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**RHEOLOGICAL CHARACTERIZATION OF
COMPLEX MATERIALS
AND
MODELING OF SHEAR – FREE FLOWS**

by

© Michel A. Beaulne

B.A.Sc. Chemical Engineering

A Thesis

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the Degree of Master of Applied Science**

in

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Abstract

The behaviour of complex materials, the main study of rheology, is investigated in this work. In an effort to better understand these materials, a two-step process was undertaken. First, the nonlinear behaviour of such materials was determined in a laboratory. Second, experimental measurements were extracted from the literature with respect to shear-free flows of complex materials and simulations were performed for the shear-free flows in question. These flows involve uniaxial extension in the case of fiber spinning and film casting, and biaxial extension in the case of film blowing.

Rheological experiments were conducted on polymer solutions, namely poly(ethylene oxide) and polyacrylamide, at room temperature and on a polypropylene (PP) polymer melt at high temperature, with a Weissenberg rheogoniometer in a laboratory. The shear viscosity and first normal stress difference were measured at varying shear rates. An integral constitutive equation of the K-BKZ type was used to predict the nonlinear behaviour of these materials. Transient regression was performed to find the parameters of the K-BKZ model for the L8-Stamylan low-density polyethylene (LDPE), and predictions for steady-state materials functions were given.

Fiber-spinning simulations were undertaken for a series of complex materials at a wide range of operating conditions. A one-dimensional approach was used in the development of the code, F-SPIN, used for the simulations. The Newtonian and upper-convected Maxwell (UCM) models were first used to ensure the numerical scheme was accurate. Isothermal simulations were then undertaken with the use of the K-BKZ model for the M1 polymer solution. The results were compared to previous experimental data, and an attempt was made to predict the elongational viscosity from fiber-spinning experiments. Good overall agreement between the simulations and experiments was achieved. Isothermal simulations were also performed with a PP melt. Good overall agreement was obtained with experimental measurements for the fiber radius and velocity, but not with the drawing force. Poor agreement for the drawing force was attributed to non-isothermal influences in the experiments. Non-isothermal simulations were conducted for a poly(ethylene terephthalate) (PET) melt and the IUPAC-A LDPE

melt. In the case of the PET melt, good agreement was obtained with previous non-isothermal simulations, while a fair agreement was obtained with experimental data. The effects of inertia, gravity, and especially air drag were found to be significant. In the case of the IUPAC-A LDPE melt, good agreement was obtained with previous simulations when an assumption concerning the extrudate swell effect was made. However, only a fair agreement was obtained with the experimental data, which could be due to other effects not taken into account, such as two-dimensional effects.

Film-casting simulations were also undertaken for a series of complex materials. Again, a one-dimensional approach was used in the development of the code, F-CAST, used in the simulations. The Newtonian and UCM models were first used to ensure the numerical scheme was accurate. Comparisons were made with previous two- and three-dimensional simulations for the Newtonian and UCM models. Very good agreement was obtained with the previous two-dimensional simulations with the UCM model. The K-BKZ model was then used for viscoelastic simulations of a PP melt and comparisons were made with previous experimental data. Good overall agreement was obtained with the experimental data. A parametric study was performed for two polymer melts, namely PET and the IUPAC-A LDPE, due to a lack of experimental data in the literature. The PET melt behaved much like a Newtonian fluid, while the IUPAC-A LDPE melt behaved much like a UCM fluid. This was explained by calculating the Trouton ratio (T_R) for each material.

Film-blowing simulations were undertaken for complex materials. A one-dimensional approach was used in the development of the code, F-BLOW, used in the simulations. The Newtonian and UCM models were first used to ensure the numerical scheme was accurate. The UCM model was also used in an investigation of using two non-isothermal approaches: the Morland-Lee hypothesis and the shifting of relaxation times. Both methods gave similar predictions at low temperature drops, but gave moderately different predictions at higher temperature drops. Non-isothermal simulations were conducted for the L8-Stamylan LDPE, and comparisons were made with previous non-isothermal simulations and experimental data. Good agreement was obtained with the previous simulations, but poor agreement was obtained with the experimental data.

The poor agreement with experimental data was attributed to a deficiency in the one-dimensional approach to take into account all the forces acting on the blown film. Comments were also made regarding a previous simulation study and questions were raised concerning its validity.

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Nomenclature

a	relaxation modulus (Pa)
	limit of integration
a_T	Arrhenius shift factor
a(x)	variable
	velocity gradient for film casting
A	aspect ratio
	dimensionless force
A_s	surface area (cm ²)
b	coefficient in air drag relation
	limit of integration
b(x)	velocity gradient for film casting
B	aspect ratio
	dimensionless pressure
c	speed of rotation (rev s ⁻¹)
	stress conservation parameter
c_i	i th guess for the bisection method
c_p	specific heat capacity (erg g ⁻¹ K ⁻¹)
C_f	air drag coefficient
$\overline{C}_t$	Cauchy-Green tensor
$\overline{C}_t^{-1}$	Finger strain tensor
d	diameter (cm)
D	diameter (cm)
D_R	draw ratio
$\overline{D}$	rate-of-deformation tensor (s ⁻¹)
E	activation energy (J mole ⁻¹)
	error

f	function dimensionless force
$\overline{f}$	extra force vector
F	take-up force (dynes) force on lower plate (dynes) function
$\overline{F}$	deformation tensor
$\overline{g}$	acceleration due to gravity (cm s^{-2})
g	function
G'	storage modulus (Pa)
G''	loss modulus (Pa)
h	thickness (cm) function
h_c	convective heat transfer coefficient ($\text{erg cm}^{-2} \text{K}^{-1}$)
H	strain-memory function (s)
I	integral
$\overline{I}$	identity tensor
I_C	first invariant of the Cauchy-Green tensor
$I_{C^{-1}}$	first invariant of the inverse Cauchy-Green tensor
$I_{C^{-1}}$	first invariant of the Finger strain tensor
$II_{C^{-1}}$	second invariant of the Finger strain tensor
$\overline{J}$	Jacobian matrix
k	thermal conductivity ($\text{erg s}^{-1} \text{cm}^{-1} \text{K}^{-1}$)
k_i	i^{th} Runge-Kutta equation
k_1	heat capacity empirical constant
k_2	heat capacity empirical constant (K^{-1})
k_T	modulus of torsion bar ($\text{dynes cm } \mu\text{m}^{-1}$)
k_N	modulus of normal force leaf spring ($\text{dynes } \mu\text{m}^{-1}$)
l	position within element

l_e	length of element
L	characteristic length (cm) length (cm) degree of Gauss-Legendre quadrature
M	time-memory function ($\text{Pa}\cdot\text{s}^{-1}$) number of nodes
n	moving normal coordinate (cm)
$\bar{n}$	outward unit normal
N	number of modes in relaxation spectrum
N_1	first normal stress difference (Pa)
N_1^+	transient first normal stress difference (Pa)
N_2	second normal stress difference (Pa)
p	hydrostatic pressure (Pa)
P	pressure (Pa)
$\bar{q}$	heat flux vector ($\text{erg cm}^{-2} \text{s}^{-1}$)
Q	volumetric flow rate ($\text{cm}^3 \text{s}^{-1}$)
r	radius (cm) radial coordinate (cm)
R	ideal gas constant ($\text{J mole}^{-1}\cdot\text{K}^{-1}$) radius (cm)
$\{R\}$	residual vector
R_i	residual
R_s	principal radius in s -coordinate (cm)
R_t	principal radius in t -coordinate (cm)
s	moving axial coordinate (cm)
S_k	substitution for Gauss-Laguerre quadrature
$\{S\}$	set of unknowns
t	moving transverse coordinate (cm)
t	present time (s)
t'	past time relative to the present (s)

t''	a time between present time t and past time t' (s)
T	temperature (K, °C)
T_f	film temperature (K, °C)
T_{ref}	reference temperature (K)
T_∞	ambient temperature (K, °C)
u	axial velocity (cm s ⁻¹)
v	velocity (cm s ⁻¹)
$\vec{v}$	velocity vector
w	width (cm)
w_i	Gauss-Legendre integration weights
	Gauss-Laguerre integration weights
x	axial coordinate (cm)
x_i	Gauss-Legendre integration points
$\vec{x}$	position vector of the present state (cm)
$\vec{x}'$	position vector of the past state relative to the present (cm)
y	transverse coordinate (cm)
z	axial coordinate (cm)
	position at present time (cm)
z_i	Gauss-Laguerre integration points
z'	position at past time (cm)
z''	a position between present position z and past position z'

Greek Letters

α	shear material parameter for the K-BKZ model
	angle of conical upper plate (radians)
β	elongational material parameter for the K-BKZ model
γ	shear strain (cm cm ⁻¹)

$\dot{\gamma}$	rate-of-strain tensor (s^{-1})
γ	shear rate (s^{-1})
δ	expansion coefficient (K^{-1})
Δl	streamline segment (cm)
Δ_N	deflection of normal force leaf spring (μm)
ΔP	blow-up pressure (Pa) pressure drop (Pa)
$\{\Delta S\}$	change in unknowns
Δ_T	deflection of torsion bar (μm)
Δx	step increase in distance (cm)
ε	extensional strain ($cm\ cm^{-1}$) emissivity
$\dot{\varepsilon}$	extensional rate (s^{-1})
$\dot{\varepsilon}_B$	biaxial extensional rate (s^{-1})
$\dot{\varepsilon}_E$	uniaxial extensional rate (s^{-1})
$\dot{\varepsilon}_P$	planar extensional rate (s^{-1})
η	viscosity (Pa·s)
η_0	zero-shear-rate viscosity (Pa·s)
η_B	biaxial elongational viscosity (Pa·s)
η_E	uniaxial elongational viscosity (Pa·s)
η_P	planar elongational viscosity (Pa·s)
η_S	steady-state shear viscosity (Pa·s)
η_S^+	transient shear viscosity (Pa·s)
θ	azimuthal coordinate (degrees) normal stress material parameter for the K-BKZ model interpolation function, dimensionless
κ_1	dimensionless heat transfer coefficient
κ_2	dimensionless heat transfer coefficient

λ	relaxation time (s)
μ	Newtonian constant viscosity (Pa·s)
ξ	local elemental coordinate
	particle's internal time (s)
ρ	density (g cm ⁻³)
σ_{SB}	Stefan-Boltzmann constant (erg s ⁻¹ cm ⁻² K ⁻⁴)
$\bar{\sigma}$	total stress tensor (Pa)
$\bar{\tau}$	extra stress tensor (Pa)
τ	shear stress (Pa)
τ_{ij}	stress in j -direction normal to i -direction (Pa)
$\mathfrak{T}$	torque (dynes cm)
ϕ	angle from tangent of inner bubble surface to origin (degrees)
ψ	interpolation function
Ψ_i	i^{th} interpolation function
Ω	real (physical) domain
ω	frequency (s ⁻¹)

Subscripts

a	at ambient conditions
air	at air conditions
B	biaxial
E	elongational (uniaxial)
i	present iteration
	i^{th} node
	i^{th} coordinate
j	j^{th} coordinate
ij	components of a tensor

L	take-up conditions
max	maximum value
n	n-direction
o	exit-die conditions
	reference temperature conditions
P	planar
s	s-direction
S	shear
t	t-direction
x	x-direction
y	y-direction
z	z-direction
θ	θ-direction
0+	immediately outside of the die
0-	immediately inside of the die
∞	infinite
	ambient conditions

Superscripts

e	element
(e)	element
i	present iteration
'	past state relative to the present
"	state between present state and past state
-1	the inverse of a matrix
*	dimensionless quantity
T	transpose of a vector

Overscripts

–	characteristic value
–	average value
–	vector
=	matrix, tensor
·	rate
∇	upper-convective derivative

Dimensionless Groups

Fr Froude number = $\frac{u}{gD}$

Pr Prandtl number = $\frac{c_{p,a}\mu_a}{k_a}$

Ra Raleigh number = $\frac{g(T - T_a)L^3 c_{p,a}\rho_a^2}{T_f k_a \mu_a}$

Re Reynolds number = $\frac{Du\rho}{\eta}$

T_R Trouton ratio = $\frac{\eta_E(\dot{\epsilon})}{\eta_S(\dot{\gamma})}$

Ws Weissenberg number = $\frac{\lambda}{t} = \frac{\lambda U}{R}$

Mathematical Symbols

·	dot product
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:	double-dot product
Δ	increment
∂	differential operator
∇	vector differential operator
$\frac{D}{Dt}$	substantial derivative
$\sum_i$	summation over i
Γ	multiplication series
{ }	column vector
[]	matrix
 	magnitude
	determinant
e	natural exponential
exp	natural exponential
tr	trace of a tensor

Abbreviations

FEM	Finite Element Method
IUPAC	International Union for Pure and Applied Chemistry
K-BKZ	Kaye; Bernstein, Kearsley, and Zapas
LDPE	Low-Density Polyethylene
PET	Poly(Ethylene Terephthalate)
PP	Polypropylene
PS	Polystyrene
PTT	Phan-Thien, Tanner
UCM	Upper-Convected Maxwell

Chapter 1

Introduction

1.1 Polymer Processing

The manufacturing of a polymeric material into a useful product, known as *polymer processing*, is the subject matter of the *plastics industry*. This industry has become one of today's largest industries, contributing \$3.5 billion to Canada's annual gross domestic product (GDP) in 1997, compared to \$6.6 billion contributed from the paper industry (Statistics Canada, 1997). The paper industry has an average annual growth rate (AAGR) of 1%, while the plastics industry has an AAGR of 5% (Industry Canada, 1997). The growth of the plastics industry is expected to double the economic growth rate beyond the year 2000 (Industry Canada, 1997). The continuing growth of the polymer industry is due, in part, to the applicability of plastics in other major industries (e.g., reinforced polymer side-panels in the automotive industry). It is also due to the low cost of the polymeric material and the ease with which the material can be manipulated. This manipulation of a polymeric material into a useful product is the main embodiment of polymer processing. To fully understand a polymer process, the polymer engineer must know the mechanics, kinematics, and any other extra effects the polymer is exposed to, while undergoing its transformation.

For the modern polymer engineer, the computer has become an integral tool to analyze, design, and control the polymer from a hot material (called the *melt*) to a final product. To do so, a mathematical model is needed, which incorporates all the forces and effects (e.g., pressure and temperature) exerted on the polymer to predict the final characteristics of the product (e.g., processing speed and strength of the material). Hence, the model must take into account such principles as mass, momentum, and energy conservation, as well as any extra effects from the polymer.

1.2 Rheology

Most of the materials under consideration for a polymer process are *viscoelastic*. By definition, a viscoelastic material possesses both viscous and elastic properties. In a short time-scale they respond elastically, but due to the material's fading memory they respond like fluids on a long-time scale. The elastic response of these materials causes unusual flow phenomena and can complicate the polymer process. Hence, the viscoelastic properties of the polymeric material can be the most important of the transport properties in the design of a polymer process.

The study of the elastic and viscous effects of different materials is known as *rheology*, where the formal definition of rheology is “*the science of deformation and flow of materials*” (Bird et al., 1960). In the field of rheology, there exist many material functions used to describe the significance of the elastic and viscous forces present in different flows.

a) Shear Viscosity

One rheologically significant material function used to characterize forces within a flowing material is the *shear viscosity*. The shear viscosity can be viewed as the resistance of the material (fluid) to flow. In terms of the stresses within the fluid, the definition of the shear viscosity is:

$$\eta_s = \frac{\tau_{xy}}{\dot{\gamma}} \quad (1.1)$$

where τ_{xy} is the shear stress, η_s is the shear viscosity, and $\dot{\gamma}$ is the shear rate. The shear stress τ_{xy} can be interpreted as the viscous flux of x -momentum in the y -direction.

A mathematical relationship that provides the stresses in a liquid, given the flow history, is known as a *constitutive equation*. A very simple constitutive equation is Newton's law of viscosity, which states for simple shear flow

$$\tau_{xy} = \mu \dot{\gamma} \quad (1.2)$$

where μ is a constant viscosity. Water is the most common fluid obeying the Newtonian model. The shear viscosity of the viscoelastic materials used in a polymeric process can

be very high compared to water (e.g., a polystyrene (PS) melt at 160°C has a viscosity $\eta_s = 1 \times 10^5$ Pa·s, while water at room temperature has a viscosity $\eta_s = 1 \times 10^{-3}$ Pa·s). Viscoelastic materials also possess a characteristic behaviour known as *shear-thinning*, i.e., the material's viscosity decreases at higher shear rates. The experimental variations of the shear viscosity with respect to the shear rate are shown in Figure 1.1(a) for a typical low-density polyethylene (LDPE) melt (Meissner, 1975). It is noted that at a shear rate higher than about $\dot{\gamma} = 0.01 \text{ s}^{-1}$, the shear viscosity of the LDPE melt starts decreasing (shear-thinning). Shear-thinning is known to be caused by the molecules in the material aligning due to shear deformation.

b) Normal Stress Differences

Another set of significant rheological material functions used to characterize forces within a flowing material are the *normal stress differences*. For their definition we have to use a three dimensional perspective, where the stresses (force per unit area) experienced by a flowing material in rectangular Cartesian coordinates can be expressed as:

$$\underline{\sigma} = \begin{pmatrix} -p + \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & -p + \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & -p + \tau_{zz} \end{pmatrix} \quad (1.3)$$

where p is called the *isotropic pressure*. The components $-p + \tau_{xx}$, $-p + \tau_{yy}$, and $-p + \tau_{zz}$ are called the *normal stresses*, while the other components are called the *shear stresses*. Since the isotropic pressure p is usually unknown, convenient rheological expressions for the normal stresses are:

$$N_1 = (-p + \tau_{xx}) - (-p + \tau_{yy}) = \tau_{xx} - \tau_{yy} \quad (1.4)$$

$$N_2 = (-p + \tau_{yy}) - (-p + \tau_{zz}) = \tau_{yy} - \tau_{zz} \quad (1.5)$$

where N_1 and N_2 are called the *first* and *second normal stress differences*, respectively. The quantity N_1 can be measured quite accurately for low shear rates, while the quantity N_2 is, in general, difficult to determine. The variation of N_1 with respect to the shear rate is shown in Figure 1.1(b) for a typical LDPE melt (Meissner, 1975). The normal forces within a flowing polymeric material play a major role in rheological phenomena such as

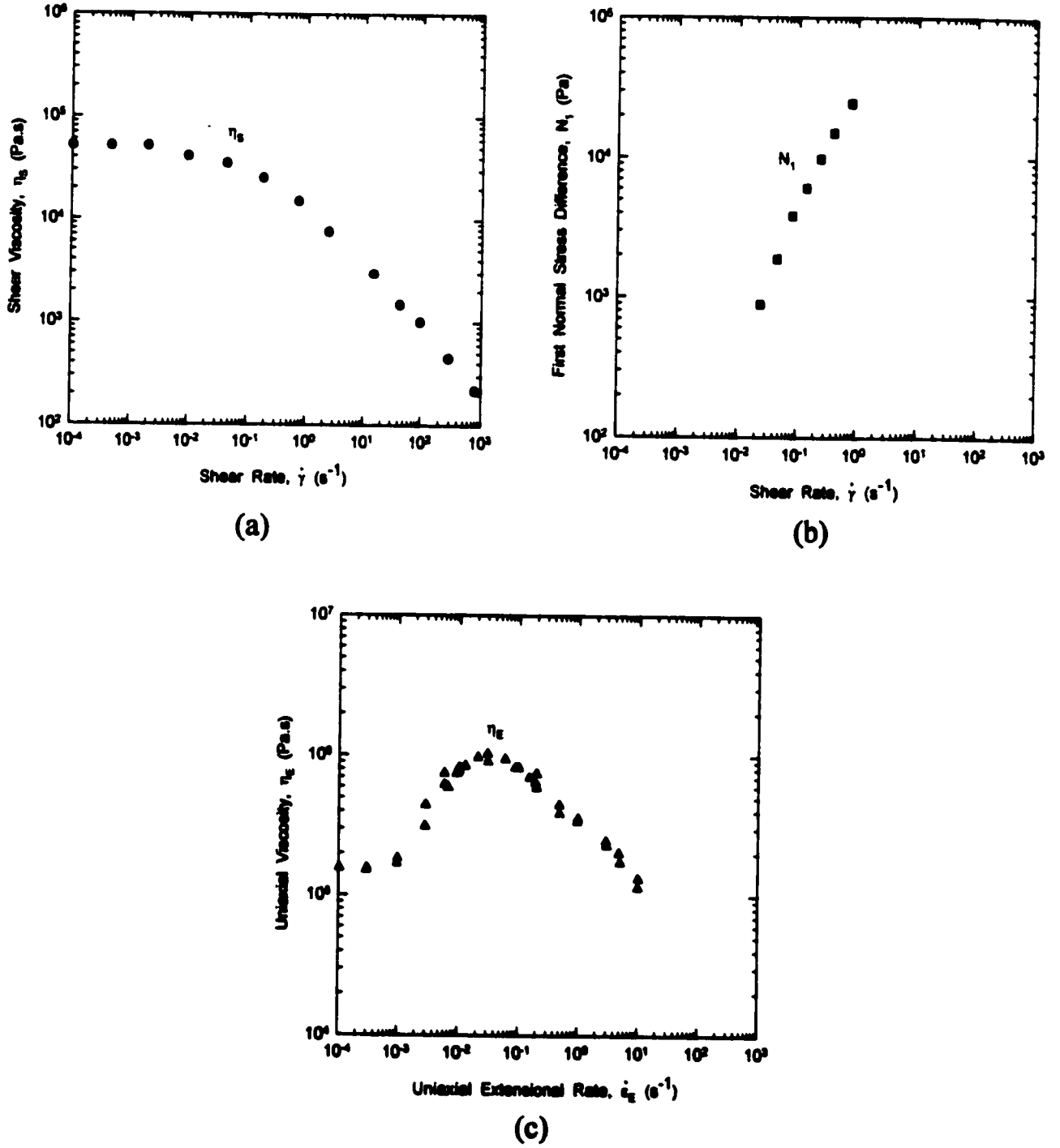


Figure 1.1: Rheological material functions for a typical LDPE melt at 150°C (Meissner, 1975): (a) Shear viscosity vs. shear rate; (b) first normal stress difference vs. shear rate; (c) elongational viscosity vs. elongational rate.

