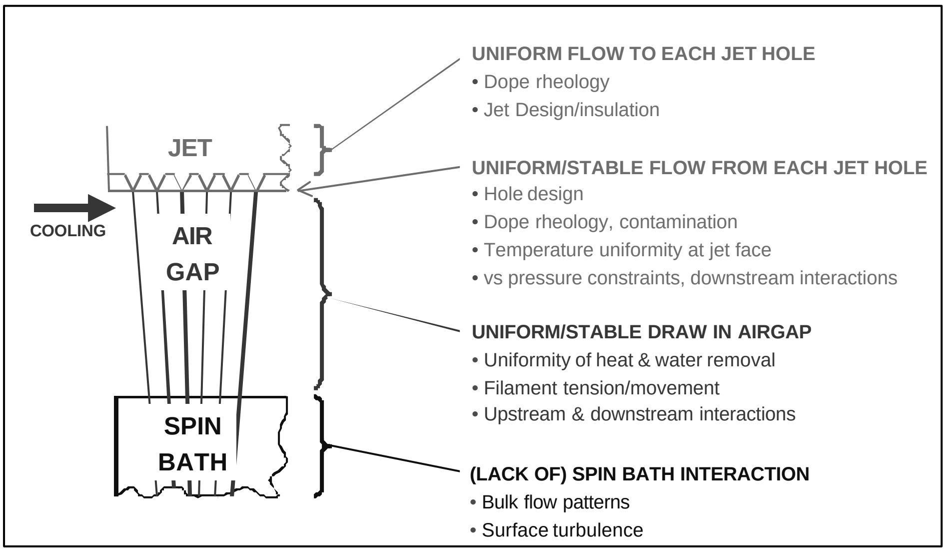

Figure 1. Examples of parameters that influence spinning stability

Tencel has developed a multi-faceted strategy to understand the fundamentals of lyocell fibre formation. Key elements are:

- Empirical pilot scale practical/iterative studies
- In-depth investigations of model systems (often single filament)
- Development of computer simulations

At the core of the programme is the development of a computer model of the air-gap spinning system.

The Air Gap Model

There are three key stages in the development of the air-gap model.

STAGE 1 is to decide what we need the model to predict. Ideally we would like the model to tell us when filaments will not spin. Rather than trying to construct a theoretical model of spinnability, we have used empirical experiments to define the spinnability of a filament in terms of its environmental variables such as the air temperature and line speed.

STAGE 2 is to apply the data on the failure criteria to develop a model of an individual filament that will interact with its environment in an appropriate manner. As will be made clear shortly, we need a model that will predict the exchange of heat, moisture and momentum with its environment. The model must also allow obvious process parameters such as line speed, spinneret hole size, polymer concentration and temperature to be included. As far as possible, model predictions are validated against experiment.

STAGE 3 is to incorporate the single filament model into a model that takes account of larger scale features such as air injection systems, the shape and temperature of the jet bodies etc. This is an area that can be treated by conventional computational fluid dynamics packages (CFD). Again, simulation performance is tested, as far as possible, against practical observation.

The key challenge from a modelling perspective is the combination of the small-scale details of the individual filament model and the larger scale CFD model. Constructing a CFD model at the smallest scale would require much computational effort.

When validated, the aim was to couple the air gap model with simulations of other key process sections (jet design, spin bath liquor flow) and apply predictions from this exercise to optimising overall spinning productivity.

Each of the stages is now considered in more detail

STAGE 1 – What are key spinning failure criteria?

Practical methods of characterising the stability and failure modes of lyocell filaments have been devised. For a single filament we can define a set of independent parameters that characterise the spinning process. We can use these parameters to characterise a surface in many dimensions that divides the "spinning space" into spinning and non-spinning regions. We refer to this as a stability surface. We have found that the filament spinnability is quite insensitive to some of the parameters but highly sensitive to others. We can illustrate the results by fixing all the parameters except two. This leads to the stability surface conveniently being represented by a curve. An example is shown if figure 2.

In this example we spin a single filament through an air gap into which we feed air that has been conditioned. For a given air temperature we increase the absolute humidity until the filament fails. The absolute humidity falls as the air temperature is raised. We have mapped out many such curves for different parameters such as line speeds and jet hole diameter.

