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MODELING OF NONISOHERMAL CHANNEL FLOWS AND ELONGATIONAL FLOWS IN POLYMERIC PROCESSES

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

By

Dongbu Cao, M.S., B.S.

The Ohio State University

1995

Dissertation Committee:
Professor Stephen E. Bechtel
Professor Brian D. Harper
Professor Somnath Ghosh

Approved by
Adviser
Engineering Mechanics
To My Mother
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VITA

November 22, 1965 .................................. Born - Nanning, China

June, 1986 .......................................... B.S.
     The Zhongshan University
     Guangzhou, China

January, 1989 ..................................... M.S.
     The Harbin Civil Engineering Institute
     Harbin, China

September, 1991 - present .................. Graduate Research Associate
     The Ohio State University
     Columbus, Ohio

Fields of Study

Major Field: Engineering Mechanics
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CHAPTER I

Introduction

In an industrial polymer process, polymer experiences thermal and mechanical treatments to form the final product. The maximum temperature in the process is concerned because the polymer degradation happens at excessive temperatures. Also, the temperature effects on the material behavior are often significant. Modeling of flow behavior, stress, and temperature in the processes is crucial for process control and optimization. The model consists of the conservation laws of mass, momentum, and energy, together with material-dependent constitutive equations for stress, internal energy, and heat flux.

In general, the material properties involved in these constitutive equations are functions of state variables such as stress and temperature. In the literature, assumptions have been made to simplify the problem. An example is the incompressible theory, in which density is assumed to be constant and a constraint pressure is introduced to maintain the mechanical constraint imposed by the assumption.

In nonisothermal processes, the temperature changes are often so large that the effects of shrinkage or expansion of material can no longer be neglected. In these cases polymer density must be modeled as a temperature-dependent property. The
common practice is to *a posteriori* substitute an expression for density as a function of temperature into models derived for an incompressible material to account for the effects of temperature-dependent density. This ad hoc approach is examined and corrected in this work. The assumption of density as a function of temperature amounts to imposition of a thermomechanical constraint which is fundamentally different from the incompressibility constraint. Here, the form of the constraint response is deduced by requiring it to maintain the constraint while producing no entropy. The theory of a material with temperature-dependent density is contrasted with the theory of an incompressible material. In this work the balance equations governing a constrained material with prescribed temperature-dependent density are derived under a thermomechanically constrained theory and the effects of constraint response on the flow behavior in channel flows and elongational flows are investigated.

Channel flows are a class of viscometric flows which have extensive applications in viscometry and industrial processes. At high shear rates, it is known that viscous heating has significant effects on the flow behavior, causing the fluid temperature to vary across the channel in spite of any effort to maintain a uniform fluid temperature. The effects of viscous heating have been studied extensively in the literature. In contrast, expansion cooling due to the temperature-dependent density, which has a contrary effect on the fluid temperature, has been studied by few researchers.

Based on the thermomechanically constrained theory for a material with prescribed temperature-dependent density, we show that there should be a term in the energy equation governing the temperature distribution to account for the effects of
temperature-dependent density. This term causes a direct coupling of the governing equations for velocity and temperature fields, in contrast to the one-way coupling equations derived under the ad hoc theory. The constrained theory captures the phenomenon of expansion cooling which is missed by the ad hoc theory. Expansion cooling has the effect of depressing the fluid temperature at the middle of the channel. Our studies show that even for a material with moderate temperature dependence of density the effects of expansion cooling on both velocity and temperature distributions are significant. This results in a considerable difference in predicted flow curves, and leads to the argument that when the viscous heating is considered in high shear rate process, the effects of temperature-dependent density should also be included in the context of the thermomechanically constrained theory.

The study is extended from the slit die flows with isothermal wall condition to flows with finite heat loss coefficient, a more realistic thermal boundary condition. An interesting observation is that varying thermal boundary condition has an effect on the flow curve similar to that of temperature-dependent density. The study is also extended to capillary flows and flows in annular dies.

Polymer fibers, with end uses in textiles and reinforced composites, are manufactured in nonisothermal spinning processes in which molten polymer is extruded from a circular hole into cooling air and drawn continuously into a solidified thin filament. Thin filament models are used in industry to numerically simulate fiber spinning processes to predict the physical properties of filaments produced under different operation conditions and thereby optimize the process. A large part of this
work is devoted to improving the modeling of nonisothermal fiber spinning process by developing thin-filament models that can account for i) the effects of shrinkage due to cooling and ii) radial temperature variation within the filament.

Existing thin-filament models are based on the incompressible theory. It is recognized that it is necessary to specify the polymer density as a function of temperature in fiber spinning processes, in which the molten polymer experiences large temperature change, but this important feature has not been incorporated correctly into thin-filament models. The common practice is to \textit{a posteriori} substitute the expression of temperature-dependent density into the thin-filament equations for an incompressible material. A robust approach to deriving \textit{thin-filament models for nonisothermal melt spinning of polymer with prescribed temperature-dependent density} is given in this work.

The conservation equations of mass, momentum, and energy in the thermomechanically constrained theory constitutes our 3-dimensional mathematical model for the fiber spinning. To derive the 1-dimensional thin-filament equations, we employ perturbation techniques and the concept of process regime. The dimensionless components of velocity and dimensionless pressure are expanded into power series of dimensionless radial variable and slenderness parameter. The leading order problem can be obtained for any specified process regime. In this approach, we are able to avoid presuming \textit{radial independence of temperature}, which is used as basis for thin-filament equations in the literature. It is found that the assumption of radial independence of temperature is erroneous despite of its common use. A parabolic shape
function for radial temperature distribution is proposed to replace this assumption. The proposed shape function is examined in a simplified rigid rod model where an exact solution can be obtained. The numerical solution calculated from the proposed shape function is extremely close to the exact solution.

The prediction by the thin-filament model which incorporates both temperature dependence of density and radial temperature variation is compared to that by the conventional thin-filament model. A phenomenon that there exists a stress relaxation zone near the fiber's glass transition position is discovered. The tensile stress in the fiber reaches its peak near the fiber's glass transition position and then drops almost 50 percent. Explanations are given for the mechanism underlying the phenomenon that is related to the effects of shrinkage and the stretching process of fiber. Overall, the new model predicts a slower stretching and cooling of the fiber, a lower maximum tensile stress, and a stress relaxation zone near the fiber's glass transition position in the process.

The dissertation is organized as follows:

In Chapter 2 the balance equations of mass, momentum, and energy governing a constrained material with prescribed temperature-dependent density are derived in the context of a thermomechanically constrained theory. In contrast to that for the incompressible theory, the constraint pressure is present not only in the momentum equation but also in the energy equation.

In Chapter 3 the constrained theory is applied to study the competing effects of viscous heating and expansion cooling in channel flows. The ad hoc theory, in
which a temperature-dependent expression for density is inserted \textit{a posteriori} into the equations for an incompressible material, cannot model the effect of expansion cooling and results in qualitative and quantitative errors in prediction. The flow rate vs. wall shear stress curves predicted by the constrained theory and the ad hoc theory are close to each other in low shear rate region but deviate from each other in high shear rates. The study is extended to flows in slit dies, capillaries, and annular dies, with varying thermal boundary condition.

In Chapter 4 the study of fiber spinning modeling begins with a rigid rod model to reveal the importance of radial temperature variation. It is shown that the conventional assumption of radially independent temperature is incorrect no matter how slender the fiber is. Based on an exact solution for the rigid rod problem, a parabolic shape function is proposed to model the radial temperature variation and found satisfactory.

In Chapter 5 mathematical models for fiber spinning are developed to account for radial temperature variation. They predict substantially lower tensile stresses in the fiber and longer cooling length compared to the conventional modeling. Effects of inertia, rheological force, surface tension, gravity, heat conduction, heat loss, and viscous heating are included in the model. The local values of dimensionless numbers are utilized to track the relative importance of these competing effects down the spinline.

In Chapter 6 the thin-filament equations are derived to model the effect of shrinkage in fiber spinning in the context of a thermomechanically constrained theory. The
thin-filament equations predict that there exists a stress relaxation zone near the fiber’s glass transition area. The relation of incompressibility in elongational flows, \( u_{rr} = -\frac{1}{2} v_{r,z} \), is invalid in this stress relaxation zone, and the conventional thin-filament model which is based this relation fails to predict this phenomenon.

Chapter 7 is a conclusion and summary of results.

Appendix A presents an alternative pointwise perturbation theory for the modeling of fiber spinning. It shows the conventional assumption of radially independent temperature is incorrect, and provides the motivation to study the effect of radial temperature variation.
CHAPTER II

The Thermomechanically Constrained Theory for a Material with Prescribed Temperature-Dependent Density

In general, the properties of material depend on both thermal and mechanical state variables. Nonetheless, in some industrial processes such as polymer extrusion and fiber spinning, the general problem can be reasonably simplified by neglecting the pressure dependence of density, specific heat, viscosity, and thermal conductivity. This is because the mechanical dependence of material properties is weak at the low to moderate pressure levels encountered in these processes (Lodge & Ko [53], Winter [76], Cox & Macosko [18], Spencer & Gilmore [67]). In contrast, temperature in these processes is high enough and temperature change and temperature gradient are sufficiently large so that the thermal dependence of material properties may have a significant effect on process behavior. At a fundamental as well as practical level, models for design or optimization of these processes must incorporate this temperature dependence.

Specification of material density as a function of temperature amounts to the imposition of a thermomechanical constraint, i.e. a condition on the temperature
and deformation state of the material that must be satisfied \textit{a priori} by any motion. The presence of a constraint results in a mathematical model different from the corresponding models from unconstrained theories, e.g. in Bird \textit{et al.} [10] and Toor [69]. In this chapter, the balance equations governing the behavior of a material with prescribed temperature-dependent density are derived in the context of a thermomechanical constraint and its corresponding constraint response.

2.1 Literature Review

The concept of mechanical constraints in the form of incompressibility and inextensibility has a long history in classical mechanics. The first general mechanical theory of internal constraints was developed by Noll [59]. The generalization to thermomechanical constraints was made by Green, Naghdi & Trapp [32] and Gurtin & Guidugli [33]. Trapp [71] further generalized the form of thermomechanical constraints given by Green \textit{et al.} [32], and applied the general theory to the special case of an inextensible material with an additional thermal constraint on the temperature gradient, in the context of small deformations and a linear elastic constitutive assumption. Reddy [62] constructed a theory of constrained elastic materials which was a slight modification of that proposed by Trapp [71].

The general form of the thermomechanical constraint adopted by Green \textit{et al.} [32] and Trapp [71] is

\[ A \cdot \mathbf{D} + b \cdot \text{grad} \theta + a \dot{\theta} = 0, \]  

(2.1)
where $A$, $b$ and $\alpha$ are specified functions which do not depend on $D$, $\text{grad} \theta$ and $\dot{\theta}$. $D$ is the symmetric part of the Eulerian velocity gradient $L = \text{grad} v$ and $\dot{\theta}$ denotes the material derivative of $\theta$,

$$D = \frac{1}{2}(L + L^T) = \frac{1}{2}[\text{grad} v + (\text{grad} v)^T], \quad \dot{\theta} = \frac{\partial}{\partial t} \theta + \text{v} \cdot \text{grad} \theta,$$

(2.2)

where $\frac{\partial}{\partial t}$ is the Eulerian partial derivative with respect to time and $v$ is velocity vector.

Prescribed temperature-dependent density was first recognized as a material constraint by Green et al. [32], but neither they nor any subsequent researchers have studied the resulting balance equations governing a material subject only to this constraint (for example: Green & Naghdi [31], Naghdi & Srinivasa [58], Batra [4, 3], Cohen & Wang [17], Rubin [63], Casey [14], Ahmadi [1], Atkin & Craine [2], Hutter [42], Chen & Nunziato [16], Chadwick [15]). As we shall see, the constraint demanded by prescribed temperature-dependent density $\rho = \rho(\theta)$ is the special case of (2.1) with

$$A = I, \quad b = 0, \quad \alpha = \frac{\rho'}{\rho},$$

(2.3)

where $\rho'$ denotes the derivative of $\rho(\theta)$ with respect to $\theta$,

$$\rho' = \frac{d}{d\theta} \rho(\theta).$$

(2.4)

This thermomechanically constrained theory yields a problem formulation that is simpler to solve than the unconstrained theory, yet predicts temperature-induced volume-change effects that are missed by both the incompressible theory and the ad hoc theory of incompressibility combined with temperature-dependent density. In
this chapter, we derive the balance equations governing the behavior of materials with temperature-dependent density in the context of a thermomechanically constrained theory. Then in the next chapter we will compare solutions of our thermomechanically constrained theory in plane Poiseuille flows with solutions of the ad hoc theory, i.e. the incompressible equations with \textit{a posteriori} substitution of temperature-dependent density.

2.2 The \textit{a Posteriori} Treatment of Temperature-Dependent Density

We first present the straightforward, but inconsistent, extension of incompressibility that was employed elsewhere (Hayashi \textit{et al.} [37], Dutta [23], Sabhapathy & Cheng [64]) to model nonisothermal processes with temperature dependence of material density.

The governing equations for all thermomechanical continua are the conservation laws of mass, linear momentum and energy:

\begin{align*}
\dot{\rho} + \rho \text{div} \mathbf{v} &= 0, \\
\rho \dot{\mathbf{v}} &= \text{div} \mathbf{T} + \rho \mathbf{g}, \\
\rho \dot{\varepsilon} &= \mathbf{T} : \mathbf{D} + \rho \gamma - \text{div} \mathbf{q},
\end{align*}

where \( \rho \) and \( \mathbf{g} \) are the material density and body force, respectively; \( \mathbf{v}, \mathbf{D} \) and \( \mathbf{T} \) are the velocity vector, symmetric part of the Eulerian velocity gradient \( \mathbf{L} = \text{grad} \mathbf{v} \), and Cauchy stress tensor, respectively; \( \varepsilon, \gamma \) and \( \mathbf{q} \) are the internal energy, heat supply
per unit mass, and heat flux vector, respectively; "div" is the Eulerian divergence operator and "\( \dot{\epsilon} \)" the material derivative with respect to time, e.g.

\[
\dot{\epsilon} = \frac{\partial \epsilon}{\partial t} + \mathbf{v} \cdot \text{grade} \epsilon.
\]  

(2.8)

A process must also satisfy the second law of thermodynamics in the form of Clausius-Duhem inequality,

\[
s \equiv \dot{s} - \frac{\gamma}{\rho} + \frac{1}{\rho} \text{div} \left( \frac{\mathbf{q}}{\theta} \right) \geq 0,
\]  

(2.9)

where \( s \) is the internal entropy production rate per unit mass and \( \theta \) denotes absolute temperature. In a particular application these equations are accompanied by boundary conditions, constitutive equations, and perhaps material constraint equations.

The most familiar constrained theory is that for an incompressible material. The constraint for an incompressible material is

\[
\text{div} \mathbf{v} = 0.
\]  

(2.10)

We briefly review how the constraint response is deduced for an incompressible material: From the thermodynamics second law considerations that the constraint response produces no entropy, it is deduced that the internal energy and heat flux vector are determined completely by constitutive functions \( \dot{\epsilon} \) and \( \dot{\mathbf{q}} \), respectively, but the Cauchy stress \( \mathbf{T} \) consists of a constitutive part \( \mathbf{T} \) plus an additive workless constraint response \( \mathbf{\tilde{T}} \),

\[
\mathbf{T} = \mathbf{T} + \mathbf{\tilde{T}},
\]  

(2.11)

with

\[
\mathbf{\tilde{T}} \cdot \mathbf{D} = 0.
\]  

(2.12)
Condition (2.12) must hold for all rate of strain tensors $D$ satisfying the incompressibility constraint (2.10), i.e., for all symmetric tensors $D$ perpendicular to the identity tensor $I$, since constraint (2.10) can be rewritten as

$$\text{div } v = I \cdot D = 0. \quad (2.13)$$

Since $\hat{T}$ must therefore be perpendicular to all $D$ which are perpendicular to $I$, we conclude that the constraint response $\hat{T}$ must be parallel to $I$,

$$\hat{T} = -p I. \quad (2.14)$$

Combining the governing equations (2.6) and (2.7) for the continuum with the constraint (2.10) and the result (2.14), we see that the field equations for an incompressible material are

$$\text{div } v = 0, \quad (2.15)$$

$$\rho \dot{v} = \text{div } \hat{T} - \text{grad } p + \rho g, \quad (2.16)$$

$$\rho \dot{\varepsilon} = \hat{T} \cdot D + \rho \gamma - \text{div } \dot{q}. \quad (2.17)$$

The 3-dimensional initial/boundary value problem consists of field equations (2.15)-(2.17), constitutive equations for $\hat{T}, \varepsilon, \dot{\varepsilon}, \dot{q},$ and initial and boundary conditions. Note that the constraint response $p$ necessary to maintain the condition (2.15) of incompressibility enters only in the momentum equation (2.16) and is absent from the energy equation (2.17).

Recall that for modeling many processes it is necessary to account for temperature dependence of density since the temperature-induced volume change is considerable.
In Hayashi *et al.* [37], Dutta [23] temperature dependence of density is merely substituted *a posteriori* into (2.15)-(2.17). Although these incompressible 3-dimensional equations are correct for constant density, they are invalid for prescribed temperature-dependent density. In Kase & Matsuo [47] the incompressibility constraint (2.15) was replaced with equation (2.5), which takes into account thermal expansion, but temperature dependence of density was again incorrectly substituted *a posteriori* in the incompressible momentum and energy equations (2.16) and (2.17):

\[
\text{div } \mathbf{v} = -\frac{\rho'(\theta)}{\rho(\theta)} \dot{\theta}, \quad (2.18)
\]

\[
\rho(\theta) \dot{\mathbf{v}} = \text{div } \mathbf{\dot{T}} - \text{grad } p + \rho(\theta) \mathbf{g}, \quad (2.19)
\]

\[
\rho(\theta) \dot{\mathbf{\varepsilon}} = \mathbf{\dot{T}} : \mathbf{D} + \rho(\theta) \gamma - \text{div } \mathbf{\dot{q}}. \quad (2.20)
\]

### 2.3 The Thermomechanically Constrained Theory for Materials with Temperature-Dependent Density

We now derive the correct equations for a material with temperature-dependent density, by taking this nonconstant density into account *a priori* in the derivation.

For a material with prescribed temperature-dependent density,

\[
\rho = \rho(\theta), \quad (2.21)
\]

conservation of mass becomes the thermomechanical constraint

\[
\frac{\rho'}{\rho} \dot{\theta} + \mathbf{I} : \mathbf{D} = 0. \quad (2.22)
\]
In our discussion it is convenient to replace internal energy $\epsilon$ with Helmholtz free energy $\psi$, defined by a Legendre transformation through

$$\psi = \epsilon - \theta \eta,$$  

(2.23)

where $\eta$ is entropy per unit mass. We first assume that there is an additive constraint response to all dependent quantities, i.e. we assume

$$T = \tilde{T} + \hat{T}, \quad q = \tilde{q} + \tilde{q}, \quad \psi = \tilde{\psi} + \psi, \quad \eta = \tilde{\eta} + \tilde{\eta},$$  

(2.24)

where "*" denotes the constitutive response as a function of deformation and temperature, and "−" denotes the constraint response. We postulate that the additive constraint response maintain the constraint while producing no entropy. Therefore we have

$$- \rho \dot{\psi} - \rho \tilde{\eta} \dot{\theta} + \tilde{T} \cdot D - \frac{1}{\theta} \tilde{q} \text{grad} \theta = 0,$$  

(2.25)

for all processes satisfying the constraint (2.22).

In particular (2.25) must hold for the subset of processes with grad$\theta \equiv 0$, $D \equiv 0$ and $\dot{\theta} \equiv 0$, which necessarily satisfy the constraint (2.22). For this subset, condition (2.25) reduces to

$$\dot{\psi} = 0,$$  

(2.26)

or, without loss of generality,

$$\bar{\psi} = 0.$$  

(2.27)

Since the constraint response must be independent of the particular process which satisfies the constraint, equation (2.27) must hold for all processes, not just the above subset.
We next consider all processes with $D = 0$, $\theta = 0$, but $\text{grad} \theta \neq 0$ and arbitrary. Again, each process in this family satisfies the constraint (2.22), so that condition (2.25) must hold; for this family (2.25) reduces to
\[
\frac{1}{\theta} \bar{q} \cdot \text{grad} \theta = 0, \quad (2.28)
\]
from which follows
\[
\bar{q} = 0. \quad (2.29)
\]

To summarize our results so far, there can be no additive constraint response to the free energy and heat flux vector if the constraint response is not to produce entropy; said differently, for a material with temperature-dependent density, $\psi$ and $q$ are determined entirely by constitutive functions of deformation and temperature.

All that remains from condition (2.25) is
\[
-\rho \dot{q} + \bar{T} : D = 0. \quad (2.30)
\]
We note that the subset of processes with $D = 0$ but $\dot{\theta} \neq 0$ and arbitrary, which is used to reach the result (2.14) in the above section, is not possible for the thermally-constrained material: $D$ and $\dot{\theta}$ are not independent, but instead are related through the constraint (2.22). If we regard $(\dot{\theta}, D)$ and $(\xi', I)$ as vectors in the seven-dimensional inner product space $\mathcal{E}^7$, the constraint (2.22) demands that the only admissible vectors $(\dot{\theta}, D)$ are those perpendicular to $(\xi', I)$, since the constraint (2.22) in $\mathcal{E}^7$ is
\[
(\xi', I) \cdot (\dot{\theta}, D) = 0. \quad (2.31)
\]
The condition (2.30), which we rewrite as
\[
(-\rho \bar{q}, \bar{T}) \cdot (\dot{\theta}, D) = 0, \quad (2.32)
\]
indicates that the response \((-\rho \bar{\eta}, \bar{T})\) must be perpendicular to all \((\dot{\varepsilon}, D)\) which are perpendicular to \((\xi^I, I)\). Hence we deduce that \((-\rho \bar{\eta}, \bar{T})\) is parallel to \((\xi^I, I)\), i.e.

\[
(-\rho \bar{\eta}, \bar{T}) = -p \left( \frac{\xi^I}{\rho}, I \right),
\]

where \(p\) is a scalar function of position and time. The total response (constitutive plus constraint) is therefore

\[
T = \dot{T} - p I, \quad q = \dot{q}, \quad \psi = \dot{\psi}, \quad \eta = \dot{\eta} + \frac{p}{\rho^2} \frac{\rho'}{\rho}.
\] (2.34)

Using the relation (2.23) between \(\psi, \varepsilon,\) and \(\eta,\) we obtain

\[
\varepsilon = \dot{\varepsilon} + p \theta \frac{\rho'}{\rho^2},
\]

where we have defined

\[
\dot{\varepsilon} = \dot{\varepsilon} + \theta \dot{\eta}.
\] (2.36)

We see from (2.35) that the term \(p \theta \frac{\rho'}{\rho^2}\) is needed in the internal energy to offset the entropy created by the constraint pressure in the stress, so that the net entropy generated by the entire response maintaining the constraint (2.22) is zero.

Combining the governing equations (2.6) and (2.7) with the constraint (2.22) and the results (2.34) and (2.35), we see that the field equations for a material with temperature-dependent density are

\[
\text{div} \ v = -\frac{\rho'}{\rho} \dot{\theta},
\]

\[
\rho \dot{v} = \text{div} \ \dot{T} - \text{grad} \ p + \rho g,
\] (2.38)

\[
\rho \ddot{v} + \frac{\rho'}{\rho} \theta \dot{p} + \frac{p \theta}{\rho} \dot{\theta} \frac{\rho'' - 2}{\rho} = \dot{T} \cdot D + \rho \gamma - \text{div} \ \dot{q}.
\] (2.39)
Comparing these with the equations (2.15)-(2.17) for an incompressible material, we note that the response $p$ necessary to maintain the constraint enters in both the momentum equation (2.38) and the energy equation (2.39), and there is a new term on the right hand side of the constraint (2.37). The a posteriori substitution of temperature-dependent function of density into equations (2.15), (2.16) and (2.17) for incompressible materials produces incorrect mass and energy equations. As stated before, some references (Hayashi et al. [37], Dutta [23], Sabhapathy & Cheng [64]) used (2.15), (2.16) and (2.17) directly with temperature-dependent density, and hence miss the new terms in both equations. Kase and Matsuo [47] correctly took into account thermal expansion or shrinkage in the mass conservation, i.e. they used (2.37) instead of (2.15), but left out the necessary constraint response terms in the energy equation. Hahn and Kettleborough [34, 35] positted a new term in the energy equation, but it was incomplete.

As shown, the response necessary to maintain the constraint (2.22) is an additive term not only to the stress but also to the internal energy of the material. The constraint of temperature-dependent density is fundamentally different from incompressibility: one cannot merely insert a temperature-dependent function for density a posteriori in the conventional incompressible theory, derived under the assumption of constant density. Constraint response terms must be included in the energy equation as well as the momentum equation, and the incompressibility constraint must be modified. Also, the constrained theory with a specified temperature-dependent density is different from the compressible theory. The constrained response $p$ is de-
d\hat{\varepsilon} = c(\theta)d\theta, \hspace{1cm} (2.40)

where \( c \) is the specific heat, and the energy balance equation (2.39) becomes

\[
\rho \left[ c + \frac{p_0}{\rho^2} (\rho'' - 2\frac{\rho'^2}{\rho}) \right] \dot{\theta} + \frac{\rho'}{\rho} \theta \dot{\rho} = \mathbf{T} \cdot \mathbf{D} + \rho \gamma - \text{div} \mathbf{q}, \hspace{1cm} (2.41)
\]

with both \( c \) and \( \rho \) specified functions of temperature.
CHAPTER III

The Effects of the Constraint Response for Temperature-Dependent Density in Poiseuille Flows

In Chapter 2 a mathematical model for the large-deformation processing of a material with prescribed temperature-dependent density has been developed in which the correct constraint response maintaining the thermomechanical constraint is included in both the momentum equation and the energy equation. We now investigate the effects of the constraint response on mechanical and thermal phenomena in viscometric flows. To determine the effects of the constraint response, not present in other models, we compare solutions of our thermomechanically constrained theory in plane Poiseuille flows with solutions of the ad hoc theory, i.e. the incompressible equations with *a posteriori* substitution of temperature-dependent density.

