MODELLING OF MOLECULAR ORIENTATION AND CRYSTALLIZATION IN THE MANUFACTURE OF SEMI–CRYSTALLINE COMPOUND FIBRES

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Conference on Thermal and Environmental Issues in Energy Systems

16–19 May 2010, Sorrento, Italy

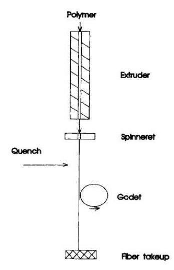
Outline

Introduction

- Bi–component compound fibres are manufactured by MELT SPINNING processes.
- Applications
  1. Telecommunications: Data transmission.
  2. Chemical industry: Filtration and separation processes.
  3. Biomedical industry.
  4. Textile industry.
- Necessary: modelling of the drawing process for both hollow and solid semi–crystalline compound fibres.
- Previous studies are based on one–dimensional models of amorphous, slender fibres at low Re.
- NO INFORMATION ABOUT RADIAL VARIATIONS.
- Use of a hybrid model for fibre spinning.

Melt spinning

Involves the extrusion and drawing of a polymer cylinder. Four zones.



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2. Flow Rearrangement Region.
3. **Melt Drawing Zone.**
4. **Solidification region.**

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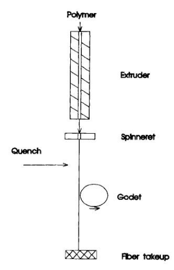

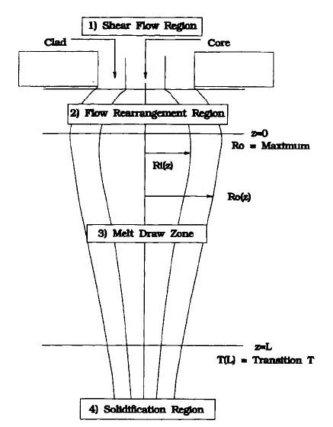

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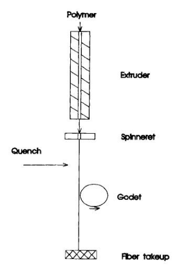

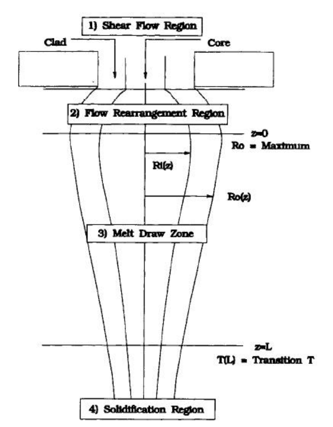

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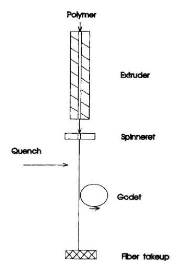

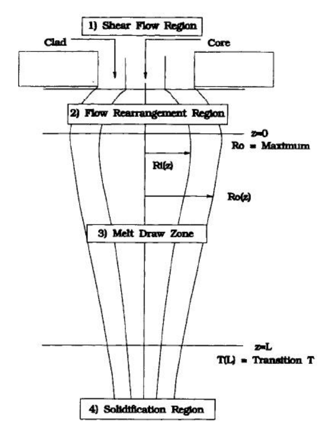

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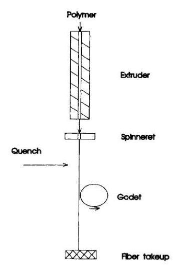

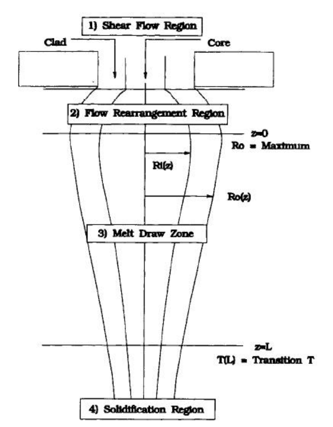

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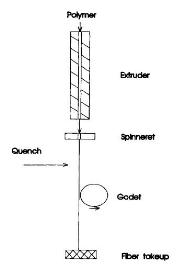