A key conclusion from these studies was that if the air gap model can predict the temperature and humidity of the air surrounding the filaments then we could make a decision on the spinnability of the filaments.

STAGE 2 – The single filament model

Given that we recognised the importance of humidity we felt it important to develop a filament model that could adequately describe the transfer of moisture from the nascent filaments to the air. The model was therefore developed from a 2-dimensional model of dry spinning. (Many filament models are 1-dimensional, i.e. a uniform temperature gradient is assumed to exist along the filament. This is not appropriate for moisture transport on time scales of process. The 1-D approximation is good for temperature but not water)

The model solves the transport equations for moisture and temperature in the radial direction (diffusive transport in the axial direction is considered negligible).

$$V\frac{\partial C}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD(C,T)\frac{\partial C}{\partial r}\right)$$

The dope is treated as a Newtonian fluid, with temperature and concentration dependent on viscosity. (We estimated that the thermal effects would dominate any non-linear rheological effects.)

$$r\,C_p V\frac{\partial T}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk(C,T)\frac{\partial T}{\partial r}\right)$$

$$b_{av} = \frac{2p\int_0^R b(C,T)rdr}{p\,R^2}$$

The diffusion coefficients and vapour pressure of the water above dope were determined experimentally. The heat and mass transfer coefficients were those developed by the workers in the dry spinning field. The temperature dependence of the viscosity was determined from in-house rheometry. The model works by estimating the initial tension in the filament and propagating along the filament to determine the final (take up) velocity. This is an iterative process and finishes when the boundary conditions are matched. At each step in the filament direction the transport equations are solved using a finite difference scheme. Output is predicted profiles of, for example, temperature and moisture content through the filament at various conditions.

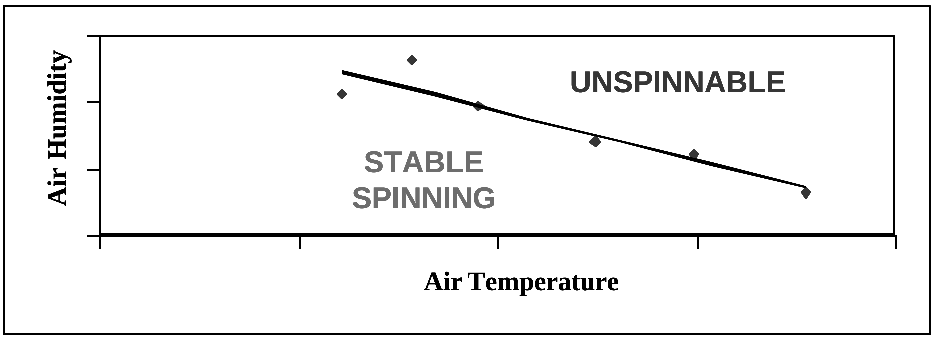

Figure 2. Example of 'response surface' generated via single filament measurements