3.1 Literature Review

The nonisothermal flows in capillary and slit die have been studied extensively because of its importance in industrial processes and viscometric measurements (Vergnes *et al.*
Brinkman [12] appears to be the first to give a rigorous treatment for capillary flow with consideration of the effect of viscous heating. The flow was assumed incompressible, Newtonian model was used and the viscosity was assumed independent of temperature. Bird [9] extended Brinkman's work to describe heat effects for some types of non-Newtonian fluid. To recognize the effects of compressibility and thermal expansion, Toor [70, 69] gave an excellent discussion on the energy balance for the compressible flow and qualitatively showed the expansion cooling effect on the temperature distribution in capillaries. Cox and Macosko [18] studied the heat effect numerically and experimentally. The effects of compressibility and thermal expansion were examined, but they used a bulk temperature that was inadequate to describe the expansion cooling effects. In addition, an error was made when transferring the pressure and temperature dependence of density from Donovan [21].

Due to its capability in high shear rate measurements, flows in slit dies have received increasing attention. In high shear rate measurements, the effect of viscous heating becomes predominant. Neglecting viscous heating and temperature dependence of viscosity may lead to meaningless results (Duda et al. [22], Ybarra & Eckert...
Lodge and Ko [53, 51] studied fully-developed and developing flow in a slit die and derived a factor to correct for the viscous heating in the slit die viscometry with shear rates up to $5 \times 10^3 \text{s}^{-1}$. Button [13] studied the fully-developed flow with dissipative heating for different fluid models and the effect of viscous heating on fluidity. The importance of compressibility is recently recognized in slit die viscometers by Rauwendaal & Fernandez [61] and Hatzikiriakos [36].

In this chapter the competing effects of thermal expansion cooling and viscous heating in channel flows are investigated in the context of the thermomechanically constrained theory. We will show the effects of thermal expansion on the distributions of temperature and velocity and its interplay with viscous heating. In particular, we discover that our constrained theory is able to predict thermomechanical flow features that are unattainable in the incompressible treatments.

### 3.2 Plane Poiseuille Flows with Isothermal Walls

We now investigate the effects of the constraint response on mechanical and thermal phenomena in the case of plane Poiseuille flows with isothermal walls. In the following, solutions for velocity and temperature distributions in plane Poiseuille flows are obtained from the constrained theory, eqs.(2.37)-(2.39), and compared to the solutions of the ad hoc, incorrect extension of incompressibility, eqs.(2.15)-(2.17) with $\rho = \rho(\theta)$. We shall show that the use of the ad hoc theory may result in considerable error and can miss qualitative features of physical response.
3.2.1 The Boundary Value Problem

To complete the boundary value problem formulation for a material with temperature-dependent density, we must specify: (i) the constitutive functions \( \hat{T}, \hat{\varepsilon}, \) and \( \hat{q} \) for the determinate parts of stress, internal energy, and heat flux, respectively; (ii) the body force \( g, \) heat source \( \gamma, \) and density function \( \rho(\theta), \) that appear in the governing equations (2.37)-(2.39); and (iii) appropriate boundary conditions.

Here we model the steady flow between two infinite horizontal planes, depicted in Figure 1. We assume that the flow is two dimensional, laminar, and hydrodynamically and thermally fully-developed. Then, the velocity and temperature fields are of the form

\[
v_1 = v_1(x_2), \quad v_2 = 0, \quad v_3 = 0, \quad \theta = \theta(x_2),
\]

subject to the boundary conditions

\[
v = 0, \quad \theta = \theta_w,
\]
at the planes $x_2 = \pm h/2$, where $\theta_w$ is a specified constant temperature. This is a case of slit die flows with isothermal walls and no slip at the walls.

For simplicity, we assume constant specific heat and constant thermal conductivity in the constitutive functions for internal energy and heat flux,

$$d\varepsilon = c \, d\theta, \quad \dot{q} = -k \, \text{grad}\theta,$$

(3.3)

although $c$ and $k$ could just as well be taken as functions of temperature and will not change the form of governing equations, unlike the situation with temperature dependence of density. We also employ the Newtonian model for stress constitutive response of the fluid,

$$\dot{T} = 2\mu(\theta)D,$$

(3.4)

where viscosity $\mu(\theta)$ is a specified function of temperature $\theta$.

The body force is

$$g = -g e_2,$$

(3.5)

where $g$ is the acceleration of gravity and $e_2$ is a unit vector in the $x_2$ direction, and we assume no heat supply, i.e.

$$\gamma = 0.$$

(3.6)

3.2.2 Solution of the Boundary Value Problem in the Constrained Theory

With (3.1) the constraint equation (2.37) is identically satisfied for any specified function $\rho(\theta)$, the $x_1$, $x_2$, and $x_3$ components of the momentum equation (2.38) simplify
to
\[
\frac{dT_{12}}{dx_2} - \frac{\partial p}{\partial x_1} = 0, \quad -\frac{\partial p}{\partial x_2} - g = 0, \quad 0 = 0,
\] (3.7)
and the energy equation (2.39) becomes
\[
\frac{\rho'(\theta)}{\rho(\theta)} v_1 \theta \frac{\partial p}{\partial x_1} = T_{12} \frac{dv_1}{dx_2} + k \frac{d^2 \theta}{dx_2^2}.
\] (3.8)
Equations (3.7) imply
\[
p = C - \beta x_1 - gx_2,
\] (3.9)
\[
-T_{12} \tau_w = \frac{x_2}{h/2},
\] (3.10)
where \(\beta\) is the constant rate of pressure drop (positive when the pressure gradient is negative), \(C\) is a constant and \(\tau_w\) is the absolute value of shear stress at wall. The shear stress at wall is related to the rate of pressure drop \(\beta\) by
\[
\tau_w = \frac{1}{2} h \beta.
\] (3.11)

With the use of linear distribution of shear stress, eq. (3.10), and the Newtonian constitutive equation (3.4), the reduced one-dimensional equations governing the velocity and temperature distributions across the channel are then
\[
\frac{dv_1}{dx_2} = -\frac{\beta}{\mu(\theta)} x_2,
\] (3.12)
\[
\frac{d^2 \theta}{dx_2^2} = -\frac{\beta}{k \mu(\theta)} x_2^2 - \frac{\beta \rho'(\theta)}{k \rho(\theta)} v_1 \theta.
\] (3.13)
In eq.(3.13), the term \(-\frac{\beta \rho'(\theta)}{k \rho(\theta)} v_1 \theta\) represents the effect of constraint response; this term is absent if the temperature-dependent density is inserted \textit{a posteriori}. 

To proceed further we must be specific in the forms of the temperature dependence of density and viscosity. Here we assume a linear dependence of density on temperature,

$$\rho(\theta) = \rho_0 - \rho_1 \theta,$$  \hspace{1cm} (3.14)

where $\rho_0$ and $\rho_1$ are constants, and an Arrhenius form for viscosity,

$$\mu(\theta) = \mu_w \exp \left[ \frac{E}{R} \left( \frac{1}{\theta_0} - \frac{1}{\theta_w} \right) \right], \hspace{1cm} (3.15)$$

where the constants $E$, $R$, and $\theta_w$ are the activation energy, gas constant, and wall temperature, respectively, and $\mu_w$ is the viscosity at the wall temperature. The constants $\rho_0$, $\mu_w$, $E$, $R$, and $\theta_w$ must be positive; $\rho_1$ will also be positive in a usual case that material expands while being heated.

To nondimensionalize eqs.(3.12) and (3.13), we scale temperature to the wall temperature $\theta_w$, length to the wall separation $h$, and velocity to

$$v_0 = \frac{\beta h^2}{8 \mu_w}, \hspace{1cm} (3.16)$$

which is the maximum velocity in the isothermal solution of eq.(3.12), i.e.

$$\frac{dv_1}{dx_2} = -\frac{\beta}{\mu_w} x_2, \hspace{1cm} (3.17)$$

with the condition of no-slip at wall. The dimensionless transverse coordinate is then

$$\tilde{x}_2 = \frac{x_2}{h}, \hspace{1cm} (3.18)$$

and dimensionless temperature and velocity are

$$\tilde{\theta} = \frac{\theta}{\theta_w}, \hspace{0.5cm} \tilde{v}_1 = \frac{v_1}{v_0} = \frac{8 \mu_w v_1}{\beta h^2}. \hspace{1cm} (3.19)$$
Using the material density at the wall temperature, \( \rho_w \), as the characteristic value of density, the dimensionless form of the density function (3.14) becomes

\[
\hat{\rho}(\hat{\theta}) = \frac{\rho(\hat{\theta})}{\rho_w} = \frac{1 - P\hat{\theta}}{1 - \hat{\theta}},
\]

(3.20)

where the dimensionless thermal expansion number,

\[
P = \frac{\rho_1\theta_w}{\rho_0},
\]

(3.21)

is a measure of the degree of temperature dependence of the material's density at the processing conditions.

The dimensionless forms of equations (3.12) and (3.13) are

\[
\frac{d\tilde{v}_1}{d\tilde{x}_2} = -8\tilde{x}_2\exp \left[ -E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right],
\]

(3.22)

\[
\frac{d^2\tilde{\theta}}{d\tilde{x}_2^2} = -64B_r\tilde{x}_2^2\exp \left[ -E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] + 8B_rP\frac{\tilde{v}_1\tilde{\theta}}{1 - P\tilde{\theta}},
\]

(3.23)

where

\[
B_r = \frac{\mu_\infty v_\infty^2}{k\theta_w} = \frac{\tau_\infty^2 h^2}{16k\mu_\infty \theta_w}, \quad E = \frac{E}{R\theta_w}.
\]

(3.24)

\( B_r \) is the Brinkman number indicating the balance of the competing effects of viscous heating and thermal conduction, and \( E \) is a dimensionless number quantifying the degree of viscosity variation with temperature. The dimensionless boundary conditions are

\[
\tilde{v}_1 = 0, \quad \tilde{\theta} = 1 \quad \partial \tilde{x}_2 = \pm \frac{1}{2}.
\]

(3.25)

The two-point coupled boundary value problem (3.22), (3.23), and (3.25), involving the three dimensionless parameters \( B_r, E \) and \( P \), is solved with a relaxation
method. The exact, unique solution of the two point boundary value problem with temperature-independent viscosity and density, i.e. equations (3.22), (3.23), and (3.25) with $E = P = 0$, is used as the initial guess in the ODE solver. This solution is

$$
\tilde{u}_1(\tilde{x}_2) = 1 - 4\tilde{x}_2^2, \quad \tilde{\theta}(\tilde{x}_2) = 1 + \frac{Br}{3} (1 - 16\tilde{x}_2^4).
$$

(3.26)

The governing equations for the fields of velocity and temperature are coupled when the effects of expansion cooling are taken into account. The ordinary differential equations (3.22), (3.23) have to be solved for velocity and temperature distributions simultaneously. If viscous heating is considered but the expansion effect term is suppressed, the temperature distribution can be obtained first and then used to determine the velocity profile as done by Burton [13]. The rearrangement and effect on temperature of velocity due to thermal expansion are consequently omitted, however, if one proceeds in this manner. The boundary value problem from the ad hoc theory also decouples velocity from temperature, as is shown in the next section.

### 3.2.3 Solution of the Boundary Value Problem in the Ad Hoc Theory

If the same plane Poiseuille flow shown in Figure 1 is modeled with the ad hoc theory, in which a temperature-dependent density function is substituted *a posteriori* in the incompressible equations (2.15)–(2.17), the dimensionless governing equations reduce to

$$
\frac{d\tilde{u}_1}{d\tilde{x}_2} = -8\tilde{x}_2 \exp \left[ -E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right],
$$

(3.27)
subject to the boundary conditions (3.25). The parameter $P$ describing the temperature dependence of density does not appear in equations (3.27) and (3.28); in fact, the equations are exactly the same as the governing equations derived for an incompressible material in nonisothermal plane Poiseuille flows in this particular case. Hence, this a posteriori approach leads to an erroneous result that, no matter how strong the temperature dependence of density is, it can not effect velocity, temperature and stress distributions. The only effect of temperature-dependent density is on the density itself: once $\tilde{\theta}$ is determined from the boundary value problem (3.27), (3.28), and (3.25), the nondimensional density is obtained from

$$\tilde{\rho}(\tilde{x}_2) = \frac{1 - P\tilde{\theta}(\tilde{x}_2)}{1 - P}.$$  

In fact, temperature dependence of density has strong effects on the velocity and temperature distributions.

### 3.2.4 Comparison of the Solutions and Discussion

The effects in the constrained theory of temperature-dependent density on the velocity and temperature fields are shown in Figure 2. As the temperature dependence of density becomes more pronounced (i.e. as $P$ becomes greater), a depression develops at the center of the temperature profile, and the difference between the wall temperature and mean temperature of the flow decreases. At $P = 0.3$, the temperature at mid-channel is even lower than the wall's temperature, which completely changes the
Figure 2: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows with isothermal walls as predicted by the constrained theory, showing the effects of varying the level of temperature dependence of density: \( E = 5.0, \, Br = 0.2, \) varying \( P \). The vertical coordinate is the dimensionless transverse coordinate \( \tilde{x}_2 \). The solution for all values of \( P \) from the ad hoc theory, with \textit{a posteriori} substitution of temperature-dependent density into the incompressible theory, is the same for all values of \( P \) as the solution to the constrained theory with \( P = 0 \).
temperature profile from that predicted by the ad hoc theory. This effect is due to the phenomenon of expansion cooling (Winter [76], Cox & Macosko [18], Toor [69]). In the plane Poiseuille flow we model, the fluid interior undergoes viscous heating, which tends to increase fluid temperature in the center. The viscous heating also tends to expand the fluid when the fluid is heated, and the work done in this expansion leads to loss of temperature. These competing effects lead to the temperature profiles in Figure 2. The inflection points observed in these temperature profiles from our constrained theory are also predicted in all compressible analyses of fully-developed nonisothermal Poiseuille flows in the literature. There are no inflection points in the temperature distribution curve predicted by the ad hoc theory, however. The ad hoc theory cannot reflect the competing effects of viscous heating and expansion cooling. Although viscous heating is included in the ad hoc model through the right hand side of eq.(3.28), the expansion work term $8B\rho \frac{d}{d\rho} \left( \frac{5\rho}{1-\rho} \right)$ is missing when the temperature-dependent density function is inserted \textit{a posteriori} in the incompressible equations. The solutions for the velocity and temperature distributions in the ad hoc theory are not affected by the degree of temperature dependence of density: the predicted distributions for temperature-dependent density and constant density are identical, and given by the solutions with $P = 0$ in Figure 2. When modeling plane Poiseuille flows with the ad hoc theory the temperature dependence of density decouples from the temperature and velocity problem, and only affects the density distribution itself.

The ad hoc theory therefore makes both qualitative and quantitative errors. The bulk temperature and maximum temperature of fluid can be much lower than these
predicted when the thermal expansion is disregarded. The ad hoc theory overestimates the fluid maximum absolute temperature by 5.3 percent and the velocity at the mid-channel by 16.7 percent for the case with thermal expansion number $P = 0.2$. Polymers are typically processed at fairly large $P$, ranging from 0.1 to 0.3 (Toor [70]). Even with a lesser value of $P$, say $P = 0.05$, the effects of thermal expansion on the distributions of velocity and temperature are significant. In these cases, taking the thermal expansion into account is essential for an accurate modeling.

The density distributions across the channel predicted by the two theories are shown in Figure 3. In our constrained theory the density has a local maximum in the center of channel, reflective of the depressed temperature there due to expansion cooling. In the ad hoc theory, the density minimum is in the center of the channel. Since the ad hoc theory cannot model the lowering of temperature at mid-channel due to expansion cooling, it underestimates fluid density there.

The errors in material density and velocity distributions that result from the use of the ad hoc theory have contrary effects on the mass flow rate: the overestimated fluid temperature lowers fluid viscosity and thus leads to higher velocity, as shown in Figure 2, and therefore too high a volume flow rate; on the other hand, the underestimated density distribution in the ad hoc theory underpredicts mass flow rate. In the simulation shown in Figure 4, with $E = 5.0$ and $Br=0.2$, the net result of the two competing errors in the ad hoc theory is an overprediction of the mass flow rate. Figure 4 compares the dimensionless mass flow rates, $\int_0^1 \tilde{\rho} \tilde{v} \, d\tilde{z}$, resulting from the velocity and density profiles predicted by the two theories as functions of parameter
Figure 3: The density distribution across the channel for different levels of temperature dependence of density: $E = 5.0$, $Br = 0.2$, varying $P$. The horizontal coordinate is the dimensionless density, and the vertical coordinate is the dimensionless transverse coordinate $\tilde{x}_2$. Solid lines are the predictions from the constrained theory, and dashed lines are the predictions from the ad hoc formulation.
Table 1: PET properties and flow conditions used in the simulations of channel flows and the corresponding dimensionless numbers

<table>
<thead>
<tr>
<th>Material properties for PET</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Density coefficient $\rho_0 =$</td>
<td>1493 $\text{kg \cdot m}^{-3}$ 1</td>
</tr>
<tr>
<td>Density coefficient $\rho_1 =$</td>
<td>0.5 $\text{kg \cdot m}^{-3} \cdot \text{K}^{-1}$ 1</td>
</tr>
<tr>
<td>Thermal conductivity $k =$</td>
<td>0.147 $\text{W \cdot m}^{-1} \cdot \text{K}^{-1}$ 2</td>
</tr>
<tr>
<td>Intrinsic viscosity [$\eta =$</td>
<td>0.6450 $\text{dl} \cdot \text{g}^{-1}$ 2</td>
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<tr>
<td>Activation energy $\mathcal{E} =$</td>
<td>$56.54 \times 10^3$ $\text{J \cdot mole}^{-1}$ 1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flow conditions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall separation $h =$</td>
<td>0.2 $\text{mm}$</td>
</tr>
<tr>
<td>Wall temperature $\theta_w =$</td>
<td>285 °C = 558.2 K</td>
</tr>
<tr>
<td>Viscosity $\mu_w$ at wall temperature $=</td>
<td>204.6 \text{ Pa} \cdot \text{s}^3 $</td>
</tr>
<tr>
<td>shear stress at wall $\tau_w =$</td>
<td>variable</td>
</tr>
</tbody>
</table>

<table>
<thead>
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<th>Dimensionless numbers</th>
<th></th>
</tr>
</thead>
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<tr>
<td>Arrhenius number $E =$</td>
<td>12.18</td>
</tr>
<tr>
<td>Brinkman number $\mathcal{B} = \mathcal{B}(\tau_w) =$</td>
<td>$0.1489\tau_w^2$ $\text{MPa}^{-2}$</td>
</tr>
<tr>
<td>Dimensionless expansion number $P =$</td>
<td>0.1869</td>
</tr>
</tbody>
</table>

1 Hayashi et al [37].
2 Polymer Handbook [1].
3 Calculated by $\mu(\theta) = [\eta]^{0.18}\exp\left\{\frac{J}{R} - 2.3\right\} \text{poise}.$

$P$. Note that the incorrect ad hoc theory overestimates the mass flow rate for any material with temperature-dependent density. The difference is significant even for moderate temperature dependence of density: e.g. when $P = 0.1$, the dimensionless mass flow rate predicted by the ad hoc theory is 5.9 percent higher than the correct value predicted by the constrained theory.

As an explicit example, when Poly(Ethylene Terephthalate) (PET) is melt processed in a steady nonisothermal plane Poiseuille flow with a wall temperature $\theta_w$ of 558.2K, the dimensionless numbers $E$ and $P$ are calculated to be 12.18 and 0.1869, respectively (see Table 1).
Figure 4: The dimensionless mass flow rate as a function of the level of temperature dependence of density in plane Poiseuille flows: $E = 5.0$, $Br = 0.2$, varying $P$. 
The Brinkman number is in addition a function of the shear stress at wall, \( \tau_w \), or equivalently, the imposed pressure gradient \( \beta = 2\tau_w/h \). When \( Br = 0.1 \) (\( \tau_w = 0.82 \text{ MPa}, \beta = 8.2 \text{ MPa/mm} \)), the dimensionless mass flow rate predicted by the constrained theory is 0.7983 and by the ad hoc theory is 0.9574, respectively. The ad hoc theory then overestimates the mass flow rate at this pressure gradient by 19.93 percent.

The relation between volume flow rate and either pressure drop or shear stress at wall is important in many processes and viscometric measurements. To study this relation, we compute the dimensional volume flow rate per unit channel width, as a function of shear stress at wall \( \tau_w \), predicted by the two theories for the process described in Table 1. For comparison, we also compute the volume flow rate per width given by the exact solution for a flow with "effective" constant values of density and viscosity. The exact solution follows from setting \( E = P = 0 \) in the boundary value problem (3.22), (3.23), and (3.25), and is given in equations (3.26). The effective constant values of density and viscosity in this modeling are taken as their values at the wall temperature, i.e. \( \rho = \rho_w, \eta = \eta_w \).

Figure 5 shows that the ad hoc theory underestimates the shear stress at walls \( \tau_w \) which is calculated from a specified the volume flow rate, or, viewed differently, the ad hoc theory overestimates the volume flow rate under an imposed pressure gradient necessary to produce a flow. On the other hand, assuming no temperature dependence of viscosity or neglecting the effect of viscous heating (isothermal flow), the isothermal "effective" model results in overestimates \( \tau_w \) with a specified volume
Figure 5: The relation between volume flow rate per unit width of the channel and shear stress at wall $\tau_w$ in the flow direction for the PET melt processing of Table 1, calculated from the constrained theory with comparison to the isothermal "effective" solution.
flow rate. Therefore, one will overdo the correction of viscometric measurements when considering the effect of viscous heating but neglecting the effect of thermal expansion. In Figure 5, the flow rate increases nearly linearly with \( \tau_w \) when \( \tau_w \) is small. In the lower range of shear stress, in other words, small shear rate, the three theories give close results. The correction with the viscous heating to the result given in the "exact" solution can broaden the valid range of measurements without consideration of thermal expansion. That has been tried by Lodge & Ko [53]. As the pressure gradient increases, both the constrained and ad hoc theories predict that the relations between volume flow rate and shear stress at walls are nonlinear, the isothermal "effective" model gives a linear function. But the mass flow rate predicted by the ad hoc theory increases much too rapidly with increasing pressure gradient. At the specified volume flow rate 0.15 cm\(^3\)/s/cm, the isothermal "effective" model produces an error of +4.57 percent in the wall shear stress, and the ad hoc theory produces an error of -2.46 percent. As the flow rate increases, so do the errors: for 0.38 cm\(^2\)/s the isothermal "effective" model and ad hoc theory give errors of +27.7 and -10.8 percent, respectively. For such flow rates, process modeling based on either the ad hoc theory or the isothermal "effective" model can lead to serious design flaws.

Another important phenomenon is that there is no solution to the boundary value problem of the steady, fully-developed nonisothermal flow from the constrained theory when the pressure gradient exceeds a certain level. That also be noticed in the incompressible flow (the same as the ad hoc theory in the presented case) by Martin [54] and Sukanek [68]. The solution with constant density and viscosity cannot predict
The effects of temperature dependence of density are augmented by large $\text{Br}$, as shown in Figure 6. When there is viscous heating in the flow of a fluid with poor thermal conductivity (and hence large $\text{Br}$), the concavity in the temperature distribution at mid-channel deepens, the bulk temperature and mean velocity in the channel increase, and the temperature and velocity gradients at wall become greater, relative to a fluid with good thermal conductivity. The effect of temperature dependence of viscosity, or equivalently $E$, on the temperature distribution is similar to that of $\text{Br}$ just described, but much less pronounced (see Figure 7). The development of concavity in temperature profile is a consequence of temperature dependence of density, strongly affected by the Brinkman number of the flow.

Figure 8 illustrates the danger of neglecting temperature dependence of density and viscosity altogether in the modeling of a process. The isothermal "effective" solution for temperature-independent viscosity and density differs greatly from the result given by the constrained theory for a process with $\text{Br} = 0.1$, $E = 10$ and $P = 0.2$, and cannot capture the phenomenon of expansion cooling. The maximum dimensionless temperature predicted by the constant density/constant viscosity theory is 1.033 at the middle of the channel, and by the constrained theory is 1.020 at dimensionless transverse coordinate 0.3. If the material is processed at a wall temperature of 558.2 K, this means the mid-channel temperature predicted by the constant density/constant viscosity solution is 7.1 K higher than the correct temperature given by the constrained theory. For comparison, the mid-channel temperature predicted by
Figure 6: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows with isothermal walls as predicted by the constrained theory, showing the effect of varying the thermal conductivity of the fluid: $E = 5.0, P = 0.1$, varying $Br$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{z}_2$. 
Figure 7: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows with isothermal walls as predicted by the constrained theory, showing the effects of temperature dependence of viscosity: $Br = 0.1$, $P = 0.1$, varying $E$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{x}_2$. 
Figure 8: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows as predicted by the constrained theory and the ad hoc theory, which model temperature dependence of density and viscosity: $E = 10.0, Br = 0.1, P = 0.2$; and by the exact solution for a fluid which replaces density and viscosity with effective constant values: $Br = 0.1$. 
the ad hoc theory is 15.3 K too high.