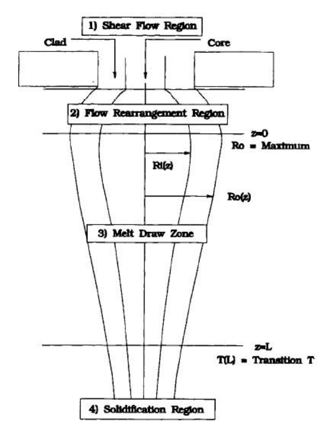

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Mathematical formulation (I)

- **Mass conservation equation**

$$\nabla \cdot \mathbf{v}_i = 0 \qquad i = 1, 2,$$

where $\mathbf{v} = u(r,x)\,\mathbf{e_x} + v(r,x)\,\mathbf{e_r}$

- **Linear Momentum conservation equation**

$$\rho_i \left(\frac{\partial \mathbf{v}_i}{\partial t} + \mathbf{v}_i \cdot \nabla \mathbf{v}_i \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau}_i + \rho_i \cdot \mathbf{f}^m \qquad i = 1, 2,$$

where $\mathbf{f}^m = g\,\mathbf{e_x}$

- **Energy conservation equation**

$$\rho_i\, C_i \left(\frac{\partial T_i}{\partial t} + \mathbf{v}_i \cdot \nabla T_i \right) = -k_i \Delta T_i \qquad i = 1, 2,$$

- **Constitutive equations**
  - Rheology

$$\boldsymbol{\tau} = \mu_{eff} \left(\nabla \mathbf{v} + \nabla \mathbf{v}^T \right) + \boldsymbol{\tau}_p,$$

where

$$\boldsymbol{\tau}_p = 3c\, k_B\, T \left[-\frac{\lambda}{\phi} F(\mathbf{S}) + 2\lambda \left(\nabla \mathbf{v}^T : \mathbf{S} \right) \left(\mathbf{S} + \mathbf{I}/3 \right) \right]$$

Mathematical formulation (II)

- **Molecular orientation tensor equation: Doi–Edwards theory**

$$\mathbf{S}_{(1)} = F(\mathbf{S}) + G(\nabla\mathbf{v}, \mathbf{S}),$$

$$F(\mathbf{S}) = -\frac{\phi}{\lambda}\left\{(1 - N/3)\,\mathbf{S} - N\,(\mathbf{S}\cdot\mathbf{S}) + N\,(\mathbf{S} : \mathbf{S})\,(\mathbf{S} + \mathbf{I}/3)\right\}$$

$$G(\nabla\mathbf{v}, \mathbf{S}) = \frac{1}{3}\left(\nabla\mathbf{v} + \nabla\mathbf{v}^T\right) - 2\left(\nabla\mathbf{v}^T : \mathbf{S}\right)(\mathbf{S} + \mathbf{I}/3)\,.$$

where subscript (1) denote UCTD operator

$$\Lambda_{(1)} = \frac{\partial\Lambda}{\partial t} + \mathbf{v}\cdot\nabla\Lambda - \left(\nabla\mathbf{v}^T\cdot\Lambda + \Lambda\cdot\nabla\mathbf{v}\right)$$

- **Molecular orientation scalar order parameter**

$$\mathcal{S} \equiv \sqrt{\frac{3}{2}\,(\mathbf{S} : \mathbf{S})} \qquad \mathbf{S} = \mathrm{diag}\,(S_{rr},\, S_{\theta\theta},\, S_{xx})\,,$$

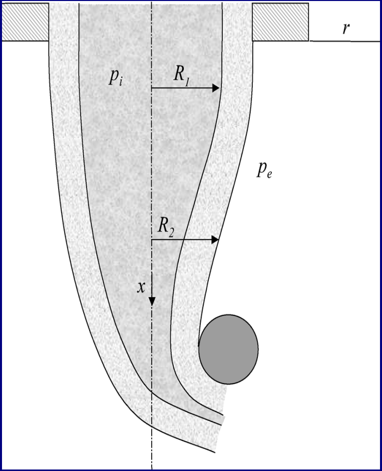
- **Crystallization: Avrami–Kolmogorov's theory & Ziabicki's model**

$$\frac{\partial\mathcal{X}_i}{\partial t} + \mathbf{v}\cdot\nabla\mathcal{X}_i = k_{Ai}(\mathcal{S}_i)\,(\mathcal{X}_{\infty,i} - \mathcal{X}_i) \qquad i = 1, 2,$$

where

$$k_{Ai}(\mathcal{S}_i) = k_{Ai}(0)\exp\left(a_{2i}\mathcal{S}_i^2\right), \qquad i = 1, 2.$$

