TWO–DIMENSIONAL ANALYSIS OF THE CRYSTALLIZATION OF HOLLOW COMPOUND PLASTIC FIBERS

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Index

1. Introduction

2. Formulation

3. Results and discussion
   - Numerical results of the two-dimensional model
   - Comparisons with results of one-dimensional model

4. Conclusions
Index

1. Introduction

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4. Conclusions
1 Introduction

2 Formulation

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   - Comparisons with results of one–dimensional model

4 Conclusions
Index

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2 Formulation

3 Results and discussion
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   - Comparisons with results of one–dimensional model

4 Conclusions
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- Bi–component hollow compound fibers may be manufactured by MELT SPINNING processes.

Applications

- Chemical industry: Filtration and separation processes.
- Textile industry.
- Optics: Data transmission.
- Biomedical industry.


Previous studies are based on one–dimensional models of amorphous, slender fibers at very low \( Re \) and \( Bi \) numbers.

NO INFORMATION ABOUT TEMPERATURE NON–UNIFORMITIES IN THE RADIAL DIRECTION.

Use of a two–dimensional model for fiber spinning.
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Use of a two–dimensional model for fiber spinning.
Melt spinning

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

1. Shear Flow Region.
2. Flow Rearrangement Region.
3. Melt Drawing Zone.
4. Solidification region.
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About the authors...
Mass conservation equation

\[ \nabla \cdot \mathbf{v}_i = 0 \quad i = 1, 2, \]

where \( \mathbf{v} = u(r, x) \mathbf{e}_x + v(r, x) \mathbf{e}_r \)

Linear Momentum conservation equation

\[ \rho_i \left( \frac{\partial \mathbf{v}_i}{\partial t} + \mathbf{v}_i \cdot \nabla \mathbf{v}_i \right) = -\nabla p_i + \nabla \cdot \tau_i + \rho_i \cdot \mathbf{f}^m \quad i = 1, 2, \]

where \( \mathbf{f}^m = g \mathbf{e}_x \)

Energy conservation equation

\[ \rho_i C_i \left( \frac{\partial T_i}{\partial t} + \mathbf{v}_i \cdot \nabla T_i \right) = -K_i \Delta T_i \quad i = 1, 2, \]

Constitutive equations

Rheology

\[ \tau = \mu \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) + \tau_p, \]

where

\[ \tau_p = 3ck_BT \left[ -\frac{\lambda}{\phi} F(S) + 2\lambda (\nabla \mathbf{v}^T : S) (S + I/3) \right] \]
Governing equations

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Molecular orientation and crystallinity models

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

\[ \frac{\partial Y_i}{\partial t} + v_i \cdot \nabla Y_i = k_{A_i}(S_i) (Y_{\infty,i} - Y_i) \quad i = 1, 2, \]

where

\[ k_{A_i}(S_i) = k_{A_i}(0) \exp \left( a_2 S_i^2 \right), \quad i = 1, 2. \]

- **Molecular orientation scalar order parameter**

\[ S \equiv \sqrt{\frac{3}{2}} (S : S) \quad S = \frac{1}{3} \cdot \text{diag} \left( S_{rr}, - (S_{rr} + S_{xx}), S_{xx} \right), \]

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

\[ S_{(1)} = F(S) + G(\nabla v, S), \]

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

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

where subscript (1) denote UCTD operator

\[ \Lambda_{(1)} = \frac{\partial \Lambda}{\partial t} + v \cdot \nabla \Lambda - \left( \nabla v^T \cdot \Lambda + \Lambda \cdot \nabla v \right) \]
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Kinematic, dynamic and thermal boundary conditions are required:

- Initial conditions \((t = 0)\)
- Die exit conditions \((x = 0)\)
- Take-up point conditions \((x = L)\)
- Conditions on free surfaces of hollow compound fiber \((r = R_1(x), r = R(x)\) and \(r = R_2(x)\))
Boundary and initial conditions

Kinematic, dynamic and thermal boundary conditions are required:
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Non–dimensionalize

- **Non–dimensional variables**

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

\[
\hat{u} = \frac{u}{u_0} \quad \hat{v} = \frac{v}{(u_0 \epsilon)} \quad \hat{p} = \frac{p}{(\mu_0 u_0 / L)} \quad \hat{T} = \frac{T}{T_0}
\]

\[
\hat{\rho} = \frac{\rho}{\rho_0} \quad \hat{C} = \frac{C}{C_0} \quad \hat{\mu} = \frac{\mu}{\mu_0} \quad \hat{K} = \frac{K}{K_0}
\]