3.3 Plane Poiseuille Flows with Finite Heat Loss Coefficient

3.3.1 The Boundary Value Problem

The condition of isothermal wall, which has been used in the analysis in Section 3.2, is an idealized thermal boundary condition that assumes an infinite thermal conductivity for the wall material. In this section we model the more realistic and industrially-practical boundary condition

\[
\frac{d\theta}{dx_2} = H(\theta - \theta_w), \quad x_2 = \pm \frac{h}{2},
\]

(3.30)

where \(\theta_w\) is a specified constant temperature. There are two limiting cases for this boundary condition: when \(H\) approaches zero, the walls are adiabatic (i.e. perfectly insulated); when \(H\) approaches infinity, the walls are isothermal (as in the previous section). In the modeling of real industrial processes, the heat loss coefficient \(H\) is a finite number.

In this section, the flow behaviors are studied as the heat loss coefficient is varied. The governing equations (3.12) and (3.13) for the velocity and temperature fields within the channel remain the same, and the no-slip condition (3.2) is kept, but the isothermal condition (3.2) is replaced with condition (3.30). Since the heat loss coefficient \(H\) is included in the newly defined boundary value problem, in addition to the Brinkman number, \(E\) number, and \(P\) number, one more dimensionless number,
the Biot number

$$\text{Bi} = \frac{H \delta}{k},$$

(3.31)
is needed to complete the nondimensionalized boundary value problem. This dimensionless boundary value problem consists of eqs. (3.22), (3.23) and the boundary conditions

$$\bar{v}_1 = 0, \quad \frac{d\bar{\theta}}{d\bar{x}_2} = \text{Bi}(1 - \bar{\theta}) \quad \bar{\theta}(\bar{x}_2) = \pm \frac{1}{2}. \quad (3.32)$$

The exact, unique solution of the two point boundary value problem with temperature-independent viscosity and density, i.e. with $E = P = 0$, is used as the initial guess in the ODE solver. This solution is

$$\tilde{v}_1(\tilde{x}_2) = 1 - 4\tilde{x}_2^2, \quad \tilde{\theta}(\tilde{x}_2) = 1 + \frac{8\text{Br}}{3\text{Bi}} + \frac{\text{Br}}{3}(1 - 16\tilde{x}_2^4). \quad (3.33)$$

### 3.3.2 Comparison of the Solutions and Discussion

The effects of thermal boundary condition on the velocity and temperature fields are shown in Figure 9. The velocity and temperature distributions are plotted for fixed $E, \text{Br}, P$, and varied $\text{Bi}$, to focus on the effects of the heat loss condition at the walls of slit die. An increase of $\text{Bi}$ is equivalent to an increase of $H$ with all other flow conditions held constant. The solution for a large Biot number approaches the solution for the isothermal wall case, as shown in Figure 9. With a smaller $\text{Bi}$, the bulk temperature and the average velocity of fluid increases. The phenomenon of depression in temperature profile becomes more significant for a smaller Biot number. Approaching the adiabatic case ($\text{Bi} \to 0$), the effect of expansion cooling dominates.
Figure 9: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows with varying heat loss conditions as predicted by the constrained theory, showing the effects of thermal boundary condition at the die walls: $E = 5.0$, $Br = 0.2$, $P = 0.2$, varying $Bi$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{x}_2$. 
the distributions of velocity and temperature (see Figure 10). For flows in slit die with adiabatic walls (Bi = 0), the fluid temperature and velocity continuously increase down the channel, and fully-developed flow conditions are not established.

For a fixed Biot number, the effects of temperature-dependent density on the velocity and temperature fields are shown in Figure 11. Although the temperature profiles have the same shapes as the temperature profiles with the same $E$ and $Br$ in the isothermal wall case, there are significant increases in the maximum values of temperature and velocity due to temperature dependence of viscosity, as can be seen from a comparison with Figure 2. Together with Figure 9, Figure 11 shows the importance of the interplay of the heat loss condition and the thermal expansion on the velocity and temperature distributions. Failing to take into account thermal expansion and the appropriate thermal boundary condition, i.e. the heat loss coefficient $H$, can lead to erroneous results.

We show in Figure 12 the effect of varying Bi on the volume flow rate. Specifically, Figure 12 demonstrates that how finite heat loss condition at the die walls influences the relation between volume flow rate per unit width of the channel and shear stress at wall $\tau_w$ for the PET melt processing of Table 1. The capacity of flow passing the die becomes larger as the heat loss coefficient gets smaller. This is because the viscosity decreases with the increase of fluid temperature, i.e. the fluidity (inverse of viscosity) is improved. For a specified volume flow rate in viscometric measurements, the corresponding shear stress at wall $\tau_w$ is larger with the improved condition of heat loss through the die walls (i.e. higher $H$). The isothermal “effective” solution with
Figure 10: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows with varying heat loss conditions as predicted by the constrained theory, showing the effects of thermal boundary condition at the die walls: $E = 5.0$, $Br = 0.2$, $P = 0.2$, varying Bi. The vertical coordinate is the dimensionless transverse coordinate $\tilde{x}_2$. 
Figure 11: The transverse velocity and temperature distributions in nonisothermal plane Poiseuille flows as predicted by the constrained theory, showing the effects of varying the level of temperature dependence of density: $E = 5.0$, $Br = 0.2$, $Bi = 20$, varying $P$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{x}_2$. 
Figure 12: The effect of varying heat loss conditions on the relation between volume flow rate per unit width of the channel and shear stress at wall $\tau_w$ in the flow direction for the PET melt processing of Table 1.
Figure 13: Fully-developed nonisothermal capillary flow with varying thermal wall conditions.

no temperature dependence of viscosity and density is included for comparison.

As can be seen by comparing Figure 12 to Figure 5, the curve calculated from the constrained theory with a prescribed thermal expansion and a particular nonzero value of $Bi$ is close to the curve calculated from the ad hoc theory without thermal expansion with isothermal walls. It seems that two mistakes (neglect of thermal expansion and neglect of heat loss through the walls) combine to produce the right answer in this particular case, but it is not true for general situation for thermal expansion and heat loss conditions.

3.4 Nonisothermal Capillary Flows

Capillary flows is another type of channel flows. In particular, it is the flow in the die proceeding the process of fiber spinning that we will study in Chapters 4, 5, 6. Capillary flows in fully-developed conditions are shown in Figure 13. We employ the
cylindrical coordinates \((r, \phi, z)\) with the \(z\)-axis in the flow direction, denote the radius of the capillary by \(r_0\).

Repeating the procedure of Section 3.2 we obtain the dimensionless boundary value problem. The dimensionless forms of governing equations are

\[
\frac{d\hat{v}_z}{d\hat{r}} = -2\hat{r}\exp\left[-E\left(\frac{1}{\hat{\theta}} - 1\right)\right],
\]

\[
\frac{d^2\hat{\theta}}{d\hat{r}^2} + \frac{1}{\hat{r}} \frac{d\hat{\theta}}{d\hat{r}} = -Br\hat{r}^2\exp\left[-E\left(\frac{1}{\hat{\theta}} - 1\right)\right] + BrP\frac{\hat{v}_z\hat{\theta}}{1 - P\hat{\theta}},
\]

where \(\hat{r} = \frac{r}{r_0}, \hat{\theta} = \frac{\theta}{\theta_w}, \hat{v}_z = \frac{v_z}{\nu_w r_0},\) and

\[
Br = \frac{\tau_w r_0^2}{k \mu_w \theta_w}, \quad Bi = \frac{H r_0}{k}, \quad E = \frac{\mathcal{E}}{R \theta_w}, \quad P = \frac{\rho_1 \theta_w}{\rho_0}.
\]

The dimensionless boundary conditions are two symmetry conditions at the centerline,

\[
\frac{d\hat{v}_z}{d\hat{r}} = 0, \quad \frac{d\hat{\theta}}{d\hat{r}} = 0 \quad \forall \hat{r} = 0,
\]

and no-slip and heat loss at the wall,

\[
\hat{v}_z = 0, \quad \frac{d\hat{\theta}}{d\hat{r}} = Bi(1 - \theta) \quad \forall \hat{r} = 1.
\]

The relation of the shear stress at the wall \(\tau_w\) and the pressure drop rate \(\beta\) in this case is

\[
\tau_w = \frac{1}{2} \beta r_0.
\]

The effects of temperature-dependent density on the velocity and temperature fields are shown in Figure 14. The curve with \(P = 0\) represents the predicted temperature distribution without consideration of thermal expansion, which is the same as that predicted by the \textit{a posteriori} treatment of temperature-dependent density or
Figure 14: The transverse velocity and temperature distributions in nonisothermal capillary flows as predicted by the constrained theory, showing the effects of varying the level of temperature dependence of density: $E = 5.0$, $Br = 0.2$, $Bi = 20$, varying $P$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{r}$. 
by the incompressible theory. As noted elsewhere (Duda et al. [22], Winter [75]), the temperature profile in this case has a broad, flat plateau in the center of the capillary. In contrast, the constrained theory predicts a local minimum at the center and an average temperature that can be much lower. Comparing Figure 14 to Figure 2, we see similar patterns of the effect of temperature-dependent density on the velocity and temperature distributions in the capillary flow and in the slit die flow, but with less sensitivity of velocity to the effect of temperature-dependent density in the capillary.

The effects on the velocity and temperature fields in the capillary from varying the heat loss condition are shown in Figure 15. The shape of temperature profiles does not change much for a wide range of Biot number, but there is a significant increase in the fluid average temperature. The velocity profiles are changed through the temperature-dependent viscosity.

For a case of isothermal wall, Figure 16 shows that the incompressible theory overestimates the volume flow rate through the capillary, as does it in the slit die case. In viscometric measurements, too high a value of shear stress will be predicted for a specified volume flow rate by the incompressible theory with no temperature dependence of density. This tendency is similar to the observation in slit die flows. Figure 17 shows that the effect of varying heat loss condition on the relation between volume flow rate and wall shear stress. Again, the need to separate the effects of the thermal expansion cooling from the effects of varying heat loss condition is demonstrated. The isothermal “effective” solution with no temperature dependence of viscosity and density is included in Figure 16 and 17 for comparison.
Figure 15: The transverse velocity and temperature distributions in nonisothermal capillary flows with finite heat loss coefficient as predicted by the constrained theory, showing the effects of thermal boundary condition: $E = 5.0$, $Br = 0.2$, $P = 0.2$, varying $Bi$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{r}$. 
Figure 16: The relation between volume flow rate and shear stress at wall $\tau_w$ in the flow direction for the PET melt processing of Table 1, calculated from the constrained theory with comparison to the isothermal "effective" solution: capillary flows with isothermal walls.
Figure 17: The relation between volume flow rate and shear stress at wall $\tau_w$ in the flow direction for the PET melt processing of Table 1, calculated from the constrained theory: the effect of varying Biot number in capillary flows.
The outer wall has radius $r = r_2$, and the inner wall has radius $r = r_1$.

The dimensionless form of momentum and energy equations is for the annular flow

$$\frac{d^2\tilde{v}_z}{dr^2} + \frac{1}{r} \frac{d\tilde{v}_z}{dr} = -Br (\frac{d\tilde{v}_z}{dr})^2 \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] + 8BrP \frac{\tilde{v}_z \tilde{\theta}'}{1 - P\tilde{\theta}'}.$$  \hspace{1cm} (3.41)

where $\tilde{r} = \frac{r}{r_1}, \tilde{\theta} = \frac{\theta}{\theta_\infty}, \tilde{v}_z = \frac{\tilde{v}_z}{\mu h^2},$ where $h = r_2 - r_1$, and

$$Br = \frac{\beta^2 h^4}{64k\mu \theta_\infty}, \quad Bi = \frac{Hh}{k}, \quad E = \frac{E}{R\theta_\infty}, \quad P = \frac{\rho_1\theta_\infty}{\rho_0}.$$  \hspace{1cm} (3.42)

The heat loss conditions at the walls in dimensionless form are described through the Biot numbers, where $Bi = 0$ corresponds to a perfectly insulated adiabatic wall.
and $\text{Bi} = \infty$ to an isothermal wall. No-slip conditions are assumed at both the inner and outer cylindrical walls. Therefore the dimensionless boundary conditions are

$$\begin{align*}
v_z &= 0, \quad \frac{d\tilde{\theta}}{d\tilde{r}} = \text{Bi}_1(1 - \tilde{\theta}) \quad @ \tilde{r} = \tilde{r}_1, \\
v_z &= 0, \quad \frac{d\tilde{\theta}}{d\tilde{r}} = \text{Bi}_2(1 - \tilde{\theta}) \quad @ \tilde{r} = \tilde{r}_2. \quad (3.43)
\end{align*}$$

The inner wall is usually modeled with a small Biot number since heat loss through the inner cylinder is difficult.

The boundary value problem stated above is the modeling of the flow in a die for film blowing and coextrusion processes. The effects of temperature-dependent density on the velocity and temperature fields in the annular flow with boundary conditions (3.43) for a fixed Biot numbers are shown in Figure 19. It is evident that the ad hoc theory is inapplicable in the modeling even for a very moderate temperature dependence of density since the temperature and velocity profiles are very sensitive to the effects of temperature dependence of density.

The effects of the thermal boundary condition at outer wall on the velocity and temperature fields are shown in Figure 20. The effect of thermal expansion cooling produces an inflection point in the temperature profile. The asymmetric velocity and temperature profiles are due to the geometry of annular dies and the different heat loss conditions at the inner and outer walls. Figure 21 compares the predictions of volume flow rate by the constrained theroy and the \textit{a posteriori} treatment for prescribed temperature dependence of density with the isothermal outer wall/adiabatic inner wall case. Figure 22 shows that the effect of the varying the outer wall Biot number on the volume flow rate through the annular die.
Figure 19: The transverse velocity and temperature distributions in nonisothermal annular flows between an adiabatic inner wall and an outer wall with finite heat loss coefficient as predicted by the constrained theory, showing the effects of varying the level of temperature dependence of density: \( E = 3.0, \ Br = 0.2, \ Bi_1 = 0, \ Bi_2 = 10.0, \) varying \( P; \) inner radius vs. wall separation \( \frac{r}{R} = 0.5. \) The vertical coordinate is the dimensionless transverse coordinate \( \hat{r}. \)
Figure 20: The transverse velocity and temperature distributions in nonisothermal annular flows between an adiabatic inner wall and an outer wall with finite heat loss coefficient as predicted by the constrained theory, showing the effects of thermal boundary condition: $E = 5.0$, $Br = 0.2$, $Bi_1 = 0$, $P = 0.2$, varying $Bi_2$; $\frac{h}{a} = 0.5$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{r}$.
Figure 21: The relation between volume flow rate and pressure drop rate $\beta$ in the flow direction for the PET melt processing of Table 1, calculated from the constrained theory with comparison to the isothermal "effective" solution: the adiabatic inner wall isothermal outer wall case ($B_i = 0$ and $B_o = \infty$); $\frac{T_e}{T_i} = 0.5$. 
Figure 22: The relation between volume flow rate and pressure drop rate $\beta$ in the flow direction for the PET melt processing of Table 1, calculated from the constrained theory: the effect of a varying outer wall Biot number in the adiabatic inner wall case ($Bi_1 = 0$); $\frac{h}{k} = 0.5$. 
For comparison to plane Poseuille flows, the results for the inner and outer wall with the same heat transfer conditions are shown in Figures 23–26. Shown is the case with the ratio of the inner radius to the wall separation equal to 0.5. The distortion in the velocity and temperature profiles is more pronounced with the smaller ratio of the inner radius to wall separation. When the inner radius is more than twice the wall separation, the profiles of temperature and velocity approach those for the plane flow with the same wall separation.
Figure 23: The transverse velocity and temperature distributions in nonisothermal annular flows with heat loss conditions same for both inner and outer walls as predicted by the constrained theory, showing the effects of varying the level of temperature dependence of density: $E = 5.0$, $Br = 0.2$, $Bi_1 = Bi_2 = 20$, varying $P$; $\frac{r}{R} = 0.5$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{r}$.
Figure 24: The transverse velocity and temperature distributions in nonisothermal annular flows with heat loss conditions same for both inner and outer walls as predicted by the constrained theory, showing the effects of thermal boundary conditions: $E = 5.0$, $Br = 0.2$, $P = 0.2$, varying $Bi_1 = Bi_2 = Bi$; $\beta = 0.5$. The vertical coordinate is the dimensionless transverse coordinate $\tilde{r}$. 
Figure 25: The relation between volume flow rate and pressure drop rate \( \beta \) in the flow direction for the PET melt processing of Table 1, calculated from the constrained theory with comparison to the isothermal "effective" solution: isothermal inner and outer walls (\( B_i = B_i = \infty \)).
Figure 26: The relation between volume flow rate and pressure drop rate $\beta$ in the flow direction for the PET melt processing of Table 1, calculated from the constrained: the effect of varying Biot number.
CHAPTER IV

The Rigid Rod Model for Solidified Fibers in the Melt Spinning Process

In the fiber spinning of polymers, fibers continue to cool down beyond the glass transition and the processing length is usually long enough to allow the fiber temperature to cool to the ambient temperature. A rigid rod model can be used directly to model the fiber behavior in the range from solidification point to take-up location (the solidified zone in Figure 27).

The rigid rod model will also be useful in modeling the molten zone in melt spinning, where the cooling polymer is still a fluid (see Figure 27). The temperature field in the slender cooling filament is fundamentally different from the axial velocity and normal stress fields. The radial distributions of axial velocity and normal stresses can effectively be assumed uniform to leading order, with zero radial gradients. In contrast, although the temperature difference between the centerline and the surface is small, this difference is important, and the temperature gradient in radial direction is large and a leading order effect since the fiber is slender. The rigid rod solution will be employed to develop a 1-dimensional leading order thin filament model for the polymer melt which can account for this radial temperature variation.
Figure 27: Schematic configuration of melt spinning process with cooling ambient
4.1 The Steady 3-Dimensional Boundary Value Problem for Solidified Fibers

The concept of rigid rod here is based on the theory of constrained material and its constraint response. In the present rigid rod model, the material properties of density, specific heat, and thermal conductivity are assumed constant when body temperature changes. For the rigid fiber the constraint is six mechanical constraint equations

\[ A_i \cdot D = 0, \quad (4.1) \]

where

\[ A_i = e_1 \otimes e_1, e_1 \otimes e_2, e_1 \otimes e_3, e_2 \otimes e_2, e_2 \otimes e_3, e_3 \otimes e_3, \quad (4.2) \]

where \( e_1, e_2, e_3 \) is a basis of \( E^3 \) space. Then, the six scalar constraint equations reduce to the tensor equation

\[ D = 0. \quad (4.3) \]

The corresponding constraint response is

\[ T = \text{arbitrary}. \quad (4.4) \]

In the torsionless axisymmetric case, the constraint eq. (4.3) in cylindrical coordinates becomes

\[ D = \begin{bmatrix} \frac{\partial \nu_r}{\partial r} & 0 & \frac{\partial \nu_r}{\partial \theta} \\ 0 & \frac{\nu_r}{r} & 0 \\ \frac{\partial \nu_r}{\partial r} & 0 & \frac{\partial \nu_r}{\partial \theta} \end{bmatrix} = 0, \quad (4.5) \]

which in the steady state implies

\[ \nu_r = 0, \quad \nu_\theta = \text{constant}, \quad (4.6) \]
and
\[ \phi = \text{constant}. \] \hspace{1cm} (4.7)

As a consequence of constant radius and spinning velocity of the rigid fiber, the heat loss coefficient \( h \) is a constant if the quenching ambient conditions are held unchanged. The governing equation then reduces in the steady case to
\[ \rho c v_z \frac{\partial \theta}{\partial z} = k \nabla^2 \theta, \] \hspace{1cm} (4.8)

with boundary conditions
\[ -k \left( \frac{\partial \theta}{\partial r} \right) \bigg|_{0} = h(\theta - \theta^o)|_0, \quad \left( \frac{\partial \theta}{\partial r} \right) \bigg|_{r=0} = 0, \] \hspace{1cm} (4.9)

\[ \theta|_{z=0} = \theta_0(r), \quad \theta|_{z=l} = \theta_1(r). \] \hspace{1cm} (4.10)

The origin of the coordinate system is set up at the solidification point; \( l \) is the length from the solidification point to the take-up position.

### 4.2 The Exact Solution for the Temperature Field

We now obtain an exact solution for the 2-dimensional distribution of temperature in the \( r \) and \( z \) directions in the cooling rigid fiber. We start by nondimensionalizing the reduced thermal boundary value problem, eqs. (4.8)-(4.10). Let \( r_c, z_c, v_c, \theta_c \) be the characteristic values for transverse length, axial length, velocity, and absolute temperature, respectively. Since the radius and velocity of the rigid fiber are constant, they are naturally chosen as the characteristic values \( r_c \) and \( v_c \). The glass transition temperature of polymer is also chosen as the characteristic temperature \( \theta_c \). The
length of the rigid filament from solidification point to take-up position is used as the characteristic axial length $z_c (= l)$. We use these characteristic values to scale all dimensional quantities in the rigid rod boundary value problem: the dimensionless independent variables $\tilde{r}$ and $\tilde{z}$ are defined as

$$\tilde{r} = \frac{r}{r_c}, \quad \tilde{z} = \frac{z}{z_c},$$

and the dimensionless dependent variable temperature (a function of $r$ and $z$ only, due to axisymmetry) is defined as

$$\theta(r, z) = \theta_0(\tilde{r}, \tilde{z}).$$

Quantities without tildes are dimensional and the quantities with tildes are dimensionless. The slenderness parameter is defined as

$$\epsilon = \frac{r_c}{z_c}.$$

With the above definition of $z_c$, the end boundaries of the rigid fiber are temperature at $\tilde{z} = 0$ (the solidification point) and $\tilde{z} = 1$ (the take-up position).

The dimensionless form of the boundary value problem is

$$\tilde{\theta}_{,\tilde{z}} = \frac{1}{Gz} \left( \tilde{\theta}_{,\tilde{r}} + \frac{1}{\tilde{r}} \tilde{\theta} + \epsilon^2 \tilde{\theta}_{,\tilde{z}^2} \right) \text{ for } 0 \leq \tilde{r} \leq 1, 0 \leq \tilde{z} \leq 1,$$

$$\tilde{\theta}_{,\tilde{r}}\big|_{\tilde{z}=1} = -Bi (\tilde{\theta} - \tilde{\theta}^*)\big|_{\tilde{z}=1}, \quad \tilde{\theta}_{,\tilde{r}}\big|_{\tilde{z}=0} = 0,$$

$$\tilde{\theta}\big|_{\tilde{z}=0} = \tilde{\theta}_0(\tilde{r}), \quad \tilde{\theta}\big|_{\tilde{z}=1} = \tilde{\theta}_1(\tilde{r}).$$

Two dimensionless numbers, the Graetz number and the Biot number, are involved,

$$Gz = \frac{\rho cv_c r_c^2}{k z_c}, \quad Bi = \frac{hr_c}{k}.$$
We seek a solution to (4.14)–(4.16) of the form

\[ \hat{\theta} = \hat{\theta}_a + \hat{\theta}_R(\hat{r}) \hat{\theta}_Z(\hat{z}). \]  

(4.18)

This separation of spatial variables leads to a second-order ODE for the axial temperature variation,

\[ \frac{d^2 \hat{\theta}_Z}{d\hat{z}^2} - \frac{\epsilon^2}{Gz} \frac{d^2 \hat{\theta}_Z}{d\hat{z}^2} + \frac{A^2}{Gz} \hat{\theta}_Z = 0, \]  

(4.19)

and a second-order ODE and boundary conditions for the radial temperature variation,

\[- \left( \frac{d^2 \hat{\theta}_R}{d\hat{r}^2} + \frac{1}{\hat{r}} \frac{d \hat{\theta}_R}{d\hat{r}} \right) - A^2 \hat{\theta}_R = 0, \]  

(4.20)

\[ \left. \frac{d \hat{\theta}_R}{d\hat{r}} \right|_{\hat{r}=1} = -Bi \hat{\theta}_R|_{\hat{r}=1}, \]  

(4.21)

\[ \left. \frac{d \hat{\theta}_R}{d\hat{r}} \right|_{\hat{r}=0} = 0, \]  

(4.22)

where \( A^2 \) is the separation of variables parameter.