extrudate swell (Larson, 1988), which is the swelling of the polymer as it exits from a die into the atmosphere.

c) Extensional Viscosities

Significant rheological material functions used to characterize forces within a flowing material in shear-free flows (absence of walls) are the *extensional viscosities*. These are defined by the first normal stress difference, N_1 , and the extensional rates, $\dot{\epsilon}$. Geometrically, there are three different ways of stretching a fluid, i.e., uniaxial extension, planar extension, and biaxial extension (Dealy and Wissburn, 1980). There are three corresponding definitions of extensional viscosity:

$$\eta_E = \frac{N_1}{\dot{\epsilon}_E} \quad (\text{uniaxial extensional viscosity}) \quad (1.6)$$

$$\eta_P = \frac{N_1}{\dot{\epsilon}_P} \quad (\text{planar extensional viscosity}) \quad (1.7)$$

$$\eta_B = \frac{N_1}{\dot{\epsilon}_B} \quad (\text{biaxial extensional viscosity}) \quad (1.8)$$

where $\dot{\epsilon}_E, \dot{\epsilon}_P, \dot{\epsilon}_B$ are the equivalent extensional rates. Figure 1.1(c) shows experimental data for the variation of one of the extensional viscosities (η_E , the uniaxial viscosity) with respect to the extensional rate, $\dot{\epsilon}_E$, for a typical LDPE melt (Meissner, 1975). Different polymers can exhibit very different extensional viscosities; they can rise sharply at a certain extensional rate or they can remain constant for a large range of extensional rates. The extensional viscosities for polymer melts are extremely difficult to measure (Larson, 1988) and a subject of active research.

d) Dynamic Functions

There also exist significant rheological material functions, in several tests where the material is under oscillatory deformation. Similar to the shear viscosity, which is related to the material's resistance to shear flow, the dynamic functions of the material relate to its ability to either resist or yield oscillatory motion. Thus, two functions known as the *storage modulus* (G') and the *loss modulus* (G'') are defined. The moduli of the material can also be viewed as the rigidity of the material. For a *perfectly elastic* material, which

stores all mechanical energy imparted to it, $G'' = 0$. For a *perfectly viscous* material, which instantly loses all mechanical energy, $G' = 0$. Figure 1.2 shows the experimental variation of the storage and loss modulus (G', G'') as a function of frequency for the same LDPE melt used by Meissner (1975). The variation of the moduli can be very different for different materials.

1.3 Extrusion and Extrusion Dies

The majority of polymer processes (roughly 95%) require an *extruder* to compress, convey, and melt the polymer before it is shaped into a final product. A schematic representation of a typical extruder is shown in Figure 1.3(a) (Baird and Collias, 1995). Also shown in Figure 1.3(b) is the *die*, which usually accompanies the extruder. The first part of the extruder is the feed hopper, where the polymer in solid form (usually in the form of pellets) is fed into the extruder. The polymer pellets are then conveyed by the extruder *screw* down the barrel of the extruder through the *solids conveying zone* to the *melting zone*. It is here that the barrel is equipped with heaters in order to change the phase of the polymer from a solid form into a liquid or melt form. Once the polymer melt passes through the *melt conveying zone*, it is fed into the die. The die usually consists of a *manifold*, to distribute the polymer melt evenly throughout the die, and a *restrictor* to control the flow rate and the pressure of the polymer melt as it exits the die. The die lips are used to control the final shape of the polymer melt as it exits the die. It is here that extrudate swell occurs, and it is caused by the relaxation of stresses accumulated within the extruder and the die. The existence of extrudate swell must be taken into account in the process and is an important aspect in die design.

1.4 Polymer Processing of Fibers and Films

Three important polymer processes used in the plastics industry to manufacture fibers and films are the processes of (a) *fiber spinning*, (b) *film casting*, and (c) *film blowing*. The three processes are shown in Figure 1.4 (Baird and Collias, 1995). Each process is

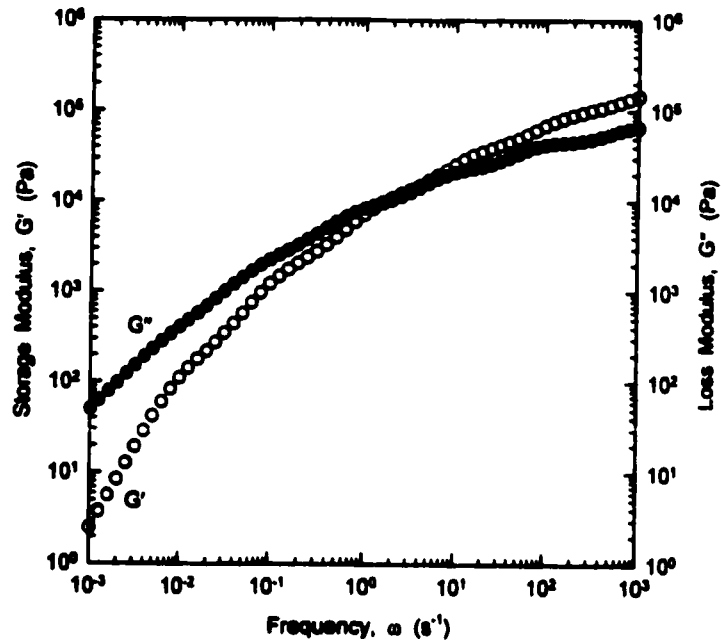


Figure 1.2: Storage and loss modulus (G' , G'') as a function of frequency for a typical LDPE melt at 150°C (Meissner, 1975).

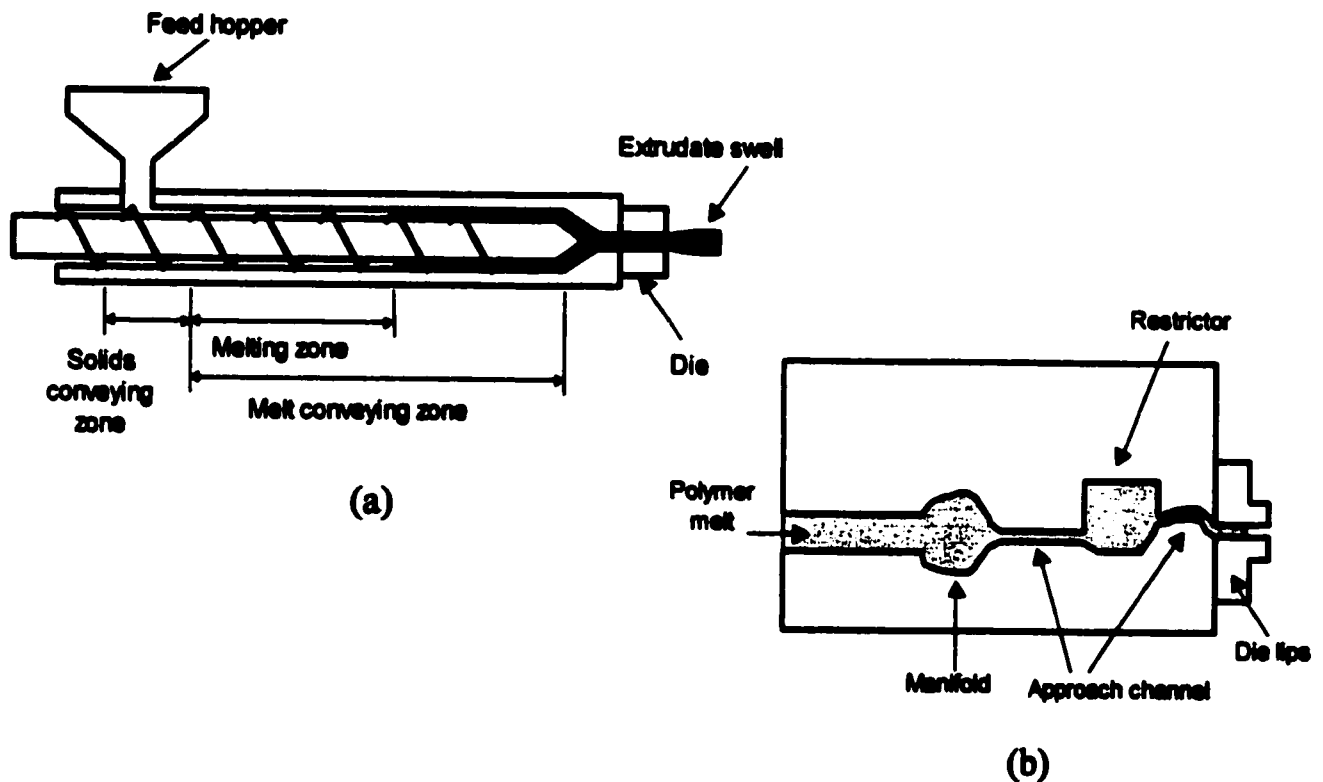


Figure 1.3: Schematic representation of (a) a typical extruder and (b) an extruder die (from Baird and Collias, 1995).

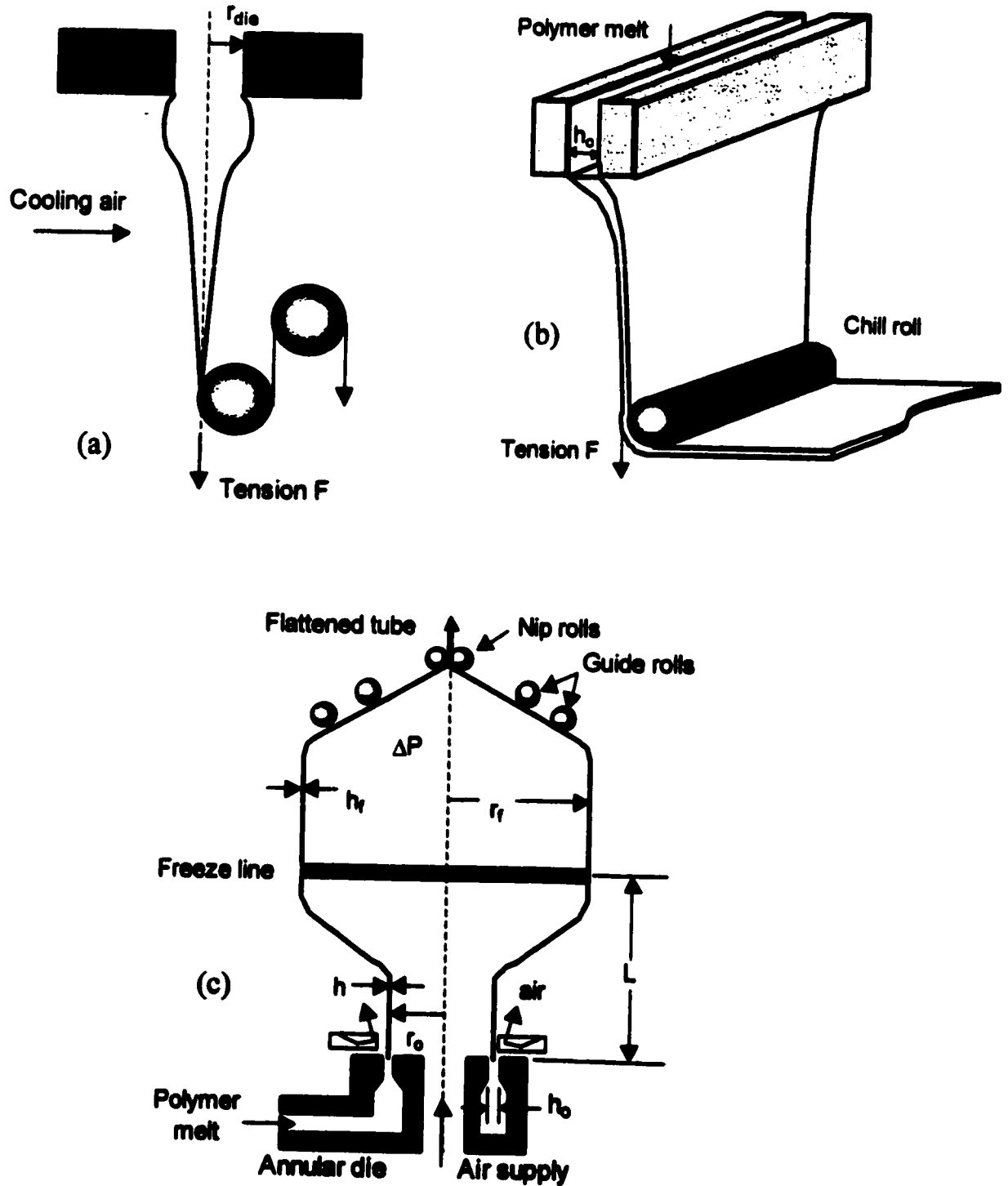


Figure 1.4: Schematic representation of the three polymer processes considered: (a) fiber spinning, (b) film casting, (c) film blowing (from Baird and Collias, 1995).

considered as a *post-die* process, since the transformation of the polymer into a fiber or film occurs outside the die. Each process is also considered as a *free-surface* process, since no walls are interrupting the transformation. The final characteristics of the fiber or film are determined by the rheological properties of the melt as well as the processing conditions such as take-up speed, cooling rate, extrusion rate, and die dimensions. *Optical properties* such as haze, gloss, and opacity, and *physical properties* such as tear and modulus, are greatly affected by the conditions of flow inside and outside the die.

1.4.1 Fiber Spinning

Fiber spinning consists of pulling a polymeric material from the die to produce a long, thin, tough plastic filament that is taken up at the chill roll (see Figure 1.4(a)). The fibers are generally used in the textile industry, but new uses have been identified to produce *reinforced composite plastics*. The fibers are produced by the extrusion of the polymer through a plate containing many small holes, known as the *spinneret plate*. Extrudate swell usually occurs after the melt passes through the spinneret plate due to the relaxation of stresses accumulated within the die. Two main types of procedures can be used to spin the material: (i) *melt spinning*, if the material is thermally stable with a high fluidity at the extrusion temperature, or (ii) *solution spinning*, if the material does not meet the above criteria. Of the two, melt spinning is the simplest and most economical. Different filaments can have different take-up speeds at the chill roll (Baird and Collias, 1995).

- *Very-low-speed* spinning has a filament speed at take-up ranging from 30 to 100 m/min, and is usually reserved for thick monofilaments.
- *Low-speed* spinning ranges from 100 to 750 m/min, where the tension along the filament is constant.
- *Intermediate-speed* spinning, ranging from 750 to 3500 m/min, has an increased tension in the filament due to inertia and air drag.
- *High-speed* spinning has take-up speeds exceeding 3500 m/min, where the filament can undergo stress-induced crystallization.

The fiber-spinning process, besides its uses in industry, can also be used as an elongational rheometer to measure the elongational viscosity of the material (Rheotens test) (Larson, 1988).

1.4.2 Film Casting

Thin flat sheets or films are produced by the film-casting process, whereby a polymeric material is extruded through a rectangular die or slit and taken up at the drum or chill roll (see Figure 1.4(b)). Afterwards, the film is usually subjected to additional processes, such as biaxial extension or thermoforming, to increase its tensile strength. The term *film* is reserved for thicknesses less than 250 μm , while the term *sheet* refers to higher thicknesses. Typical thicknesses range from 10 μm to 2500 μm , whereas lateral dimensions can vary from 40 to 320 cm. Cast films are primarily used in the packaging industry for either foodstuffs or other consumer products, but other uses include magnetic strips for audio- and videotapes. Film casting is very similar to the fiber-spinning process, except that while a fiber is drawn uniaxially (stretching of a cylindrical rod), the film or sheet is drawn planarly (stretching of a flat surface). After the film reaches the drum or chill roll, it is trimmed at the sides to remove thick edges, known as *edge beads*.

1.4.3 Film Blowing

Film blowing is a process by which a polymeric material is extruded through an annular die, stretched and blown to produce a biaxially drawn film called the *bubble*, collapsed by guide rolls, then flattened at the nip rolls to form an air-tight seal (see Figure 1.4(c)). The film is either sold as "lay-flat" tubing or trimmed at the edges and wound into two rolls as flat film. This process is much faster and economical than the film casting process and is preferred for thinner films. Unlike fiber spinning and film casting, which are processed in the downward direction, film blowing is normally processed in the upward direction. Biaxial extension is affected by slight internal pressurization and by axial drawing. The two processing directions are the axial direction (machine direction, MD) due to the drawing of the tube, and circumferential direction (transverse

direction, TD) due to blow-up of the tube. Typical thicknesses of the tubes are usually in the order of 50 μm .

1.5 Objectives

The objectives of this work are to study the three aforementioned shear-free processes by using numerical simulation methods. To that effect it is necessary to solve the governing conservation equations along with proper rheological constitutive equations for the three processes of fiber spinning, film casting and film blowing. In particular, computer programs will be developed based on the finite element method (FEM) for the analysis of each process. For each FEM program, appropriate interpolation functions will be used to approximate the unknown variables (e.g., radius, thickness, width, velocity and/or temperature).

The rheological behaviour of polymer melts and solutions will first be examined in the experimental section of the thesis. The rheological constitutive equation used to model the viscoelastic behaviour of the polymeric materials will be an integral constitutive model having a spectrum of relaxation times. This model has the ability to predict well experimental data for the shear and elongational viscosities and the normal stresses measured in shear flow.

The programs developed will be tested against known analytical and numerical solutions, and thus their accuracy will be established. They then will be used for the simulation and analysis of several known polymer flows for the three aforementioned processes available in the literature. The predictive properties of each program will be investigated, and their importance in simulating the processes will be established.

1.6 Outline of Thesis

This thesis is organized in chapters with the following content matter for each chapter:

Chapter 2: Rheological Characterization

The rheological behaviour of polymer solutions and melts available in our laboratory will be studied by testing the materials with a typical rheometer to determine their shear viscosity and first normal stress difference in shear flow. Experimental data for our own polymeric materials as well as data for other materials available through the literature will be fitted to an integral constitutive equation using a nonlinear regression procedure for determining the coefficients of the model. The steady and time-dependent behaviour of the materials will be analyzed.

Chapter 3: Mathematical Modelling

The equations of conservation of mass, momentum and energy will be introduced and simplified using the appropriate assumptions. The models and the constitutive equation available for the description of the extensional flow of the polymer melts will also be presented. The appropriate boundary conditions will be given.

Chapter 4: Method of Solution

The numerical methods used to solve the equations presented in Chapter 3 will be explained in detail. Computational schemes used to numerically evaluate integral constitutive equations will be presented. Several other numerical issues will also be addressed.

Chapter 5: Fiber Spinning

The FEM formulation of the continuity, momentum and energy equations will be presented specifically for the fiber-spinning process. The program F-SPIN will be tested against known analytical and numerical solutions, and thus its accuracy will be established. The program will then be used for the simulation and analysis of experimental data from fiber-spinning experiments.

Chapter 6: Film Casting

The FEM formulation of the continuity, momentum and energy equations will be presented specifically for the film-casting process. The program F-CAST will be tested

against known analytical and numerical solutions, and thus its accuracy will be established. The program will then be used for the simulation and analysis of experimental data from film-casting experiments.

Chapter 7: Film Blowing

The FEM formulation of the continuity, momentum and energy equations will be presented specifically for the film-blowing process. The program **F-BLOW** will be tested against known analytical and numerical solutions, and thus its accuracy will be established. The program will then be used for the simulation and analysis of experimental data from film-blowing experiments.

Chapter 8: Conclusions and Recommendations

The results of this thesis will be summarized for the various problems examined and the different methods used. Conclusions and recommendations for future work will be presented.

Chapter 2

Rheological Characterization

This chapter describes the experimental part of the thesis, concerning rheological characterization experiments conducted in a typical rheometer for polymer solutions and melts. Experiments were carried out for polymer solutions at room temperature and for a polymer melt at high temperature. Modifications were made to the existing equipment to handle high temperature measurements with good accuracy. Measurements for the shear viscosity (η_s) and the first normal stress difference (N_1) were taken at varying shear rates, so as to capture a wide range of deformations.

2.1 Experimental Methods for Determining Rheological Behaviour of Viscoelastic Fluids

As mentioned in Chapter 1, viscoelastic materials can respond unusually and cause difficulties in polymer processing. Thus, a good knowledge of how materials will respond to certain deformations is crucial. The material in question can be deformed in two ways:

- *Shear deformation* occurs when the material is rearranged in the presence of walls.
- *Extensional deformation* occurs when the material is rearranged in the absence of walls.