- **Non–dimensional numbers**

\[
Re = \frac{\rho_0 u_0 R_0}{\mu_0}, \quad Fr = \frac{u_0^2}{g R_0}, \quad Ca = \frac{\mu_0 u_0}{\sigma},
\]

\[
Pr = \frac{\mu_0 C_0}{K_0}, \quad Pe = Re Fr, \quad Bi = \frac{h R_0}{K_0}
\]
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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 fiber slenderness,** $\epsilon \ll 1$, **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 steady** $(\frac{\partial}{\partial t} = 0)$ jets and

  \[ Re = \epsilon \bar{R}, \quad Fr = \frac{\bar{F}}{\epsilon}, \quad Ca = \frac{\bar{C}}{\epsilon}, \]

  \[ Pe = \epsilon \bar{P}, \quad Bi = \epsilon^2 \bar{B} \]

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

One–dimensional equations of the 2D model

**Asymptotic one–dimensional mass conservation equation**

\[ A_1 B = V_1, \]
\[ A_2 B = V_2, \]
\[ \frac{d}{d\hat{x}} \left( \frac{R_0^2}{2} B \right) = C(\hat{x}) \]

where

\[ A_1 = \frac{R_0^2 - R_1^2}{2}, \quad A_2 = \frac{R_2^2 - R_0^2}{2}, \]

and

\[ C(\hat{x}) = \left( \frac{1}{2C} \right) \left( \frac{\sigma_1}{\sigma} \right) \frac{1}{R_1} + \frac{1}{R_0} + \left( \frac{\sigma_2}{\sigma} \right) \frac{1}{R_2} <\hat{\mu}_{e1,0}> \left( \frac{1}{R_0^2} - \frac{1}{R_1^2} \right) + <\hat{\mu}_{e2,0}> \left( \frac{1}{R_2^2} - \frac{1}{R_0^2} \right), \]
One–dimensional equations of the 2D model

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

\[
(\hat{\rho}_1 V_1 + \hat{\rho}_2 V_2) \overline{R} \frac{dB}{d\hat{x}} = (\hat{\rho}_1 A_1 + \hat{\rho}_2 A_2) \frac{\overline{R}}{F} \\
+ \frac{d}{d\hat{x}} \left( 3 (\hat{\mu}_{e,0} > A_1 + \hat{\mu}_{e,0} > A_2) \frac{dB}{d\hat{x}} \right) \\
+ 2 C (\hat{x}) \left( -\frac{<\hat{\mu}_{e,0}>}{R_1} \frac{dR_1}{d\hat{x}} + \frac{<\hat{\mu}_{e,0}>}{R_0} \frac{dR_0}{d\hat{x}} + \frac{<\hat{\mu}_{e,0}>}{R_2} \frac{dR_2}{d\hat{x}} \right) \\
- \left( A_1 \frac{dD_1}{d\hat{x}} + A_2 \frac{dD_2}{d\hat{x}} \right),
\]

where

\[
D_1 = -<\hat{\mu}_{e,0}> \frac{2 C (\hat{x})}{R_1^2} - \frac{1}{C'} \left( \frac{\sigma_1}{\sigma} \right) \frac{1}{R_1}, \\
D_2 = -<\hat{\mu}_{e,0}> \frac{2 C (\hat{x})}{R_2^2} + \frac{1}{C'} \left( \frac{\sigma_2}{\sigma} \right) \frac{1}{R_2}
\]

- **Incompressibility condition**

\[
\mathcal{V}(\hat{r}, \hat{x}) = \frac{C (\hat{x})}{\hat{r}} - \frac{\hat{r}}{2} \frac{dB}{d\hat{x}},
\]
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\[ + 2 \mathcal{C}(\hat{x}) \left( - \frac{\hat{\mu}_{e1,0}}{R_1} \frac{dR_1}{d\hat{x}} + \frac{\hat{\mu}_{e1,0}}{R_0} \frac{dR_0}{d\hat{x}} + \frac{\hat{\mu}_{e2,0}}{R_2} \frac{dR_2}{d\hat{x}} \right) \]

\[ - \left( A_1 \frac{dD_1}{d\hat{x}} + A_2 \frac{dD_2}{d\hat{x}} \right), \]

where

\[ D_1 = - \frac{\hat{\mu}_{e1,0}}{R_1} \frac{2\mathcal{C}(\hat{x})}{\mathcal{C}} \frac{1}{\sigma} \frac{1}{R_1}, \]

\[ D_2 = - \frac{\hat{\mu}_{e2,0}}{R_2} \frac{2\mathcal{C}(\hat{x})}{\mathcal{C}} \frac{1}{\sigma} \frac{1}{R_2}. \]