The solution of (4.20), subject to the boundary conditions (4.21) and (4.22), is

\[ \hat{\theta}_R = C J_0(A\hat{r}), \]  

(4.23)

where \( J_0 \) denotes the zeroth Bessel function, and \( A \) is an eigenvalue which satisfies the characteristic equation

\[ -AJ_0(A) = BiJ_0(A). \]  

(4.24)

Solving (4.19) gives

\[ \hat{\theta}_Z = C_1 \exp(\lambda_1 \hat{z}) + C_2 \exp(\lambda_2 \hat{z}), \]  

(4.25)

where

\[ \lambda_1 = \frac{Gz - \sqrt{Gz^2 + 4\epsilon^2 A^2}}{2\epsilon^2}, \quad \lambda_2 = \frac{Gz + \sqrt{Gz^2 + 4\epsilon^2 A^2}}{2\epsilon^2}. \]  

(4.26)
With combination of (4.23) and (4.25), the complete solution in the separation of variables form is

\[ \tilde{\theta} = \tilde{\theta}_0 + \sum_{i=0}^{\infty} J_0(A_i \tilde{r}) [C_{1i} \exp(\lambda_{1i} \tilde{z}) + C_{2i} \exp(\lambda_{2i} \tilde{z})], \quad (4.27) \]

where \( A_i \) is \( i \)-th eigenvalue of the characteristic equation (4.24) and corresponding to each eigenvalue \( A_i \) are the pair of parameters \( \lambda_{1i} \) and \( \lambda_{2i} \),

\[ \lambda_{1i} = \frac{Gz - \sqrt{Gz^2 + 4\epsilon^2 A_i^2}}{2\epsilon^2}, \quad \lambda_{2i} = \frac{Gz + \sqrt{Gz^2 + 4\epsilon^2 A_i^2}}{2\epsilon^2}, \quad (4.28) \]

The first three eigenvalues of eq.(4.24) as functions of \( B_i \) are shown in Figure 28. The orthogonality of the eigenfunctions states that

\[ \int_0^1 J_0(A_i \tilde{r}) J_0(A_j \tilde{r}) \tilde{r} d\tilde{r} = 0, \quad i \neq j. \quad (4.29) \]

The coefficients \( C_{1i} \) and \( C_{2i} \) in (4.27) are determined by the temperature distributions (4.16) at the two axial boundaries of the fiber:

\[ C_{1i} = \frac{\int_0^1 J_0(A_i \tilde{r})(\tilde{\theta}_i - \tilde{\theta}_0) \tilde{r} d\tilde{r}}{C_i (e^{A_{1i} \tilde{r}} - e^{A_{2i} \tilde{r}})}, \quad C_{2i} = \frac{\int_0^1 J_0(A_i \tilde{r})(\tilde{\theta}_1 - e^{A_{1i} \tilde{r}} \tilde{\theta}_0) \tilde{r} d\tilde{r}}{C_i (e^{A_{1i} \tilde{r}} - e^{A_{2i} \tilde{r}})}, \quad (4.30) \]

where

\[ C_i = \int_0^1 J_0^2(A_i \tilde{r}) \tilde{r} d\tilde{r}. \quad (4.31) \]

We now study the convergence property of the solution (4.27) with respect to the summed terms. For typical parameters \( B_i = 0.65, Gz = 0.3 \), slenderness parameter \( \epsilon = 0.02 \), and axial boundary conditions \( \tilde{\theta}_0 = 1.0 \) and \( \tilde{\theta}_i = 0.92 \), the second term is very small compared to first term: in Figure 29 the plots of the single term truncation and two term truncation of solution (4.27) overlay one another. (For a temperature
Figure 28: The first three eigenvalues as functions of the Biot number.
Figure 29: The cross-sectionally averaged temperature profile: $Bi=0.65$, $Gz=0.3$, $\varepsilon=0.02$; The take-up temperature and ambient temperature are 0.92 and 0.8912, respectively.
scale of 67°C (PET glass transition temperature), the dimensionless temperature 0.92 and ambient temperature 0.8912 represent 39.8 and 30°C, respectively.) For a smaller \( \epsilon \) the second and higher terms are even more confined to the small neighborhood of the take-up position. We conclude that for slender jet spinning the accuracy of the first term solution is sufficient. Further, notice from (4.28) that the exponential coefficients \( \lambda_{2i} \) is of order \( O(\epsilon^2) \). When the rigid rod is slender, i.e. \( \epsilon \) is very small, it is evident in (4.28) and (4.30) that \( \lambda_{2i} \) is very large and the corresponding coefficient \( C_{2i} \) is very small. Thus, for spinline temperature distribution not in the neighborhood of take-up point, the only term in summation (4.27) needed is the one with coefficient \( C_{11} \), i.e.

\[
\tilde{\theta}(\bar{r}, \bar{z}) = \bar{\theta}^a + C_{11} J_0(A_1 \bar{r}) \exp(\lambda_{11} \bar{z}). \tag{4.32}
\]

Figure 30 shows the effect of Biot number on the radial temperature distribution. The radial temperature distribution is determined by the Biot number through parameter \( A_1 \) in equation (4.32). The distribution is normalized by the average temperature. Shown in Figure 28, \( A_1 \) is a highly nonlinear, monotonous function of Biot number. For a larger Biot number, \( A_1 \) increases and the radial temperature variation is more pronounced. The temperature may be considered as radially uniform only for a very small Biot number. For a typical Biot number, the radial temperature variation is considerable.

Figure 31 shows the evolution of the centerline, surface and average temperature from the exact solution for the solidified fiber. Notice that the radial temperature varies across the fiber even though the temperature at the starting point is assumed uniform. The radial temperature difference is evident along the fiber when the fiber...
Figure 30: The radial temperature distribution varies with the Biot number. The dimensionless ambient temperature is 0.8912. Shown are the normalized radial temperature distributions at $\tilde{z} = 0$. 
Figure 31: The average, centerline, and surface filament temperature vs. axial distance: $\text{Bi}=0.65$, $\text{Gz}=0.3$, $\epsilon=0.02$; The dimensionless take-up temperature and ambient temperature are 0.92 and 0.8912, respectively.
temperature is considerably higher than the ambient quench air temperature. Only when the fiber has cooled to the ambient temperature are the average, centerline, and surface temperatures of the fiber equal, where they are all equal to the ambient temperature. The temperature difference between the centerline and the surface of the fiber is

\[ \hat{\theta}(\hat{r} = 0, \hat{z}) - \hat{\theta}(\hat{r} = \hat{\phi}, \hat{z}) = \sum_{i=1}^{\infty} (1 - J_0(A_i)[C_1\exp(\lambda_{1i}\hat{z}) + C_2\exp(\lambda_{2i}\hat{z})]). \] (4.33)

4.3 The Leading Order Problem

In the modeling of fiber spinning, it is usually assumed the axial thermal conductivity can be ignored. We now quantitatively analyze the validity of this assumption by solving the leading order problem from (4.14)–(4.16), which neglects the order \( \varepsilon^2 \) axial conduction term \( \frac{\partial^2 \hat{\theta}}{G_Z \frac{d^2}{dz^2}} \) in equation (4.19), but retains the radial conduction:

\[ \hat{\theta}_z = \frac{1}{G_Z} (\hat{\theta}_{,r} + \frac{1}{\hat{r}} \hat{\theta}_{,r}), \] (4.34)

\[ \hat{\theta}_{,r}|_{r=\hat{r}} = -Bi (\hat{\theta} - \hat{\theta}^n)|_{r=\hat{r}}, \] (4.35)

\[ \hat{\theta}_{,r}|_{r=0} = 0. \] (4.36)

Again, we assume

\[ \hat{\theta} = \hat{\theta}^n + \hat{\theta}_R(\hat{r}) \hat{\theta}_Z(\hat{z}). \] (4.37)

Separating spatial variables leads to

\[ \frac{d\hat{\theta}_Z}{d\hat{z}} + \frac{A^2}{G_Z} \hat{\theta}_Z = 0, \] (4.38)
The complete solution is

\[ -\left(\frac{d^2\hat{\theta}_R}{d\bar{r}^2} + \frac{1}{\bar{r}} \frac{d\hat{\theta}_R}{d\bar{r}}\right) - A^2\hat{\theta}_R = 0, \quad (4.39) \]

\[ \frac{d\hat{\theta}_R}{d\bar{r}}|_{\bar{r}=1} = -Bi \hat{\theta}_R|_{\bar{r}=1}, \quad (4.40) \]

\[ \frac{d\hat{\theta}_R}{d\bar{r}}|_{\bar{r}=0} = 0. \quad (4.41) \]

The complete solution is

\[ \hat{\theta} = \hat{\theta}^a + \sum_{i=0}^{\infty} C_{oi} J_0(A_i\bar{r})\exp\left(-\frac{A_i^2}{Gz}\bar{z}\right), \quad (4.42) \]

where \(A_i\) is \(i\)-th eigenvalue which satisfies equation (4.24). The coefficients \(C_{oi}\) are determined by the temperature distribution \(\tilde{\theta}_0(\bar{r})\) at the solidification point of the fiber,

\[ C_{oi} = \frac{\int_0^1 J_0(A_i\bar{r})\tilde{\theta}_0\bar{r}d\bar{r}}{C_i}, \quad (4.43) \]

where \(C_i\) is defined in (4.31).

When the higher order axial conduction term is eliminated from equation (4.34), the axial boundary condition at the downstream boundary \(\bar{z} = 1\) of the fiber is lost. In fiber spinning, the take-up temperature is not controlled and therefore is about the ambient temperature. In Figure 32, we see that the take-up temperature does not effect on the upstream fiber temperature except in a small neighborhood of the take-up point, even when we specify the take-up temperature to be much higher than the ambient temperature. The leading order equation omitting the axial thermal conduction is therefore sufficient except near the take-up point in the spinning process. The temperature distribution across the rigid fiber is largely determined by the first
Figure 32: The average, centerline, and surface temperature profile obtained from 1-dimensional modeling: $Bi=0.65$, $Gz=0.3$; The ambient temperature is 0.8912.
eigenfunction,
\[ \tilde{\theta} = \tilde{a} + C_0 J_0(A_1 \tilde{r}) \exp(-\frac{A_1^2 \tilde{z}}{Gz}). \]  \hspace{1cm} (4.44)

### 4.4 Solving for the Average Temperature Profile with Assumed Radial Temperature Variations

We now use the exact solution to test three formulae for radial temperature variation which we shall use in the modeling of melt spinning.

Integrating the steady state equation (4.34) from \( \tilde{r} = 0 \) to \( \tilde{r} = 1 \) and using (4.35) produces

\[ \tilde{\theta}, \tilde{r} = -2Z(\tilde{\theta}|_0 - \tilde{\theta}^a), \]  \hspace{1cm} (4.45)

where \( \tilde{\theta}|_0 \) is the surface temperature and \( \tilde{\theta} \) is the radially averaged temperature of the fiber, i.e.

\[ \tilde{\theta}|_0 = \tilde{\theta}|_0(\tilde{z}) = \tilde{\theta}|_{\tilde{r}=1}, \quad \tilde{\theta} = \tilde{\theta}(\tilde{z}) = 2 \int_0^1 \tilde{\theta} \tilde{r} d\tilde{r}, \]  \hspace{1cm} (4.46)

and \( Z \) is the combination of the Biot number and the Graetz number,

\[ Z = \frac{Bi}{Gz} = \frac{h_k}{\rho c_v k/\varepsilon} = \frac{h_c z_c}{\rho c_v u_c r_c}. \]  \hspace{1cm} (4.47)

There are two unknowns, \( \tilde{\theta}|_0 \) and \( \tilde{\theta} \), in only one governing equation (4.45). As in the melt-spinning model, the integrated equation (4.45) must be accompanied by an assumption relating the surface temperature \( \tilde{\theta}|_0 \) to the average temperature \( \tilde{\theta} \),

\[ \tilde{\theta}|_0 = f(\tilde{\theta}, Bi). \]  \hspace{1cm} (4.48)
Note that in equation (4.45) the only dimensionless number involved is the $Z$ number, from which the thermal conductivity coefficient $k$ cancels. Thus, the only way to reflect the influence of thermal conductivity on the temperature distribution is through the relation of surface and average temperature.

In the modeling of fiber spinning it is conventional to set the surface temperature equal to average temperature, i.e.

$$\tilde{\theta}|_0 = \tilde{\theta}.$$  \hspace{1cm} (4.49)

This assumption, which results in an approximate solution insensible to the material's thermal conductivity, is too simple, as we now show:

Learning from the study of exact solution in Section 4.2, the first term in the expansion (4.42) is the dominating factor in determining the radial temperature distribution across the filament. With the use of equation (4.44) we obtain the relation of the surface temperature and the radially averaged temperature,

$$\tilde{\theta}|_0 = \tilde{\theta}^a + \frac{A_1^2}{2 \text{Bi}} (\tilde{\theta} - \tilde{\theta}^a),$$  \hspace{1cm} (4.50)

where $J_0$ is the zeroth Bessel function and $A_1$ is the first eigenvalue for the characteristic equation (4.24).

We may also assume a parabolic shape for the radial temperature distribution,

$$\tilde{\theta}(\tilde{r}, \tilde{z}) = \tilde{\theta}^a + (1 - S\tilde{r}^2)C(\tilde{z}),$$  \hspace{1cm} (4.51)

where $S$ is a function of the Biot number and is determined by requiring the heat loss boundary condition (4.35) satisfied,

$$S = \frac{\text{Bi}}{2 + \text{Bi}}.$$  \hspace{1cm} (4.52)
The surface temperature is then related to average temperature through

\[
\hat{\theta}|_\theta = \hat{\theta}^a + \frac{1 - S}{1 - \frac{8}{3}} (\hat{\theta} - \hat{\theta}^a) = \hat{\theta}^a + \frac{4}{4 + \text{Bi}} (\hat{\theta} - \hat{\theta}^a). \tag{4.53}
\]

We examine these three approximations (4.49), (4.50), and (4.53) by plotting the solutions of the integrated governing equation (4.45) together with each of these approximations for the average temperature profiles in Figure 33. The very small difference between the cross-sectionally averaged temperature of the exact 2-dimensional solution (4.42) and the solution of (4.45) together with (4.50) is another indication that first mode in the summation (4.42) is dominant. The use of the assumption (4.53) which follows from a parabolic radial temperature distribution yields results very close to the exact solution. This form has the merits of simplicity without sacrificing accuracy. The conventional assumption (4.49), which is insensible to the material’s thermal conductivity, results in a solution significantly deviating from the exact solution.

4.5 Results and Discussion

The following observations have been obtained from the analytical solutions of the heat transfer problem in the rigid filament:

1. The leading order problem (4.34)-(4.36) which omits the axial thermal conduction models the temperature distribution well for a slender jet away from the take-up point. The specified take-up temperature in the complete problem
Figure 33: The comparison of performance of the three approximations in 1-dimensional modeling by showing the average temperature profiles: $Bi=0.65$, $Gz=0.3$; The ambient temperature is 0.8912.
(4.14)-(4.16) has little effect upstream except for in a narrow axial boundary layer near the take-up position.

2. After reaching the position of the glass transition, the fiber cools down exponentially in the axial direction. The cooling rate depends on the fiber's take-up speed and thermal conductivity through the Graetz number, and the coefficient $A_1$, which in turn is determined by the Biot number. The exponential cooling rate is $\frac{A_1^2}{GZ}$.

3. The first eigenfunction truncation sufficiently represents the radial temperature variation for the slender jet.

4. The coefficient $A_1$, which largely determines the radial temperature variation, has a strongly nonlinear relation with the Biot number (see Figures 28 and 30). When the Biot number is very small, $A_1$ increases rapidly with the Biot number. When the Biot number is large, it reaches a limit of about 2.22.

5. The approximate solution which follows from assuming a parabolic form of radial temperature achieves high accuracy in the integrated problem for the cross-sectionally averaged temperature, and has the merit of simplicity. The conventional assumption of surface temperature equal to average temperature is qualitatively and quantitatively incorrect.
CHAPTER V

The Thin-Filament Models with Radial Temperature Variation

In modeling the fiber spinning processes it is of interest to predict the temperature, stress, and velocity profiles along a spinline. Considering the complexity of the problem and slenderness of the fibers, 1-dimensional thin-filament equations are commonly employed to obtain cross-sectionally averaged values of these quantities. Importantly, the assumptions of radial independence of temperature, and radial independence of normal stresses and axial velocity are made in the derivation of the thin-filament equations in the literature, citing the slenderness of the filaments.

Although the assumption of radial independence of normal stresses and axial velocity is good for leading order calculations, the assumption of radial independence of temperature is not justified (see Appendix A). As discussed in Chapter 4, the temperature field is fundamentally different from the velocity and stress fields. Although the axial velocity and normal stresses are uniform to leading order in the slender filament problem, we show in this chapter that the radial temperature gradient must be accounted for in the leading order problem. We demonstrate through numerical examples that the effects of incorporating this radial temperature gradient in the
modeling are significant, even though the temperature difference between core and surface of the fiber is found to be small. Ignoring this effect results in a very different temperature profile along the spinline, and thus erroneous velocity and stress profiles.

In this chapter, we focus on the modeling with the effect of radial variation of temperature within the filament. Hence we assume here that the density is a constant and employ the incompressible theory. This assumption will be relaxed in Chapter 6 to model fiber processing with temperature-dependent density as well as radial dependence of temperature.

5.1 Literature Review

Many researchers have produced nonisothermal process models for melt spinning in which energy transport governed by the energy equation is coupled with the mechanical phenomena governed by the conservation laws of mass and momentum (Bechtel & Forest [6], Vassilatos et al. [72], Schoene & Bruenig [65], Zahorski [78], Ziabicki & Kawai [80], Keunings et al. [50], George [27], Fisher et al. [25], Petrie [60], Fisher & Denn [24], Ziabicki [79], Kase & Matsuo [47, 48]). The assumption of radially independent temperature is employed in all models in these works.

In the process modeling of Vassilatos et al. [72], Schoene & Bruenig [65], Zahorski [78], George [27], Fisher & Denn [24], and Matovich & Pearson [55] the underlying theory is strictly incompressible, i.e. the material is assumed incompressible, the constraint response appears only in the momentum equation, and density is taken as constant. In the resulting incompressible theory, the pressure $p$ appears only in
the momentum equation and not in the energy equation. These models run the risk of missing important physical behavior traceable to the temperature dependences that have been neglected. Even though the coefficients of these dependences are very small, they can have significant effects on the energy balance and flow behavior (Hatzikiriakos [36], Cox & Macosko [18], Toor [69, 70]).

In the process models of Hayashi et al. [37], Dutta [23], the incompressibility constraint and incompressible equations, which follow rigorously from the assumption of constant density, were retained, but a temperature-dependent expression for density is inserted *a posteriori* into these equations. In Kase & Matsuo [47] the density is assumed to be temperature dependent and the incompressibility constraint is modified to account for temperature-induced shrinkage or expansion, but the constraint response and governing equations of an incompressible material were still employed. Both of these approaches are not self-consistent.

In this work we will derive the self-consistent thin-filament equations and provide a comparison to evaluate the conventional assumption and illustrate errors in the resulting models.

5.2 The 3-Dimensional Boundary Value Problem for Melt Spinning

The melt spinning process was shown schematically in Figure 27. The thin-filament equations of this chapter are used to model the deformation and stress state of the filament and its heat transfer to the ambient air in the region beyond the extrudate
swell and before fiber's solidification point. We will illustrate our development with
the use of Newtonian fluid model, which is generally accepted for PET fiber spinning.

The governing equations for incompressible fluid are the incompressibility con­
straint and the conservation laws of momentum and energy:

\[ \text{div} \mathbf{v} = 0, \quad (5.1) \]
\[ \rho \dot{\mathbf{v}} = \text{div} \dot{T} - \text{grad} p + \rho \mathbf{g}, \quad (5.2) \]
\[ \rho \dot{\mathbf{e}} = \dot{T} \cdot \mathbf{D} - \text{div} \mathbf{q}, \quad (5.3) \]

where \( \mathbf{g}, \mathbf{e}, \) and \( \mathbf{q} \) are the body force, internal energy, and heat flux vector, respec­
tively, and \( \dot{T} \) and \( \rho \mathbf{I} \) are determinate part and constraint pressure in the Cauchy
stress tensor.

The boundary conditions at the free surface

\[ F = \phi(z, t) - r = 0 \quad (5.4) \]

of an axisymmetric fiber are the kinematic free surface boundary condition,

\[ \{ \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) F \} |_{\sigma} = 0, \quad (5.5) \]

the stress boundary condition,

\[ (T^a - T) |_{\sigma \cdot n} = \sigma_{kn}, \quad (5.6) \]

and the convective heat loss boundary condition,

\[ \mathbf{q} |_{\sigma \cdot n} = h(\theta - \theta^a) |_{\sigma}, \quad (5.7) \]
where the heat loss coefficient $h$ is a specified function of the free surface geometry and velocity. In (5.5)–(5.7) $|\partial|$ denotes the value of the function at the surface, $n$ denotes the outward unit normal vector at the surface, $\kappa$ is the mean curvature of the surface, $\sigma$ is the surface tension, assumed constant, and $\theta$ is absolute temperature. The symbols with superscript $a$, namely $T^a$ and $\theta^a$, are the stress tensor and the temperature of the ambient air, respectively. We assume that the quench air is maintained at constant temperature. For the axisymmetric surface (5.4) we compute,

$$n = \frac{1}{(1 + \phi_z^2)^{1/2}}(e_r - \phi_z e_z),$$

(5.8)

$$\kappa = \frac{1}{\phi(1 + \phi_z^2)^{1/2}} - \frac{\phi_{zz}}{(1 + \phi_z^2)^{1/2}}.$$

(5.9)

We assume the boundary ambient stress $T^a$ in this axisymmetric problem is of the form

$$T^a = \begin{bmatrix} -p^a & 0 & T^a_{rz} \\ 0 & -p^a & 0 \\ T^a_{rz} & 0 & -p^a \end{bmatrix},$$

(5.10)

where $p^a$ and $T^a_{rz}$ are specified functions of $\phi, v$, and $\theta$.

We assume the internal energy is assumed determined by the constitutive equation

$$d\dot{e} = c(\theta) d\theta.$$  

(5.11)

For an incompressible fluid, the specific heat $c$ at constant pressure and constant volume are equal. It is further assumed that the specific heat $c$ is a linear function of temperature,

$$c(\theta) = C_0 + C_1 \theta.$$  

(5.12)

Heat conduction is modeled by the Fourier law,

$$\dot{q} = -k \nabla \theta.$$  

(5.13)
where the thermal conductivity $k$ is a specified constant. A Newtonian constitutive model for the fluid is written as

$$\dot{T} = 2\mu(\theta)D,$$  \hspace{1cm} (5.14)

with viscosity $\mu(\theta)$ specified as a function of absolute temperature $\theta$ by the Arrhenius form

$$\mu(\theta) = \mu_0 \exp \left( \frac{\mathcal{E}}{R\theta} \right),$$  \hspace{1cm} (5.15)

where $R$ is the gas constant, and $\mu_0$ and $\mathcal{E}$ are material constants. For convenience we express the Arrhenius form as

$$\mu(\theta) = \mu_c \exp \left[ \frac{\mathcal{E}}{R\theta} \left( \frac{1}{\theta} - \frac{1}{\theta_c} \right) \right],$$  \hspace{1cm} (5.16)

where $\theta_c$ is a characteristic absolute temperature of the process being modeled, and $\mu_c$ is the viscosity of that temperature,

$$\mu_c = \mu_0 \exp \left( \frac{\mathcal{E}}{R\theta_c} \right).$$  \hspace{1cm} (5.17)

We also define the characteristic value $c_c$ of specific heat to be its values at the characteristic temperature,

$$c_c = C_0 + C_1 \theta_c.$$  \hspace{1cm} (5.18)

In the next two sections we produce 1-dimensional fiber-spinning equations from the 3-dimensional boundary value problem (5.1)-(5.3), (5.5)-(5.7), together with the constitutive equations (5.11)-(5.15).
5.3 The Dimensionless Boundary Value Problem for the Axisymmetric Slender Fiber, and Regimes of Fiber Behavior

In the boundary value problem (5.1)–(5.7), (5.11)–(5.15) for fiber spinning processes, many physical effects such as temperature distribution, fiber’s axial tension, surface tension and air drag at the interface, viscosity, and inertia contribute to the final state of the fiber. Not all of these competing physical effects are equally important, e.g. for a particular process viscosity and inertia may be more important than gravity and surface tension. We call the relative importance of the physical effects in the particular process the regime of fiber behavior. It is important to emphasize that different fiber-spinning processes operate in different regimes; effects that are dominant in one process may be negligible in another. Our model for fiber spinning processes is sufficiently general to allow for the analysis of fiber behavior in any regime, as will be seen.