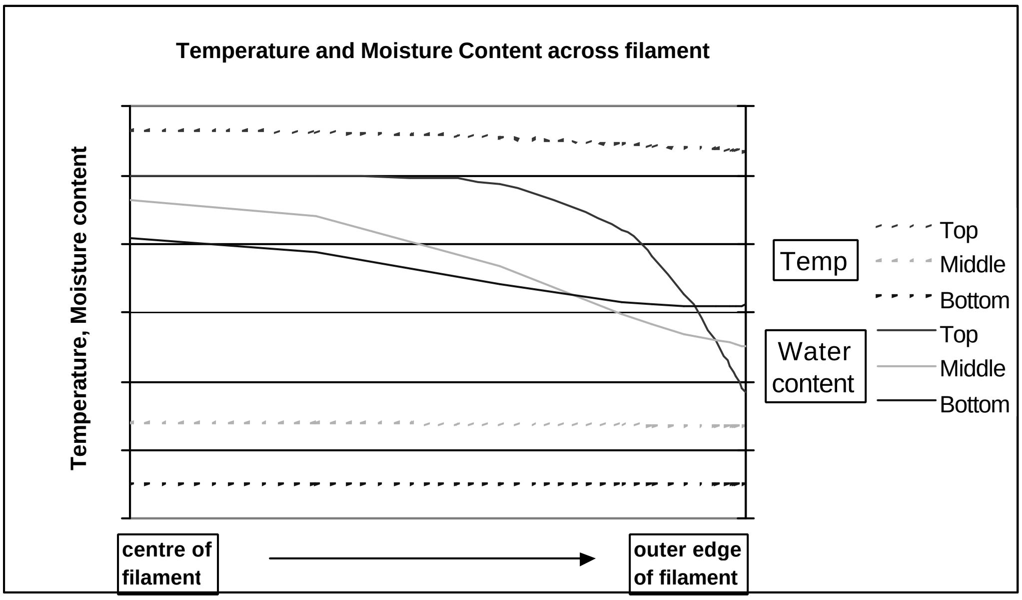

Figure 3. Example of output from single filament model

In figure 3, the x-axis runs from the centre to the edge of the filament. The solid lines show the water concentration in the filament and the dashed lines the temperature. The three curves correspond to different distances from the jet face. The temperature profiles are flat indicating that a 1-D model would have been adequate. The sharper gradients that exist in the water curves demonstrate the need for a 2-D model.

So far as possible, model predictions are tested against practical measurement. We cannot measure moisture/temperature variation within filament directly, so measure the radius of the filament using a high magnification telescope and plotted the results against the model predictions, figure 4.

The agreement is good. We have further tested against IR camera measurements of filament temperature and the agreement is again satisfactory.

STAGE 3 – The CFD model

Several "representative" filaments from stage 2 have been coded into a computational fluid dynamics (CFD) programme. The filaments interact with the air velocity, temperature and humidity of the cell in which they are placed.

The amount of heat, moisture and momentum (fibre drag) exchanged with the filament is added as a source term to the equations that the CFD package solves. The filament calculation sits inside the iterative loop of the CFD program and the combined program iterates until a converged solution is reached. The contribution of each filament is scaled to represent the filament density in the jet. The number of representative filaments is varied to