Unfortunately, the shear properties of a viscoelastic fluid do not give any insight into its extensional properties. Thus, different techniques must be devised which can predict the material's response in both shear and extension. Two such devices to measure the shear and elongational properties of a polymeric material are the *Weissenberg rheogoniometer* (also called *cone-and-plate rheometer*) and the *Meissner rheometer* (also called *extensional rheometer*), respectively.

A schematic representation of a cone-and-plate rheometer is shown in Figure 2.1. The fluid sample is placed between the rotating cone and the stationary bottom plate. The shear viscosity (η_s) is calculated by measuring the torque imposed on the upper plate from the rotating fluid, while the first normal stress difference (N_1) is calculated by measuring the force exerted on the bottom plate. The cone-and plate rheometer has the advantage of a constant shear rate, $\dot{\gamma}$. This is accomplished by having the lower flat plate stationary, while the cone-shaped upper plate is rotated. Thus a constant shear rate is achieved for different radii, which would not be true if the upper plate were flat. The cone-and-plate rheometer is widely used and preferred for shear measurements and is capable of obtaining measurements for shear rates up to $\dot{\gamma} = 10 \text{ s}^{-1}$ for polymer melts.

A schematic representation of the *Meissner rheometer* (also called *extensional rheometer*) is shown in Figure 2.2. A sample is placed between the two sets of rotating nip rolls and the sample is stretched. Both ends of the sample are pulled at a constant velocity to achieve either a uniform extensional rate or a constant stress. Normally, a constant extensional rate is chosen, and the *time-dependent uniaxial viscosity* (η_E^+) is measured until a steady-state value is reached. The full uniaxial viscosity curve as a function of extensional rate can be obtained by performing multiple tests at different constant extensional rates until the steady-state value is reached. The Meissner rheometer is the preferred instrument to measure extensional data and is capable of reaching fairly high extensional rates ($\dot{\epsilon} = 10 \text{ s}^{-1}$) depending on the test material and the temperature of testing.

2.1.1 Experimental Setup

The device used in the experiments was the cone-and-plate rheometer, as described above, for measurements of the shear viscosity and first normal stress difference. Unfortunately, experiments were not conducted with the Meissner rheometer since this equipment was unavailable due to cost (> \$150,000 US). The exact configuration of the cone-and-plate rheometer is illustrated in Figure 2.3. The means by which the shear viscosity and first normal stress difference are measured with the cone-and-plate rheometer is described below.

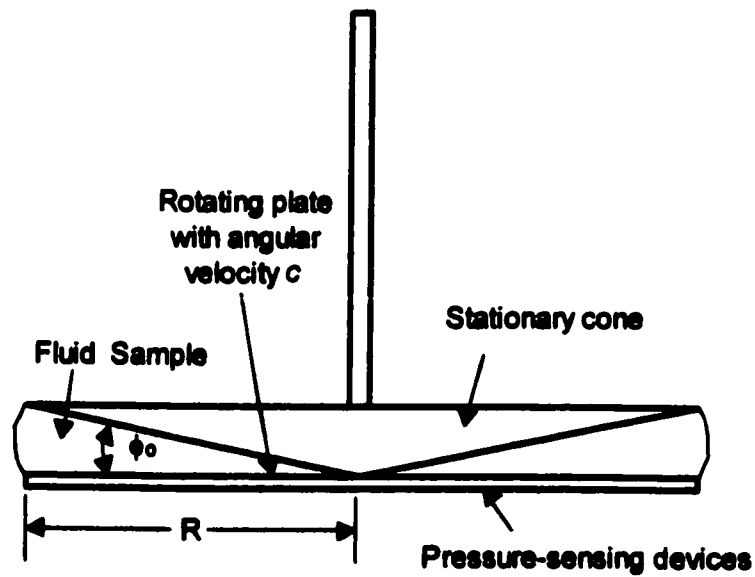


Figure 2.1: Schematic diagram of the *Weissenberg rheogoniometer* (also called *cone-and plate rheometer*).

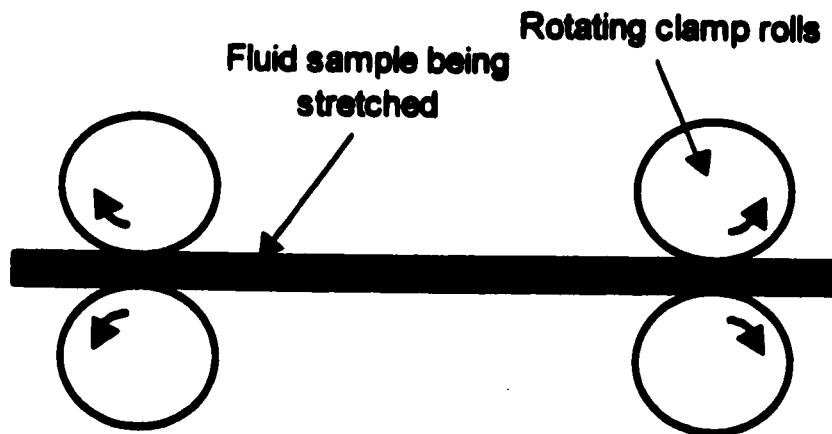


Figure 2.2: Schematic representation of the *Meissner rheometer* (also called *extensional rheometer*).

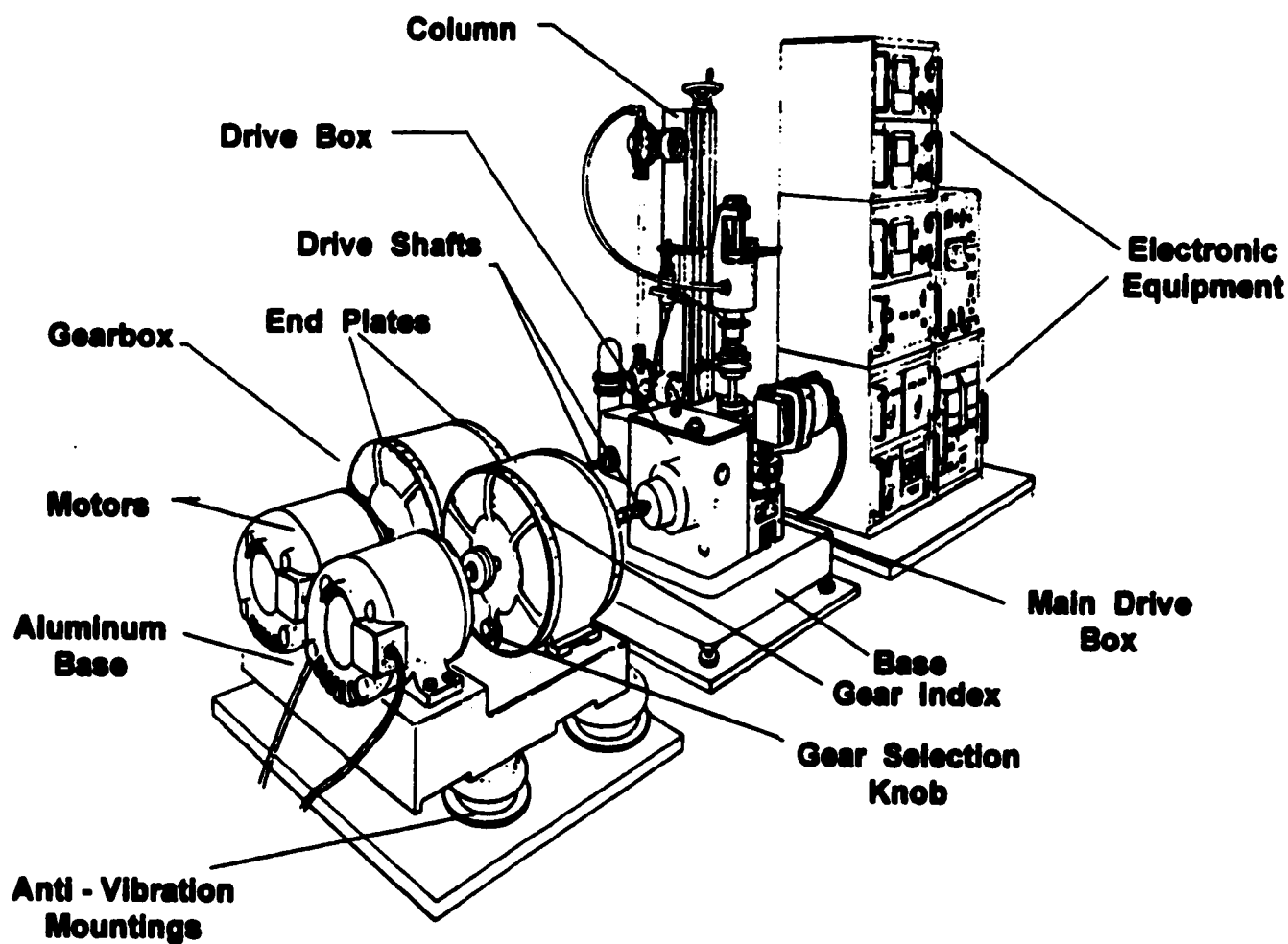


Figure 2.3: Experimental configuration of the cone-and-plate rheometer used in the experiments (from Sangamo Controls Ltd., 1967).

2.1.2 Shear Viscosity (η_s)

The mechanism by which the shear viscosity is measured within the cone-and-plate rheometer is illustrated in Figure 2.4. Before making any measurements, the gap between the conical upper plate and flat lower plate must be measured. The cone on the upper plate is slightly sectioned off as to avoid friction from contact (see Figure 2.5). Thus, the amount of cone removed, measured in the vertical direction, must be set as the gap between the upper and lower plate. The amount of shear produced by the sample occupying the space, which would otherwise be taken up by the sectioned amount of cone, is assumed negligible. A transducer fixed to the base assembly of the cone-and-plate rheometer is used to measure the gap (in units of μm). The gap transducer is calibrated to zero simply when the upper plate touches the lower plate.

The conical upper plate, which is supported by a torsion bar, is positioned within a frictionless air bearing, which allows the plate to move freely. When a sample is placed between the lower and upper plates, and the lower plate is set in rotation, the upper plate is subject to deflection. The amount of deflection depends on the modulus of the torsion bar. The modulus of the torsion bar was measured by the manufacturer (Sangamo Controls Ltd., England) and given in *dynes-cm / (μm deflection)*. The amount of deflection in μm is measured by a transducer, which sends a signal to a meter. The transducer is calibrated to zero simply when the upper plate was at rest. The viscosity of the sample being rotated between the upper and lower plates can be measured in terms of torque. The torque for the system is easily found by the following formula

$$\mathfrak{I} = \int_0^R \tau_{xy} \cdot 2 \cdot \pi r^2 dr \quad (2.1)$$

where $\mathfrak{I}$ is the torque, τ_{xy} is the shear stress, and r is the radius. Using the relation $\tau_{xy} = \eta_s \dot{\gamma}$ and integrating, one obtains the relation for viscosity

$$\eta_s = \frac{3\mathfrak{I}}{2\pi R^3 \dot{\gamma}} \quad (2.2)$$

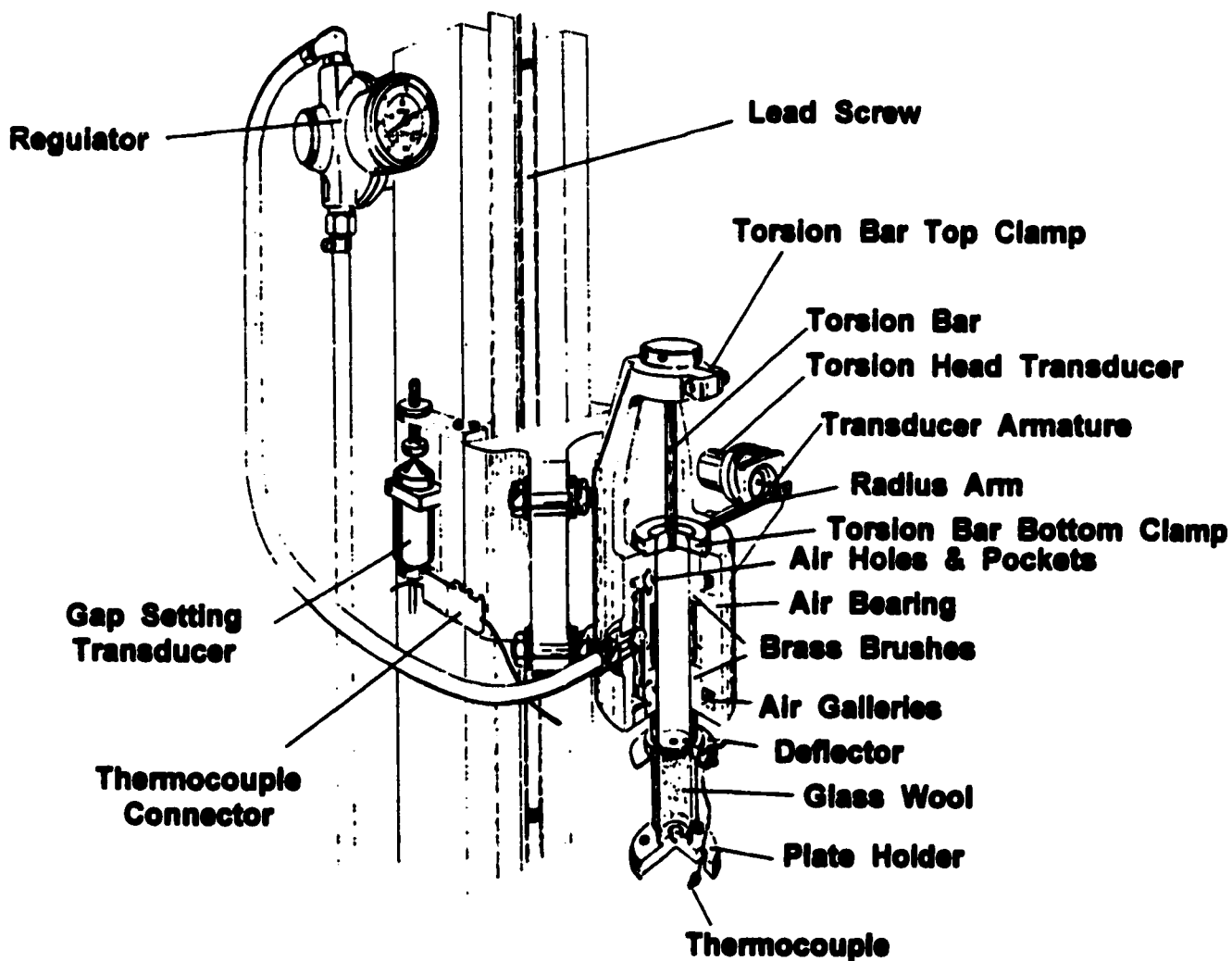


Figure 2.4: Mechanism for measuring the shear viscosity (η_s) for the cone-and-plate rheometer (from Sangamo Controls Ltd., 1967)

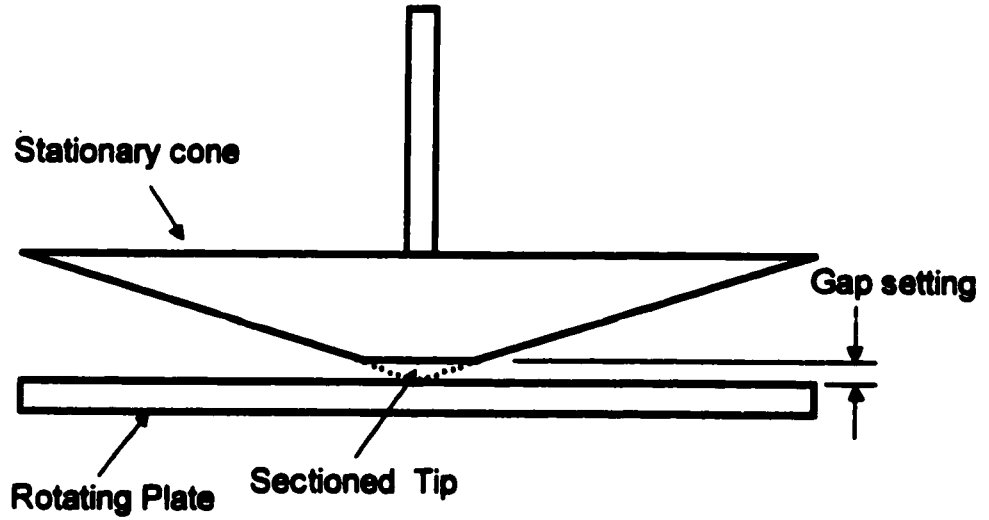


Figure 2.5: Arrangement of the upper and lower plates for the cone-and-plate rheometer.

The torque $\mathfrak{J}$ is measured by the deflection of the upper plate and is simply the product of the modulus of the torsion bar and the amount of deflection. The shear rate, $\dot{\gamma}$, is given by

$$\dot{\gamma} = \frac{360}{\alpha c} \quad (2.3)$$

where α is the angle of the conical upper plate and c is the speed of rotation in revolutions/second. The final formula used in the laboratory to determine the viscosity is

$$\eta_s = \frac{c \alpha \Delta_T k_T}{94.25 d^3} \quad (2.4)$$

where Δ_T is the measurement of deflection of the upper plate in μm , k_T is the modulus of the torsion bar, and d is the diameter of the upper and lower plates.

2.1.3 First Normal Stress Difference (N_1)

The mechanism by which the first normal stress difference is measured within the cone-and-plate rheometer is illustrated in Figure 2.6. As mentioned above, before making any measurements, the gap between the conical upper plate and flat lower plate must be measured. The method of measuring the gap between the upper and lower plates is explained in section 2.2.2. The lower plate is supported by a diaphragm, which is attached to a shaft and rests on the normal force leaf spring. Below the leaf spring where the shaft is located, a servo-transducer is positioned. The purpose of the servo-mechanism is to elevate the free-end of the leaf spring, such that the reading on the servo-transducer is zero (i.e., the free-end is raised to account for the downward pressure caused by the first normal stress difference). The normal force transducer is also located at the free-end of the leaf spring and measures the amount by which the leaf spring is raised. The servo-transducer and normal force transducer are simply calibrated to zero before the sample is placed on the lower plate (i.e., no force on the lower plate).

The amount of downward force caused by the sample in rotation is a product of the deflection of the leaf spring in μm and the modulus of the leaf spring. The manufacturer did not give the modulus of the leaf spring, unlike the torsion bar for shear viscosity measurements. Thus, the modulus was measured by applying known weights to the lower plate and measuring the deflection on the normal force meter. The calibration curve obtained is shown in Figure 2.7, which displays a linear trend. The modulus of the leaf spring is then found by finding the slope of this curve, with units in *dynes* / (μm deflection). The first normal stress difference is simply given as

$$N_1 = \frac{2F}{\pi R^2} = \frac{8\Delta_N k_N}{\pi d^2} \quad (2.5)$$

where Δ_N is the normal force measurement of deflection in μm , k_N is the modulus of the leaf spring, and d is the diameter of the upper and lower plates.

2.2 Rheological Characterization of Viscoelastic Fluids Using a K-BKZ Integral Model

In order to simulate successfully the flow of viscoelastic fluids, it is necessary to know first the rheological behaviour of the polymeric fluid. This is done by conducting

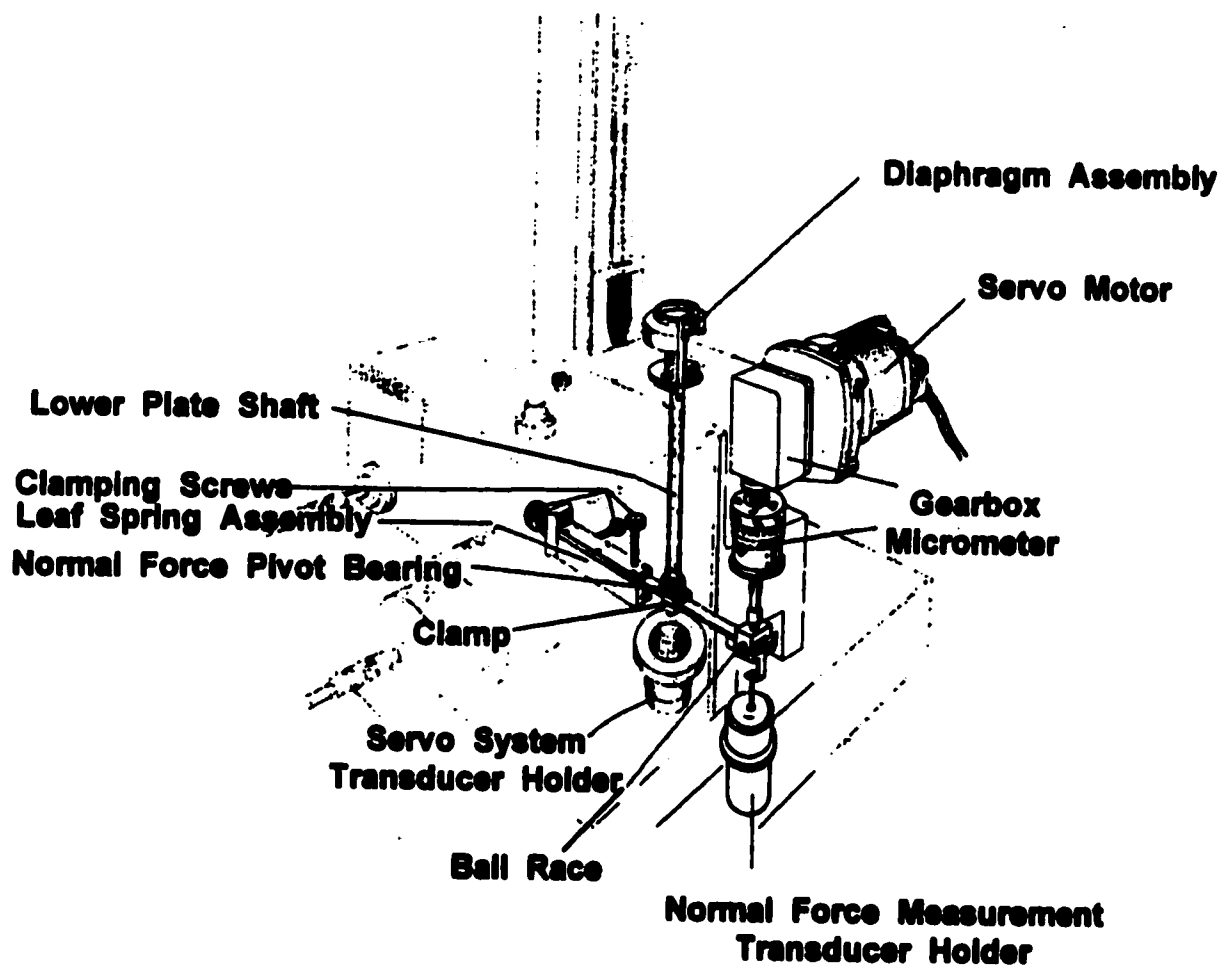


Figure 2.6: Mechanism for measuring the first normal stress difference (N_1) for the cone-and-plate rheometer (from Sangamo Controls Ltd., 1967).