Mathematical formulation (III)



Kinematic, dynamic and thermal boundary conditions are required:

- Initial conditions $(t = 0)$
- Symmetry conditions $(r = 0)$
- Die exit conditions $(x = 0)$
- Take–up point conditions $(x = L)$
- Conditions on free surfaces of compound fibre $(r = R_1(x)$ and $r = R_2(x))$

Non–dimensionalize

- Non–dimensional variables

$$\hat{t} = \frac{t}{(L/u_0)} \qquad \hat{r} = \frac{r}{R_0} \qquad \hat{x} = \frac{x}{L} \quad \Rightarrow \quad \epsilon = \frac{R_0}{L}$$

$$\hat{u} = \frac{u}{u_0} \qquad \hat{v} = \frac{v}{(u_0\,\epsilon)} \qquad \hat{p} = \frac{p}{(\mu_0 u_0/L)} \qquad \hat{T} = \frac{T}{T_0}$$

$$\hat{\rho} = \frac{\rho}{\rho_0} \qquad \hat{C} = \frac{C}{C_0} \qquad \hat{\mu} = \frac{\mu}{\mu_0} \qquad \hat{k} = \frac{k}{k_0}$$

- Non–dimensional numbers

$$Re = \frac{\rho_0 u_0 R_0}{\mu_0}, \quad Fr = \frac{u_0^2}{g R_0}, \quad Ca = \frac{\mu_0 u_0}{\sigma_2},$$

$$Pr = \frac{\mu_0 C_0}{k_0}, \quad Pe = Re\,Pr, \quad Bi = \frac{h R_0}{k_0}$$

Asymptotic analysis: 1D model

- **Asymptotic method using the fibre slenderness, $\epsilon << 1$, as perturbation parameter**

$$\Psi_i = \Psi_{i,0} + \epsilon^2 \Psi_{i,2} + O(\epsilon^4) \, ,$$

for the variables $\hat{R}_i$, $\hat{u}_i$, $\hat{v}_i$, $\hat{p}_i$ and $\hat{T}_i$ where $i = 1, 2$.

- **Flow regime considered for steady ($\frac{\partial}{\partial \hat{t}} = 0$) jets**

$$Re = \epsilon \, \bar{R}, \qquad Fr = \frac{\bar{F}}{\epsilon}, \qquad Ca = \frac{\bar{C}}{\epsilon},$$

$$Pe = \epsilon \, \bar{P}, \qquad Bi = \epsilon^2 \, \bar{B}$$

where $\bar{\Upsilon} = O(1)$.

One–dimensional equations of the $1 + 1/2$D model

- **Asymptotic one–dimensional mass conservation equation**

$$\mathcal{A}_1 \mathcal{U} = Q_1, \qquad \mathcal{A}_2 \mathcal{U} = Q_2$$

where

$$\mathcal{A}_1 = \frac{\mathcal{R}_1^2}{2}, \qquad \mathcal{A}_2 = \frac{\mathcal{R}_2^2 - \mathcal{R}_1^2}{2},$$

- **Asymptotic one–dimensional linear momentum equation**

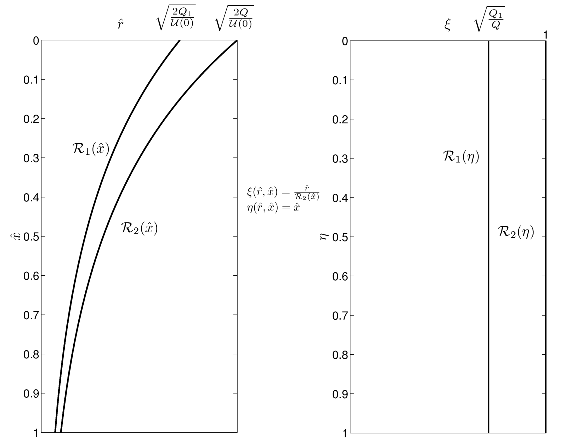
$$\begin{aligned}\bar{R}(\hat{\rho}_1 \mathcal{A}_1 + \hat{\rho}_2 \mathcal{A}_2)\mathcal{U}\frac{d\mathcal{U}}{d\hat{x}} &= \frac{d}{d\hat{x}}\left(3\left(< \hat{\mu}_{eff,1} > \mathcal{A}_1 + < \hat{\mu}_{eff,2} > \mathcal{A}_2\right)\frac{d\mathcal{U}}{d\hat{x}}\right) \\ &+ \frac{1}{2\bar{C}}\left(\frac{d\mathcal{R}_2}{d\hat{x}} + \frac{\sigma_1}{\sigma_2}\frac{d\mathcal{R}_1}{d\hat{x}}\right) \\ &+ (\hat{\rho}_1 \mathcal{A}_1 + \hat{\rho}_2 \mathcal{A}_2)\frac{\bar{R}}{\bar{F}}\end{aligned}$$