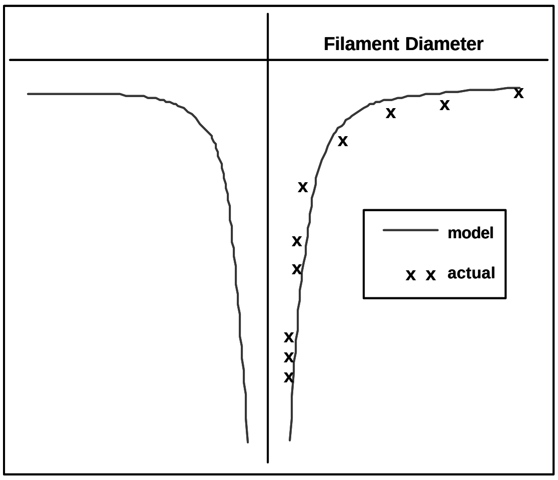

Figure 4. Example of model validation

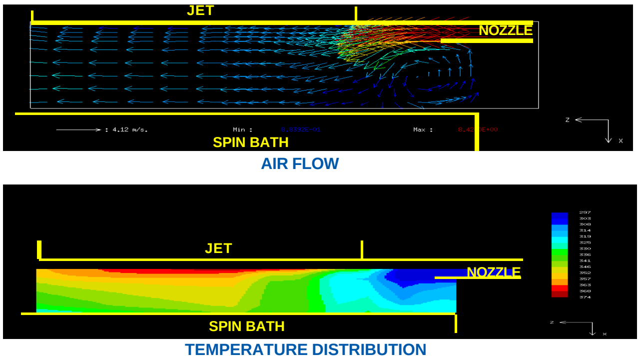

Figure 6. Air flow and temperature predictions, cross-section

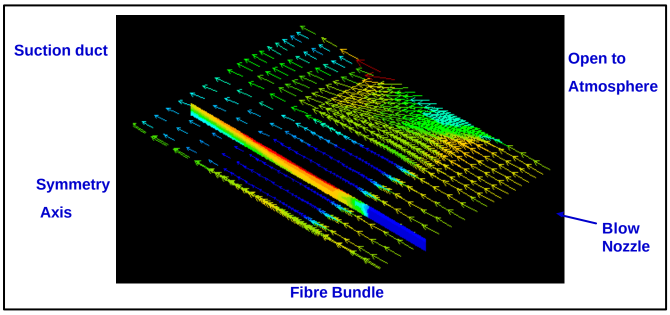

Figure 5. CFD representation of air-gap air flow & temperature distribution

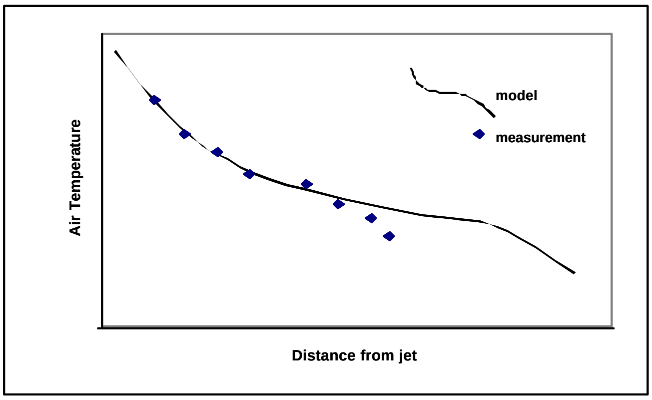

Figure 7. Validation of CFD model of air-gap-air-temperature

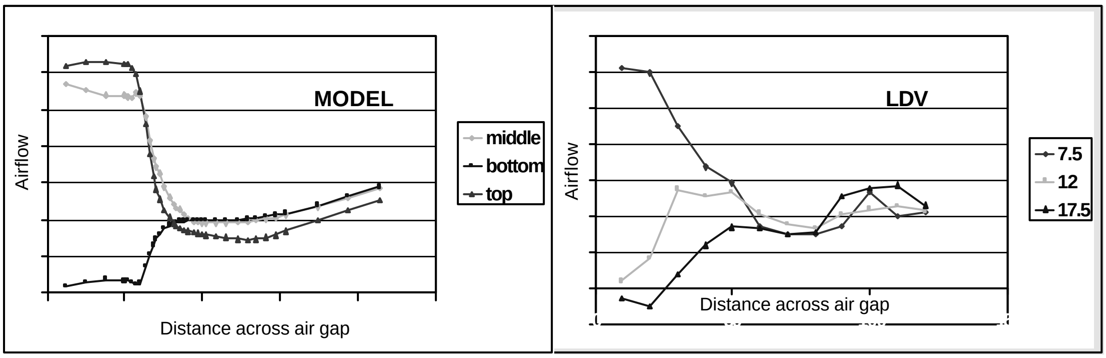

Figure 8. Validation of CFD model. Comparison of predicted and measured air-flow

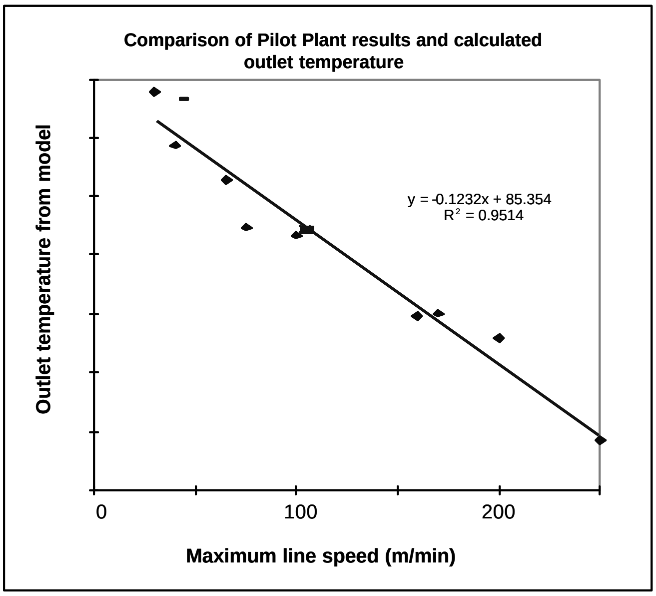

Figure 9. Validation of CFD model. Prediction of spinning failure

ensure that the final solution is independent of the number of representative filaments.