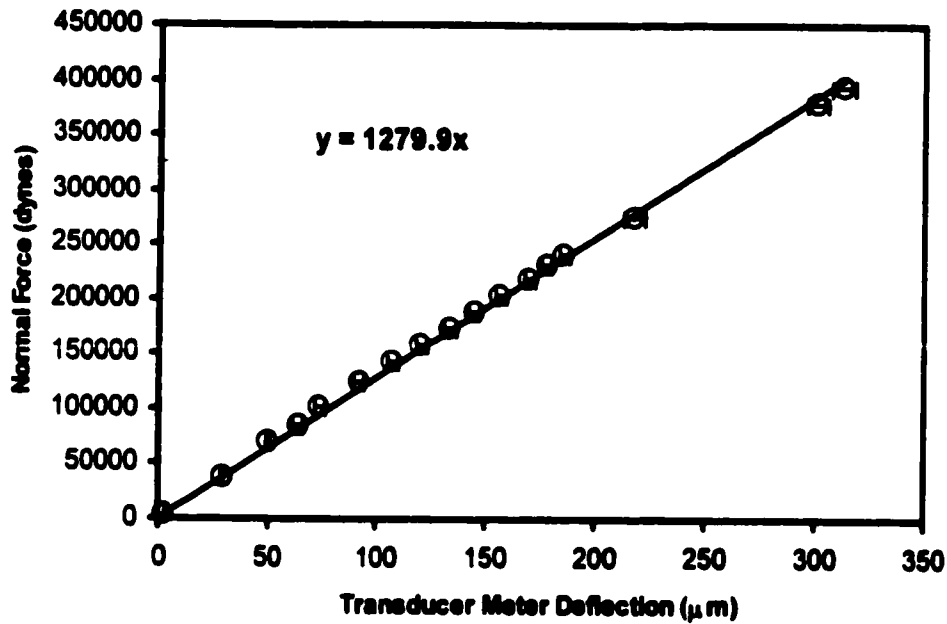


Figure 2.7: Normal force leaf spring calibration curve.

experiments on the material to measure rheologically significant material functions, such as the shear viscosity (η_s), the first normal stress difference (N_1), the extensional viscosities (η_E , η_P , η_B), and the dynamic functions (G' , G''). However, as mentioned earlier, it is extremely difficult to measure some of these material functions, and thus not all of the material behaviour may be known.

The next step in viscoelastic flow simulations is choosing a suitable constitutive model, which describes well the rheologically significant material functions. One such class of constitutive equations is the K-BKZ integral class of equations, where the K-BKZ equation was derived independently by Kaye (1962), and by Bernstein, Kearsley, and Zapas (1963) (hence its abbreviation from the initials of the researchers' names). The particular constitutive model was modified by Papanastasiou et al. (1983) and further modified by Luo and Tanner (1988). In this work, the modified K-BKZ constitutive model is used along with a nonlinear regression technique to determine the appropriate coefficients in the model to give good predictions for the rheological material functions.

2.2.1 Constitutive Equation

The constitutive equation used for the prediction of the rheological material functions is an integral constitutive equation of the K-BKZ type modified by Papanastasiou et al. (1983) and further modified by Luo and Tanner (1988). It is written as

$$\bar{\tau}(t) = \frac{1}{1-\theta} \int_{-\infty}^t \sum_{k=1}^N M(t-t') H(I_C, I_{C^{-1}}) \left[\left\{ \bar{C}_t^{-1}(t') - \bar{I} \right\} + \theta \left\{ \bar{C}_t(t') - \bar{I} \right\} \right] dt' \quad (2.6)$$

where $\bar{I}$ is the identity matrix,

$$M(t-t') = \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) \quad (2.7)$$

is a linear time-memory function with N modes, and $H(I_C, I_{C^{-1}})$ is a nonlinear strain-memory function given by

$$H(I_C, I_{C^{-1}}) = \frac{\alpha_k}{(\alpha_k - 3) + \beta_k I_{C^{-1}} + (1 - \beta_k) I_C} \quad (2.8)$$

where λ_k and a_k are relaxation times and relaxation modulus coefficients at a reference temperature T_{ref} , respectively. The parameters α_k and β_k are material parameters chosen to fit the material's response in high shear and elongation, respectively. The invariants I_C and $I_{C^{-1}}$ are the first invariants of the Cauchy-Green tensor $\bar{C}_t(t')$ and its inverse $\bar{C}_t^{-1}(t')$, the Finger strain tensor. The parameter θ has been incorporated by Luo and Tanner (1988) to take into account the second normal stress difference, N_2 , and is related to the first normal stress difference, N_1 , via the formula

$$\frac{N_2}{N_1} = \frac{\theta}{1-\theta} \quad (2.9)$$

Since N_2 is a negative quantity defined by $N_2 = \tau_{22} - \tau_{33}$, θ must have a negative value. Its usual range for polymer solutions and melts is $-0.4 \leq \theta \leq 0$ (Tanner, 1985). Unless otherwise specified, the value of θ used in this work is $-1/9$ (or $N_2/N_1 = -0.1$).

The rheological material functions used in the regression of the modified K-BKZ constitutive model are: (i) the shear functions (the shear viscosity, η_s , and the first normal stress difference, N_1), (ii) the extensional functions (the uniaxial, η_E , planar, η_P , and

biaxial, η_B , extensional viscosities), and (iii) the dynamic functions (the storage modulus, G' , and the loss modulus, G''). The nonlinear strain-memory function, eq. (2.8), and the Finger and Cauchy-Green tensors in eq. (2.6) are expressed differently based on the type of deformation and type of function. The expressions for each type of deformation were derived by Kajiwar et al. (1995) and used in a regression program developed by Barakos (1994). The program by Barakos (1994), named BESTFIT[®], was extended in this study to handle multiple α 's (α_k) and β 's (β_k), to better fit the rheological functions. The derivations by Kajiwar et al. (1995) were also extended to handle transient rheological material functions, and gave rise to the creation of a computer program developed during the course of this work, named TIMEFIT[®].

The steady-state material functions for the modified K-BKZ model, eq. (2.6), are described in detail by Barakos (1994). The procedure for the nonlinear regression, based on the Levenberg-Marquardt method, is also given by Barakos (1994), and the reader is referred to that work for more detailed information.

2.2.2 Transient Material Functions for the K-BKZ Integral Constitutive Equation

The steady-state rheological material functions for the modified K-BKZ integral constitutive equation, derived by Kajiwar et al. (1995), are extended to produce the transient rheological material functions. This is done by assuming that the deformation imparted to the material begins at time $t=0$ and the rate of deformation is constant. This assumption is common in experimental procedures when measuring the time-dependent rheological material functions. The relaxation spectrum, λ_k and a_k in eq. (2.6), do not change since they are found in the steady-state regression of the modified K-BKZ model. That is to say, these parameters are highly dependent on the steady-state predictions and *should not* be regressed with the transient rheological material functions. This would cause the steady-state predictions to change unpredictably. However, the nonlinear parameters in the modified K-BKZ model, α_k and β_k in eq. (2.6), can be altered without major changes in the steady-state predictions. Therefore, only the nonlinear parameters

are used in the regression of the modified K-BKZ integral constitutive model for predicting the transient rheological material functions.

In the case of the shear viscosity, the steady-state rheological material function for the shear stress (and hence the shear viscosity from $\eta_s = \tau_{xy}/\dot{\gamma}$) is given as (Barakos, 1994)

$$\tau_{12} = \int_{-\infty}^t \sum_{k=1}^N \left[\frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) \right] \left[\frac{\alpha_k \gamma}{\alpha_k + \gamma^2} \right] dt' \quad (2.10)$$

where γ is the shear strain defined as

$$\gamma = \dot{\gamma}(t-t') \quad (2.11)$$

To simplify this equation, the domain of integration is transformed from $0 \rightarrow t$ instead of $-\infty \rightarrow t$, since it is assumed that no deformation is imparted to the material before $t = 0$.

With this in mind, the first normal stress difference is given as (Barakos, 1994):

$$N_1 = \int_0^t \sum_{k=1}^N \left[\frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) \right] \left[\frac{\alpha_k \gamma^2}{\alpha_k + \gamma^2} \right] dt' \quad (2.12)$$

The extensional viscosities are also given in short form as:

$$\eta = \frac{1}{1-\theta} \int_0^t \sum_{k=1}^N \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) \left[H(I_C, I_{C^{-1}}) \left\{ \left(\bar{C}_t^{-1}(t') - \bar{I} \right) + \theta \left(\bar{C}_t(t') - \bar{I} \right) \right\} \right] dt' \quad (2.13)$$

Note that η refers to any extensional viscosity (η_E , η_P , η_B), and that the above formula results after integration-by-parts has been performed. The term in square brackets in eq. (2.13) (the strain-memory function with contributions from the Finger and Cauchy-Green tensors) for each extensional rheological material function is given as (Barakos, 1994):

Uniaxial extension:

$$\frac{\alpha_k}{(\alpha_k - 3) + \beta_k(e^{2\varepsilon} + 2e^{-\varepsilon}) + (1 - \beta_k)(e^{-2\varepsilon} + 2e^{\varepsilon})} \left[(e^{2\varepsilon} - e^{-\varepsilon}) + \theta(e^{-2\varepsilon} - e^{\varepsilon}) \right] \quad (2.14)$$

Planar extension:

$$\frac{\alpha_k}{(\alpha_k - 3) + e^{2\varepsilon} + e^{-2\varepsilon} + 1} \left[(e^{2\varepsilon} - e^{-2\varepsilon}) + \theta(e^{-2\varepsilon} - e^{2\varepsilon}) \right] \quad (2.15)$$

Biaxial extension:

$$\frac{\alpha_k}{(\alpha_k - 3) + \beta_k(2e^{2\varepsilon} + e^{-4\varepsilon}) + (1 - \beta_k)(2e^{-2\varepsilon} + e^{4\varepsilon})} \left[(e^{2\varepsilon} - e^{-4\varepsilon}) + \theta(e^{-2\varepsilon} - e^{4\varepsilon}) \right] \quad (2.16)$$

where ε is the extensional strain defined in the same manner as the shear strain, i.e.,

$$\varepsilon = \dot{\varepsilon}(t - t') \quad (2.17)$$

The above rheological material functions are those used in the regression of the modified K-BKZ integral constitutive model when transient data are available.

2.3 Results and Discussion

The programs for the nonlinear regression analysis were tested against experimental data for the rheological material functions. Steady-state predictions were made for the polymer solutions and the polymer melt tested experimentally as described in section 2.1. Steady-state and transient predictions were made for the Stamylan-L8 low-density polyethylene (LDPE) with experimental data from Tas (1994).

2.3.1 Experimental Measurements and Steady-State Predictions for Polymer Solutions

Measurements of the steady-state shear viscosity (η_s) and first normal stress difference (N_1) were conducted for two polymeric materials in an aqueous solvent (polymer solutions). The two polymeric materials used were a poly(ethylene oxide) resin provided by Union Carbide, Inc., and a polyacrylamide resin provided by Polysciences, Inc. Both solutions were prepared at a 2% w/w concentration and were mixed with extreme care (i.e., slow mixing) as not to degrade the polymer by breaking the molecular chains. For the polyacrylamide solution, the measurements were conducted at low light conditions, since polyacrylamide is reported to degrade when in direct contact with light (Dhahir and Walters, 1989).

Figure 2.8 shows the results of conducting experiments with the poly(ethylene oxide) resin. The shear viscosity shows a great deal of thinning at a shear rate of $\dot{\gamma} = 10 \text{ s}^{-1}$, which is expected for polymeric materials. The first normal stress difference also behaves as expected with a slope of 2 (quadratic) at very small shear rates, but measurements at low shear rates were very difficult. This was due to machine sensitivity, where a first normal stress difference measurement below 1000 dyne/cm^2 is considered difficult (Dhahir and Walters, 1989). Also shown in Figure 2.8 are the predictions for the

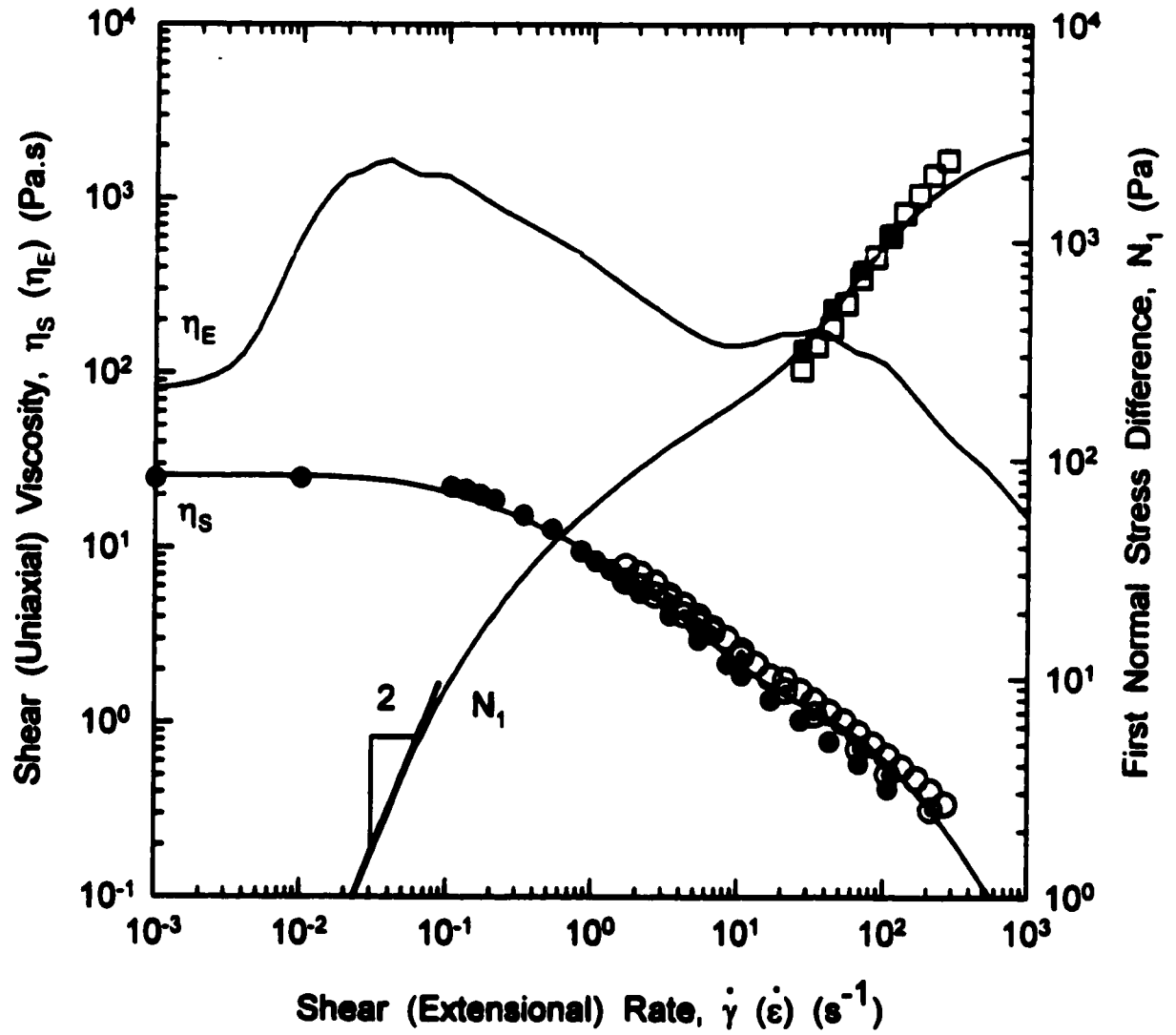


Figure 2.8: Steady-state shear viscosity (η_s), uniaxial viscosity (η_E), and first normal stress difference (N_1) for poly(ethylene oxide) at 21°C. Symbols represent experiments with the cone-and-plate rheometer, while lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum given in Table 2.1. Open symbols correspond to additional experiments.

shear viscosity and first normal stress difference from eq. (2.6). The relaxation times, with the relaxation spectrum given in Table 2.1, were chosen from 1×10^{-1} s to $1 \times 10^{+3}$ s. A sufficiently good fit could not be obtained with a single α -value for this material. Therefore, multiple α_k -values were used, which gave a much better fit.

Figure 2.9 shows the predictions for the storage and loss moduli (G', G'') from eq. (2.6) with the relaxation spectrum of Table 2.1. The storage modulus at low frequencies increases quadratically (slope of 2), while the loss modulus at low frequencies increases linearly (slope of 1). This is also indicative of a good fit, since linear viscoelastic theory (see, e.g., Larson, 1988) predicts that at low frequencies the storage modulus increases quadratically while the loss modulus increases linearly.

Table 2.1: Relaxation spectrum and associated parameters for a poly(ethylene oxide) resin at 21°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\beta = 0.2$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)	α_k
1	0.1	11.4	271
2	1	6.31	21.6
3	10	0.859	67.8
4	100	9.76×10^{-2}	348
5	1000	9.54×10^{-7}	13000

Figure 2.10 shows the results of conducting experiments with the polyacrylamide solution with predictions from eq. (2.6). The shear viscosity shows thinning behaviour at a shear rate of $\dot{\gamma} = 0.1 \text{ s}^{-1}$. The first normal stress difference also behaves as expected with a slope of 2 (quadratic). Again, a first normal stress difference measurement below 1000 dyne/cm^2 was unattainable. The relaxation times, with the relaxation spectrum given in Table 2.2, were also chosen from 1×10^{-1} s to $1 \times 10^{+3}$ s. For this material, a single α gave a sufficiently good fit for the shear viscosity (η_s) and the first normal stress difference (N_1).