- **Radial velocity field**

$$\mathcal{V}(\hat{r}, \hat{x}) = -\frac{\hat{r}}{2}\frac{d\mathcal{U}}{d\hat{x}},$$

Mapping: 2D model

$(\hat{r},\hat{x}) \mapsto (\xi,\eta)$ maps $\Omega_{\hat{r}\hat{x}} = \{[0,\,\mathcal{R}_2(\hat{x})] \times [0,\,1]\}$ into a rectangular domain $\Omega_{\xi\eta} = \{[0,\,1] \times [0,\,1]\}$



Two–dimensional equations of the $1 + 1/2$D model

- **Two–dimensional energy equation**

$$\frac{\partial \hat{T}_i}{\partial \eta} = \frac{1}{2\,Q}\,\frac{1}{\bar{P}_i}\,\frac{1}{\xi}\,\frac{\partial}{\partial \xi}\left(\xi \frac{\partial \hat{T}_i}{\partial \xi}\right) \qquad i = 1, 2,$$

- **Two-dimensional degree of crystallinity equation**

$$\hat{U}\,\frac{\partial \mathcal{X}_i}{\partial \eta} = k_{Ai}(0)\exp\left(a_{2i}\mathcal{S}_i^2\right)\,\left(\mathcal{X}_{\infty,i} - \mathcal{X}_i\right), \qquad i = 1, 2,$$

- **Effective dynamic viscosity**

$$\hat{\mu}_{eff,i} = \hat{G}_i\,\exp\left(\hat{E}_i\left(1 - \hat{T}_i\right) + \beta_i\left(\frac{\mathcal{X}_i}{\mathcal{X}_{\infty,i}}\right)^{n_i}\right) \qquad i = 1, 2.$$

Molecular orientation tensor components equations

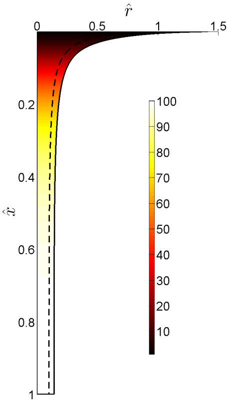
$$\mathcal{U}\,\frac{\partial S_{i\,rr}}{\partial \eta} = \left(S_{i\,rr} + \frac{1}{3}\right)\left(S_{i\,rr} + S_{i\,\theta\theta} + S_{i\,xx} - 1\right)\frac{d\mathcal{U}}{d\eta}$$
$$-\frac{\phi}{\hat{\lambda}}\left\{S_{i\,rr} - N\left[\left(S_{i\,rr} + \frac{1}{3}\right)\left(S_{i\,rr} - \Pi_{i\,s}\right)\right]\right\}, \qquad i = 1, 2,$$

$$\mathcal{U}\,\frac{\partial S_{i\,\theta\theta}}{\partial \eta} = \left(S_{i\,\theta\theta} + \frac{1}{3}\right)\left(S_{i\,rr} + S_{i\,\theta\theta} + S_{i\,xx} - 1\right)\frac{d\mathcal{U}}{d\eta}$$
$$-\frac{\phi}{\hat{\lambda}}\left\{S_{i\,\theta\theta} - N\left[\left(S_{i\,\theta\theta} + \frac{1}{3}\right)\left(S_{i\,\theta\theta} - \Pi_{i\,s}\right)\right]\right\}, \qquad i = 1, 2,$$