To compare the importance of each physical effect relative to the others in the spinning process we must nondimensionlize the boundary value problem (5.1)–(5.7), (5.11)–(5.15). We select characteristic values \( r_c, z_c, \nu, \tau_c, p_c, \theta_c \) for transverse length, axial length, velocity, stress, pressure, and absolute temperature, respectively. The particular values of this choice depend on the particular process. In the next section we will exploit the fact that the fiber is slender. To this end we define as the slenderness parameter \( \varepsilon \) the ratio of the characteristic transverse length to the characteristic
axial length, i.e.

\[ \epsilon = \frac{r_c}{z_c} \]  

(5.19)

for a particular process \( \epsilon \) is a small, fixed, positive number. (Note the subtly different symbols for internal energy \( \varepsilon \) and slenderness ratio \( \epsilon \).) A characteristic time scale is defined through

\[ t_c = \frac{z_c}{v_c} \]  

(5.20)

We use these characteristic values to scale all dimensional quantities in the boundary value problem: the dimensionless independent variables \( \hat{r}, \hat{z}, \hat{t} \) are defined as

\[ \hat{t} = \frac{t}{t_c}, \quad \hat{r} = \frac{r}{r_c}, \quad \hat{z} = \frac{z}{z_c}, \]  

(5.21)

and the dimensionless dependent variables, namely the polar cylindrical components of velocity and stress, pressure, temperature (functions of \( r, z \) and \( t \) only, due to axisymmetry) and free surface radius (a function of \( z \) and \( t \)) are defined through

\[ u_r(r, z, t) = \epsilon u_c \hat{u}_r(\hat{r}, \hat{z}, \hat{t}), \]
\[ u_z(r, z, t) = u_c \hat{u}_z(\hat{r}, \hat{z}, \hat{t}), \]
\[ \hat{T}_{rr}(r, z, t) = \tau_c \hat{T}_{rr}(\hat{r}, \hat{z}, \hat{t}), \]
\[ \hat{T}_{\theta\theta}(r, z, t) = \tau_c \hat{T}_{\theta\theta}(\hat{r}, \hat{z}, \hat{t}), \]
\[ \hat{T}_{zz}(r, z, t) = \tau_c \hat{T}_{zz}(\hat{r}, \hat{z}, \hat{t}), \]
\[ \hat{T}_{rz}(r, z, t) = \epsilon \tau_c \hat{T}_{rz}(\hat{r}, \hat{z}, \hat{t}), \]
\[ p(r, z, t) - p^o = p_c \hat{p}(\hat{r}, \hat{z}, \hat{t}), \]
\[ \theta(r, z, t) = \theta_c \hat{\theta}(\hat{r}, \hat{z}, \hat{t}), \]
\[ \phi(z, t) = r_c \hat{\phi}(\hat{z}, \hat{t}). \]  

(5.22)
We also define
\[
T^a_{rr}(z,t) = \epsilon r \tilde{T}^a_{rr}(\tilde{z},\tilde{t})
\]
\[
p^a(z,t) = \rho_c \tilde{p}^a(\tilde{z},\tilde{t}),
\]
\[
h(z,t) = h_c \tilde{h}(\tilde{z},\tilde{t}).
\]  

In (5.21), (5.22) and (5.24) the quantities without tildes are dimensional and the quantities with tildes are dimensionless. The radial velocity of melt fiber and the shear stress in the fiber and on the interface are scaled as order \( \epsilon \). This is due to the features of slenderness geometry and general processing conditions of fiber spinning. The melt spinning is elongational in character, so that the transverse velocity is much smaller than the axial velocity and the normal stresses are larger in magnitude than the shear stress.

When the scalings (5.21) and (5.22) are inserted into the axisymmetric case of the boundary value problem (5.1)-(5.7), (5.11)-(5.15), we obtain the dimensionless boundary value problem in polar form,

**Dimensionless field equations:**

\[
\tilde{v}_{r,\tilde{r}} + \frac{\tilde{v}_r}{\tilde{r}} + \tilde{v}_{z,\tilde{t}} = 0,
\]

\[
\epsilon^2(\tilde{v}_{r,\tilde{t}} + \tilde{v}_{r,\tilde{r}} + \tilde{v}_{z,\tilde{t}}) = B \left[ \tilde{T}_{rr,\tilde{r}} + \frac{\tilde{T}_{rr} - \tilde{T}_{r\theta}}{\tilde{r}} + \epsilon^2 \tilde{T}_{xz,\tilde{r}} - \alpha(\tilde{p}_r + \tilde{p}_z) \right],
\]

\[
\tilde{v}_{z,\tilde{t}} + \tilde{v}_{r,\tilde{r}} + \tilde{v}_{z,\tilde{t}} = B \left[ \tilde{T}_{zx,\tilde{r}} + \tilde{T}_{xz,\tilde{r}} + \frac{\tilde{T}_{zz}}{\tilde{r}} - \alpha(\tilde{p}_r + \tilde{p}_z) \right] + \frac{1}{F_T},
\]

\[
(1 - C + C \tilde{\theta})(\tilde{\theta}_{,\tilde{t}} + \tilde{v}_r \tilde{\theta}_{,\tilde{r}} + \tilde{v}_z \tilde{\theta}_{,\tilde{t}}) = \frac{1}{GZ} \left( \tilde{\theta}_{,\tilde{t}} + \frac{1}{\tilde{r}} \tilde{\theta}_{,\tilde{r}} + \epsilon^2 \tilde{\theta}_{,\tilde{t},\tilde{r}} \right)
\]

\[
+ U \left[ \tilde{T}_{rr,\tilde{r}} + \tilde{T}_{r\theta,\tilde{r}} + \tilde{T}_{xz,\tilde{r}} \tilde{\theta}_{,\tilde{t}} + \frac{1}{2} \tilde{T}_{rs}(\epsilon^2 \tilde{v}_{r,\tilde{r}} + \tilde{v}_{z,\tilde{t}}) \right],
\]

(5.24)
\[ \tilde{T}_{rr} = E_s \tilde{u}_r \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (5.28) \]
\[ \tilde{T}_{\theta\theta} = E_s \tilde{v}_r \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (5.29) \]
\[ \tilde{T}_{zz} = E_s \tilde{u}_z \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (5.30) \]
\[ \tilde{T}_{rz} = \frac{E_s}{2} (\tilde{u}_{r,z} + \epsilon^{-2} \tilde{u}_{z,r}) \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (5.31) \]

**Dimensionless boundary conditions:**

**Kinematic boundary condition:**

\[ (\tilde{\phi}_{,r} - \tilde{v}_r + \tilde{u}_z \tilde{\phi}_{,z})|_{\tilde{r} = \tilde{\delta}} = 0, \quad (5.32) \]

**Stress boundary condition:**

\[ \left( \alpha \tilde{p} - \tilde{T}_{rr} + \epsilon^2 \tilde{T}_{rz} \tilde{\phi}_{,z} \right)|_{\tilde{r} = \tilde{\delta}} = \gamma \tilde{\kappa} + \epsilon^2 \tilde{T}_{rz} \tilde{\phi}_{,z}, \quad (5.33) \]
\[ \left[ \tilde{T}_{rz} + (\alpha \tilde{p} - \tilde{T}_{zz}) \tilde{\phi}_{,z} \right]|_{\tilde{r} = \tilde{\delta}} = \gamma \tilde{\kappa} \tilde{\phi}_{,z} + \tilde{T}_{rz}, \quad (5.34) \]

where

\[ \tilde{\kappa} = \tau_0 \kappa = \frac{1}{\tilde{\phi}(1 + \epsilon^2 \tilde{\phi}_{,zz})^{1/2}} - \frac{\epsilon^2 \tilde{\phi}_{,zz}}{(1 + \epsilon^2 \tilde{\phi}_{,zz})^{1/2}}, \quad (5.35) \]

is the dimensionless mean curvature of the free surface.

**Convective heat boundary condition:**

\[ \frac{1}{(1 + \epsilon^2 \tilde{\phi}_{,zz})^{1/2}} \left( \partial_{,r} - \epsilon^2 \tilde{\phi}_{,z} \partial_{,z} \right)|_{\tilde{r} = \tilde{\delta}} = -\text{Bi} \tilde{\kappa} (\tilde{\theta} - \tilde{\theta}^a)|_{\tilde{r} = \tilde{\delta}}, \quad (5.36) \]

The dimensionless boundary value problem (5.24)-(5.36) involves the following dimensionless combinations of material properties and characteristic scales:

\[ B = \frac{\tau_c}{\rho \nu_c^2}, \quad \text{Fr} = \frac{v_c^2}{g z_c}, \quad Y = \frac{\sigma}{\tau_c f_c}, \quad E_s = \frac{2 \mu_c v_c}{\tau_c z_c}, \quad \alpha = \frac{p_c}{\tau_c}. \]
Some of these numbers are recognizable: $E_s$ is the Ellis number, $F_r$ is the Froude number, and $B_i$ is the Biot number, $G_z$ is the Graetz number, $E$ is the Arrhenius number. Also, combinations of these numbers give familiar dimensionless groups. For instance, the combination of $B$ and $E_s$ gives

$$Re = \frac{1}{BE_s},$$

which is the Reynolds number. The combination of $B$ and $Y$ is the Weber number,

$$W = \frac{1}{BY}.$$  

$X$ is a half of the combination of $U$ and $E_s$,

$$X = \frac{UE_s}{2}.$$  

$Z$ is the combination of $B_i$ and $G_z$,

$$Z = \frac{B_i}{G_z}.$$  

Each of the dimensionless number in (5.37) can be expressed through its order in slenderness parameter $\epsilon$. For example we may write

$$K = \tilde{K}\epsilon^n,$$

where $\tilde{K}$ is a scalar of $O(\epsilon^0)$, i.e.

$$\epsilon < \tilde{K} < \epsilon^{-1}.$$
The relative magnitudes in $\epsilon$ of the numbers (5.37) indicate the relative importance of the competing physical effects in a specific process, and provide an explicit description of the regime of fiber behavior.

### 5.4 Reduction to One-Spatial-Dimensional Thin-Filament Equations

We now reduce the 3-dimensional boundary value problem to a 1-dimensional leading order thin-filament model through integration over the filament cross section and extracting the leading order terms in the slenderness ratio $\epsilon$. To obtain closure in the resulting 1-dimensional equations, however, we must first make necessary assumptions on spatially-dependent unknowns occurring nonlinearly in the 3-dimensional equations, to relate cross-sectional averages of products to products of averages.

In the purely mechanical theory (i.e. no energy equation, thermal boundary condition, or temperature dependence) all nonlinear terms in the 3-dimensional field equations involve only the velocity components $v_r$, $v_z$ and the free surface radius $\phi$. Therefore, to produce closure in the mechanical problem it is sufficient to postulate the following radial dependence in the velocity field

\[
\tilde{u}_z(\tilde{r}, \tilde{z}, \tilde{\ell}) = \sum_{n,m \geq 0} \epsilon^{2n+m} \tilde{r}^{2n} v_{z,n,m}(\tilde{z}, \tilde{\ell})
\]

\[
= v_{z,0}^{0,0} + \epsilon v_{z,1}^{0,1} + \epsilon^2 (v_{z,2}^{0,2} + \tilde{r}^2 v_{z,1}^{1,0}) + O(\epsilon^3),
\] (5.44)

\[
\tilde{u}_r(\tilde{r}, \tilde{z}, \tilde{\ell}) = \sum_{n,m \geq 0} \epsilon^{2n+m} \tilde{r}^{2n+1} v_{r,n,m}(\tilde{z}, \tilde{\ell})
\]

\[
= \tilde{r} v_{r,0}^{0,0} + \epsilon \tilde{r} v_{r,1}^{0,1} + \epsilon^2 \tilde{r}^2 (v_{r,2}^{0,2} + \tilde{r}^2 v_{r,1}^{1,0}) + O(\epsilon^3),
\] (5.45)
and expansion of the free surface radius

\[ \hat{\phi}(\tilde{z}, \tilde{t}) = \sum_{m \geq 0} \epsilon^m \phi^{(m)}(\tilde{z}, \tilde{t}) \]

\[ = \phi^{(0)} + \epsilon \phi^{(1)} + \epsilon^2 \phi^{(2)} + O(\epsilon^3). \]  

(5.46)

With these expansions, integration of the mechanical 3-dimensional field equation over the cross section produces, in most regimes, closed sets of one-space, one-time differential equations at each order in the perturbation theory in \( \epsilon \) (Bechtel et al. [7, 8]). The leading order problem usually consists of seven one-space, one-time differential equations; the 1-dimensional unknowns in this leading order problem are the first terms in the velocity expansions,

\[ v_z^{0,0}(\tilde{z}, \tilde{t}), \quad v_r^{0,0}(\tilde{z}, \tilde{t}), \]  

(5.47)

the averages of the diagonal components of the determinate part \( \hat{T} \) of the Cauchy stress tensor,

\[ \int \hat{T}_{rr} da, \quad \int \hat{T}_{\theta\theta} da, \quad \int \hat{T}_{zz} da, \]

(5.48)

the average constraint pressure,

\[ \int \hat{p} da, \]  

(5.49)

and the leading order term in the free surface radius,

\[ \phi^{(0)}(\tilde{z}, \tilde{t}). \]  

(5.50)

Shear stress does not appear in the leading order problem of the integrated form; we will only be concerned with the leading order problem here.
We emphasize that if one does not explicitly assume a form for the radial dependence of the velocity components, as we did in (5.44) and (5.45), one still obtains seven leading order equations, but for ten unknowns, since the two velocity quantities (5.47) are replaced by the five integrations
\[
\int v_r da, \quad \int v_\theta da, \quad \int v_\phi^2 da, \quad \int v_t^2 da, \quad \int v_r v_\phi da.
\] (5.51)

This classic loss-of-closure situation is avoided by our perturbation expansions (5.44)-(5.46). The first term of each velocity expansion in the assumption is a function of \(z\) and \(t\) only, which is a classical assumption for the modeling of slender fiber spinning as seen in (Petrie [60], Fisher & Denn [24], Ziabicki [79], Matovich & Pearson [55], Kase & Matsuo [47]). The expansions (5.44)-(5.46) enable us to obtain higher order governing equations as we wish. Similar perturbation expansions are adopted by Dewynne et al. [19] and Matovich & Pearson [55]. We note that in many purely mechanical regimes, the \(r\) expansions in (5.44)-(5.46) can be deduced from the \(\epsilon\) expansion, i.e. slenderness and the 3-dimensional boundary value problem demand the radial expansions in (5.44)-(5.46) (Schultz & Davis [66]).

When we generalize from the purely mechanical theory to the thermomechanical theory, closure difficulties arise again, even with assumptions (5.44)-(5.46): integration of the energy equation over the filament cross section produces one additional one-space, one-time differential equation, but two additional unknowns,
\[
\bar{\theta}(z, t) = \frac{\int_{\text{cross-section}} \theta da}{\int_{\text{cross-section}} da} = \text{average temperature,} \quad (5.52)
\]
\[
\theta_{0}(z, t) = \theta(r = \phi, z, t) = \text{surface temperature,} \quad (5.53)
\]
(the surface temperature occurs through the convective heat boundary condition (5.36)).

To recover closure it is necessary to introduce a relation between the surface temperature $\theta|_\partial$ and average temperature $\bar{\theta}$. In all existing nonisothermal thin-filament models surface temperature is simply equated to average temperature. There are problems with this simple identification:

- It ignores the significant radial temperature gradients that are necessarily present in cooling slender filaments, as demonstrated in Chapter 4.

- In the slender filament problem with this assumptions there is nowhere any appearance of the conductive property $k$ of the filament, which certainly is important in the cooling of the filament since it reflects the ease at which heat is conducted to the filament surface, from where it is convected away by the quench air.

To remedy both these problems, we instead recover closure by postulating a relation between the average temperature, surface temperature, and the Biot number:

$$\theta|_\partial = f(\bar{\theta}, \text{Bi})_t. (5.54)$$

This relation takes into account the evolution in $z$ direction of the radial temperature distribution in the filament by introducing the local value of the Biot number, $\text{Bi}_t$

$$\text{Bi}_t = \text{Bi}_t(z,t) = \frac{h}{k}\phi(z,t), (5.55)$$

in which the length scale is now replaced with the local value of the free surface radius $\phi$. The particular form of the relation (5.54) depends on the temperature distribution
over the fiber cross-section. One of the results in this chapter is the demonstration that the inclusion (5.54) of the local Biot number in the relation is necessary, both theoretically and numerically.

To recover closure it is also necessary to make the assumption that specific heat and viscosity are functions of average temperature over cross-section rather than pointwise temperature,

\[ c = C_0 + C_1 \bar{\theta}, \quad (5.56) \]

\[ \mu = \mu_c \exp \left[ E \left( \frac{1}{\theta} - \frac{1}{\theta_c} \right) \right]. \quad (5.57) \]

If the pointwise expression (5.18) for specific heat as a linear function of temperature were inserted into the energy equation (5.27), and then the resulting equation were to be integrated over the filament cross section, an additional 1-dimensional unknown \( \int \theta^2 da \) would be introduced without an accompanying additional equation. Also, a pointwise dependence of viscosity on temperature in the constitutive equations (5.17) would produce a leading order transverse variation of velocity, destroying the perturbation structure (5.44)–(5.46). We avoid both of these situations by the assumptions (5.56) and (5.57) that the material properties \( c \) and \( \mu \) depend on average rather than pointwise temperature.

To obtain the 1-dimensional leading order problem, we (i) insert expansions (5.44)–(5.46) into the boundary value problem (5.24)–(5.36), (ii) introduce assumptions (5.56) and (5.57), (iii) integrate the field equations (5.24)–(5.31) over the fiber cross section, (iv) incorporate the free surface conditions and convective heat loss using the boundary conditions (5.32)–(5.36), and (v) attach equation (5.54). We denote the
nondimensional stress resultants (5.48) and (5.49) that appear as a result of integration of the field equations as

\[ A_{rr}(\tilde{r}, \tilde{t}) = 2\pi \int_0^{\phi(0)} \tilde{T}_{rr}(\tilde{r}, \tilde{z}, \tilde{t}) \tilde{r} d\tilde{r}, \]

\[ A_{\theta\theta}(\tilde{r}, \tilde{t}) = 2\pi \int_0^{\phi(0)} \tilde{T}_{\theta\theta}(\tilde{r}, \tilde{z}, \tilde{t}) \tilde{r} d\tilde{r}, \]

\[ A_{zz}(\tilde{r}, \tilde{t}) = 2\pi \int_0^{\phi(0)} \tilde{T}_{zz}(\tilde{r}, \tilde{z}, \tilde{t}) \tilde{r} d\tilde{r}, \]

\[ \beta(\tilde{z}, \tilde{t}) = 2\pi \int_0^{\phi(0)} p(\tilde{r}, \tilde{z}, \tilde{t}) \tilde{r} d\tilde{r}. \]

(5.58)

The integral of shear stress \( T_{rz} \) is not defined because it does not enter in the leading order problem. The dimensionless average temperature and surface temperature are denoted as \( \tilde{\theta} \) and \( \tilde{\theta}|_\partial \), i.e.

\[ \tilde{\theta}(\tilde{z}, \tilde{t}) = \frac{2}{\phi(0)^2} \int_0^{\phi(0)} \tilde{T}(\tilde{r}, \tilde{z}, \tilde{t}) \tilde{r} d\tilde{r}, \]

(5.59)

\[ \tilde{\theta}|_\partial = \tilde{\theta}(\tilde{r} = \tilde{z}, \tilde{t}) = \tilde{f}(\tilde{\theta}, \text{Bi}). \]

(5.60)

We produce the thin-filament equations in the regime in which all physical effects with all dimensionless numbers in (5.37), namely \( B, Fr, Y, Es, \alpha, Gz, Bi, U, E, \) and \( C \), are order \( \epsilon^0 \). The 1-dimensional leading order problem in our regime is

\[ v_{z,\xi}^{0,0} + v_z^{0,0} v_{z,\xi}^{0,0} = \frac{1}{W} \frac{\phi(0)}{\phi(0)^2} \tilde{T}_{zz} - \frac{2B}{\phi(0)} \tilde{T}_{rz} - \alpha \tilde{B} \tilde{p}_{\xi,\xi} + \frac{1}{F_{rr}} \]

\[ + \frac{3}{\text{Re}} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] \left[ v_{z,\xi,\xi}^{0,0} + v_{z,\xi}^{0,0} \left( 2\frac{\phi(0)}{\phi(0)} - E \frac{\tilde{\theta}_{\xi,\xi}}{\tilde{\theta}_{\xi}^2} \right) \right], \]

(5.61)

\[ (1 - C + C \tilde{\theta})(\tilde{\theta}_{,\xi} + v_{z,\xi,\xi}^{0,0}) = 3X \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] \left( v_{z,\xi,\xi}^{0,0} \right)^2 - 2Z \frac{\tilde{\theta}_{,\xi}}{\phi(0)} (\tilde{\theta}|_\partial - \tilde{\theta}^s), \]

(5.62)

\[ \phi(0) + v_{z,\xi,\xi}^{0,0} \phi_{,\xi}^{0,0} + \frac{1}{2} \phi(0) v_{z,\xi,\xi}^{0,0} = 0, \]

(5.63)
This dimensionless initial/boundary value problem can be reduced to the $4 \times 4$ matrix form

$$G(u)u_{,t} + M(u)u_{,t} = f(u),$$

with

$$u = (\phi^{(0)}, v^{0,0}, \tilde{\theta}, \omega)^T,$$

$$G(u) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$M(u) = \begin{bmatrix} v^{0,0} & \frac{1}{2} v^{(0)} & 0 & 0 \\ M_{21} & v^{0,0} & \frac{3E}{\omega} D_3 & -\frac{3}{\text{Re}} D_3 \\ 0 & 0 & v^{0,0} & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

and

$$f(u) = \begin{pmatrix} 0 \\ \frac{1}{\text{Re}} + 2B \frac{\tilde{\theta}}{\omega} - \alpha \beta \tilde{\theta} \\ -2 \frac{\tilde{\theta}}{D_3} [f(\tilde{\theta}, \text{Bi}) - \tilde{\theta}] + 3X \frac{D_4}{\omega} \omega^2 \end{pmatrix},$$

where

$$D_2 = 1 - C + C \tilde{\theta},$$

and

$$\beta = \frac{1}{\alpha} A_{rr} + \frac{\pi Y}{\alpha} \phi^{(0)},$$

$$A_{rr}(\tilde{z}, \tilde{t}) = A_{\theta\theta}(\tilde{z}, \tilde{t}) = 2\pi E v^{0,0} \phi^{(0)} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right],$$

$$A_{zz}(\tilde{z}, \tilde{t}) = 2\pi E v^{0,0} \phi^{(0)} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right],$$

$$\tilde{\theta} |_{\theta} = f(\tilde{\theta}, \text{Bi}).$$
The remaining variables, $v_{r}^{0,0}$, $\beta$, $A_{rr}$, $A_{\theta\theta}$, $A_{zz}$, and $\tilde{\theta}|_{\theta}$, are calculated by algebraic equations.

In the fiber spinning, a solidification zone follows the molten zone. The 1-dimensional modeling of fiber spinning consists of a 1-dimensional thin-filament model for the polymer melt slender filament and a 1-dimensional rigid rod model for the solidified fiber. Since axial thermal conduction is neglected in all stages of fiber spinning, only the extrudate temperature can be specified in our 1-dimensional model, which proceeds the 1-dimensional rigid rod model for the solidified fiber discussed in Chapter 1. The temperature at the take-up point is not controlled and usually close to the ambient temperature in the process, and does not effectively affect the processing except in the neighborhood of the take-up point. Therefore, this modeling is appropriate for obtaining the numerical results for velocity, stress, and temperature distributions along the spinline except a small region near the take-up position. Especially, this approximation is applicable for the melt spinning region, which is of most interest.

For the steady state problem, the industrially relevant boundary conditions are specifying the fiber radius, axial velocity, and temperature at $\bar{z} = 0$, and take-up velocity at $\bar{z} = 1$.

$$\phi^{(0)}(0) = \phi_{0}^{(0)}, \quad v_{r}^{0,0}(0) = \bar{v}_{0}, \quad \tilde{\theta}(0) = \bar{\theta}_{0}, \quad (5.77)$$
and

\[ v_s^{0,0}(1) = 1. \]  \hspace{1cm} (5.78)

It should be noticed that in equations (5.61)-(5.68) the thermal conductivity \( k \) implicitly appears through the proposed relation (5.54). In contrast, the conventional thin-filament equations requires no value of the thermal conductivity \( k \) in the calculation.

**5.5 Investigation of the Effects of Radial Temperature Variation**

We now return to the assumption (5.54) relating the surface temperature \( \tilde{\theta}|_o \) to the average temperature,

\[ \tilde{\theta}|_o = f(\tilde{\theta}, Bi), \]  \hspace{1cm} (5.79)

necessary to obtain closure in the 1-dimensional thin-filament model. We will compare three different forms of this function:

1. The common practice in the modeling of fiber spinning sets the surface temperature equal to average temperature, i.e.

\[ \tilde{\theta}|_o = \tilde{\theta}. \]  \hspace{1cm} (5.80)

Relation (5.80), in which the surface temperature of the filament is assumed to be the same as its average temperature, is used to obtain closure in all existing 1-dimensional nonisothermal filament-spinning models. There are serious physical flaws with this assumption; in particular, assumption (5.80) does not allow for the temperature of the
ambient atmosphere surrounding the filament to be different from the temperature of the filament itself, in contrast to the result in thermodynamics that the heat cannot be conducted in the absence of a temperature gradient (detail in Appendix A). The error in measurement of heat loss coefficient $h$ resulting from the assumption is discussed by Vassilatos et al. [72].

2. Motivated by the exact 2-dimensional solution for a rigid circular rod problem of Chapter 4, instead of (5.80) we propose relation (5.81) from the rigid solution, but using the local Biot number $Bi_l$,

$$\theta |_{\theta_0} = \hat{\theta}_0 + \frac{A_l^2}{2Bi_l}(\hat{\theta} - \hat{\theta}_0).$$

In (5.81) $A_l$ is the first root of the equation

$$-A_l J_0'(A_l) = Bi_l J_0(A_l).$$

The number $A_l$ is a function of local value of the Biot number. It accounts for the changing profile of radial temperature distribution: the smaller $Bi_l$, the smaller $A_l$ (Figure 28) and the flatter the radial temperature profile (Figure 30). The use of the local Biot number allows the relation between the surface temperature and average temperature to reflect the evolution of the temperature profile down the filament.