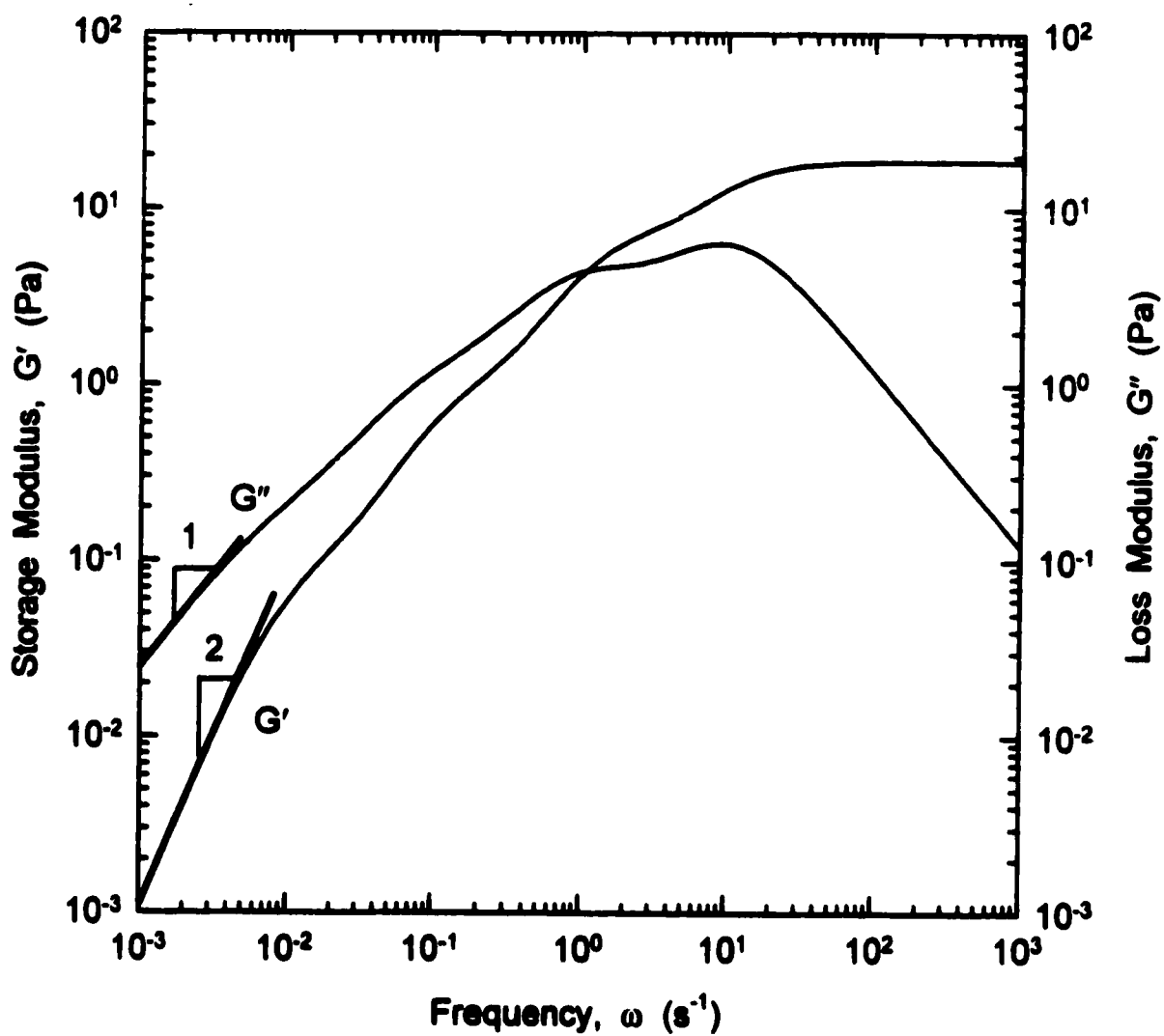


Figure 2.9: Predictions of the modified K-BKZ constitutive model, eq. (2.6), for the storage and loss moduli (G' , G'') of poly(ethylene oxide) at 21°C, with the relaxation spectrum of Table 2.1.

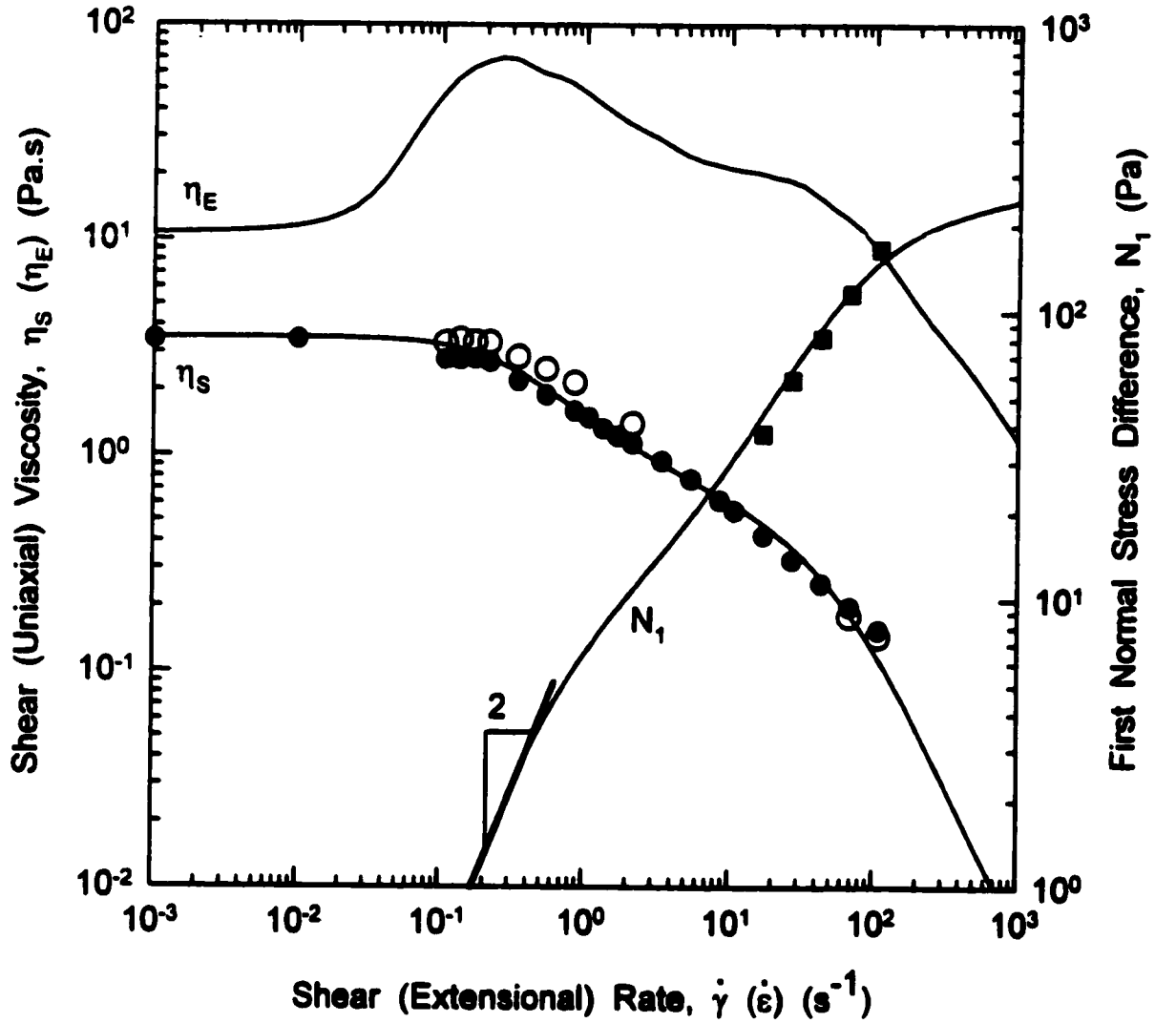


Figure 2.10: Steady-state shear viscosity (η_s), uniaxial viscosity (η_E), and first normal stress difference (N_1) for polyacrylamide at 21°C. Symbols represent experiments with the cone-and-plate rheometer, while lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum given in Table 2.2. Open symbols correspond to additional experiments.

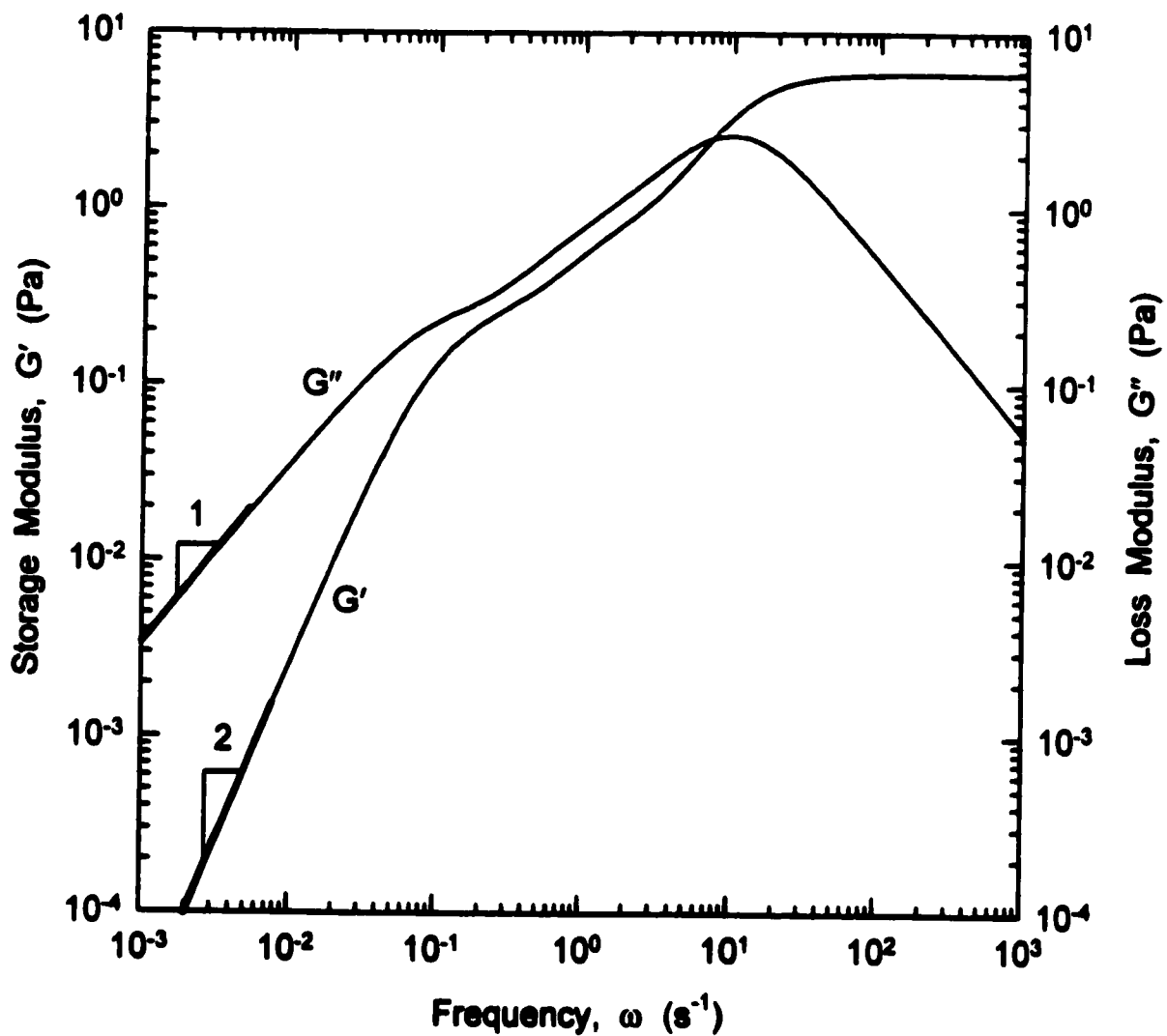


Figure 2.11: Predictions of the modified K-BKZ constitutive model, eq. (2.6), for the storage and loss moduli (G' , G'') of polyacrylamide at 21°C, with the relaxation spectrum of Table 2.2.

Table 2.2: Relaxation spectrum and associated parameters for a polyacrylamide resin at 21°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 44.5, \beta = 0.2, \theta = -0.111$).

K	λ_k (s)	a_k (Pa)
1	0.1	5.15
2	1	0.497
3	10	0.249
4	100	4.29×10^{-5}
5	1000	3.34×10^{-6}

Figure 2.11 shows the predictions for the storage and loss moduli (G', G'') from eq. (2.6) with the relaxation spectrum of Table 2.2. Again, the storage modulus increases quadratically and the loss modulus increases linearly, indicative of a good fit from linear viscoelastic theory.

2.3.2 Experimental Measurements and Steady-State Predictions for a Polymer Melt

Measurements of the steady-state shear viscosity (η_s) and first normal stress difference (N_1) were conducted for a polymer melt at a temperature of 230°C. The material was acquired from the University of Waterloo, and it was a virgin polypropylene (PP) melt supplied by Shell Canada (Oakville, Ontario). The material was in pellet form and was placed between the cone-and-plate systems, while the temperature was increased to 230°C. Once this temperature was reached, experiments were first conducted for the shear viscosity. Another sample was afterwards placed between the cone-and-plate system for measurements of the first normal stress difference. Measurements could only be made up to a shear rate of 1.0 s^{-1} for the shear viscosity, since the melt had a very high viscosity, which in turn produced a very high torque. Other devices, such as a capillary rheometer (Baird and Collias, 1995), can be used to measure viscosities above 10 s^{-1} . Again, this device was unavailable due to cost (> \$100,000 US).

Figure 2.12 shows the results of conducting experiments with the PP melt at 230°C. The shear viscosity shows thinning behaviour at a shear rate around 0.01 s⁻¹. Also shown in Figure 2.12 are the results for the PP melt from Barakos et al. (1996), where a capillary rheometer was used to measure the shear viscosity at high shear rates. The current results at low shear rates with the cone-and-plate rheometer extend the results given by Barakos et al. (1996) at high shear rates obtained with a capillary rheometer, while they overlap for the normal stresses in a certain range. The agreement between the two sets of data also validates the current experimental procedure. The first normal stress difference also behaves as expected with a slope of 2 (quadratic) and agreed well with the predictions by Barakos et al. (1996). The predictions by Barakos et al. (1996) for the first normal stress difference were obtained from the following recursive formula (Laun, 1986)

$$N_1 = 2G' \left[1 + \left(\frac{G'}{G''} \right)^2 \right]^{0.7} \quad (2.18)$$

where measurements for the storage modulus (G') and the loss modulus (G'') were also conducted by Barakos et al. (1996). Figure 2.12 also shows the predictions from eq. (2.6). The relaxation spectrum was first obtained by Barakos et al. (1996) with limited experimental data, especially at low shear rates. The results from the cone-and-plate rheometer provided the necessary data at low shear rates to confirm the earlier predictions. Only a single α - and β -values were needed to predict well the shear viscosity and first normal stress difference. The relaxation spectrum is given in Table 2.3. Figure 2.13 shows the predictions of the storage and loss moduli (G', G''), along with the experimental data by Barakos et al. (1996), where again a good fit is obtained.

2.3.3 Transient Predictions

For the transient predictions, experiments could not be conducted due to lack of the necessary equipment. However, transient experiments have been conducted by Tas (1994), for three different grades of LDPE. Only one grade (Stamylan L8 LDPE) was chosen for the transient predictions of eq. (2.6). Figure 2.14 shows the experimental data for the transient shear viscosity (η_s^+) along with the modified K-BKZ equation

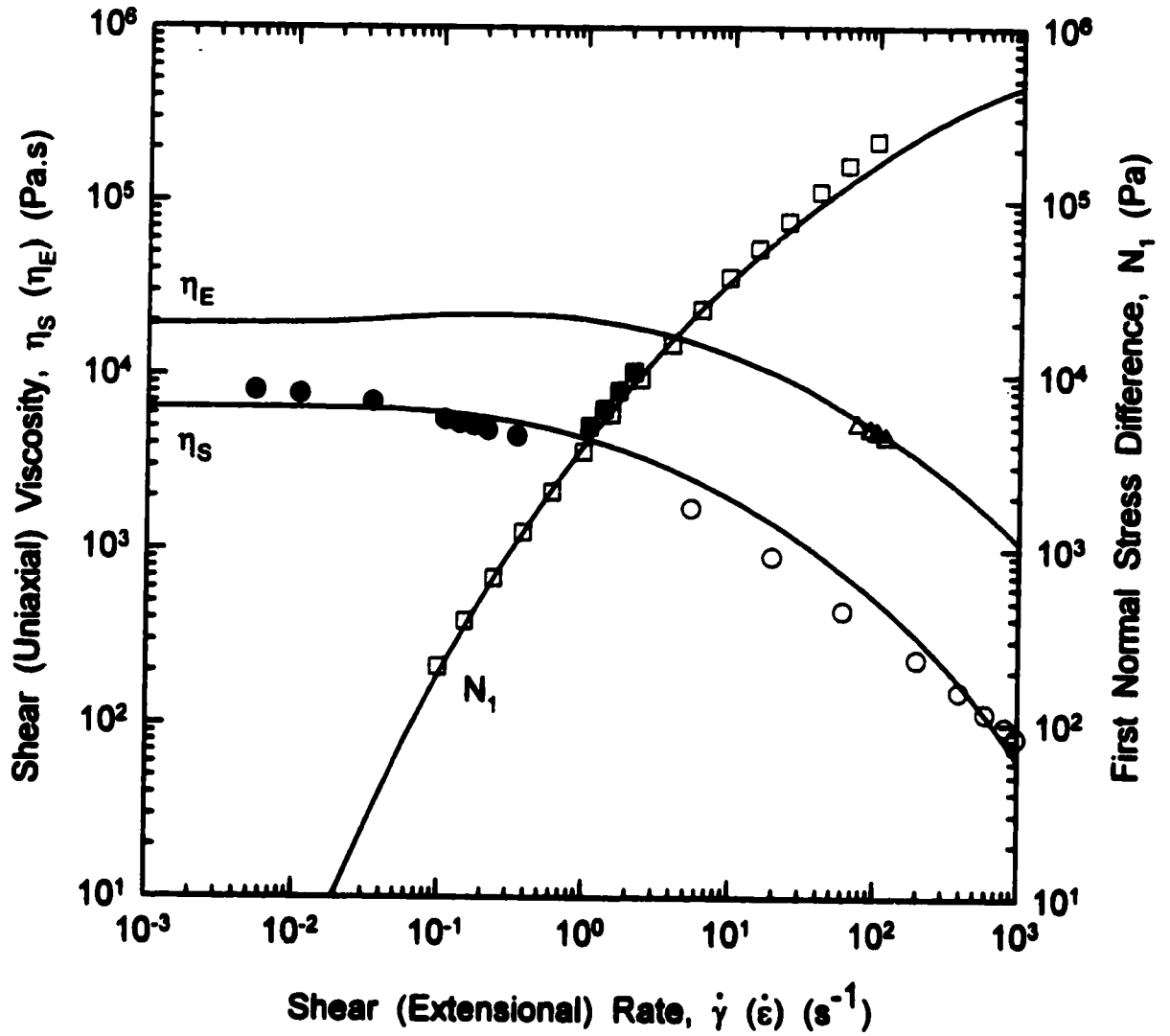


Figure 2.12: Steady-state shear viscosity (η_s), uniaxial viscosity (η_E), and first normal stress difference (N_1) for the PP melt at 230°C. Open symbols represent experimental data obtained with a capillary rheometer by Barakos et al. (1996), closed symbols represent current experimental data with the cone-and-plate rheometer, and lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum given in Table 2.3.

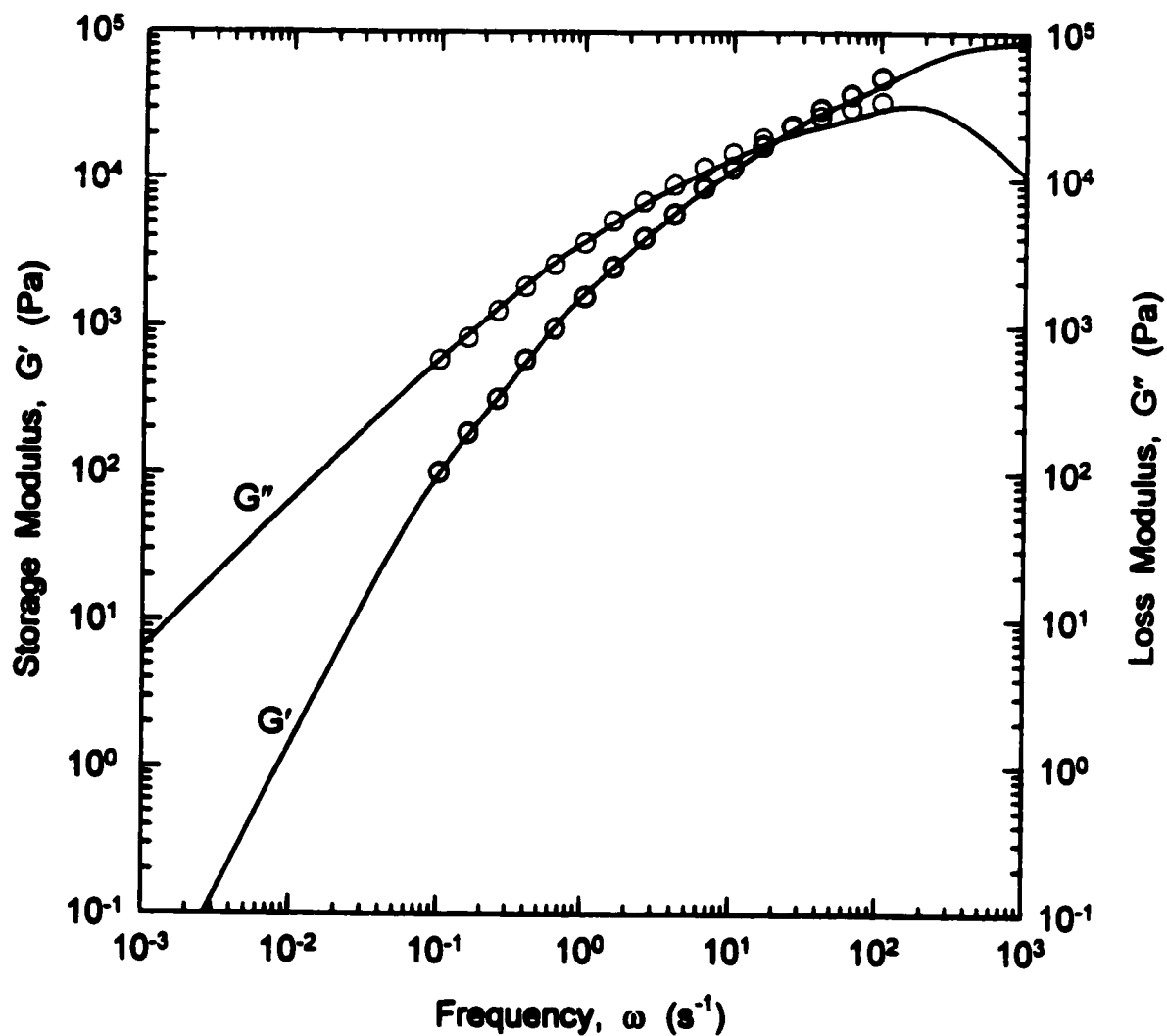


Figure 2.13 Storage and loss moduli (G' , G'') for the PP melt at 230°C. Open symbols represent experimental data obtained by Barakos et al. (1996), while lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum given in Table 2.3.