The CFD model of the air gap is three-dimensional. Model output for a typical rectangular jet configuration is shown in figure 5. This represents an air gap with a horizontal blow nozzle located close to the jet face and only partially extending down the air gap depth, a suction nozzle that extends over the entire air gap depth and two jets in the air gap (symmetry implies we only need model one). The outer edge of the assembly is open to atmosphere.

The results are showing the velocity vectors in a horizontal plane and the temperature profile in a vertical plane. Note, for this configuration:

- the way that the air slows on moving through the bundle –due to the fibre drag
- the air coming in from the outside,
- development of the thermal profile within the bundle.

Looking at CFD predictions in cross-section, figure 6. Figure 6 shows the velocity contours in the area of the fibres. Note the way the velocity initially appears faster closer to the jet face but as we move to the suction side of the bundle the profile appears to invert.

The second shows the thermal profile in the bundle. The contour arises because of the combination of heat loss by the filaments, the initial downward flow of the air and the impact of the incoming atmospheric air impinging on the latter part of the jet.

As with the single filament model, so far as possible the CFD predictions have been tested by practical measurement. For example, an array of thermocouples was mounted on a carriage and traversed across a full-size jet assembly with the probe ~2cm away from the filaments. Actual thermal profiles are compared with model predictions. Plotting the expected thermal profile from jet to spin bath at one particular position against the experimental results, figure 7:

In addition to good overall agreement, the measurements confirmed CFD predictions, showing a temperature profile down the air gap, from jet to spin bath. The more detailed data also shows interesting looking “peaks”, located inside the fibre bundles. For this particular trial configuration, many filament failures occurred within these peak temperature zones.

We have further tested the model by using Laser Doppler Velocimetry (LDV) to measure the air velocity within the air gap. The results for air velocities across the air gap at various heights from the jet are shown, figure 8, for both model and experiment. It is worth noting that the inversion of the velocity profile occurs experimentally as well as theoretically.

The validation tests built confidence that the model that could predict air velocities, temperatures and humidity within the air gap with reasonable precision. We can now ask how well the model relates to spinning performance. Various full-scale jet configurations have been tested by evaluating the maximum line speed (before filament failure). The model was used to predict temperature/spinning failure at a given line speed for each configuration. The correlation is good.

Interaction with other process models

The work outlined above has resulted in a robust 'stand-alone' computer model of interactions occurring within the air-gap during formation of lyocell fibre. The value of this model has been further enhanced by coupling with simulations of process interactions directly before and directly after the air-gap, i.e.:

- Dope flow stability & uniformity from spinneret holes
- Spin bath liquor flows, impact on filament deflection in air gap

However, this work is beyond the scope of this paper.

Benefits derived from the Air Gap Model

There have been many benefits to Tencel from the computer simulation programme. At a management level, it has imposed a discipline and focus on the practical studies and prompted important discussions to develop key hypotheses.

In terms of scientific learning, the programme highlighted the significance of air gap humidity and provided an explanation of the flow patterns of the cooling air. The hypothesis regarding the importance of water removal for filament stabilisation (as opposed to a simple thermoplastic cooling mechanism) was first developed from the modelling results.

At a more detailed level, the excellent agreement with practical measurements gave confidence that model could be used as a 'design tool' in optimising the spinning cell, removing need for many costly and time-consuming large-scale practical iterations. 'Weak points' were identified via the model, for example appearance of temperature/humidity peaks and many concepts to remove these weak points could be assessed very easily on the computer.

Conclusions

- Tencel have developed computer simulations which accurately predict temperature, humidity and velocity profiles in the air-gap during lyocell fibre formation.
- The model is based on a combination of single filament and CFD approaches, validated by practical measurements.
- The air-gap model has been central to improving our understanding of the key fundamental parameters which must be controlled to enable viable commercial production of lyocell.
- In particular, maximising efficiency of water removal and uniformity of conditions in air gap
- Many questions concerning formation of lyocell fibres remain unresolved, but current state-of-the-art understanding has allowed successful commercialisation ~120,000 tonnes of lyocell capacity in Europe and USA.
- The robust, high productivity technology gives an excellent platform for the introduction of new product variants.