- **Incompressibility condition**

\[ \mathcal{V}(\hat{r}, \hat{x}) = \frac{\mathcal{C}(\hat{x})}{\hat{r}} - \frac{\hat{r}}{2} \frac{dB}{d\hat{x}}, \]
Two–dimensional equations of the 2D model

- **Two–dimensional energy equation**

\[ B \frac{\partial \hat{T}_1}{\partial \hat{x}} + \left( \frac{C (\hat{x})}{\hat{r}} - \hat{r} \frac{dB}{2 \hat{x}} \right) \frac{\partial \hat{T}_1}{\partial \hat{r}} = \frac{1}{P_1} \frac{1}{\hat{r}} \frac{\partial}{\partial \hat{r}} \left( \hat{r} \frac{\partial \hat{T}_1}{\partial \hat{r}} \right) \]

\( R_1 \leq \hat{r} \leq R_0, \)

\[ \hat{T}_1 (\hat{r}, 0) = \hat{T}_1 (\hat{r}), \]
\[ -\hat{K}_1 \frac{\partial \hat{T}_1}{\partial \hat{r}} (R_1, \hat{x}) = 0, \]
\[ \hat{T}_1 (R_0, \hat{x}) = \hat{T}_2 (R_0, \hat{x}) \]

\[ B \frac{\partial \hat{T}_2}{\partial \hat{x}} + \left( \frac{C (\hat{x})}{\hat{r}} - \hat{r} \frac{dB}{2 \hat{x}} \right) \frac{\partial \hat{T}_2}{\partial \hat{r}} = \frac{1}{P_2} \frac{1}{\hat{r}} \frac{\partial}{\partial \hat{r}} \left( \hat{r} \frac{\partial \hat{T}_2}{\partial \hat{r}} \right) \]

\( R_0 \leq \hat{r} \leq R_2, \)

\[ \hat{T}_2 (\hat{r}, 0) = \hat{T}_2 (\hat{r}), \]
\[ -\hat{K}_2 \frac{\partial \hat{T}_2}{\partial \hat{r}} (R_2, \hat{x}) = B h_2 \left( \hat{T}_2 (R_2, \hat{x}) - \hat{T}_{2, \infty} \right), \]
\[ -\hat{K}_2 \frac{\partial \hat{T}_2}{\partial \hat{r}} (R_0, \hat{x}) = -\hat{K}_2 \frac{\partial \hat{T}_2}{\partial \hat{r}} (R_0, \hat{x}) \]
Two–dimensional equations of the 2D model

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

\[
B \frac{\partial Y_i}{\partial \hat{x}} + \left( \frac{C(\hat{x})}{\hat{r}} - \frac{\hat{r} \, dB}{2 \, d\hat{x}} \right) \frac{\partial Y_i}{\partial \hat{r}} = k_{Ai}(0) \exp \left( a_{2i} S_i^2 \right) (Y_{\infty,i} - Y_i), \quad i = 1, 2,
\]

\[
Y_i(\hat{r}, 0) = \tilde{Y}_i(\hat{r}), \quad i = 1, 2,
\]

- **Effective dynamic viscosity**

\[
\hat{\mu}_{ei,0}(\hat{r}, \hat{x}) = \hat{G}_i \exp \left( \hat{E}_i \left( 1 - \hat{T}_i \right) + \beta_i \left( \frac{Y_i}{Y_{\infty,i}} \right)^{n_i} \right) + \frac{2}{3} \alpha_i \hat{\lambda}_i S_i^2 \quad i = 1, 2.
\]

- **Cross-sectionally averaged effective dynamic viscosity**

\[
< \hat{\mu}_{e1,0} > (\hat{x}) = \int_{\mathcal{R}_1}^{\mathcal{R}_0} \hat{\mu}_{e1,0}(\hat{r}, \hat{x}) \hat{r} \, d\hat{r} / A_1,
\]

\[
< \hat{\mu}_{e2,0} > (\hat{x}) = \int_{\mathcal{R}_0}^{\mathcal{R}_2} \hat{\mu}_{e2,0}(\hat{r}, \hat{x}) \hat{r} \, d\hat{r} / A_2.
\]
Two–dimensional equations of the 2D model