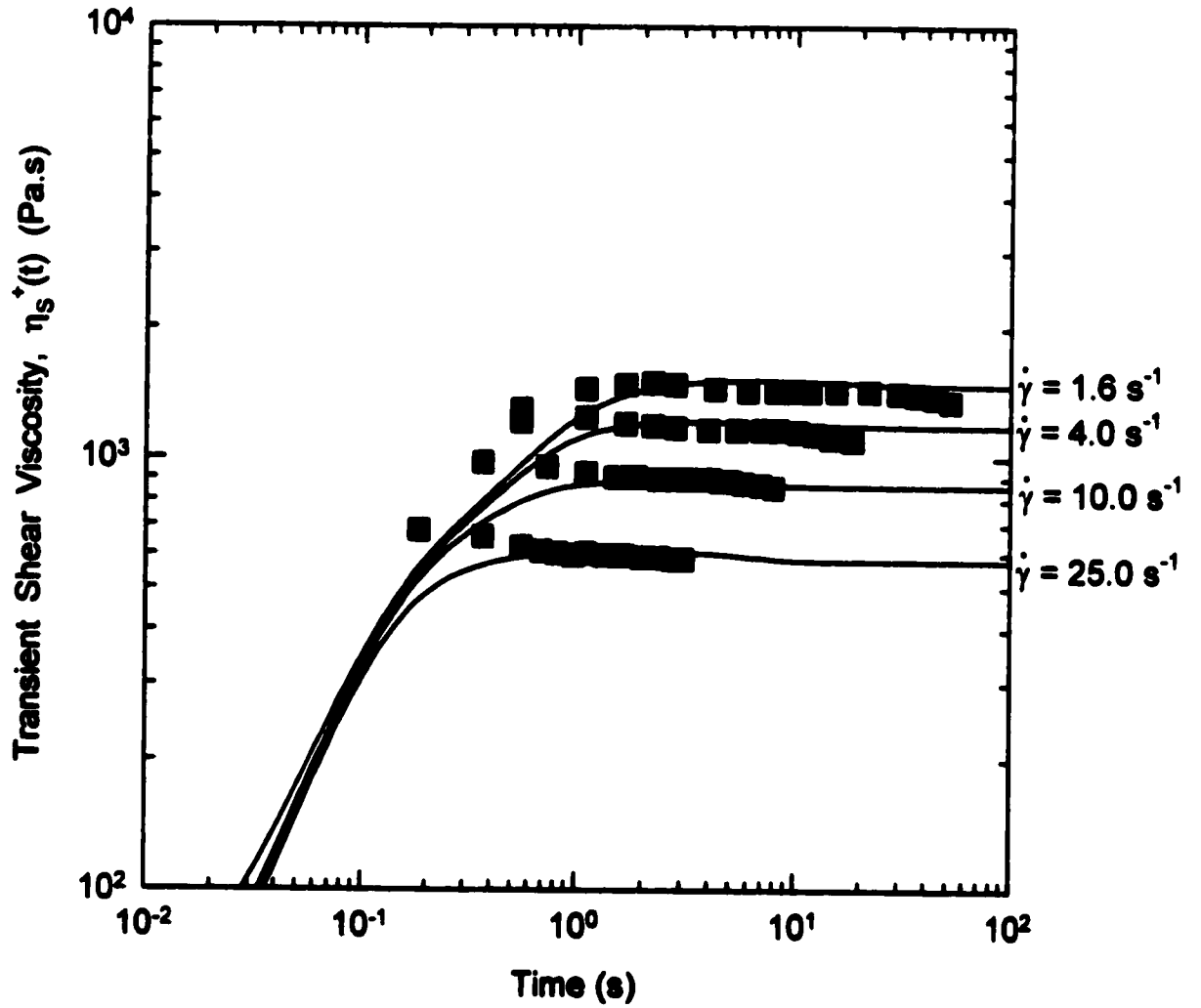


Figure 2.14: Transient shear viscosity (η_s^+) for the Stamylan-L8 LDPE at 190°C. Symbols represent experiments from Tas (1994), while lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum given in Table 2.4.

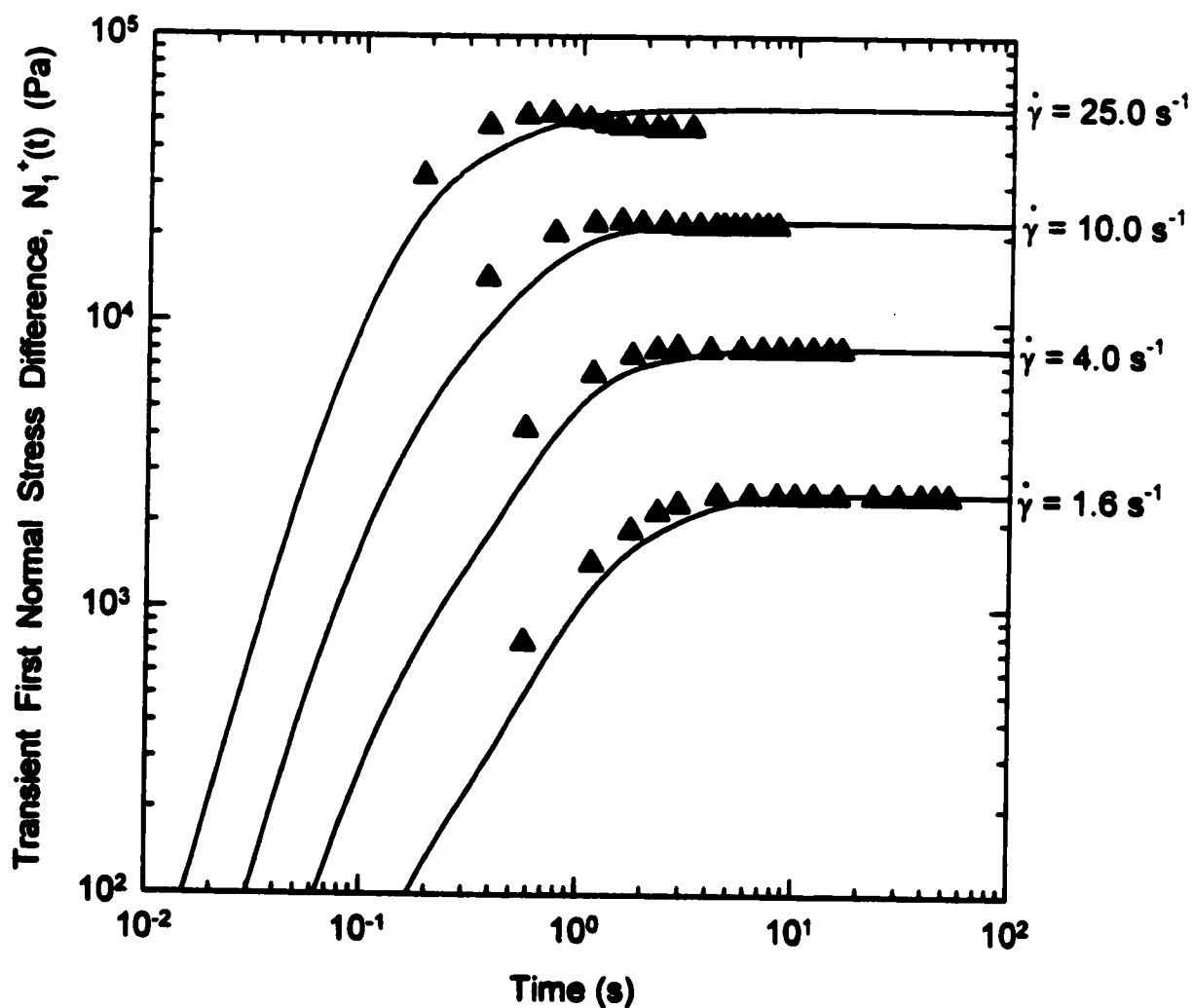


Figure 2.15 Transient first normal stress difference (N_1^*) for the Stamylan-L8 LDPE at 190°C. Symbols represent experiments from Tas (1994), while lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum given in Table 2.4.

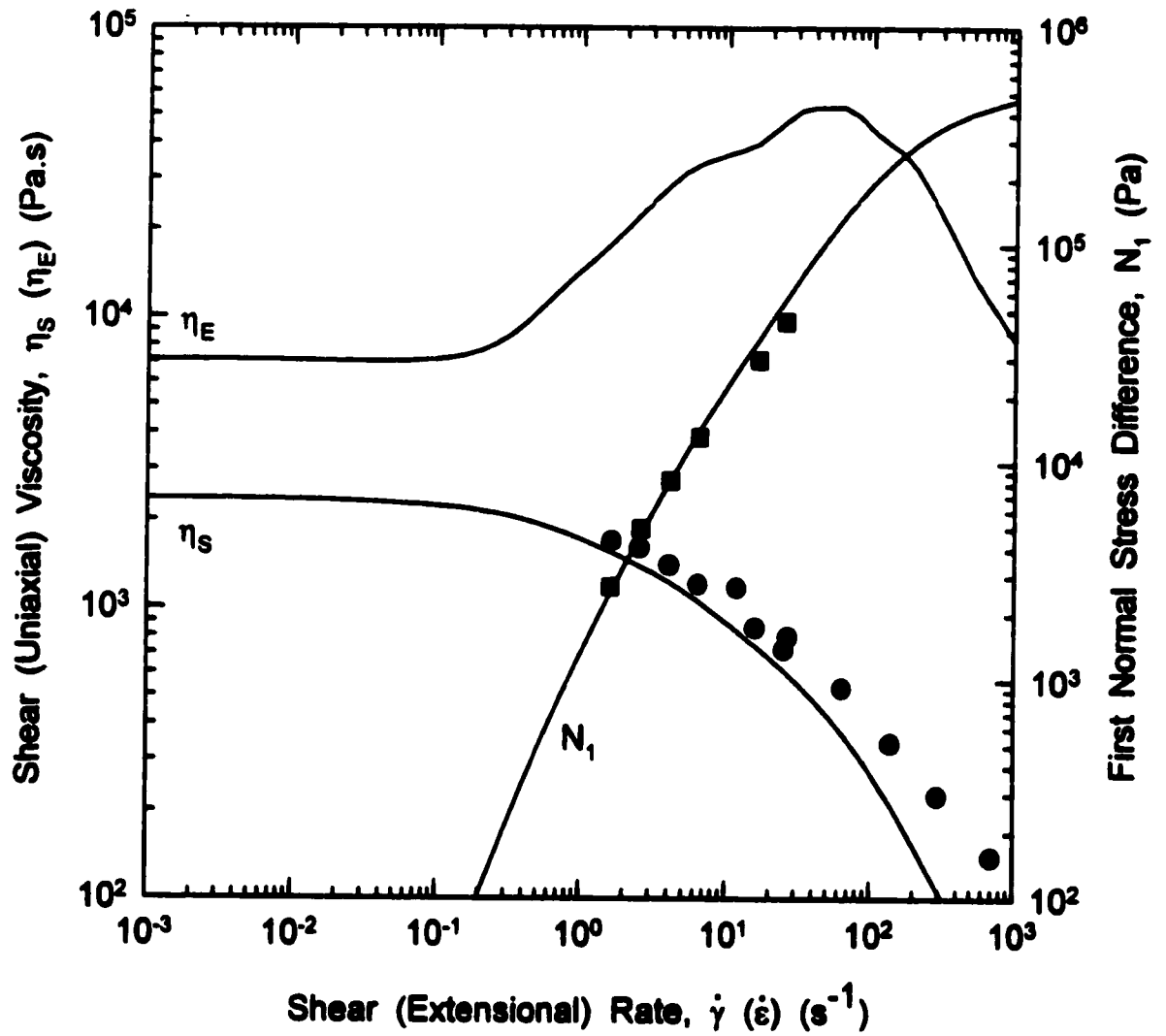


Figure 2.16: Steady-state shear viscosity (η_s), uniaxial viscosity (η_E), and first normal stress difference (N_1) for the Stamylan-L8 LDPE at 190°C. Symbols represent experiments from Tas (1994), while lines represent predictions from the modified K-BKZ constitutive model, eq. (2.6), with the relaxation spectrum from transient regression given in Table 2.4.

Table 2.3: Relaxation spectrum and associated parameters for the virgin PP melt at 230°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 7.32$, $\beta = 0.448$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)
1	5.59×10^{-3}	$5.70 \times 10^{+5}$
2	4.04×10^{-2}	$2.19 \times 10^{+5}$
3	0.223	77100
4	1.24	17700
5	8.23	1650

Table 2.4: Relaxation spectrum and associated parameters for the Stamylan L8 LDPE at 190°C found from transient nonlinear regression for the modified K-BKZ integral constitutive equation ($\beta = 5.80 \times 10^{-3}$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)	α_k
1	4.28×10^{-5}	$2.17 \times 10^{+5}$	12.8
2	2.07×10^{-4}	91800	12.8
3	1.34×10^{-3}	57500	1.81×10^{-6}
4	9.02×10^{-3}	24300	4.87×10^{-5}
5	5.69×10^{-2}	8910	55.9
6	0.353	2340	19.7
7	1.82	321	8.94
8	9.94	12.4	0.438

predictions. Figure 2.15 shows the experimental data and predictions for the transient first normal stress difference (N_1^+). Both the transient shear viscosity and transient first normal stress difference were used in finding the multiple α_k -values to sufficiently predict the experimental data. The relaxation spectrum is given in Table 2.4.

Figure 2.16 shows the influence on the steady-state predictions when using transient experimental data in the regression process. The multiple α_k spectrum gives good steady-

state predictions at low shear rates, but predicts poorly the shear viscosity at higher shear rates. This is due to a lack of transient data at the higher shear rates. Transient data at higher shear rates would give better steady-state predictions.

2.4 Concluding Remarks

Experiments were conducted for polymer solutions at room temperature and for a polymer melt at high temperature with a cone-and-plate rheometer. Measurements for the shear viscosity (η_s) and the first normal stress difference (N_1) were made at a wide range of shear rates for the polymer solutions, but they were limited to about 1.0 s^{-1} for the very viscous polymer melt. The experiments for the polymer melt, which is the most difficult to measure, agreed well with previous experiments and predictions. The agreement with previous results validates the experimental procedure used with the current equipment.

A nonlinear regression program was developed, based on the Levenberg-Marquardt method, for the regression of the modified K-BKZ integral constitutive equation with respect to transient rheological material functions. The program was tested against data for a typical LDPE melt, and good predictions were obtained. However, the relaxation spectrum obtained from the transient regression gave less than fair predictions for the steady-state material functions. This was attributed to a lack of transient data at higher shear rates. Thus, a substantial amount of data is required at a wide range of shear rates in order to accurately predict the steady-state material functions from transient data.

Chapter 3

Mathematical Modeling

The first step in solving any problem involving fluid flow is to describe the process with governing equations, namely field equations and constitutive equations. The field equations in this case are the principles of conservation of momentum, mass, and energy. The constitutive equations are microscopic or phenomenological models, which relate deformation to stress for the fluid in question. This chapter presents the general conservation equations and simplifications made to them for the specific processes under study. This chapter also presents the particular integral constitutive equation used in the viscoelastic modelling of polymeric materials encountered in these processes.

3.1 Conservation Equations

The field equations presented here are the classical ones, namely, the *equation of continuity*, the *equation of motion*, and the *equation of energy*. In vector notation, these equations are respectively written as

$$\frac{\partial \rho}{\partial t} + (\bar{\nabla} \cdot \rho \bar{v}) = 0 \quad (3.1)$$

$$\rho \frac{D\bar{v}}{Dt} = -\bar{\nabla} p + \bar{\nabla} \cdot \bar{\tau} + \rho \bar{g} + \bar{f} \quad (3.2)$$

$$\rho c_p \frac{DT}{Dt} = -\bar{\nabla} \cdot \bar{q} + \bar{\tau} : \bar{\nabla} \bar{v} \quad (3.3)$$

Here, ρ is the density, t is the time, $\bar{v}$ is the velocity vector, p is the pressure, $\bar{\tau}$ is the extra stress tensor, $\bar{g}$ is the vector of acceleration due to gravity, and $\bar{f}$ are extra forces (e.g., air drag). Also, c_p is the heat capacity, T is the temperature, and $\bar{q}$ is the heat flux vector. The substantial derivative, D/Dt is given as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{\mathbf{v}} \cdot \bar{\nabla} \quad (3.4)$$

The extra stress tensor, $\bar{\boldsymbol{\tau}}$, is related to the velocity and its gradients through a *rheological constitutive equation*, where the choice of the constitutive equation is usually at one's disposal. The following assumptions are made to the conservation equations for the present study:

- First, the flow is steady ($\partial/\partial t = 0$), which is valid for the operations of fiber spinning, film casting, and film blowing.
- Second, the fluid is incompressible (constant density), which is valid for the free-surface flows under consideration. The equation of continuity then reduces to

$$\bar{\nabla} \cdot \bar{\mathbf{v}} = 0 \quad (3.5)$$

- The pressure term is set to zero due to the free-surface flows under consideration. The equation of motion then becomes

$$\rho \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{\mathbf{v}} = \bar{\nabla} \cdot \bar{\boldsymbol{\tau}} + \rho \bar{\mathbf{g}} - \rho_a \bar{\mathbf{v}}^2 C_f \quad (3.6)$$

where ρ_a is the density of ambient air, and C_f is the drag coefficient.

- Viscous dissipation ($\bar{\boldsymbol{\tau}} : \bar{\nabla} \bar{\mathbf{v}}$) is usually assumed to be negligible for free-surface flows (Alaie, 1991; Tas, 1994), and radiation from the surface of the fluid to ambient air becomes considerable. Also, conduction for a polymeric material is negligible compared to the effects of convection and radiation. The equation of energy now becomes

$$\rho c_p \bar{\mathbf{v}} \cdot \bar{\nabla} T = -h_c A_s (T - T_\infty) \bar{\mathbf{n}} - \sigma_{SB} \varepsilon A_s (T^4 - T_\infty^4) \bar{\mathbf{n}} \quad (3.7)$$

where T_∞ is the ambient air temperature, h_c is the heat transfer coefficient, A_s is the exposed surface area, $\bar{\mathbf{n}}$ is the outward unit normal vector to a surface, σ_{SB} is the Stefan-Boltzmann constant for radiation, and ε is the emissivity.

A further simplification can be applied to the processes of fiber spinning, film casting, and film blowing. Since the thickness of the fiber or film is small compared to the domain of operation ($L \gg D$), the above equations can be averaged over the cross-

sections to yield one-dimensional expressions for the equations of continuity, momentum and energy. Since the domain of each process differs in terms of geometry, each simplification will be presented separately. Also, the processes of fiber spinning and film blowing are cylindrical in nature, while the film casting process is rectangular in nature. Thus, a cylindrical (polar) coordinate system (r, z, θ) will be used for fiber spinning and film blowing, while a Cartesian coordinate system (x, y, z) will be used for film casting.

3.1.1 The One - Dimensional Model for Fiber Spinning

The domain of interest is portrayed in Figure 3.1, along with the location of the cylindrical (polar) coordinate system (r, z, θ) with respect to the fiber. An axisymmetric filament of viscoelastic fluid is extruded through a die and is continuously taken up at the chill roll. The area of concern is the region downstream from the maximum swell to the location where the filament becomes solid on the chill roll. The distance between maximum swell and solidification or take-up is denoted as L , the force required to draw the fiber is denoted as F , and the final velocity of the filament is denoted as u_L . The current analysis of the fiber-spinning process follows that of the analysis first performed by Denn et al. (1975), where the velocity and stress within the fiber is assumed to be equal over the cross-sectional area. The assumptions used in the analysis are given here for completeness.