3. Finally, we assume a parabolic shape for the radial temperature distribution

$$\theta (\vec{r}, \hat{z}) = \theta_0 + [1 - S(\hat{z})\vec{r}^2]C(\hat{z}),$$

where $S(\hat{z})$ is a function of $\hat{z}$ which determines the shape evolution of radial temperature distribution, and $C(\hat{z})$ describes the cooling along the fiber. The parabolic
representation (5.83) is the simplest form to account for radial temperature variation in the filament, but we found in our comparison with the exact solution of the previous chapter that this simplest form is sufficient to accurately model both the axial and radial temperature profiles in the filament.

From the definition of average temperature \( \tilde{\theta} \),

\[
\tilde{\theta} = \frac{2}{\phi^2} \int_0^\phi \left[ \tilde{\theta}^a + (1 - S r^2) C(\tilde{\varphi}) \right] \tilde{\varphi} d\tilde{\varphi},
\]

we deduce

\[
C(\tilde{\varphi}) = \frac{\tilde{\theta} - \tilde{\theta}^a}{1 - \frac{S}{2} \phi^2}.
\]

(5.85)

\( S \) is determined by requiring that the leading order equation from the pointwise heat loss boundary condition (5.36) is satisfied,

\[
-2S\phi C(\tilde{\varphi}) = -\frac{Bi_l}{\phi} (1 - S \phi^2) C(\tilde{\varphi}),
\]

(5.86)

so that

\[
S = \frac{Bi_l}{(2 + Bi_l) \phi^2}.
\]

(5.87)

The surface temperature is then evaluated from (5.83), which because of results (5.85) and (5.87) produces a third form of the desired relation (5.54) between \( \partial|_a, \tilde{\theta} \) and \( Bi_l \),

\[
\partial|_a = \theta(\tilde{r} = \tilde{\varphi}, \tilde{\varphi}) = \tilde{\theta}^a + \frac{4}{4 + Bi_l} (\tilde{\theta} - \tilde{\theta}^a).
\]

(5.88)

The assumed temperature distribution (5.83) does not satisfy the governing 3-dimensional equations for either the melt spinning of fibers or the rigid filament processing exactly, but we recall from Figure 33 of the previous chapter that use of this assumed form
in the rigid filament model is satisfactory, compared with the 3-dimensional exact solution.

5.6 Simulation of PET Melt Spinning

We now simulate the process of fiber spinning of poly(ethylene terephthalate) (PET). The material properties of PET and processing conditions used in the numerical simulation are listed in Table 2. Amorphous PET melt experiences glass transition at 67°C. Although in high speed fiber spinning the PET melt exhibits some viscoelastic behavior, since our purpose here is to study the heat transfer phenomena in the processing we model the polymer melt as a Newtonian fluid above glass transition and the solidified polymer as rigid.

The mass throughput $G$ is specified in the simulation and the extrudate velocity $v_0$ is calculated by

$$v_0 = \frac{G}{\pi r_0^2 \rho},$$  \hspace{1cm} (5.89)

where $r_0$ is the spinneret radius. The take-up velocity is also specified in fiber spinning process.

We use the empirical formulae for the dimensional heat transfer coefficient $h$ and the dimensional air drag $T_{rz}$ from Matsui [56, 57]

$$h(z, t) = 1.352 \times \frac{(v_0, 0)^{0.333}}{(\phi(0))^{0.667}} \frac{J/(m^2sK)/(m^{0.334} s^{0.333})}{},$$ \hspace{1cm} (5.90)

$$T_{rz}(z, t) = 4.643 \times 10^{-6} \frac{(v_0, 0)^{1.39}}{(\phi(0))^{0.81}} \text{ Pa} \cdot m^{0.61} / s^{1.39},$$ \hspace{1cm} (5.91)
Table 2: PET properties and spinning conditions used in the simulations of fiber spinning

<table>
<thead>
<tr>
<th>PET properties</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density coefficient $\rho$</td>
<td>kg·m$^{-3}$</td>
<td>1322.9</td>
</tr>
<tr>
<td>Specific heat coefficient $c_0$</td>
<td>J·kg$^{-1}$·K$^{-1}$</td>
<td>711.0</td>
</tr>
<tr>
<td>Specific heat coefficient $c_1$</td>
<td>J·kg$^{-1}$·K$^{-2}$</td>
<td>2.364</td>
</tr>
<tr>
<td>Glass transition temperature $T_g$</td>
<td>K</td>
<td>340.2</td>
</tr>
<tr>
<td>Thermal conductivity $k$</td>
<td>W·m$^{-1}$·K$^{-1}$</td>
<td>0.147</td>
</tr>
<tr>
<td>Surface tension $\sigma$</td>
<td>N·m$^{-1}$</td>
<td>25×10$^{-3}$</td>
</tr>
<tr>
<td>Intrinsic viscosity $[\eta]$</td>
<td>dl·g$^{-1}$</td>
<td>0.6450</td>
</tr>
<tr>
<td>Viscosity $\mu_0$ at 558.2K</td>
<td>Pa·s</td>
<td>204.8</td>
</tr>
<tr>
<td>Activation energy $\mathcal{E}$</td>
<td>J·mole$^{-1}$</td>
<td>56.54×10$^{3}$</td>
</tr>
<tr>
<td>Gas constant $R$</td>
<td>J·mole$^{-1}$·K$^{-1}$</td>
<td>8.314</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Spinning conditions</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spinneret hole radius $r_0$</td>
<td>m</td>
<td>0.2×10$^{-3}$</td>
</tr>
<tr>
<td>Spinline length $z_0$</td>
<td>m</td>
<td>1.2</td>
</tr>
<tr>
<td>Throughput $G$</td>
<td>kg·s$^{-1}$</td>
<td>1.5×10$^{-5}$</td>
</tr>
<tr>
<td>Extrudate temperature $T_0$</td>
<td>K</td>
<td>558.2</td>
</tr>
<tr>
<td>Take-up velocity $u_t$</td>
<td>m·s$^{-1}$</td>
<td>50</td>
</tr>
<tr>
<td>Cooling air temperature $\theta^a$</td>
<td>K</td>
<td>303.2</td>
</tr>
</tbody>
</table>

2 Density calculated by $\rho = \rho_0 - \rho_1\theta_g$, where $\rho_0 = 1493$kg·m$^{-3}$ and $\rho_1 = 0.5$kg·m$^{-3}$·K$^{-1}$, from Iiyashi et al. [37].
3 Calculated by $\mu(\theta) = [\eta]^{0.15}\exp\left\{\frac{136}{\theta} - 2.3\right\}$ poise.
Table 3: The characteristic values of physical properties and conditions for the PET melt spinning process of Table 2

<table>
<thead>
<tr>
<th>Characteristic scales</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transverse length scale $r_e = \sqrt{\frac{\rho}{\pi \rho_c}}$</td>
<td>m</td>
<td>$8.496 \times 10^{-6}$</td>
</tr>
<tr>
<td>Axial length scale $z_e$</td>
<td>m</td>
<td>0.15</td>
</tr>
<tr>
<td>Temperature scale $\theta_e = \text{glass transition} \theta_g$</td>
<td>K</td>
<td>340.2</td>
</tr>
<tr>
<td>Axial velocity scale $v_c = \text{take-up velocity} v_t$</td>
<td>m \cdot s^{-1}</td>
<td>50</td>
</tr>
<tr>
<td>Stress scale, $\tau_c = \mu \left( \frac{\theta_e + \theta_g}{2} \right) \frac{v - v_t}{r_e}$</td>
<td>MPa</td>
<td>1.310</td>
</tr>
<tr>
<td>Specific heat $c_e = c_0 + c_1 \theta_e$</td>
<td>J \cdot kg^{-1} \cdot K^{-1}</td>
<td>1515.2</td>
</tr>
<tr>
<td>Viscosity $\mu_c = \mu(\theta_e)$</td>
<td>Pa \cdot s</td>
<td>$0.5034 \times 10^6$</td>
</tr>
<tr>
<td>Nominal air drag shear $T_{rz}^0$</td>
<td>Pa</td>
<td>1.323</td>
</tr>
<tr>
<td>Nominal heat loss coefficient $h_c$</td>
<td>J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}</td>
<td>$1.199 \times 10^4$</td>
</tr>
</tbody>
</table>

1 Estimated distance from spinneret to solidification point.
2 $T_{rz}^0 = 4.643 \times 10^{-6} \frac{\theta_e}{r_e^{1.19}}$.
3 $h_c = 1.352 \frac{\theta_e}{r_e^{3.23}}$.

For the process described in Table 2, the characteristic values for nondimensionalization are selected as listed in Table 3. The dimensionless numbers and boundary conditions are computed from these characteristic scales as shown in Table 4. Note that for this typical process all of the dimensionless parameters in Table 4 are $O(\epsilon^2)$, i.e. they are between $\epsilon = 5.664 \times 10^{-5}$ and $\epsilon^{-1} = 1.766 \times 10^4$. Hence the leading order problem (5.61)–(5.68) is valid. We integrate these equations for the boundary conditions given in Table 4, and study the predicted behavior for each of the three temperature relations (5.80), (5.81), and (5.88).

The comparison of performance of the three assumptions on the radial temperature variation is shown in Figure 34. The predicted axial profiles of fiber radius, velocity, average temperature, and average tensile stress for each of the three relations are
<table>
<thead>
<tr>
<th>Dimensionless numbers</th>
<th>Formula</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slenderness parameter $\epsilon$</td>
<td>$r_c/z_c$</td>
<td>$5.664 \times 10^{-5}$</td>
</tr>
<tr>
<td>Arrhenius number $E$</td>
<td>$E/(R\theta_c)$</td>
<td>19.99</td>
</tr>
<tr>
<td>Degree of temperature dependence of specific $C$</td>
<td>$C_1\theta_c/z_c$</td>
<td>0.5308</td>
</tr>
<tr>
<td>Reynolds number $Re$</td>
<td>$\rho v_c z_c/\mu_c$</td>
<td>0.01971</td>
</tr>
<tr>
<td>Ellis number $Es$</td>
<td>$2\mu_c v_c/(\tau_c z_c)$</td>
<td>256.2</td>
</tr>
<tr>
<td>Froude number $Fr$</td>
<td>$v_c^2/(g z_c)$</td>
<td>1698.9</td>
</tr>
<tr>
<td>Weber number $W$</td>
<td>$\rho u_c^2 r_c/\sigma$</td>
<td>1124.0</td>
</tr>
<tr>
<td>$B$</td>
<td>$\tau_c/(\rho v_c^2)$</td>
<td>0.3961</td>
</tr>
<tr>
<td>$Y$</td>
<td>$\sigma/(\tau_c r_c)$</td>
<td>$2.246 \times 10^{-3}$</td>
</tr>
<tr>
<td>Graetz number $Gz$</td>
<td>$\rho c_v r_c/(k z_c)$</td>
<td>0.3281</td>
</tr>
<tr>
<td>Biot number, $Bi$</td>
<td>$h_r r_c/k$</td>
<td>0.6932</td>
</tr>
<tr>
<td>$U$</td>
<td>$\tau_c/(\rho c_v \theta_c)$</td>
<td>$1.921 \times 10^{-3}$</td>
</tr>
<tr>
<td>$X$</td>
<td>$\mu_c v_c/(\rho c_v \theta_c z_c)$</td>
<td>0.2460</td>
</tr>
<tr>
<td>$Z$</td>
<td>$h_r z_c/(\rho c_v r_c)$</td>
<td>2.113</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Dimensionless boundary conditions</th>
<th>definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upstream radius $r_0$</td>
<td>$r_0/r_c$</td>
<td>23.54</td>
</tr>
<tr>
<td>Upstream velocity $v_0$</td>
<td>$v_0/v_c$</td>
<td>$1.805 \times 10^{-3}$</td>
</tr>
<tr>
<td>Upstream temperature $\theta_0$</td>
<td>$\theta_0/\theta_c$</td>
<td>1.641</td>
</tr>
<tr>
<td>Downstream velocity $\tilde{v}_i$</td>
<td>$\tilde{v}_i/v_c$</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure 34: The axial profiles of fiber’s radius, velocity, average temperature, and tensile stress obtained from 1-dimensional thin-filament models: the conventional assumption of average temperature equal to surface temperature (dashed line); the Bessel function form of radial temperature distribution based on the rigid solution (dotted line); the parabolic form of radial temperature distribution (solid line).
plotted from the spinneret to the solidification point of the filament. The relations (5.81), (5.88) based on the assumed Bessel function radial temperature distribution and parabolic radial temperature distribution give predictions close to each other, and significantly different from the prediction from the relation (5.80) which follows from the conventional assumption that surface temperature equals average temperature. From our experience in the rigid rod modeling, we can say that the former pair of predictions are better approximate solutions. The conventional assumption predicts too rapid a cooling and a tensile stress that is too high.

The evolutions down the fiber of the radial temperature distribution, as predicted by each of the three assumptions are shown in Figure 35. The radial temperature distribution from the parabolic form is calculated with formula (5.83), or with an explicit form

\[ \tilde{T}(\hat{r}, \hat{z}) = \tilde{T}_a + \frac{1 - S \hat{r}^2}{1 - \frac{S}{2} \phi(0)^2} (\tilde{T} - \tilde{T}_a), \quad S = \frac{Bi_t}{(2 + Bi_t) \phi(0)^2}. \]  

(5.92)

The radial temperature distribution from the Bessel function form is calculated by

\[ \tilde{T}(\hat{r}, \hat{z}) = \tilde{T}_a + \frac{A_t^2}{2Bi_t} \frac{J_0(A_t \hat{r}/\phi(0))}{J_0(A_t)} (\tilde{T} - \tilde{T}_a), \]  

(5.93)

where \( A_t \) is the first root of equation (5.82). The radial temperature variations predicted by the assumed Bessel function form and parabolic form are both pronounced with no significant difference in the average temperature profiles. In contrast, the difference between these predictions and that resulting from the conventional assumption (5.80) is significant. At the position \( z = 0.078 \text{m} \) the average temperature from the conventional assumption is lower than even the surface temperatures from
Figure 35: Radial temperature distributions across the fiber at positions $z = 0.012, 0.024, 0.045, 0.078$ m, calculated from the Bessel function form (dotted line), the parabolic form (solid line), the conventional assumption of radially independent temperature (dashed line). Vertical coordinate is temperature ($^\circ$C). Horizontal coordinate is radial length (m).
the assumed Bessel function form and parabolic form. Figure 35 also shows that the predicted fiber cooling process results in a difference in the fiber stretching process. The molten polymer fiber becomes thin more quickly and the final dimension of fiber is attained earlier as predicted from conventional assumption than predicted from the assumed Bessel function form and parabolic form.

The predicted axial profiles of average temperature, centerline temperature, and surface temperature when the assumed parabolic form (5.88) is used are shown in Figure 36. The temperature difference between the core and the surface of the fiber is of magnitude $10^0$C, and the average radial gradient of temperature is of magnitude of magnitude $10^0$C/m near the solidification point. In contrast, the average axial gradient of temperature is of magnitude $10^3$C/m as the polymer temperature drops 218°C, from the melt temperature 285°C to the glass transition temperature 67°C.

The local values of dimensionless groups are computed with the parabolic form to show the change of regime for the process (Figures 37 and 5.6). Recall that the physical effects which are leading order in the slenderness ratio $\epsilon$ constitute the regime of fiber behavior. In the high-speed spinning of very thin, rapidly cooled fibers, the regime may change with distance down the spinline. For example, the surface tension of polymer melt might be a leading order effect when the jet just emerges at a high temperature from the spinneret and the flow is relatively slow, but may not be a leading order effect downstream where the axial velocity is high and the viscosity is increasing rapidly due to fiber's cooling. We monitor this possible the change of regime by tracking the local values of the dimensionless numbers, in which the local
Figure 36: The predicted temperature profiles of average, centerline, and surface temperature from the parabolic form of radial temperature variation.
Figure 37: The local values of the dimensionless numbers for the process of Table 2, calculated from the parabolic form of radial temperature variation.
Figure 37: Continued.
values of fiber radius, axial velocity, elongational stress, and average temperature are used:

\[
\begin{align*}
  P_l &= \left( \frac{\rho_l \theta}{\rho(\theta)} \right)^l, \quad C_l = \frac{C_l \theta}{c(\theta)}, \quad E_l = \frac{E}{R \theta}, \\
  B_l &= \frac{\tau(\theta)}{\rho(\theta)\nu^2}, \quad Fr_l = \frac{\nu^2}{gz_e}, \quad W_l = \frac{\sigma}{\rho(\theta)\nu^2}, \\
  Y_l &= \frac{\sigma}{\tau(\theta)\phi}, \quad Re_l = \frac{\rho(\theta)\nu z_e}{\mu(\theta)}, \quad Bi_l = \frac{h(\phi, v)\phi}{k}, \\
  X_l &= \frac{\mu(\theta)\nu}{\rho(\theta)c(\theta)\theta z_e}, \quad Z_l = \frac{h(\phi, v)z_e}{\rho(\theta)c(\theta)\nu \phi}, \quad G_l = \frac{\rho(\theta)c(\theta)\nu \phi^2}{k z_e},
\end{align*}
\]

(5.94)

where

\[
(\rho(\theta) = \rho_0 - \rho_l \theta)^l,
\]

\[
c(\theta) = C_0 + C_l \theta,
\]

\[
\mu(\theta) = \mu \exp \left[ E \left( \frac{\theta}{\theta} - 1 \right) \right],
\]

\[
\tau(\theta) = \mu(\theta) \left( \frac{dv}{dz} \right)_l,
\]

\[
h(\phi, v) = 1.352 \frac{v^{0.333}}{\phi^{0.667}} \text{ J/(m}^2\text{sK})/(m^{0.334})^{0.333},
\]

where \( \phi, v, \frac{dv}{dz}, \theta \) are the pointwise solutions of the thin-filament equations (5.69).

The changing local values of the dimensionless number show the evolution of relative importance of physical effects. We have employed an updating scheme which makes use of local value of the Biot number in the evaluation of radial temperature variation.

The effects of gravity and surface tension are important when the spinning speed is low, but quickly become secondary effects as the fiber accelerates. The effect of viscous heating which is negligible in the beginning becomes considerable when the

\[1\text{P number will be defined in Chapter 6 for a material with temperature-dependent density.}\]
highly viscous fiber is stretching. We see from the evolution of $E_\ell$ and $C_\ell$ that the temperature dependence of viscosity and specific heat are leading order effects for the whole process.

Although in this chapter we do not model the melt spinning of polymer with temperature dependent density, we plot $P$ number (which is the dimensionless number as a measure for the level of temperature dependence of density defined in next chapter) by formula $P = \frac{\rho_0 \theta}{\rho(\theta)}$ where $\rho(\theta) = \rho_0 - \rho_1 \theta$. In Figure 37 we see that the temperature dependence of density is a leading order effects for the whole process. The result from monitoring $P$ number leads to a conclusion that deriving a consistent model for melt spinning of polymer with temperature-dependent density in the modeling of fiber spinning is necessary. It is the motivation for the work presented in next chapter.
CHAPTER VI

Modeling Melt Spinning of Polymers with Prescribed Temperature-Dependent Density

In many nonisothermal processes, the temperature dependence of density is an important feature of the material response. It has been shown in Chapter 3 that the use of the thermomechanically constrained theory is necessary to account for the effects of temperature-dependent material density on the velocity, stress and temperature distributions in Poiseuille flows. In the modeling of melt spinning (Hayashi et al. [37], Dutta [23], Kase & Matsuo [47]), the effects of prescribed temperature-dependent material density has not been incorporated into the thin-filament equations correctly. A posteriori substitution of the expression of temperature-dependent material density function into the thin-filament equations for a constant density material (such as those in the previous chapter) is conventionally done; this straightforward extension of incompressibility is incorrect.

In this chapter, the thin-filament equations are rederived in the context of the thermomechanically constrained theory which follows when density is a prescribed function of temperature. The validity of the conventional thin-filament equations (i.e. with \( \rho(0) \) substituted a posteriori into the incompressible equations) will be
examined. The elongational flow in the melt spinning provides us the opportunity to complement our study of the thermomechanically constrained theory applied to Poiseuille flows in Chapter 3.

6.1 The Statement of the Boundary Value Problem

The 3-dimensional boundary value problem for the melt spinning of a material with constant density is given in Chapter 5. Here we model the melt spinning process under the constrained theory for temperature dependent density of polymer developed in Chapter 2. The incompressibility constraint (5.1) is replaced by constraint equation (2.22) involving the density function \( \rho = \rho(\theta) \). Here we assume that the density is a linear function of temperature,

\[
\rho(\theta) = \rho_0 - \rho_1 \theta. \tag{6.1}
\]

The momentum equation (5.2) holds, but with density \( \rho \) now a function of temperature \( \theta \). The energy equation (5.3) is replaced with equation (2.39). The constitutive laws for specific heat, heat flux, an stress remain (5.12), (5.13), and (5.14). The boundary conditions at the free surface of a fiber (5.4) are the kinematic free surface boundary condition (5.5), the stress boundary condition (5.6), and the convective heat loss boundary condition (5.7). The same empirical formulae (5.90) and (5.91) for the heat transfer coefficient \( h \) and the air drag \( T_{rs} \) are used.
6.2 The Dimensionless Boundary Value Problem

As in Chapter 5, we select characteristic values $r_c$, $z_c$, $v_c$, $r_c$, $p_c$, $\theta_c$ for transverse length, axial length, velocity, stress, pressure, and absolute temperature, respectively, and use the same procedure to nondimensionalize velocity components, stress components, pressure, temperature, and fiber radius. In addition, to nondimensionalize the temperature-dependent density $\rho(\theta)$ we adopt as our characteristic density $\rho_c$ the density of the material at the characteristic absolute temperature $\theta_c$,

$$\rho_c = \rho_0 - \rho_1 \theta_c. \quad (6.2)$$

The dimensionless density $\tilde{\rho}$ is then defined through

$$\tilde{\rho}(\tilde{\theta}) = \frac{\rho(\theta)}{\rho_c} = 1 + P - P\tilde{\theta}, \quad (6.3)$$

where

$$P = \frac{\rho_1 \theta_c}{\rho_c}. \quad (6.4)$$

The dimensionless number $P$ is a measure of the degree of temperature dependence of density in a process.