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

\[
\mathcal{B} \frac{\partial Y_i}{\partial \hat{x}} + \left( \frac{C(\hat{x})}{\hat{r}} - \frac{\hat{r} dB}{2 d\hat{x}} \right) \frac{\partial Y_i}{\partial \hat{r}} = k_{Ai}(0) \exp \left( a_{2;S_i^2} \right) \left( Y_{\infty,i} - Y_i \right), \quad i = 1, 2,
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\hat{\mu}_{ei,0}(\hat{r}, \hat{x}) = G_i \exp \left( \hat{E}_i \left( 1 - \hat{T}_i \right) + \beta_i \left( \frac{Y_i}{Y_{\infty,i}} \right)^{n_i} \right) + \frac{2}{3} \alpha_i \hat{\lambda}_i S_i^2 \quad i = 1, 2.
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\]
Two-dimensional equations of the 2D model

Two-dimensional equations for the molecular orientation tensor components

\[ \mathcal{B} \frac{\partial S_{irr}}{\partial \hat{x}} + \left( \frac{C (\hat{x})}{\hat{r}} - \frac{\hat{r} dB}{2 d\hat{x}} \right) \frac{\partial S_{irr}}{\partial \hat{r}} = (1 - S_{irr}) (1 + S_{ixx}) \frac{dB}{d\hat{x}} \]

\[- \frac{\phi_i}{\lambda_i} \left\{ S_{irr} + \frac{N_i}{3} [(S_{irr} - 1) (S_{irr} - O_{is})] \right\}, \quad i = 1, 2, \]

\[ \mathcal{B} \frac{\partial S_{irr}}{\partial \hat{x}} + \left( \frac{C (\hat{x})}{\hat{r}} - \frac{\hat{r} dB}{2 d\hat{x}} \right) \frac{\partial S_{irr}}{\partial \hat{r}} = (1 + S_{ixx}) (2 - S_{ixx}) \frac{dB}{d\hat{x}} \]

\[- \frac{\phi_i}{\lambda_i} \left\{ S_{ixx} - \frac{N_i}{3} [(S_{ixx} + 1) (S_{ixx} - O_{is})] \right\}, \quad i = 1, 2, \]

\[ O_{is}(\hat{r}, \hat{x}) = \frac{2}{3} \left( S_{irr}^2 + S_{ixx}^2 - S_{irr} S_{ixx} \right). \]

\[ S_{irr}(\hat{r}, 0) = -\tilde{S}_i(\hat{r}), \]

\[ S_{ixx}(\hat{r}, 0) = 2 \tilde{S}_i(\hat{r}). \]
Mapping: 2D model

\[(\hat{r}, \hat{x}) \mapsto (\xi, \eta)\] maps \(\Omega_{\hat{r}\hat{x}} = \{[\mathcal{R}_1(\hat{x}), \mathcal{R}_2(\hat{x})] \times [0, 1]\}\) into a rectangular domain \(\Omega_{\xi\eta} = \{[0, 1] \times [0, 1]\}\)
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Two–dimensional equations of the 2D model

- Two–dimensional energy equation

\[
\frac{\partial \hat{T}_1}{\partial \eta} = \frac{1}{2 (V_1 + V_2)} \frac{4}{P_1} \frac{\partial}{\partial \xi} \left( \left( \xi + \frac{R_1^2}{R_2^2 - R_1^2} \right) \frac{\partial \hat{T}_1}{\partial \xi} \right) \quad 0 \leq \xi \leq \frac{V_1}{V_1 + V_2},
\]

\[\hat{T}_1(\xi, 0) = \hat{T}_1(\xi),\]

\[-\hat{K}_1 \frac{\partial \hat{T}_1}{\partial \xi}(0, \eta) = 0,\]

\[\hat{T}_1 \left( \frac{V_1}{V_1 + V_2}, \eta \right) = \hat{T}_2 \left( \frac{V_1}{V_1 + V_2}, \eta \right)\]

\[
\frac{\partial \hat{T}_2}{\partial \eta} = \frac{1}{2 (V_1 + V_2)} \frac{4}{P_2} \frac{\partial}{\partial \xi} \left( \left( \xi + \frac{R_1^2}{R_2^2 - R_1^2} \right) \frac{\partial \hat{T}_2}{\partial \xi} \right) \quad \frac{V_1}{V_1 + V_2} \leq \xi \leq 1,
\]

\[\hat{T}_2(\xi, 0) = \hat{T}_2(\xi),\]

\[-\hat{K}_2 \frac{\partial \hat{T}_2}{\partial \xi}(1, \eta) = \frac{R_2^2 - R_1^2}{2 R_2} \hat{B} \hat{h}_2 \left( \hat{T}_2(1, \eta) - \hat{T}_{2,\infty} \right),\]

\[-\hat{K}_1 \frac{\partial \hat{T}_1}{\partial \xi} \left( \frac{V_1}{V_1 + V_2}, \eta \right) = -\hat{K}_2 \frac{\partial \hat{T}_2}{\partial \xi} \left( \frac{V_1}{V_1 + V_2}, \eta \right)\]
Two–dimensional equations of the 2D model