For free-surface flows, the velocity and stress only vary with the z -coordinate (i.e., $v_r = v_\theta = 0$). Taking into consideration that the total stress $\bar{\sigma} = -p\bar{I} + \bar{\tau}$, and setting $\sigma_{rr} = 0$, the correlation between the total stress and the extra stress becomes

$$\begin{aligned}\sigma_{zz} &= \tau_{zz} - \tau_{rr} \\ \sigma_{rr} &= 0 \\ \sigma_{\theta\theta} &= \tau_{\theta\theta} - \tau_{rr}\end{aligned}\tag{3.8}$$

Equations (3.5), (3.6), and (3.7) can then be averaged over the cross-sectional area to give the area-intensive governing equations with respect to the z -coordinate. The equation of continuity becomes

$$\rho(\pi r^2)u = \rho Q = \text{constant}\tag{3.9}$$

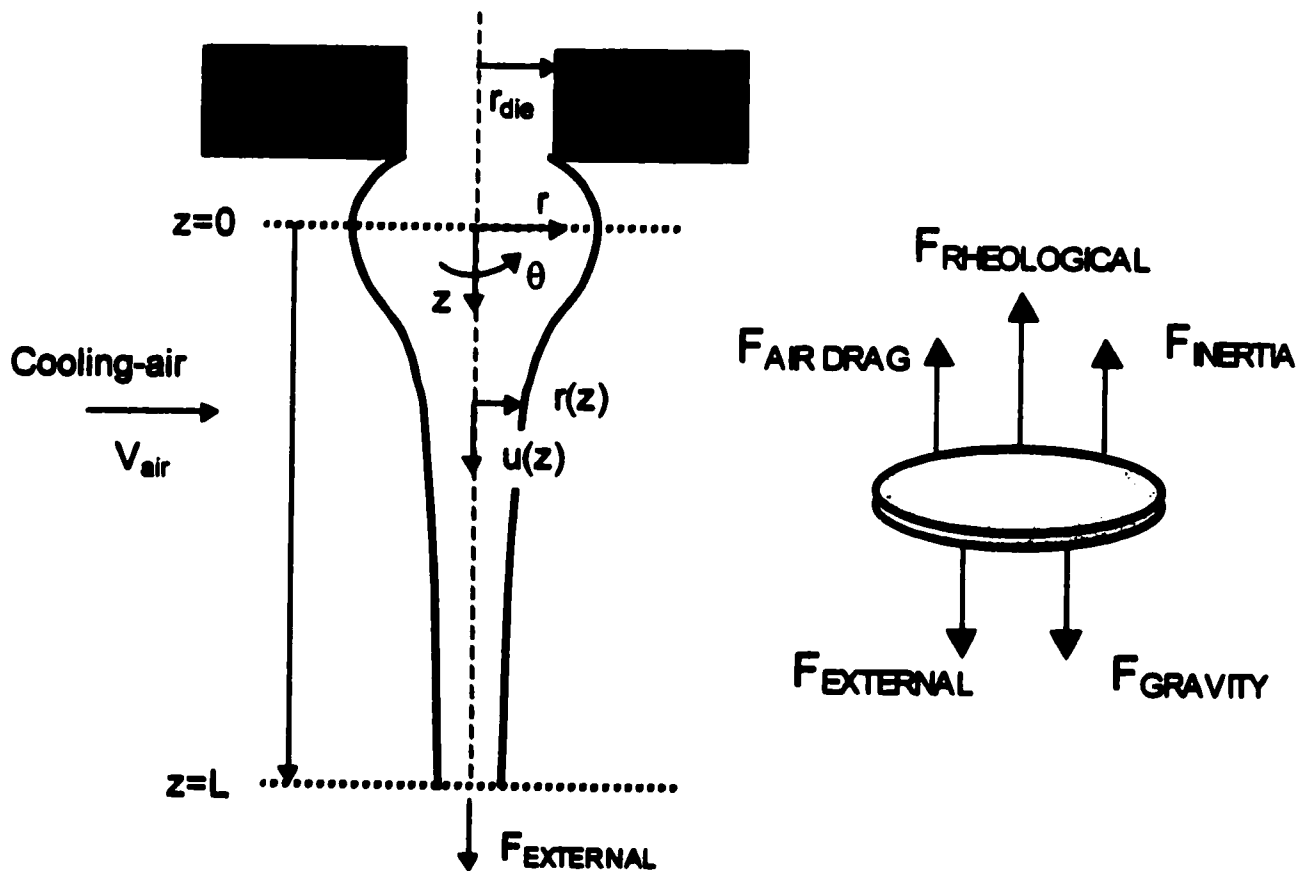


Figure 3.1: Schematic of the fiber-spinning process with the respective cylindrical coordinate system (r, z, θ) and the acting forces.

where r is the radius, u is the axial velocity, Q is the volumetric flow rate, and the term within brackets represents the cross-sectional area. The equation of momentum then becomes

$$\frac{d}{dz}[(\pi r^2)(\tau_{zz} - \tau_{rr})] - (\pi r^2)\rho u \frac{du}{dz} + (\pi r^2)\rho g - (2\pi r)C_f \rho_a \frac{u^2}{2} = 0 \quad (3.10)$$

The equation of energy in one-dimensional form is written as

$$\rho c_p Q \frac{dT}{dz} + 2\pi r h_c (T - T_\infty) + 2\pi r \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (3.11)$$

Equations (3.9) and (3.10) are combined to give

$$\frac{d}{dz} \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u} \right) - \frac{du}{dz} + \frac{g}{u} - C_f u \left(\frac{\rho_a}{\rho} \right) \sqrt{\frac{\pi u}{Q}} = 0 \quad (3.12)$$

and eqs. (3.9) and (3.11) are combined to give

$$\rho c_p Q \frac{dT}{dz} + 2\pi \sqrt{\frac{Q}{\pi u}} h_c (T - T_\infty) + 2\pi \sqrt{\frac{Q}{\pi u}} \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (3.13)$$

Equations (3.9), (3.12), and (3.13) are the final one-dimensional differential equations to be solved for in terms of the radius, r , the axial velocity, u , and the fiber temperature, T .

Single boundary conditions are required for eqs. (3.12) and (3.13), since they are first-order differential equations. These are:

1. The velocity at $z = 0$ is the velocity at the die exit, u_o :

$$u = u_o \text{ at } z = 0 \quad (3.14)$$

2. The temperature at $z = 0$ is the die temperature, T_o :

$$T = T_o \text{ at } z = 0 \quad (3.15)$$

3. The stresses $(\tau_{zz} - \tau_{rr})$ in eq. (3.12) are not known *a priori*, and thus no unique solution exists. Therefore, an additional boundary condition is required to make the solution unique. This is done by specifying the velocity at the take-up position, where the stresses depend on the velocity (through a constitutive equation):

$$u = u_L \text{ at } z = L \quad (3.16)$$

The radius, r , is easily calculated from eq. (3.9), once eq. (3.12) is solved for in terms of the velocity, u .

3.1.2 The One – Dimensional Model for Film Casting

The domain of interest for the film-casting process is portrayed in Figure 3.2, along with the location of the Cartesian coordinate system (x,y,z) with respect to the film. A thin film of viscoelastic fluid is extruded through a rectangular die and is continuously taken up at the chill roll. The area of concern is usually from the die exit to the chill roll. The distance between the die and the chill roll is denoted as L , the force required to draw the film is denoted as F , and the final velocity of the film is denoted as u_L . The current analysis of the film-casting process follows that of the analysis first performed by Denn et al. (1975) for the fiber-spinning process, as described in section 3.1.1. The changes are made from the cylindrical coordinate system for fiber spinning to the Cartesian coordinate system for film casting. Silagy et al. (1996) presented a method to calculate the variation of the width with respect to the x -coordinate, in conjunction with the velocity, and this method is used in the current analysis. The complete set of equations is presented here to describe the mathematical approach used for the simulation of the film-casting process.

For free-surface flows, the stress only varies with the x -coordinate, but the velocity in the y -direction is non-zero. Taking into consideration the total stress $\bar{\sigma} = -p \bar{I} + \bar{\tau}$, and setting $\sigma_{xx}=0$, the correlation between the total stress and the extra stress becomes

$$\begin{aligned}\sigma_{xx} &= \tau_{xx} - \tau_{xx} \\ \sigma_{yy} &= \tau_{yy} - \tau_{xx} \\ \sigma_{zz} &= 0\end{aligned}\tag{3.17}$$

The conservation equations (3.5), (3.6), and (3.7) can then be averaged over the cross-sectional area to give the area-intensive governing equations with respect to the x -coordinate. The equation of continuity becomes

$$\rho(4wh)u = \rho Q = \text{constant}\tag{3.18}$$

where w is the width, h is the thickness, u is the axial velocity, Q is the volumetric flow rate, and the term within brackets represents the cross-sectional area. With the geometry of the film as represented in Figure 3.2, the cross sectional area of the film is then $(4wh)$ while the perimeter of the film is $(4w+4h)$. The equation of momentum then becomes

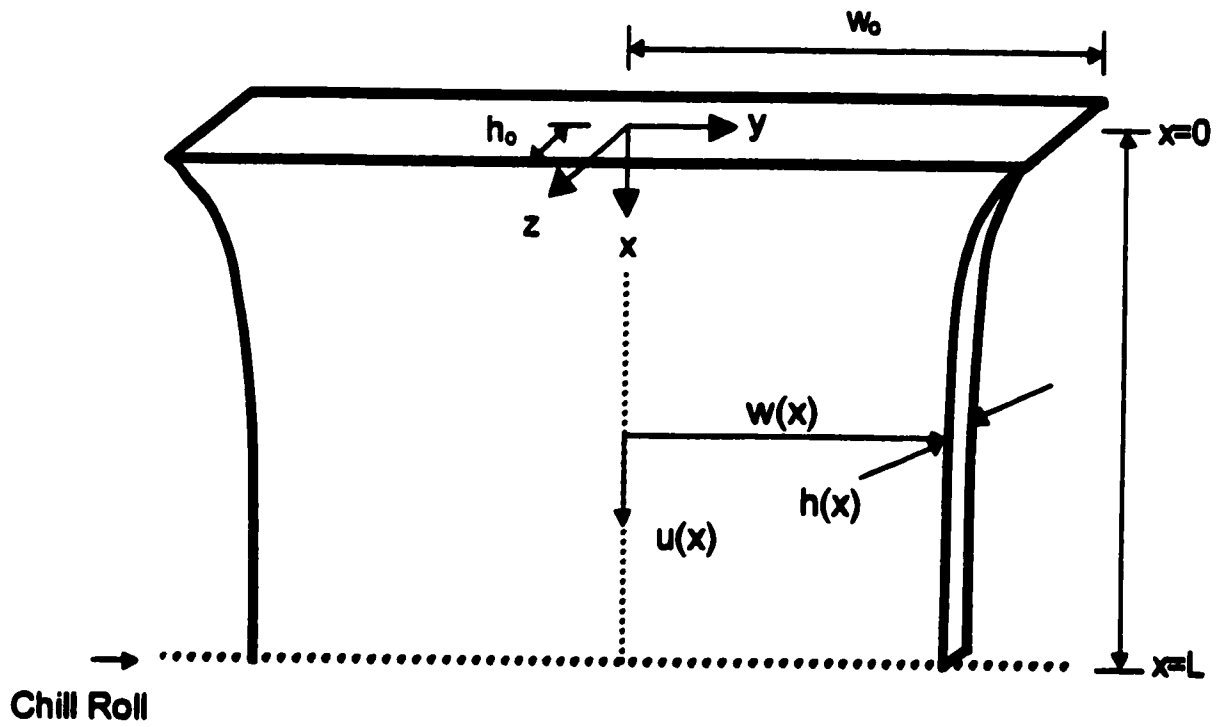


Figure 3.2: Schematic of the film-casting process with the respective Cartesian coordinate system (x,y,z) .

$$\frac{d}{dx}[(4wh)(\tau_{xx} - \tau_{zz})] - (4wh)\rho u \frac{du}{dx} + (4wh)\rho g - (4w + 4h)C_f \rho_a \frac{u^2}{2} = 0 \quad (3.19)$$

The equation of energy in one-dimensional form is given as

$$\rho c_p Q \frac{dT}{dx} + (4w + 4h)h_c(T - T_\infty) + (4w + 4h)\sigma_{SB}\epsilon(T^4 - T_\infty^4) = 0 \quad (3.20)$$

Equations (3.18) and (3.19) are combined to give

$$\frac{d}{dx}\left(\frac{\tau_{xx} - \tau_{zz}}{\rho u}\right) - \frac{du}{dx} + \frac{g}{u} - C_f u \left(\frac{\rho_a}{\rho}\right) \left(2\frac{wu}{Q} + \frac{1}{2w}\right) = 0 \quad (3.21)$$

and eqs. (3.18) and (3.20) are combined to give

$$\rho c_p Q \frac{dT}{dx} + \left(4w + \frac{Q}{4wu}\right)h_c(T - T_\infty) + \left(4w + \frac{Q}{4wu}\right)\sigma_{SB}\epsilon(T^4 - T_\infty^4) = 0 \quad (3.22)$$

So far, there are two dimensionless differential equations in terms of three variables: the velocity, u , the width, w , and the temperature, T . Hence, an additional equation is required to solve for the third unknown (the width). This extra equation was first introduced by Silagy et al. (1996), which arises from the continuity of stresses at the free-surface. In vector notation, this equation is given as

$$\bar{\sigma} \cdot \bar{n} = 0 \quad (3.23)$$

where $\bar{n}$ is the normal to the free surface on the xy free-surface plane. Expanding and solving for the width gives the third required differential equation:

$$\left(\frac{dw}{dx}\right)^2 = \frac{\sigma_{yy}}{\sigma_{xx}} = \frac{\tau_{yy} - \tau_{zz}}{\tau_{xx} - \tau_{zz}} \quad (3.24)$$

Equations (3.18), (3.21), (3.22), and (3.24) are the final one-dimensional differential equations to be solved for in terms of the thickness, h , the axial velocity, u , the width, w , and the film temperature, T .

Single boundary conditions are required for eqs. (3.21), (3.22), and (3.24) since they are first-order differential equations. These are:

1. The velocity at $x = 0$ is the velocity at the die exit, u_o :

$$u = u_o \text{ at } x = 0 \quad (3.25)$$

2. The temperature at $x = 0$ is the die temperature, T_o :

$$T = T_o \text{ at } x = 0 \quad (3.26)$$

3. The width at $x = 0$ is the width at the die exit, w_0 :

$$w = w_0 \text{ at } x = 0 \quad (3.27)$$

4. The stresses $(\tau_{xx} - \tau_{zz})$ in eq. (3.21) are not known *a priori*, and thus no unique solution exists (as in fiber spinning). Therefore, an additional boundary condition is required to make the solution unique. This is done by specifying the velocity at the take-up position, where the stresses depend on the velocity (through a constitutive equation):

$$u = u_L \text{ at } x = L \quad (3.28)$$

The thickness, h , is easily calculated from eq. (3.18), once eqs. (3.21) and (3.24) are solved for in terms of the velocity, u , and the width, w .

3.1.3 The One – Dimensional Model for Film Blowing

The equations for the film-blowing process are different from those presented for fiber spinning and film casting since they are additionally derived from *thin-shell theory*. The analysis of the film-blowing process follows the classical analysis performed by Pearson and Petrie (1970a,b) using thin-shell theory, and is restated here for completeness.

In the fiber-spinning and film-casting derivations, the curvatures of the fiber or film with respect to the axial coordinate ($\partial r / \partial z \ll 1$ for fiber spinning and $\partial y / \partial x \ll 1$ for film casting) were neglected. However, for the film-blowing process the change of the bubble radius with respect to the z -coordinate cannot be neglected, and interfacial forces must be accounted for. The equation of momentum will not be used directly, but rather a discrete method using force balances will be used to derive the governing equations for film blowing.

The domain of interest for the film-blowing process is portrayed in Figure 3.3. A thin film of viscoelastic fluid is extruded through an annular die and is continuously taken up at the nip rolls. The area of concern is from the die exit to the freezeline where the liquid polymer melt solidifies. The distance between the die and the freezeline is denoted as L , the force required to draw the film is denoted as F , the final velocity of the film is

denoted as u_L , and the final bubble radius is denoted as r_L . Also portrayed in Figure 3.3 are the locations of a *fixed* cylindrical (polar) coordinate system (r, θ) and a *moving* coordinate system (t, s, n) , with the origin on the inner surface of the film. The s -coordinate is termed the *streamline direction*, the t -coordinate is termed the *transverse direction*, and the n -coordinate is termed the *normal direction*. Industrially, the s -direction is termed the *machine direction (MD)* and the t -direction is termed the hoop direction (HD) or *transverse direction (TD)*. The correlation between the fixed and moving coordinate systems is achieved by using the variable ϕ (see Figure 3.3) where

$$ds = \sqrt{dr^2 + dz^2}$$

$$\cos \phi = \frac{dz}{ds} = \frac{1}{\sqrt{1 + \left(\frac{dr}{dz}\right)^2}} \quad (3.29)$$

For free-surface flows, the stress only varies with the s -coordinate. Taking into consideration the total stress $\bar{\sigma} = -p \bar{I} + \bar{\tau}$, and setting $\sigma_{nn}=0$, the correlation between the total stress and the extra stress becomes

$$\begin{aligned} \sigma_{ss} &= \tau_{ss} - \tau_{nn} \\ \sigma_{tt} &= \tau_{tt} - \tau_{nn} \\ \sigma_{nn} &= 0 \end{aligned} \quad (3.30)$$

The equation of continuity, eq. (3.5), can be averaged over the cross-sectional area and integrated to give

$$\rho(2\pi rh)u = \rho Q = \text{constant} \quad (3.31)$$

where r is the bubble radius, h is the film thickness, u is the film velocity in the machine direction, Q is the volumetric flow rate, and the term within brackets represents the cross-sectional area. From thin-shell theory (Pearson and Petrie, 1970a,b), the balance of pressures on both sides of the film can be expressed in terms of the balance of stresses on the free surface:

$$\bar{\sigma} \cdot \bar{n} = 0 \quad (3.32)$$

where $\bar{n}$ is the normal to the free surface. The resulting balance of forces and pressures acting on the surface in terms of σ_{ss} and σ_{tt} is given as

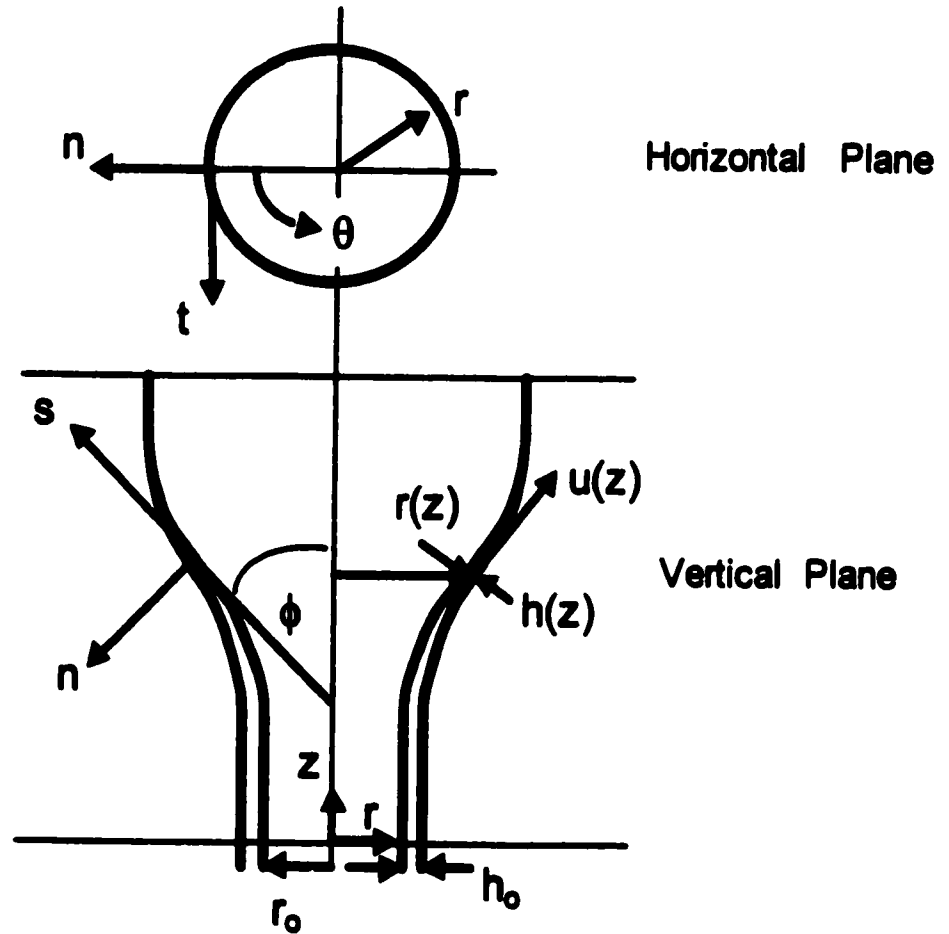


Figure 3.3: Schematic of the film-blowing process with its respective cylindrical coordinate system (r, z, θ) and moving coordinate system (t, s, n) .

$$\frac{\sigma_{ss}}{R_s} + \frac{\sigma_n}{R_t} = \frac{\Delta P}{h} \quad (3.33)$$

where R_s and R_t are the principal curvature radii, which are found from simple differential geometry principles as:

$$R_s = -\frac{\left[1 + \left(\frac{dr}{dz}\right)^2\right]^{3/2}}{\frac{d^2r}{dz^2}} \quad (3.34)$$

$$R_t = r \left[1 + \left(\frac{dr}{dz}\right)^2\right]^{1/2}$$

A z-coordinate force balance can also be performed, which results in

$$F = (2\pi rh) \cos \phi \tau_{ss} + \pi(r_L^2 - r^2) \Delta P \quad (3.35)$$

Utilizing the correlations in eq. (3.29) and eliminating h with eq. (3.31) within eqs. (3.33) and (3.35), the following equations describe the shape of the bubble:

$$\frac{\sigma_{ss}}{r} \left[1 + \left(\frac{dr}{dz}\right)^2\right]^{1/2} - \frac{d^2r}{dz^2} \sigma_n \left[1 + \left(\frac{dr}{dz}\right)^2\right]^{3/2} - \frac{2\pi r u \Delta P}{Q} = 0 \quad (3.36)$$

$$\frac{Q}{u} \sigma_{ss} \left[1 + \left(\frac{dr}{dz}\right)^2\right]^{1/2} + \pi r^2 \Delta P \left(\frac{r_L^2}{r^2} - 1\right) - F = 0 \quad (3.37)$$

The equation of energy in one-dimensional form is given as

$$\rho c_p Q \frac{dT}{dz} + 2\pi h_c (T - T_\infty) + 2\pi \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (3.38)$$

Again, using the correlations in eq. (3.29), the final form of the equation of energy is

$$\rho c_p Q \cos \phi \frac{dT}{dz} + 2\pi h_c (T - T_\infty) + 2\pi \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (3.39)$$

Equations (3.31), (3.36), (3.37), and (3.39) are the final one-dimensional differential equations to be solved for in terms of the thickness, h , the machine direction velocity, u , the bubble radius, r , and the film temperature, T .