When the scalings are inserted into the axisymmetric form of boundary value problem, we obtain the new dimensionless boundary value problem in polar form, *dimensionless field equations*:

$$\tilde{v}_{r,f} + \frac{\tilde{v}_r}{\tilde{r}} + \tilde{v}_{z,i} = \frac{P}{1 + P - P\tilde{\theta}}(\tilde{\theta}_{,i} + \tilde{v}_r \tilde{\theta}_{,f} + \tilde{v}_z \tilde{\theta}_{,z}), \quad (6.5)$$

$$\epsilon^2(1 + P - P\tilde{\theta})(\tilde{v}_{r,f} + \tilde{v}_r \tilde{v}_{r,f} + \tilde{v}_z \tilde{v}_{z,f}) =$$

$$B \left[ \tilde{T}_{rr,f} + \tilde{T}_{rr} - \tilde{T}_{\theta \theta} \right] + \epsilon^2 \tilde{T}_{rz,i} - \alpha(\tilde{p}_{,i} + \tilde{p}_{,r}^z), \quad (6.6)$$
\[ (1 + P - P\tilde{\theta})(\ddot{v}_{x,t} + \ddot{v}_{y,t} + \ddot{v}_{z,t}) = \]
\[ B \left[ \ddot{T}_{rr} + \ddot{T}_{zz} + \frac{\ddot{T}_{rz}}{\tilde{r}} - \alpha(\ddot{\tilde{p}}_{,t} + \ddot{\tilde{p}}_{,z}) \right] + \frac{1 + P - P\tilde{\theta}}{Pr}, \quad (6.7) \]
\[ (1 + P - P\tilde{\theta}) \left[ 1 - C + C\tilde{\theta} + 2P^2U \frac{(\ddot{\tilde{p}} + \ddot{\tilde{p}}_{,t})\tilde{\theta}}{(1 + P - P\tilde{\theta})^3} \right] (\ddot{\tilde{p}}_{,t} + \ddot{\tilde{p}}_{,r} + \ddot{\tilde{p}}_{,z}) \]
\[ = U \left[ \ddot{T}_{rr} + \ddot{T}_{\theta\theta} \frac{\ddot{v}_{r}}{\tilde{r}} + \ddot{T}_{zz} + \frac{1}{2} \ddot{T}_{rz}(\epsilon^2 \ddot{v}_{r,t} + \ddot{v}_{z,t}) \right] \]
\[ + \frac{1}{Gz} \left( \ddot{\tilde{p}}_{,r} + \frac{1}{r} \ddot{\tilde{p}}_{,r} + \epsilon^2 \ddot{\tilde{p}}_{,tt} \right), \quad (6.8) \]
\[ \dot{\tilde{T}}_{rr} = \frac{\text{Es} \ddot{v}_{r}}{\tilde{r}} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (6.9) \]
\[ \dot{\tilde{T}}_{\theta\theta} = \frac{\text{Es} \ddot{v}_{r}}{\tilde{r}} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (6.10) \]
\[ \dot{\tilde{T}}_{zz} = \frac{\text{Es} \ddot{v}_{z}}{\tilde{r}} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (6.11) \]
\[ \dot{\tilde{T}}_{rz} = \frac{\text{Es} \ddot{v}_{z}}{2} (\ddot{v}_{r,t} + \epsilon^{-2} \ddot{v}_{z,t}) \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (6.12) \]

**dimensionless boundary conditions:**

**kinematic boundary condition:**
\[ (\tilde{\phi}, t - \ddot{v}_{y} + \ddot{v}_{z}\tilde{\phi}, t)|_{\tilde{r}=\tilde{\phi}} = 0, \quad (6.13) \]

**stress boundary conditions:**
\[ (\alpha\ddot{\tilde{p}} - \ddot{T}_{rr} + \epsilon^2 \ddot{T}_{rz}\tilde{\phi}, t)|_{\tilde{r}=\tilde{\phi}} = Y\tilde{\kappa} + \epsilon^2 \ddot{T}_{rz}\tilde{\phi}, t, \quad (6.14) \]
\[ [\ddot{T}_{rz} + (\alpha\ddot{\tilde{p}} - \ddot{T}_{zz})\tilde{\phi}, t]|_{\tilde{r}=\tilde{\phi}} = Y\tilde{\kappa}\tilde{\phi}, t + \ddot{T}_{rz}, \quad (6.15) \]

where
\[ \tilde{\kappa} = r_0\kappa = \frac{1}{\tilde{\phi}(1 + \epsilon^2 \tilde{\phi}_{,t}^2)^{\frac{1}{2}}} - \frac{\epsilon^2 \tilde{\phi}_{,tt}}{(1 + \epsilon^2 \tilde{\phi}_{,t}^2)^{\frac{1}{2}}}. \quad (6.16) \]
convective heat boundary condition:

\[
\frac{1}{(1 + \epsilon^2 \phi_c^2)^{1/2}} \left( \partial_\phi \tilde{\phi} - \epsilon^2 \phi_c^2 \tilde{\phi}_c \right) \Big|_{\phi = \phi_c} = -B \tilde{h}(\tilde{\theta} - \tilde{\theta}_c) \Big|_{\phi = \phi_c}. \tag{6.17}
\]

The dimensionless boundary value problem (6.5)--(6.17) involves the following dimensionless combinations of material properties and characteristic scales:

\[
B = \frac{\tau_c}{\rho_c v_c^2}, \quad Fr = \frac{v_c^2}{g z_c}, \quad Y = \frac{\sigma}{\tau_c r_c}, \quad Es = \frac{2 \mu_c v_c}{\tau_c z_c}, \quad \alpha = \frac{v_c}{\epsilon},
\]

\[
Gz = \frac{\mu_c c_c v_c r_c^2}{k z_c}, \quad Bi = \frac{h_c r_c}{k}, \quad U = \frac{\tau_c}{\rho_c c_c \theta_c}, \quad P = \frac{\rho_c \theta_c}{\rho_c}, \quad C = \frac{C_l \theta_c}{c_c}, \quad E = \frac{E}{R \theta_c}. \tag{6.18}
\]

Compared with the constant-density modeling of Chapter 5, the new dimensionless number involved in the nondimensionalized boundary value problem is \(P\) for the degree of temperature dependence of density. Also, the numbers \(B, Gz,\) and \(U\) now involve the characteristic density \(\rho_c.\)

### 6.3 The Thin-Filament Model Incorporating Fiber’s Shrinkage and Radial Temperature Variation

We now reduce the 3-dimensional boundary value problem of the previous section through integration over the filament cross section. To obtain closure in the resulting 1-dimensional equations, however, we must first make necessary assumptions on spatially-dependent unknowns occurring nonlinearly in the 3-dimensional equations to relate cross-sectional averages of products to products of averages as done in Chapter 5. For a material with constant density it suffices to specify the radial dependence...
of the velocity components. When density is a function of temperature, however, the
constraint pressure \( p \) appears in the energy equation (6.8) in nonlinear combination
with temperature. Therefore, we retain the expansions (5.44) and (5.45) on the ve-
locity components, but also assume an expansion of pressure identical with the form
employed in the perturbation approach for isothermal spinning by Bechtel et al. [7],

\[
p(r, z, t) - p^a = p_c \tilde{p}(r, z, t)
\]

\[
= p_c \sum_{n,m \geq 0} \epsilon^{2n+m} \tilde{p}^{n,m}(r, z, t)
\]

\[
= p_c \{ \tilde{p}^{0,0} + \epsilon \tilde{p}^{0,1} + \epsilon^2 (\tilde{p}^{0,2} + \tilde{p}^{1,0}) \} + O(\epsilon^3). \tag{6.19}
\]

Taking advantage of the geometric property of slender jet, we assume that the
viscosity, density, and effective specific heat are functions of average temperature
over cross-section,

\[
\mu = \mu \exp \left[ E \left( \frac{1}{\tilde{\theta}} - \frac{1}{\tilde{\theta}_c} \right) \right], \tag{6.20}
\]

\[
\rho = \rho_0 - \rho \tilde{\theta}, \tag{6.21}
\]

\[
c_{eff} = C_0 + C_1 \tilde{\theta} + \frac{2\rho_1}{(\rho_0 - \rho_1 \tilde{\theta})^2} \tilde{\theta}^2 \tilde{\theta}, \tag{6.22}
\]

where \( \tilde{\theta} \) (the corresponding dimensionless form \( \tilde{\theta} \)) denotes the average temperature
over cross-section.

We obtain the 1-dimensional leading order problem by inserting the expansions
(5.44), (5.45), and (6.19), and assumptions (6.20), (6.21), and (6.22) into (6.5), (6.8)-
(6.12), then integrating over cross section of fiber and incorporating the boundary
conditions. The leading order 1-dimensional problem is

\[
2v_{r,0}^{0,0} + v_{r,0}^{0,0} = \frac{P}{1 + P - P \tilde{\theta}} (\tilde{\theta}_t + v_{r,0}^{0,0} \tilde{\theta}_r), \tag{6.23}
\]
\((1 + P - \rho \tilde{\rho})(\nu_{x_{i,t}}^{0,0} + \nu_{z_{i,t}}^{0,0}) =\)

\[\frac{2}{\Re} \exp \left[ E \left( \frac{1}{\tilde{\omega}} - 1 \right) \right] \left[ \nu_{x_{i,t}}^{0,0} - \nu_{z_{i,t}}^{0,0} + (\nu_{x_{i,t}}^{0,0} - \nu_{z_{i,t}}^{0,0}) \left( \frac{2 \phi_{i}^{(0)}}{\phi_{0}^{(0)}} - E \frac{\tilde{\omega}}{\tilde{\omega}^2} \right) \right] + \frac{1}{W} \phi_{i}^{(0)} + \frac{2B}{\phi_{0}^{(0)}} \tilde{T}_{r_{t}} - \alpha B \tilde{T}_{r_{t}} + \frac{1 + P - \rho \tilde{\rho}}{\Pr}, \tag{6.24}\]

\((1 + P - \rho \tilde{\rho}) \left[ 1 - C + C \tilde{\rho} + 2P^{2}u \frac{(p_{0,0}^{0,0} + \rho s)^{\tilde{\rho}}}{(1 + P - \rho \tilde{\rho})^{3}} \right] (\tilde{\omega}_{x_{i,t}} + \nu_{x_{i,t}}^{0,0} \rho_{x_{i,t}}) - \frac{PU \tilde{\rho}}{1 + P - \rho \tilde{\rho}} (p_{0,0}^{0,0} + \nu_{x_{i,t}}^{0,0} \rho_{x_{i,t}}) = 2X \exp \left[ E \left( \frac{1}{\tilde{\omega}} - 1 \right) \right] \left[ 2(\nu_{r_{t}}^{0,0})^{2} + (\nu_{x_{i,t}}^{0,0})^{2} \right] - 2Z \frac{\tilde{h}}{\phi_{0}^{(0)}} (\tilde{\omega}_{0} - \tilde{\omega}_{0}) \right] + \frac{PU \tilde{\rho}}{1 + P - \rho \tilde{\rho}} (\tilde{T}_{r_{t}} + \nu_{r_{t}}^{0,0} \rho_{r_{t}}), \tag{6.25}\]

\[\phi_{x_{i,t}}^{(0)} - \phi^{(0)} \nu_{x_{i,t}}^{0,0} + \nu_{x_{i,t}}^{0,0} \phi_{x_{i,t}}^{(0)} = 0, \tag{6.26}\]

\[p_{0,0}^{0,0} = \frac{A_{rr}}{\pi \phi_{0}^{(0)}} + \frac{Y}{\alpha \phi_{0}^{(0)}}, \tag{6.27}\]

\[A_{rr}(\tilde{z}, \tilde{t}) = A_{\tilde{r}_{t}}(\tilde{z}, \tilde{t}) = E \nu_{r_{t}}^{0,0} \phi_{r_{t}}^{(0)} \exp \left[ E \left( \frac{1}{\tilde{\omega}} - 1 \right) \right], \tag{6.28}\]

\[A_{xz}(\tilde{z}, \tilde{t}) = E \nu_{x_{i,t}}^{0,0} \phi_{x_{i,t}}^{(0)} \exp \left[ E \left( \frac{1}{\tilde{\omega}} - 1 \right) \right]. \tag{6.29}\]

To close the system, we postulate

\[\tilde{\omega}_{0} = f(\tilde{\omega}, B_{ii}), \tag{6.30}\]

where \(f(\tilde{\omega}, B_{ii})\) is given by one of expressions (5.80) and (5.88). As before, \(\tilde{\omega}, \tilde{\omega}_{0}, A_{rr}, A_{\tilde{r}_{t}}, \) and \(A_{xz}\) are defined by

\[\tilde{\omega}(\tilde{z}, \tilde{t}) = \frac{2}{\phi^{(0)}} \int_{0}^{\phi^{(0)}} \tilde{\omega}(\tilde{r}, \tilde{z}, \tilde{t}) \tilde{r} d\tilde{r}, \]
\[ \delta_{\theta} = \delta(\hat{r} = \phi, \hat{z}, \hat{t}) = \hat{f}(\phi, B_{ij}), \]

\[ A_{rr}(\hat{z}, \hat{t}) = 2\pi \int_{0}^{d(\theta)} \tilde{T}_{rr}(\hat{r}, \hat{z}, \hat{t}) \hat{r} d\hat{r}, \quad (6.31) \]

\[ A_{\theta\theta}(\hat{z}, \hat{t}) = 2\pi \int_{0}^{d(\theta)} \tilde{T}_{\theta\theta}(\hat{r}, \hat{z}, \hat{t}) \hat{r} d\hat{r}, \]

\[ A_{zz}(\hat{z}, \hat{t}) = 2\pi \int_{0}^{d(\theta)} \tilde{T}_{zz}(\hat{r}, \hat{z}, \hat{t}) \hat{r} d\hat{r}, \]

For this new system, \( v_{r}^{0,0} \) and \( v_{z,i}^{0,0} \) are related by a differential equation (6.23) rather than the algebraic equation \( v_{r}^{0,0} = -\frac{1}{2} v_{z,i}^{0,0} \) in the system of Chapter 5 derived from the assumption of constant density. This algebraic relation is used everywhere in the literature. In the energy equation (6.25), the derivative of pressure \( p_{0}^{0,0} \) is now present, necessitating a boundary condition for \( p_{0}^{0,0} \) that was not needed in the model of Chapter 5. Because of these two features, the generalization of thin-filament equations from constant density to temperature-dependent density is a singular one.

To study this singularity, we eliminate \( p_{0}^{0,0} \) from the energy equation (6.25). First, we rewrite the constraint (6.23) as

\[ v_{r}^{0,0} = -\frac{1}{2} v_{z,i}^{0,0} + \frac{P}{2(1 + P - P\delta)} (\tilde{\theta}_{,i} + v_{z}^{0,0} \tilde{\theta}_{,i}). \quad (6.32) \]

Compared to the incompressibility constraint (5.64) for a material with constant density, there is an extra term \( \frac{P}{2(1 + P - P\delta)} (\tilde{\theta}_{,i} + v_{z}^{0,0} \tilde{\theta}_{,i}) \) in (6.32) that accounts for shrinkage of fibers. Then, with the use of (6.27), (6.28), and (6.32), \( p_{0}^{0,0} \) can be expressed as

\[ p_{0}^{0,0} = -\frac{1}{2} \text{E} v_{z,i}^{0,0} \exp\left[ E\left(\frac{1}{\theta} - 1\right)\right] + \frac{Y}{\alpha_{\phi}^{(0)}} \]

\[ + \frac{P \text{E}}{2(1 + P - P\delta)} \exp\left[ E\left(\frac{1}{\theta} - 1\right)\right] (\tilde{\theta}_{,i} + v_{z}^{0,0} \tilde{\theta}_{,i}). \quad (6.33) \]
The derivative of temperature in expression (6.33) brings out the second order derivative of temperature to \( \tilde{z} \) and \( \tilde{t} \) in energy equation (6.25) when expression (6.33) is substituted into equation (6.25) to eliminate \( p^{0,0} \). Recall that in Chapter 5 the second order derivative of temperature to \( \tilde{z} \) is dropped when the axial thermal conductivity is neglected. This practice is considered suitable for modeling of slender fiber spinning as shown for a rigid rod modeling in Chapter 4 when the solution from neglecting of axial thermal conductivity is compared to the exact solution.

To eliminate the singular terms in the 1-dimensional equation (6.25) we assume that \( P \) is small and retain the terms with \( O(P^0) \) or \( O(P^1) \) only in the new system. Then expressions (6.32) and (6.33) can be simplified as

\[
v_r^{0,0} = -\frac{1}{2} v_{x,t}^{0,0} + \frac{P}{2} (\tilde{t}_{,t}^{0,0} + v_x^{0,0} \tilde{t}_{,t}^{0,0}), \quad (6.34)
\]

\[
p^{0,0} = -\frac{1}{2} E su_x^{0,0} \exp \left[ E \left( \frac{1}{\delta} - 1 \right) \right] + \frac{Y}{\phi^{(0)}} + \frac{PE_s}{2} \exp \left[ E \left( \frac{1}{\delta} - 1 \right) \right] (\tilde{t}_{,t}^{0,0} + v_x^{0,0} \tilde{t}_{,t}^{0,0}). \quad (6.35)
\]

The resulting dimensionless 1-dimensional thin-filament equations are

\[
\phi_{,t}^{(0)} + v_x^{0,0} \phi_{,x}^{(0)} + \phi^{(0)} \frac{v_x^{0,0}}{2} v_{x,t}^{0,0} = \frac{P}{2} \phi^{(0)} (\tilde{t}_{,t}^{0,0} + v_x^{0,0} \tilde{t}_{,t}^{0,0}), \quad (6.36)
\]

\[
(1 + P - P\tilde{t})(v_{x,t}^{0,0} + v_x^{0,0} v_{x,t}^{0,0}) =
\]

\[
\frac{3}{Re} v_x^{0,0} \exp \left[ E \left( \frac{1}{\delta} - 1 \right) \right] + \frac{3}{Re} v_{x,t}^{0,0} \left( 2 \frac{\phi^{(0)}}{\phi^{(0)}} - \frac{E \tilde{t}_{,t}^{0,0}}{\delta^2} \right) \exp \left[ E \left( \frac{1}{\delta} - 1 \right) \right] + \frac{1}{W \phi^{(0)}} + \frac{2B}{\phi^{(0)}} \tilde{f}_{,x}^{0,0} + \frac{1 + P - P\tilde{t}}{Fr} \frac{1}{Re} \left( 2 \frac{\phi^{(0)}}{\phi^{(0)}} - \frac{E \tilde{t}_{,t}^{0,0}}{\delta^2} \right) \exp \left[ E \left( \frac{1}{\delta} - 1 \right) \right] (\tilde{t}_{,t}^{0,0} + v_x^{0,0} \tilde{t}_{,t}^{0,0})
\]
\[-\frac{P}{Re} L(\tilde{z}, \tilde{t}) \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right], \quad (6.37)\]

\[D_4(\tilde{\theta}, \tilde{t} + u^{0,0}_r \tilde{\theta}, \tilde{t}) - PX\tilde{\theta} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] \left[ (v^{0,0}_{r,z}\tilde{t} + v^{0,0}_{z,r}\tilde{t}) \right] = 3X(v^{0,0}_r)^2 \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] + PU\tilde{\theta} \left[ \tilde{\theta}^2 + v^{0,0}_z \tilde{\theta}^2 + \frac{Y v^{0,0}_z}{2 \phi(0)} \right] - 2Z \frac{\tilde{h}}{\phi(0)} (\tilde{\theta}|_0 - \tilde{\theta}^a), \quad (6.38)\]

where

\[D_4 L(\tilde{z}, \tilde{t}) = \]

\[-C\tilde{\theta}, \tilde{t} (\tilde{\theta}, \tilde{t} + u^{0,0}_r \tilde{\theta}, \tilde{t}) - 3X E \left( \frac{v^{0,0}_r}{\tilde{\theta}} \right) \tilde{\theta}, \tilde{t} \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] + 6X v^{0,0}_r v^{0,0}_z \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right] - 2Z \frac{\tilde{h}}{\phi(0)} \left[ f_{\tilde{\theta}}(\tilde{\theta}, Bt) \tilde{\theta}, \tilde{t} + f_{\tilde{B}t}(\tilde{\theta}, Bt) Bt \frac{\phi^{(0)}}{\phi(0)} - \tilde{\theta}, \tilde{t} \right] - 2Z \left( \frac{\tilde{h}}{\phi(0)^2} \phi^{(0)}(\tilde{\theta}|_0 - \tilde{\theta}^a) - \frac{\tilde{h}}{\phi(0)^2} \phi^{(0)}(\tilde{\theta}|_0 - \tilde{\theta}^a) \right), \quad (6.39)\]

where

\[D_4 = (1 + P - P\tilde{\theta})(1 - C + C\tilde{\theta}) + PX v^{0,0}_r \left( 2 - \frac{E}{\tilde{\theta}} \right) \exp \left[ E \left( \frac{1}{\tilde{\theta}} - 1 \right) \right]. \quad (6.40)\]

For the conventional assumption of radially independent temperature, \(\tilde{\theta}|_0 = f(\tilde{\theta}, Bt) = \tilde{\theta}\), we have

\[f_{\tilde{\theta}}(\tilde{\theta}, Bt) = 1, \quad (6.41)\]

\[f_{Bt}(\tilde{\theta}, Bt) = 0. \quad (6.42)\]
For the proposed parabolic form of radial temperature variation, $\frac{\partial}{\partial \theta} = f(\theta, Bi_i) = \theta^2 + \frac{4}{4+Bi_i} (\theta - \theta^2)$, we have

$$f(\theta, Bi_i) = \frac{4}{4+Bi_i},$$  \hspace{1cm} (6.43)  

$$f(\theta, Bi_i) = -\frac{4}{(4+Bi_i)^2} (\theta - \theta^2).$$ \hspace{1cm} (6.44)

For comparison, we write the steady thin-filament equations in matrix form similar to equation (5.69) for fiber spinning of polymer with constant density.

$$M(\mathbf{u})\mathbf{u}_{\theta} = g(\mathbf{u}, \mathbf{u}_{\theta}),$$  \hspace{1cm} (6.45)

with

$$\mathbf{u} = (\phi^{(0)}, v_2^{(0)}, \tilde{\theta}, \omega)^T,$$ \hspace{1cm} (6.46)

$$M(\mathbf{u}) = \begin{bmatrix} v_2^{(0)} & \frac{1}{2} \phi^{(0)} & 0 & 0 \\ M_{21} & v_2^{(0)} & \frac{3E}{Re D_1} \phi^{(0)} & -\frac{3}{Re D_1} \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$ \hspace{1cm} (6.47)

and

$$g(\mathbf{u}, \mathbf{u}_{\theta}) = (g_1, g_2, g_3, \omega)^T,$$ \hspace{1cm} (6.48)

where

$$g_1 = \frac{P}{2} \phi^{(0)} (\tilde{\theta}_{\theta} + v_2^{(0)} \tilde{\theta}_{\theta}),$$ \hspace{1cm} (6.49)

$$g_2 = \frac{1}{Fr} + 2B \frac{\tilde{T}_{\theta}}{D_1 \phi^{(0)}} - \frac{\alpha B}{D_1} \tilde{P}_{\theta}^2,$$

$$- \frac{P}{D_1 Re} \left( 2 \frac{\phi^{(0)}}{\phi^{(0)}} - \frac{\tilde{\theta}_{\theta} \theta^2}{\phi^{(0)}} \right) \exp \left[ E \left( \frac{1}{\theta} - 1 \right) \right] \left( \tilde{\theta}_{\theta} + v_2^{(0)} \tilde{\theta}_{\theta} \right),$$

$$- \frac{P}{D_1 Re} L(\tilde{z}, \tilde{t}) \exp \left[ E \left( \frac{1}{\theta} - 1 \right) \right],$$ \hspace{1cm} (6.50)
\[ g_3 = -2 \frac{Z}{D_4} \phi^{(0)} \left[ \frac{1}{h} (\partial_t \phi, \partial_t \theta_t) - \dot{\theta}^s \right] + 3X \frac{D_3}{D_4} \omega^2 \\
+ \frac{P_D}{D_1} \phi^{(0)} \left( v_z^{0,0} \dot{\theta}^s + \frac{Y \theta_z^{0,0}}{2 \phi^{(0)}} \right) \] 

(6.51)

where

\[ D_1 = 1 + P - P \hat{\theta}, \] 

(6.52)

\[ M_{21} = -\frac{1}{D_1 W \phi^{(0)}^2} - \frac{6D_3}{D_1 \text{Re} \phi^{(0)}} \omega \] 

(6.53)

The boundary conditions are the same as in that in previous chapter.

\[ \phi^{(0)}(0) = \tilde{\phi}_0, \quad v_z^{0,0}(0) = \tilde{v}_0, \quad \ddot{\theta}(0) = \ddot{\theta}_0, \] 

(6.54)

\[ v_z^{0,0}(1) = 1. \] 

(6.55)

The ODE system (6.45) is a quasi-linear system different from the ODE system (5.69) modeling the process with assumed constant density. Solving for the derivative vector \( u_z \) requires an iteration scheme. We use

\[ M(u_z)(u_z)_{i+1} = g[u_z, (u_z)_i] \] 

(6.56)

The linear solution for (5.69) is used as the starting point in the iteration. Iteration ceases while the error norm of derivatives is within the specified tolerance.

### 6.4 Comparison and Discussion

We now simulate the process of fiber spinning of poly(ethylene terephthalate) (PET) described in Table 5, in which PET density is modeled as temperature-dependent
Table 5: PET properties and spinning conditions used in the simulations of melt spinning of PET with temperature-dependent density

<table>
<thead>
<tr>
<th>PET properties</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density coefficient $\rho_0$</td>
<td>kg $\cdot$ m$^{-3}$</td>
<td>1,493 $^1$</td>
</tr>
<tr>
<td>Density coefficient $\rho_1$</td>
<td>kg $\cdot$ m$^{-3}$ $\cdot$ K$^{-1}$</td>
<td>0.5 $^1$</td>
</tr>
<tr>
<td>Specific heat coefficient $c_0$</td>
<td>J $\cdot$ kg$^{-1}$ $\cdot$ K$^{-1}$</td>
<td>711.0 $^2$</td>
</tr>
<tr>
<td>Specific heat coefficient $c_1$</td>
<td>J $\cdot$ kg$^{-1}$ $\cdot$ K$^{-2}$</td>
<td>2.364 $^2$</td>
</tr>
<tr>
<td>Glass transition temperature $T_g$</td>
<td>K</td>
<td>340.2 $^2$</td>
</tr>
<tr>
<td>Thermal conductivity $k$</td>
<td>W $\cdot$ m$^{-1}$ $\cdot$ K$^{-1}$</td>
<td>0.147 $^2$</td>
</tr>
<tr>
<td>Surface tension $\sigma$</td>
<td>N $\cdot$ m$^{-1}$</td>
<td>$25 \times 10^{-3}$ $^2$</td>
</tr>
<tr>
<td>Intrinsic viscosity $[\eta]$</td>
<td>dl $\cdot$ g$^{-1}$</td>
<td>0.6450 $^2$</td>
</tr>
<tr>
<td>Viscosity $\mu_0$ at 558.2K</td>
<td>Pa $\cdot$ s</td>
<td>204.8 $^3$</td>
</tr>
<tr>
<td>Activation energy $E$</td>
<td>J $\cdot$ mole$^{-1}$</td>
<td>$56.54 \times 10^3$ $^1$</td>
</tr>
<tr>
<td>Gas constant $R$</td>
<td>J $\cdot$ mole$^{-1}$ $\cdot$ K$^{-1}$</td>
<td>8.314</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Spinning conditions</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spinneret hole radius $r_0$</td>
<td>m</td>
<td>$0.2 \times 10^{-3}$</td>
</tr>
<tr>
<td>Spinline length $z_0$</td>
<td>m</td>
<td>1.2</td>
</tr>
<tr>
<td>Throughput $G$</td>
<td>kg $\cdot$ s$^{-1}$</td>
<td>$1.5 \times 10^{-5}$</td>
</tr>
<tr>
<td>Extrudate temperature $T_0$</td>
<td>K</td>
<td>558.2</td>
</tr>
<tr>
<td>Take-up velocity $v_t$</td>
<td>m $\cdot$ s$^{-1}$</td>
<td>50</td>
</tr>
<tr>
<td>Cooling air temperature $T_a$</td>
<td>K</td>
<td>303.2</td>
</tr>
</tbody>
</table>

$^1$ Hayashi et al. [37].