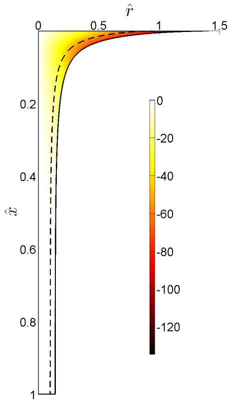
$$\mathcal{U}\,\frac{\partial S_{i\,xx}}{\partial \eta} = \left(S_{i\,xx} + \frac{1}{3}\right)\left(S_{i\,rr} + S_{i\,\theta\theta} + S_{i\,xx} + 2\right)\frac{d\mathcal{U}}{d\eta}$$
$$-\frac{\phi}{\hat{\lambda}}\left\{S_{i\,xx} - N\left[\left(S_{i\,xx} + \frac{1}{3}\right)\left(S_{i\,xx} - \Pi_{i\,s}\right)\right]\right\}, \qquad i = 1, 2,$$

$$\Pi_{i\,s} = S_{i\,rr}^2 + S_{i\,\theta\theta}^2 + S_{i\,xx}^2.$$

Two–dimensional velocity field ($\bar{B} = 5$)

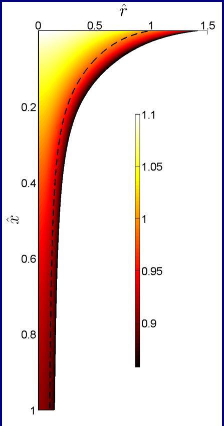


$\mathcal{U}(\hat{r}, \hat{z})$

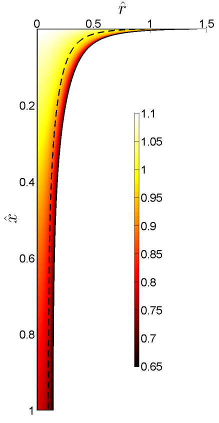


$\mathcal{V}(\hat{r}, \hat{z})$

Influence of Biot number on cooling process

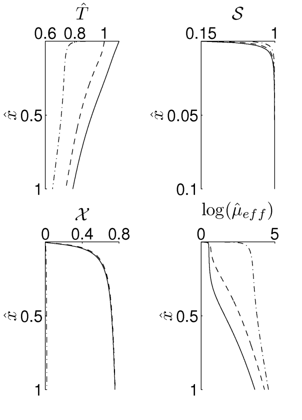


$\bar{B} = 1$

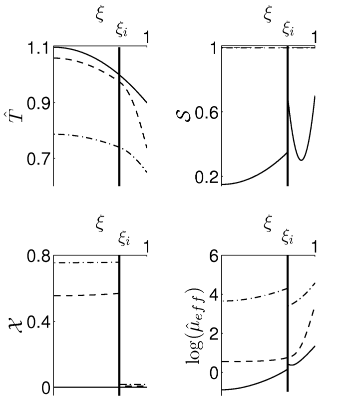


$\bar{B} = 5$

Analysis of the 2D model

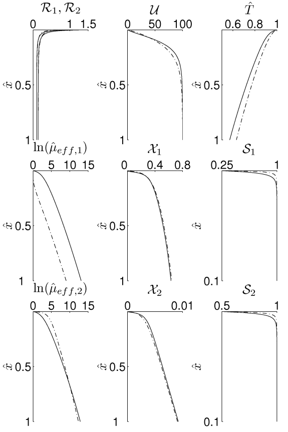


$\hat{r} = 0$ (–), $\hat{r} = \mathcal{R}_1^-$ (– –) and $\hat{r} = \mathcal{R}_2$ (– · –)



$\eta = 0$ (–), $\eta = 0{,}1$ (– –) and $\eta = 1$ (– · –)

1D model vs 2D model



1D (–) and 2D (– · –)

Conclusions

Contributions of the present work:

1. Development of a $1 + 1/2$D model for both amorphous and semicrystalline fibres with modified Newtonian rheology.
2. Validation of applicability range of the 1D model with the $1 + 1/2$D one for slender fibres.
3. Determination of the two–dimensional fields of temperature, molecular orientation tensor and degree of crystallinity for solid compound fibres.
4. Find substantial temperature non–uniformities (affect the degree of crystallization and have great effects on the properties of compound fibres) in the radial direction exist even at small Biot numbers.

About the authors...

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