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\[ B \frac{\partial Y_i}{\partial \eta} = k_{Ai}(0) \exp \left( a_2 S_i^2 \right) (Y_\infty,i - Y_i), \quad i = 1, 2, \]

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- **Effective dynamic viscosity**

\[ \mu_{e,i,0}(\xi, \eta) = \hat{G}_i \exp \left( \hat{E}_i \left( 1 - \hat{T}_i \right) + \beta_i \left( \frac{Y_i}{Y_\infty,i} \right)^{n_i} \right) + \frac{2}{3} \alpha_i \hat{\lambda}_i S_i^2 \quad i = 1, 2. \]

- **Cross-sectionally averaged effective dynamic viscosity**

\[ < \mu_{e1,0} > (\eta) = \frac{V_1 + V_2}{V_1} \int_0^{\frac{V_1}{V_1 + V_2}} \mu_{e1,0}(\xi, \eta) \, d\xi, \]

\[ < \mu_{e2,0} > (\eta) = \frac{V_1 + V_2}{V_2} \int_{\frac{V_1}{V_1 + V_2}}^1 \mu_{e2,0}(\xi, \eta) \, d\xi. \]
Two–dimensional equations of the 2D model

- Two–dimensional equations for the molecular orientation tensor components

\[
\mathcal{B} \frac{\partial S_{irr}}{\partial \eta} = (1 - S_{irr}) (1 + S_{ixx}) \frac{dB}{d\eta} \\
- \frac{\phi_i}{\lambda_i} \left\{ S_{irr} + \frac{N_i}{3} [(S_{irr} - 1) (S_{irr} - O_{is})] \right\}, \quad i = 1, 2,
\]

\[
\mathcal{B} \frac{\partial S_{ixx}}{\partial \eta} = (1 + S_{ixx}) (2 - S_{ixx}) \frac{dB}{d\eta} \\
- \frac{\phi_i}{\lambda_i} \left\{ S_{ixx} - \frac{N_i}{3} [(S_{ixx} + 1) (S_{ixx} - O_{is})] \right\}, \quad i = 1, 2,
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\[
O_{is}(\xi, \eta) = \frac{2}{3} \left( S_{irr}^2 + S_{ixx}^2 - S_{irr} S_{ixx} \right).
\]

\[
S_{irr}(\xi, 0) = -\tilde{S}_i(\xi), \quad S_{ixx}(\xi, 0) = 2 \tilde{S}_i(\xi).
\]
RESULTS AND DISCUSSION
Thermal boundary layer

\[ E_2 = 10 \]
Effect of the cladding’s viscosity parameters

\[ G_2 = 1 (-), G_2 = 0.01 (- -) \text{ and } G_2 = 100 (- - -) \]

\[ E_2 = 100 (-), E_2 = 50 (- -) \text{ and } E_2 = 10 (- - -) \]
Effect of the cladding’s viscosity parameters

$G_2 = 1 \ (-), \ G_2 = 0.01 \ (- -) \ and \ G_2 = 100 \ (- \cdot -)$

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1D model vs 2D model

1D (-) and 2D (-- - -)

$R_1, R_0, R_2$

$B$

$\dot{T}$

$\log(<\mu_{c1,0}>)$

$<Y_1>$

$<Y_2>$

$<S_1>$

$<S_2>$
CONCLUSIONS
Conclusions

Contributions of the present work:


2. 1D model (asymptotic analysis for \( \epsilon << 1 \)) for \( R_i \) and \( B \) and 2D equations for \( \hat{T}_i, S_i \) and \( Y_i \).

3. Determination of the two–dimensional fields of temperature, order parameter for molecular orientation and degree of crystallinity for hollow compound fibers.

4. Integro–differential model highly dependent on \( E_2 \) and \( G_2 \).

5. Find substantial temperature non–uniformities (may affect the degree of crystallization and have great effects on the mechanical, optical,... properties of hollow compound fibers) in the radial direction.
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THANK YOU FOR YOUR ATTENTION