$^3$ Calculated by $\mu(\theta) = [\eta]^{1.18}\exp\left(\frac{E}{RT} - 2.3\right)$ poise.
property instead of a constant “effective” value. For the process of Table 5 the characteristic scales can be chosen as in Table 3 with the additional density scale

\[
\rho_c = \rho_0 - \rho_1 \theta_c = 1322.9 \text{ kg/m}^{-3}.
\]  

The dimensionless numbers and boundary conditions to model the process of Table 5 are given in Table 6. The dimensionless number \( \mathcal{P} \) in Table 6, reflects the temperature dependence of density of PET, which could not be incorporated in the simulation in Chapter 5.

### Table 6: The dimensionless numbers and boundary conditions for the PET melt spinning process of Table 5

<table>
<thead>
<tr>
<th>Dimensionless numbers</th>
<th>Formula</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slenderness parameter ( \varepsilon )</td>
<td>( \frac{r_c}{\bar{z}_c} )</td>
<td>5.664 x 10^{-6}</td>
</tr>
<tr>
<td>Arrhenius number ( \mathcal{E}/(R\theta_c) )=</td>
<td>19.99</td>
<td></td>
</tr>
<tr>
<td>Degree of temperature dependence of density ( \mathcal{P} )</td>
<td>( \frac{\rho_t \theta_c}{\rho_c} )</td>
<td>0.1286</td>
</tr>
<tr>
<td>Degree of temperature dependence of specific ( \mathcal{C} )</td>
<td>( C_1 \frac{\theta_c}{\theta_e} )</td>
<td>0.5308</td>
</tr>
<tr>
<td>Reynolds number ( \mathcal{R} )</td>
<td>( \frac{\rho_c v_c z_c}{\mu_c} )</td>
<td>0.01971</td>
</tr>
<tr>
<td>Ellis number ( \mathcal{E} )</td>
<td>( 2\mu_c v_c/(\tau_c z_c) )</td>
<td>256.2</td>
</tr>
<tr>
<td>Froude number ( \mathcal{F} )</td>
<td>( \frac{v_c^2}{(g \rho_c) \bar{z}_c} )</td>
<td>1698.9</td>
</tr>
<tr>
<td>Weber number ( \mathcal{W} )</td>
<td>( \frac{\rho_c v_c^2 r_c}{\sigma} )</td>
<td>1124.0</td>
</tr>
<tr>
<td>( B )</td>
<td>( \frac{\tau_c}{(\rho_c v_c^2)} )</td>
<td>0.3961</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>( \frac{\sigma}{(\tau_c r_c)} )</td>
<td>2.246 x 10^{-3}</td>
</tr>
<tr>
<td>Graetz number ( \mathcal{Gz} )</td>
<td>( \frac{\rho_c c_v v_c r_c}{(k z_c)} )</td>
<td>0.3281</td>
</tr>
<tr>
<td>Biot number, ( \mathcal{Bi} )</td>
<td>( \frac{h_c r_c}{k} )</td>
<td>0.6932</td>
</tr>
<tr>
<td>( U )</td>
<td>( \frac{\tau_c}{(\rho_c c_e \theta_c)} )</td>
<td>1.921 x 10^{-3}</td>
</tr>
<tr>
<td>( X )</td>
<td>( \frac{\mu_c v_c}{(\rho_c c_e \theta z_c)} )</td>
<td>0.2460</td>
</tr>
<tr>
<td>( Z )</td>
<td>( \frac{h_c z_c}{(\rho_c c_e v_c r_c)} )</td>
<td>2.113</td>
</tr>
<tr>
<td>Dimensionless boundary conditions</td>
<td>definition</td>
<td>Value</td>
</tr>
<tr>
<td>Upstream radius ( \bar{r}_0 )</td>
<td>( r/r_c )</td>
<td>23.54</td>
</tr>
<tr>
<td>Upstream velocity ( \bar{v}_0 )</td>
<td>( v_0/v_c )</td>
<td>1.805 x 10^{-3}</td>
</tr>
<tr>
<td>Upstream temperature ( \bar{\theta}_0 )</td>
<td>( \theta_0/\theta_c )</td>
<td>1.641</td>
</tr>
<tr>
<td>Downstream velocity ( \bar{v}_t )</td>
<td>( v_t/v_c )</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure 38 shows the two step improvement we have accomplished for the modeling of fiber spinning processes: 1) we model the effects of shrinkage of the fiber due to cooling; and 2) we account for the radial temperature variation within the fiber. The solutions shown in Figure 38 are obtained from

- the commonly used model with \textit{a posteriori} substitution of expression for temperature-dependent density into the thin-filament equations derived with the use of the assumption of constant density and the assumption of surface temperature equal to average temperature,

- an intermediate model which takes into account the effects of shrinkage but retains the assumption of surface temperature equal to average temperature,

- the model which is derived under the thermomechanically constrained theory with the proposed parabolic form of radial temperature variation and can account for effects of both shrinkage and radial temperature variation.

Emphasis is put on the effects of shrinkage of polymer due to cooling on the fiber stretching, tensioning, and cooling.

Comparing the results from the intermediate model to that from the common practice reveals a phenomenon of stress relaxation which has not been observed before. The tensile stress in the fiber peaks near the glass transition position and then drops almost 50 percent. In contrast, the tensile stress calculated from the commonly used model does not have this peak value and is ever increasing. Without taking into account the effects of shrinkage, the relation $u_r^{0,0} = -\frac{1}{2}u_{r,z}^{0,0}$ is commonly borrowed from
Figure 38: The axial profiles of fiber's radius, velocity, average temperature, and tensile stress obtained from 1-dimensional thin-filament models: the conventional assumption of average temperature equal to surface temperature (dashed line); the parabolic form of radial temperature distribution (solid line); the common practice with a posteriori substitution of expression for temperature-dependent density into the thin-filament equations derived under the assumption of constant density and the assumption of surface temperature equal to average temperature (dotted line).
the classical result in isothermal elongational flows, and applied to nonisothermal fiber spinning modeling in every elsewhere in the literature. This relation approximately holds when the correction term $\frac{1}{2} P u_z^0 \delta \partial_{z} z$ is small. That is the case for the initial stage of fiber spinning where the velocity is low and the axial gradient of temperature is moderate, but the axial gradient of velocity is very high. When the velocity achieves certain level, the correction is no longer negligible. The stretching process of the fiber is almost complete when the tensile stress reaches the peak value, as can be seen from the fiber radius profile in Figure 38. Thus, at this location $v_{r}^{0,0}$ is small. Rewriting relation (6.34) as in the steady state,

$$ u_{\phi}^{0,0} = -2v_{r}^{0,0} + Pu_{z}^{0,0} \delta \partial_{z} z. $$

(6.58)

It follows that when $v_{r}^{0,0}$ is small, the correction $Pu_{z}^{0,0} \delta \partial_{z} z$ of $u_{\phi}^{0,0}$ is significant even though the negative temperature gradient is still moderate, since axial velocity has increased substantially. Neglecting effects of shrinkage results in a significant overestimate of velocity gradient and therefore results in a qualitative error in prediction of fiber tensioning behavior.

Taking into account the radial temperature variation, the tensile stress profile shifts down and the peak value of tensile stress is significantly lower. This is a result of a slower cooling predicted by the new thin-filament model with parabolic form of radial temperature variation than that predicted by the conventional, uniform temperature assumption. Therefore, the new model, compared to the commonly used model, predicts a slower stretching and cooling of the fiber, and a lower maximum tensile stress. Tensile stress also relaxes after a peak value, which is completely missed
by the common practice.

The local values of dimensionless groups are computed with the parabolic form to show the change of regime for the process (Figure 39 and 6.4). The magnitude of the local values of dimensionless numbers reveals the relative importance of each competing effect. We conclude that

1. Temperature-dependent density, as well as the temperature-dependent specific heat, is a leading order effect from the spinneret to solidification point.

2. The effects of surface tension and gravity are leading order near the spinneret where the flow is slow, and quickly decrease and can be neglected.

3. The effects of inertia and rheological force are leading order from the spinneret to solidification point.

4. The Biot number is in order $O(\epsilon^0)$ in the whole process. This implies that radial temperature variation is always a leading order effect.
Figure 39: The local values of the dimensionless numbers for the process of Table 6, calculated from the parabolic form of radial temperature variation.
Figure 39: Continued.
CHAPTER VII

Conclusion

In this dissertation the balance equations governing a constrained material with prescribed temperature-dependent density were derived under a thermomechanically constrained theory, and the effects of constraint response on the flow behavior in channel flows and elongational flows were investigated. The main findings are summarized as follows:

The constraint response $p$ accompanying the thermomechanical constraint imposed by the prescribed function of temperature-dependent density is present not only in the momentum equation but also in the energy equation,

$$
\rho \ddot{\varepsilon} + \frac{\rho'}{\rho} \dot{\rho} + \rho \dot{\theta} (\rho'' - 2 \rho'^2) = \dot{T} \cdot \mathbf{D} + \rho \gamma - \text{div} \mathbf{q}.
$$

The constraint of temperature-dependent density is fundamentally different from incompressibility: one cannot merely insert a temperature-dependent function for density \textit{a posteriori} in the conventional incompressible theory, derived under the assumption of constant density.

The effects of the constraint response on mechanical and thermal phenomena in viscometric flows were investigated. The constraint response term in the energy
equation causes a direct coupling of velocity and temperature fields. This is in contrast to the one-way coupled equations derived under the ad hoc theory (i.e. for an incompressible material, with \textit{a posteriori} substitution of a temperature-dependent expression for density). Therefore, ignoring the constraint response term leads to an erroneous result that, no matter how strong the temperature dependence of density is, it can not effect velocity, temperature and stress distributions.

The constrained theory captures the phenomenon of expansion cooling which is missed by the ad hoc theory. Expansion cooling has the effect of depressing the fluid temperature at the middle of the channel. Our studies show that even for a material with moderate temperature dependence of density the effects of expansion cooling on both velocity and temperature distributions are significant. These effects result in a considerable difference in predicted flow curves relating flow rate to pressure drop, and lead to the conclusion that when the viscous heating is considered in a high shear rate process, the effect of temperature-dependent density should also be included in the context of the thermomechanically constrained theory.

In addition to 2-dimensional channel flows with isothermal walls, flows in slit dies, capillaries, and annular dies were also studied, using the more realistic thermal boundary condition of finite heat loss coefficient. An interesting observation is that varying thermal boundary conditions have an effect on the flow curve similar to that of temperature-dependent density.

A robust approach to deriving thin-filament models for nonisothermal spinning of polymer with prescribed temperature-dependent density was given in the context
of the thermomechanically constrained theory. Thin-filament equations which can account for the effects of shrinkage and radial temperature variation were derived. Presuming radial independence of temperature, which is the basis for thin-filament equations in the literature, was avoided. It was found that the assumption of radial independence of temperature was erroneous in spite of its common use.

A parabolic shape function for radial temperature distribution was proposed to replace the conventional assumption of radially independent temperature. The proposed shape function was examined in a rigid rod model where an exact solution could be obtained, and found satisfactory.

The prediction by the thin-filament model which incorporates both temperature dependence of density and radial temperature variation was compared to that by the conventional thin-filament model. It was discovered that there existed a stress relaxation zone near the fiber's glass transition position. The tensile stress in the fiber reaches its peak near the fiber's glass transition position and then dropped almost 50 percent. The relation of incompressibility in elongational flows,

\[ v_r^{0,0} = -\frac{1}{2} v_z^{0,0}, \]  

is invalid in this stress relaxation zone, and the conventional thin-filament models which are based this relation fail to predict this phenomenon. The above relation should be replaced by

\[ v_r^{0,0} = -\frac{1}{2} v_z^{0,0} + \frac{P}{2} v_s^{0,0} \theta_s^{0,0}, \]  

for nonisothermal elongational flows, where the new term accounts for temperature-induced volume change.
Overall, the new thin-filament model predicts slower stretching and cooling of the fiber, a significant lower maximum tensile stress, and a stress relaxation phenomenon near the fiber's glass transition position in the process. The stress relaxation zone is firstly discovered in this dissertation.
Appendix A

The Pointwise Perturbation Approach to the Modeling of Nonisothermal Slender Jet

A pointwise 1-dimensional perturbation theory has been successfully applied to obtain an asymptotic solution for the isothermal free slender jet (Bechtel et al. [7]). The leading order problems obtained in different regimes of the dimensionless number groups cover all isothermal phenomenological models which have been studied before. Therefore, the pointwise 1-dimensional perturbation theory is a comprehensive approach when applied to the isothermal problem of the free slender jet. Furthermore, its higher order correction problems make the investigation of weak effects and radial dependence possible (Bechtel et al. [5]).

In this Appendix, as an alternative to the integrated theory of the main part of this work, the pointwise perturbation theory is applied to the nonisothermal problem and its limited application is shown. This theory involves asymptotic pointwise expansions of all thermal and mechanical fields. But as pointed out in Chapter 4, in most cases of application to molten polymer processing the temperature field shows a behavior very different from that of the mechanical fields of stress and velocity. As will be shown below, it is this distinct quality of temperature field that extremely limits the
extension of the 1-dimensional perturbation theory to the nonisothermal problem.

First, we assume a straightforward expansion for temperature, and then demonstrate that the valid application of the resulting theory is very limited and without relevance in real polymer fiber spinning processes. The pointwise perturbation theory produces meaningful closed ODE sets only in a few special regimes. All of these regimes are out of the range of the typical processing of the molten polymers.

A.1 A Pointwise 1-Dimensional Perturbation Theory for the Torsionless Axisymmetric Slender Jet

The fluid is assumed to be an incompressible, Maxwell fluid:

\[ \dot{T} + \lambda(\theta) \frac{D}{Dt} \dot{T} = 2\mu(\theta)D. \]  

(A.1)

The relaxation time \( \lambda \) and the viscosity \( \mu \) are assumed to depend on absolute temperature \( \theta \) through the Arrhenius forms

\[ \lambda(\theta) = \lambda_0 \exp\left(\frac{E_c}{R\theta}\right), \quad \mu(\theta) = \mu_0 \exp\left(\frac{E_v}{R\theta}\right), \]  

(A.2)

where \( R \) is the gas constant, and \( \lambda_0, \mu_0, E_c, E_v \) are the material constants. The symbol \( \frac{D}{Dt} \) denotes the material frame-invariant tensor rate:

\[ \frac{D}{Dt}(\cdot) = (\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla)(\cdot) + (\cdot) \mathbf{W} - \mathbf{W}(\cdot) - a(\cdot)\mathbf{D} + \mathbf{D}(\cdot), \]  

(A.3)

where \( \mathbf{W} \) is the skew symmetric part of velocity gradient and \( a \) is the material slip parameter. Constitutive equation (A.1) reduces to the Newtonian constitutive equation used in the main body of this work when \( \lambda_0 = 0. \)
Let $r_c, z_c, t_c, \tau_c, p_c, \theta_c, h_c$ be the jet's transverse and axial length scales, characteristic residence time, characteristic stress, characteristic pressure, characteristic absolute temperature and characteristic heat transfer loss coefficient. The geometry of slender jet is characterized by the slenderness parameter, which is chosen as the perturbation parameter:

$$\epsilon = \frac{r_c}{z_c}, \quad \epsilon \ll 1. \quad (A.4)$$

Note that $\epsilon$ is a fixed, small, positive number. The dimensionless independent variables $\tilde{r}, \tilde{z}, \tilde{t}$ are defined by

$$\tilde{t} = \frac{t}{t_c}, \quad \tilde{r} = \frac{r}{r_c}, \quad \tilde{z} = \frac{z}{z_c} \quad (A.5)$$

and the dependent variables, nonzero velocity and stress components, pressure, and temperature are similarly nondimensionalized by $\tilde{r}, \tilde{z}, \tilde{t}$, respectively. Tildes are used to denote dimensionless variables. In the following, we set $p_c = \tau_c$.

The velocity and stress components are expanded as power series of the dimensionless variable $\tilde{r}$ and small parameter $\epsilon$,

$$v_x(r, z, t) = \frac{z_c}{t_c} \sum_{n,m \geq 0} \epsilon^{2n+m+2} v_{nx}^{n,m}(\tilde{z}, \tilde{t}), \quad (A.6)$$

$$v_y(r, z, t) = \frac{z_c}{t_c} \sum_{n,m \geq 0} \epsilon^{2n+m+1} v_{ny}^{n,m}(\tilde{z}, \tilde{t}), \quad (A.7)$$

$$T_{rr}(r, z, t) = \tau_c \sum_{n,m \geq 0} \epsilon^{2n+m} T_{rr}^{n,m}(\tilde{z}, \tilde{t}), \quad (A.8)$$

$$T_{\theta\theta}(r, z, t) = \tau_c \sum_{n,m \geq 0} \epsilon^{2n+m} T_{\theta\theta}^{n,m}(\tilde{z}, \tilde{t}), \quad (A.9)$$

$$T_{zz}(r, z, t) = \tau_c \sum_{n,m \geq 0} \epsilon^{2n+m} T_{zz}^{n,m}(\tilde{z}, \tilde{t}), \quad (A.10)$$
\[ T_{rz}(r, z, t) = r_c \sum_{n,m \geq 0} \epsilon^{2n+m+1} r^{2n+1} T_{rz}^{m,n}(\hat{z}, \hat{t}), \quad (A.11) \]
\[ p(r, z, t) = p^0 + p_c \sum_{n,m \geq 0} \epsilon^{2n+m} r^{2n} p^{m,n}(\hat{z}, \hat{t}). \quad (A.12) \]

The radius of the fiber is expanded as power series of \( \epsilon \),

\[ \phi(z, t) = r_c \sum_{m \geq 0} \epsilon^m \phi^{(m)}(\hat{z}, \hat{t}). \quad (A.13) \]

The assumption that axial velocity and normal stresses are constant across fiber to leading order produces consistent 1-dimensional equations in isothermal spinning (Bechtel et al. [5]). In the nonisothermal problem, assuming the filament surface temperature equal to its average temperature is equivalent to assuming the temperature is uniform across the fiber to leading order. This assumption has been used for the 1-dimensional thin-filament equations in all published works. Here we attempt to generalize the purely mechanical 1-dimensional pointwise perturbation theory to the thermomechanical problem by adopting the following expansion for absolute temperature.

\[ \theta(r, z, t) = \theta_c \sum_{n,m \geq 0} \epsilon^{2n+m} r^{2n} \theta^{n,m}(\hat{z}, \hat{t}) \]
\[ = \theta_c \{ \theta^{0,0}(\hat{z}, \hat{t}) + \epsilon \theta^{0,1}(\hat{z}, \hat{t}) + \epsilon^2 [ \theta^{0,3}(\hat{z}, \hat{t}) + \hat{r}^3 \theta^{1,0}(\hat{z}, \hat{t}) ] + O(\epsilon^3) \}. \quad (A.14) \]

Note that in this expansion the temperature is assumed to be uniform over the fiber cross-section to leading order.

The ODE solution of this form to the 3-dimensional free surface boundary value problem is sought. The perturbation expansions of velocity and stress components,
temperature and filament radius are inserted into the field equations and the boundary conditions of Chapter 5, together with an assumed regime of filament behavior. The resulting dimensionless equations involve the parameters

\[
\begin{align*}
B &= \frac{\tau_c}{\rho c^2}, \quad Fr = \frac{v_c^2}{g z_c}, \quad W = \frac{\rho c v_c^2 r_c}{\sigma}, \quad E_3 = \frac{2\mu c v_c}{\tau_c z_c}, \\
M &= \frac{\mu c}{\tau_c r_c}, \quad \Lambda = \frac{\lambda c}{t_c}, \quad E_v = \frac{E_v}{R\theta_c}, \quad E_e = \frac{E_e}{R\theta_c}, \\
Gz &= \frac{\rho c v e r_c^2}{k z_c}, \quad Bi = \frac{h e r_c}{k}, \quad U = \frac{\tau_c}{\rho c \theta_c},
\end{align*}
\]

(A.15)

where

\[
\lambda_c = \lambda_0 \exp\left(\frac{E_v}{R\theta_c}\right), \quad \mu_c = \mu_0 \exp\left(\frac{E_v}{R\theta_c}\right).
\]

(A.16)

Like powers of \(e\) and \(r\) are equated to form the leading order and higher order problems. It turns out that closure regimes (in which the closed sets of equations for leading order and higher order problems are obtained) are very limited for the non-isothermal problem based on the temperature expansion (A.14). Only for a very small Graetz number is closure deduced. This physically means that the perturbation solution exists only if the material thermal conductivity is very large. For example, a closure regime is found with

\[
Bi = Bic^2 = O(e^2), \quad Gz = \frac{1}{K} c^2 = O(e^2),
\]

(A.17)

and the rest of the dimensionless numbers in the list (A.15) all \(O(e^0)\).

In this closure regime, the leading order problem is

\[
Du^{(0,0)}_t + M(u^{(0,0)}_t)u^{(0,0)}_x = f(u^{(0,0)}),
\]

(A.18)

with

\[
u^{(0,0)} = (\phi^{(0)}, v^{(0)}, T^{(0,0)}_r, T^{(0,0)}_z, \theta^{(0),0}, \omega),
\]

(A.19)
where

\[ A = - \left[ \frac{2B}{\phi(0)} (T_{zz}^{0,0} - T_{rr}^{0,0} + T_{rr}^a) + \frac{1}{W} \frac{1}{\phi(0)} \right], \quad (A.22) \]

\[ E = \exp \left( \frac{E_v - E_a}{\theta^{\phi(0)}} \right), \quad (A.23) \]

and

\[ f(u^{(0,0)}) = \begin{pmatrix} 0 \\ \frac{1}{F_{rr}} + B(T_{rr}^a + 2T_{rr}^a) \\ -\frac{1}{\lambda} T_{rr}^{0,0} \\ -\frac{1}{\lambda} T_{zz}^{0,0} \\ 2Bi\frac{h}{\phi(0)}(\theta^{0,0} - \theta^a) \\ \omega \end{pmatrix}, \quad (A.24) \]

where \( \tilde{h} \) denotes the dimensionless heat transfer coefficient of the fiber, which may be a function of position and velocity.

The remaining leading order unknowns are determined through the algebraic relations

\[ v_r^{0,0} = -\frac{1}{2} v_z^{0,0}, \quad (A.25) \]

\[ T_{\theta\theta}^{0,0} = T_{rr}^{0,0}, \quad (A.26) \]

\[ p^{0,0} = -T_{rr}^a + T_{rr}^{0,0} + \frac{1}{BW \phi(0)}, \quad (A.27) \]

\[ T_{rs}^{0,0} = (T_{rs}^a - T_{rs}^{0,0}) \frac{1}{\phi(0)} + (T_{zz}^{0,0} - T_{rr}^{0,0}) \frac{\phi^{(0)}}{\phi(0)}, \quad (A.28) \]
This leading order equations can be used to model the material behavior if the process regime lies in the closure regime specified above. Hence for processes with small Graetz number (e.g. involving materials with large thermal conductivity) the temperature profiles across the filament will be flat to leading order, in agreement with the assumption for (A.14). This regime is far from the conditions existing in polymer fiber spinning processes.

A.2 The Problem in the Regime of Typical Processes of Molten Polymer Spinning

Recall from Table 4 that the regime typical for fiber spinning process has

\[ Gz = O(\epsilon^0), \quad Bi = O(\epsilon^0). \]  \hspace{1cm} (A.30)

In this regime, the leading order equation in the pointwise perturbation theory from the heat loss boundary condition (5.7) is

\[ \theta^{0,0} - \theta^* = 0. \]  \hspace{1cm} (A.31)

It requires the leading order solution for temperature field matches the ambient temperature as soon as the fiber is extruded. Therefore, if a theory assumes the temperature distribution across the filament is uniform to leading order, it cannot model the cooling of the filament.
To further explain this result: in the dimensional 3-D problem the convection boundary condition is

$$- \frac{k}{h} (\text{grad}\theta \cdot n)|_\partial = \theta|_\partial - \theta^a. \quad (A.32)$$

For the slender fiber $n$ to leading order is $\epsilon r$, so that $\text{grad}\theta \cdot n$ on the boundary is $\frac{\partial \theta}{\partial r}$ to leading order. Hence the leading order convection boundary condition is

$$- \frac{k}{h} \left( \frac{\partial \theta}{\partial r} \right) |_\partial = \theta|_\partial - \theta^a. \quad (A.33)$$

With the assumption that to leading order the temperature $\theta = \theta^{0,0}(z, t)$ is uniform over the cross section, then $\frac{\partial \theta}{\partial r}$ is zero. Hence unless $\frac{k}{hk_0\epsilon}$ is very large (which is not the case in industrially fiber spinning process), equation (A.33) reduces to

$$\theta|_\partial = \theta^{0,0} = \theta^a. \quad (A.34)$$

One cannot model the cooling of filaments with a theory which ignores to leading order the radial variation of temperature in the filament. To model cooling of a filament there must be a transverse variation in temperature to leading order, no matter how slender the filament. Precisely, the radial variation of temperature must be a leading order effect in most practical regimes.

It can been seen from the relation shown in Figure 28 of the Biot number and the first eigenvalue $A_1$ in the rigid rod model that solutions of the form (A.14) do exist in some regimes. The radial temperature distribution becomes flat, i.e. radially uniform, as $A_1$ and the Biot number approach zero (Figure 30). However, $A_1$ increases rapidly with the Biot number and the radial temperature variation soon becomes considerable. Hence the regime (A.17) with $\text{Bi} = O(\epsilon^2)$ gives closed sets of equations with
temperature assumed to be uniform over the cross-section, but not in a regime such as (A.30), with Bi large enough to induce a significant radial temperature variation.
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