Two boundary conditions are required for eq. (3.36), since it is a second-order differential equation, while eqs. (3.37) and (3.39) require only one boundary condition, since they are first-order differential equations. These are:

1. The radius at $z = 0$ is the radius at the annular die exit, r_o :

$$u = u_o \text{ at } z = 0 \quad (3.40)$$

2. At the freezeline, $z = L$, the film is considered solidified and thus no further deformation occurs. This implies that the radius will no longer increase at or beyond the freezeline. Mathematically, this is written as:

$$\frac{dr}{dz} = 0 \text{ at } z = L \quad (3.41)$$

3. The velocity at $z = 0$ is the velocity at the die exit, u_o :

$$u = u_o \text{ at } z = 0 \quad (3.42)$$

4. The temperature at $z = 0$ is the die temperature, T_o :

$$T = T_o \text{ at } z = 0 \quad (3.43)$$

Since eqs. (3.36) and (3.37) involve the force, F , at the freezeline, which in turn specifies the stresses at the freezeline, no additional boundary conditions are required (unlike the fiber-spinning and film-casting boundary conditions, which do not involve the force, F). The thickness, h , is easily calculated from eq. (3.31), once eqs. (3.36) and (3.37) are solved for in terms of the radius, r , and the velocity, u .

3.2 Constitutive Equations

In order to solve the governing equations of fiber spinning, film casting, and film blowing, a constitutive equation is required to relate the extra-stress tensor, $\bar{\tau}$, to the velocity and its gradients (i.e., deformation). The three constitutive models used in this study are: (i) the *Newtonian model*, (ii) the *upper-convected Maxwell (UCM) model*, and (iii) a variant of the *K-BKZ integral model*.

(i) Elementary constitutive equations, such as the Newtonian model, which is the simplest model for *purely viscous behaviour*, help describe simple fluid behaviour and in understanding some of the more complex constitutive equations. Examples of Newtonian

fluids are water, some vegetable oils containing small molecules, and dilute suspensions. Figure 3.4 depicts the behaviour of the Newtonian model as a function of shear (extensional) rate, where the viscosities are made dimensionless by $\eta^* = \eta / \mu$. The shear viscosity predicted by the Newtonian model is constant ($\eta_S = \mu$). The uniaxial extensional viscosity is also constant ($\eta_E = 3\mu$), as is the planar extensional viscosity ($\eta_P = 4\mu$), and the biaxial extensional viscosity ($\eta_B = 6\mu$). The Newtonian model gives zero predictions for the normal force differences ($N_1 = N_2 = 0$), since the normal stresses for the Newtonian model are all equal in shear flow.

(ii) More elaborate constitutive equations include the UCM model (Maxwell, 1867), which is derived by considering viscous and elastic responses to an applied stress. The UCM model is considered simple in terms of viscoelasticity and it represents the simplest model of *linear viscoelasticity*, having a constant viscosity and a constant relaxation time, hence no material functions. It does not describe adequately the behaviour of viscoelastic solutions and melts, especially in terms of the extensional viscosities (η_E , η_P , η_B). However, the UCM model is useful in numerical simulations, since it is used as a benchmark model to ensure proper implementation of numerical methods. The UCM model is also useful in understanding simple elasticity concepts, such as particle memory (a fluid particle's ability to remember past deformations). Figure 3.5 depicts the predictions of the UCM model for various material properties as functions of shear (extensional) rate. The viscosities are made dimensionless as in the case for the Newtonian fluid ($\eta^* = \eta / \mu$). The first normal stress difference is made dimensionless by using $N_1^* = N_1 \lambda / \mu$. From Figure 3.5, the prediction for the shear viscosity is the same as for the Newtonian model (a constant shear viscosity). The extensional viscosities at low extensional rates are also similar to the Newtonian model. However, at higher extensional rates, the extensional viscosities rise infinitely, which physically is not correct. The prediction of the UCM model for the first normal stress difference, N_1 , is also shown, and it rises quadratically with shear rate (slope=2). The latter is only observed physically at very low shear rates. Thus, it becomes obvious from the deficiencies of its predictions, that *the Maxwell model is not a good model for polymer solutions and melts*.

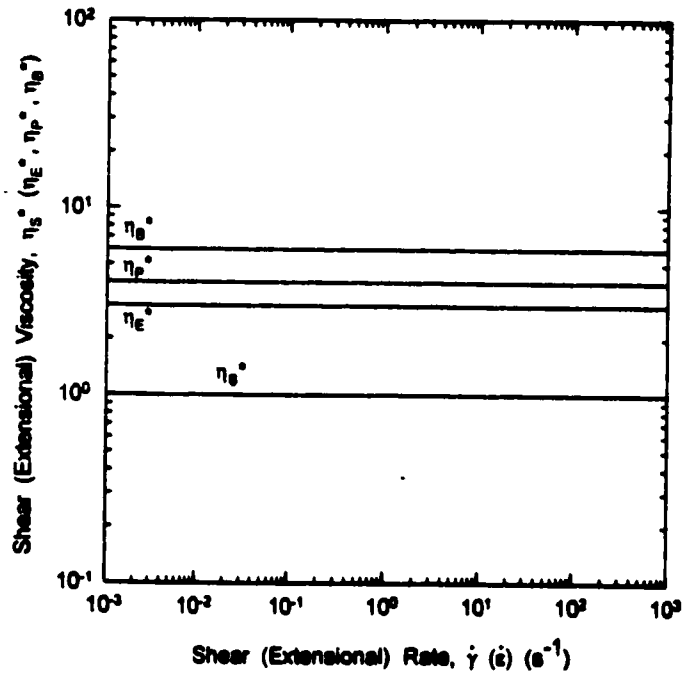


Figure 3.4: Shear and extensional viscosity predictions of the Newtonian model.

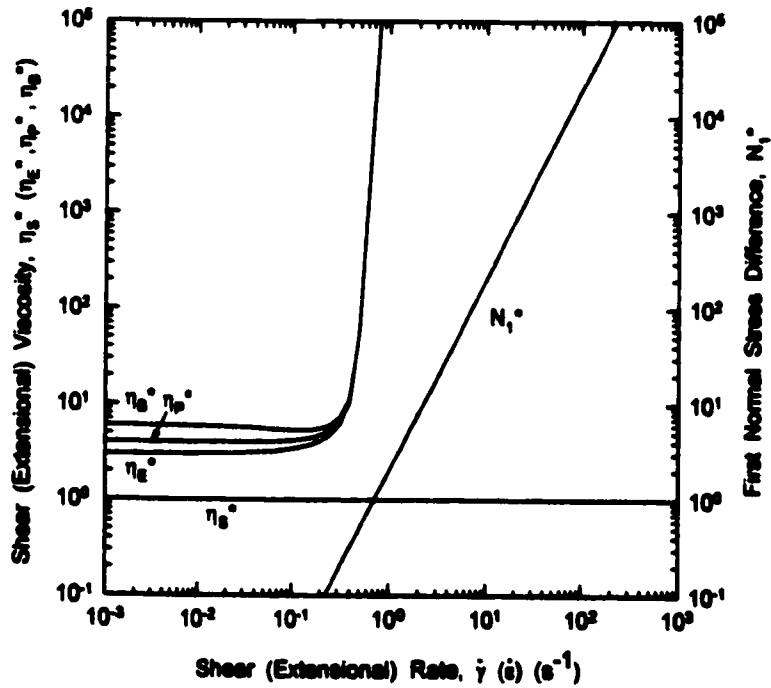


Figure 3.5: Shear viscosity, extensional viscosity, and first normal stress difference predictions of the UCM model.

(iii) A more complex constitutive equation is the K-BKZ integral constitutive equation, derived independently by Kaye (1962), and by Bernstein, Kearsley, and Zapas (1963) (note that the abbreviation comes from the initials of the researchers' names). This equation has an integral form with time limits from a present time to all past times, in order to capture the fading memory of the material. It also utilizes a spectrum of relaxation times to handle the fact that polymer solutions and melts are *polydisperse*. Polydispersity is a term used for polymer solutions and melts that have many molecules with different molecular weights. Thus, each molecule behaves differently and has its own unique relaxation time, which are grouped conveniently in a spectrum. The K-BKZ equation has the ability to predict well the behaviour of polymer melts and solutions with respect to the shear and elongational viscosities, and the normal stresses measured in shear flow. Figure 3.6 depicts the predictions of the K-BKZ equation along with experimental data for a typical low-density polyethylene (LDPE) melt at 150°C (Meissner, 1975). As shown, the K-BKZ equation predicts well the shear and uniaxial extensional viscosities, even at high shear (extensional) rates. The first normal stress difference, N_1 , is also predicted well by the K-BKZ equation.

3.2.1 The Newtonian Model

For Newtonian fluids we have:

$$\bar{\tau} = \mu \bar{\dot{\gamma}} = 2\mu \bar{D} \quad (3.44)$$

where μ is the constant Newtonian viscosity, $\bar{\dot{\gamma}}$ is the rate-of-strain tensor, and $\bar{D}$ is the rate-of-deformation tensor, given by

$$\bar{\dot{\gamma}} = 2\bar{D} = \bar{\nabla} \bar{v} + \bar{\nabla} \bar{v}^T \quad (3.45)$$

where $\bar{\nabla} \bar{v}$ is the velocity gradient tensor ($\partial u_i / \partial x_j$) and $\bar{\nabla} \bar{v}^T$ is its transpose.

3.2.2 The Upper - Convected Maxwell (UCM) Model

For the UCM model in differential form, we have:

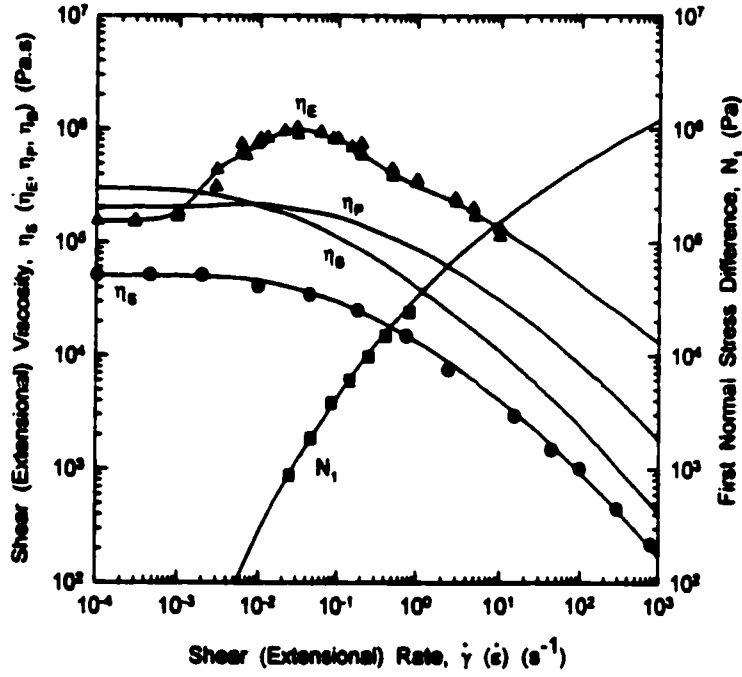


Figure 3.6: Shear (extensional) predictions of the K-BKZ integral constitutive equation along with experimental data for a typical LDPE melt at 150°C (Meissner, 1975).

$$\bar{\tau} + \lambda \bar{\nabla} \bar{\tau} = 2\eta \bar{D} \quad (3.46)$$

where $\bar{\nabla}$ is known as the *upper-convected derivative* of the extra stress tensor. The upper-convected derivative is given by

$$\bar{\nabla} \bar{\tau} = \frac{D\bar{\tau}}{Dt} - (\bar{\nabla} u)^T \cdot \bar{\tau} - \bar{\tau} \cdot \bar{\nabla} u \quad (3.47)$$

The above model is of particular importance because there exist many numerical solutions in the scientific literature, which can be used as benchmark solutions for new numerical techniques. It is also important because it leads the way to more complicated differential models, such as the Phan-Thien/Tanner (PTT) (Phan-Thien and Tanner, 1977), Leonov (Leonov, 1976), and Giesekus (Giesekus, 1982) models.

3.2.3 The K-BKZ Integral Constitutive Model

3.2.3.1 The K-BKZ Mathematical Equation

The original K-BKZ equation was modified by Papanastasiou et al. (1983), and further modified by Luo and Tanner (1988), and has the following form:

$$\bar{\tau}(t) = \frac{1}{1-\theta} \int_{-\infty}^t \sum_{k=1}^N M(t-t') H(I_C, I_{C^{-1}}) \left[\left\{ \bar{C}_t^{-1}(t') - \bar{I} \right\} + \theta \left\{ \bar{C}_t(t') - \bar{I} \right\} \right] dt' \quad (3.48)$$

where $\bar{I}$ is the identity matrix,

$$M(t-t') = \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) \quad (3.49)$$

is a linear time-memory function with N modes, and $H(I_C, I_{C^{-1}})$ is a non-linear strain-memory function given by

$$H(I_C, I_{C^{-1}}) = \frac{\alpha_k}{(\alpha_k - 3) + \beta_k I_{C^{-1}} + (1 - \beta_k) I_C} \quad (3.50)$$

where λ_k and a_k are relaxation times and relaxation modulus coefficients at a reference temperature T_{ref} , respectively. The parameters α_k and β_k are material parameters chosen to fit the material's response in strong shear and elongation, respectively. The invariants I_C and $I_{C^{-1}}$ are the first invariants of the Cauchy-Green tensor $\bar{C}_t(t')$ and its inverse $\bar{C}_t^{-1}(t')$, the Finger strain tensor. In terms of the deformation gradient tensor, $\bar{F}_t(t') = d\bar{x}'/d\bar{x}$, the Cauchy-Green and Finger tensors are

$$\begin{aligned} \bar{C}_t(t') &= \bar{F}_t(t') \cdot \left[\bar{F}_t(t') \right]^T \\ \bar{C}_t^{-1}(t') &= \left[\bar{F}_t^{-1}(t') \right]^T \cdot \bar{F}_t^{-1}(t') \end{aligned} \quad (3.51)$$

where t and t' are the present time and some time in the past, respectively, and $\bar{x}$ and $\bar{x}'$ are the present and past position vectors, respectively. Figure 3.7 illustrates the current time, t , and the past time, t' , along with the current position vector, $\bar{x}$, and the past position vector, $\bar{x}'$. The parameter θ has been incorporated by Luo and Tanner (1988) to take into account the second normal stress difference, N_2 , and is related to the first normal stress difference, N_1 , via the formula

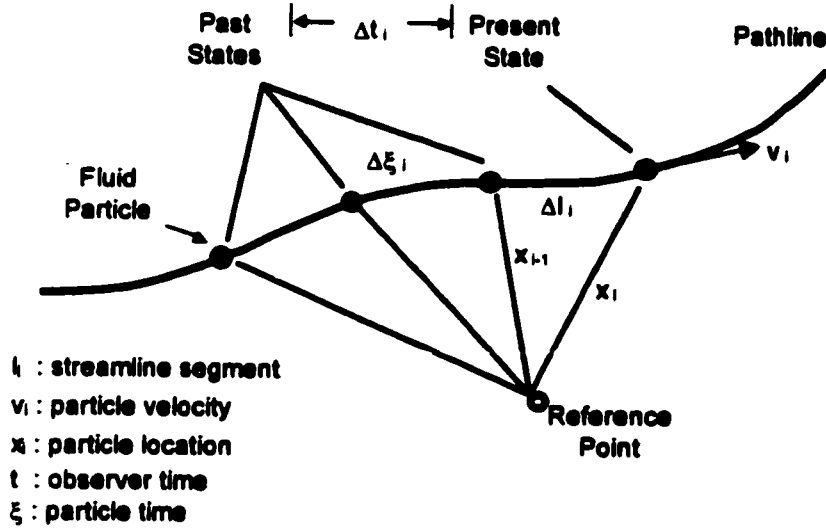


Figure 3.7: For viscoelastic fluids under flowing conditions, the present state of stress of a fluid particle is a function of the particle's stress history (past states). For the non-isothermal case, the material's internal clock is not the same as the observer's clock (Tanner, 1985).

$$\frac{N_2}{N_1} = \frac{\theta}{1 - \theta} \quad (3.52)$$

Since N_2 is a negative quantity defined by $N_2 = \tau_{22} - \tau_{33}$, θ must have a negative value. Its usual range for polymer solutions and melts is $-0.4 \leq \theta \leq 0$ (Tanner, 1985).

The Newtonian model, eq. (3.44), is readily obtained from the modified K-BKZ integral constitutive model, eq. (3.48), by setting $N=1$ and $\lambda_1 \rightarrow 0$ (or equivalently a small number, say 0.001). Also, the UCM model, eq. (3.46), is readily obtained from the modified K-BKZ integral constitutive model, eq. (3.48), by setting $N = 1$, $\lambda_i = \lambda$, and $\alpha \rightarrow \infty$ (or equivalently a very large number, say 10,000).

3.2.3.2 The Nonlinear Parameters α , β , and θ

The nonlinear parameters within the K-BKZ integral constitutive equation (namely α , β , and θ) when altered will naturally affect the rheological functions (e.g. shear

viscosity, first normal stress difference, etc.). The α parameter is normally called the *shear-thinning parameter*, while the β parameter is normally called the *extension-thinning parameter*. The θ parameter is called here the *normal stress parameter*.

Figures 3.8 (a) and 3.8 (b) show the effect of changing the shear-thinning parameter, α , on the rheological functions. A decrease in the α parameter causes an increase in the thinning effect (reduction of viscosity with increasing shear or extensional rate) for all of the viscosities (shear and extensional), with a reduction of the first normal stress difference at higher shear rates. It will be seen shortly α is the only nonlinear parameter that affects the planar extensional viscosity. The α parameter causes a less significant effect on the biaxial extensional viscosity than the other rheological functions.

Figures 3.9 (a) and 3.9 (b) show the effect of changing the extension-thinning parameter, β , on the rheological functions. The β parameter does not affect the rheological functions in shear (shear viscosity and first normal stress difference), nor does it affect the planar extensional viscosity. It does not affect the planar extensional viscosity because the first and second invariants (I_C and $I_{C^{-1}}$ in eq. (3.50)) are equal, and causes the β parameter in eq. (3.50) to vanish. An increase in the β parameter reduces the extent of thinning for the uniaxial extensional viscosity (see Figure 3.9 (a)). The *opposite* occurs with the biaxial extensional viscosity, where an increase in the β parameter causes a slight increase in the thinning effect.

Finally, Figures 3.10 (a) and 3.10 (b) show the effect of changing the normal stress parameter, θ , on the rheological functions. The θ parameter also does not affect the rheological functions in shear (shear viscosity and first normal stress difference), nor does it affect the planar extensional viscosity. As mentioned earlier, α is the only nonlinear parameter that affects the planar extensional viscosity. A decrease in the θ parameter causes a slight decrease in the uniaxial extensional viscosity. The *opposite* effect is observed with the biaxial extensional viscosity, where a decrease in the θ parameter causes a very large increase in the biaxial viscosity.

Summarizing, significant changes in the uniaxial extensional viscosity can be observed by changing either the α parameter or the β parameter, with only slight changes obtained with the θ parameter. Significant changes in the planar extensional viscosity

can be obtained by changing the α parameter only. Finally, significant changes in the biaxial extensional viscosity can be observed by changing the θ parameter, with only slight changes obtained with the α and β parameters.

3.2.3.3 The Non-Isothermal K-BKZ Equation

For the non-isothermal case, it is necessary to derive a non-isothermal constitutive equation from the isothermal one. This is done by applying the time-temperature shifting concept as explained by Luo and Tanner (1987). This concept is based on the relative difference between the observer's time scale and the material's time scale. Using ξ for the time measured by the material's own internal clock, the following relation holds between ξ and the observer's time t :

$$d\xi = \frac{dt}{a_T(T)} \quad (3.53)$$

where the denominator is the time-shifting factor. The above relationship expresses the *Morland-Lee hypothesis* in a differential form (Tanner, 1985), and it can be used to obtain the following integral relation between the particle's elapsed time and the observed period:

$$\xi = \int_0^t a_T^{-1}(T(t')) dt' \quad (3.54)$$

Thus as a fluid particle is tracked along a streamline segment Δl , the particle's time corresponding to the residence time Δt is given by

$$\Delta\xi = \frac{\Delta l}{u_l a_T(T_l)} \quad (3.55)$$

Figure 3.7 also depicts the particle's path, where the relevant times and lengths are presented for the non-isothermal case. Equation (3.53) can be used to obtain the non-isothermal form of the modified K-BKZ equation by replacing the observer's time t in eq. (3.48) with the particle's time ξ given by eq. (3.53). The resulting version of the constitutive equation becomes

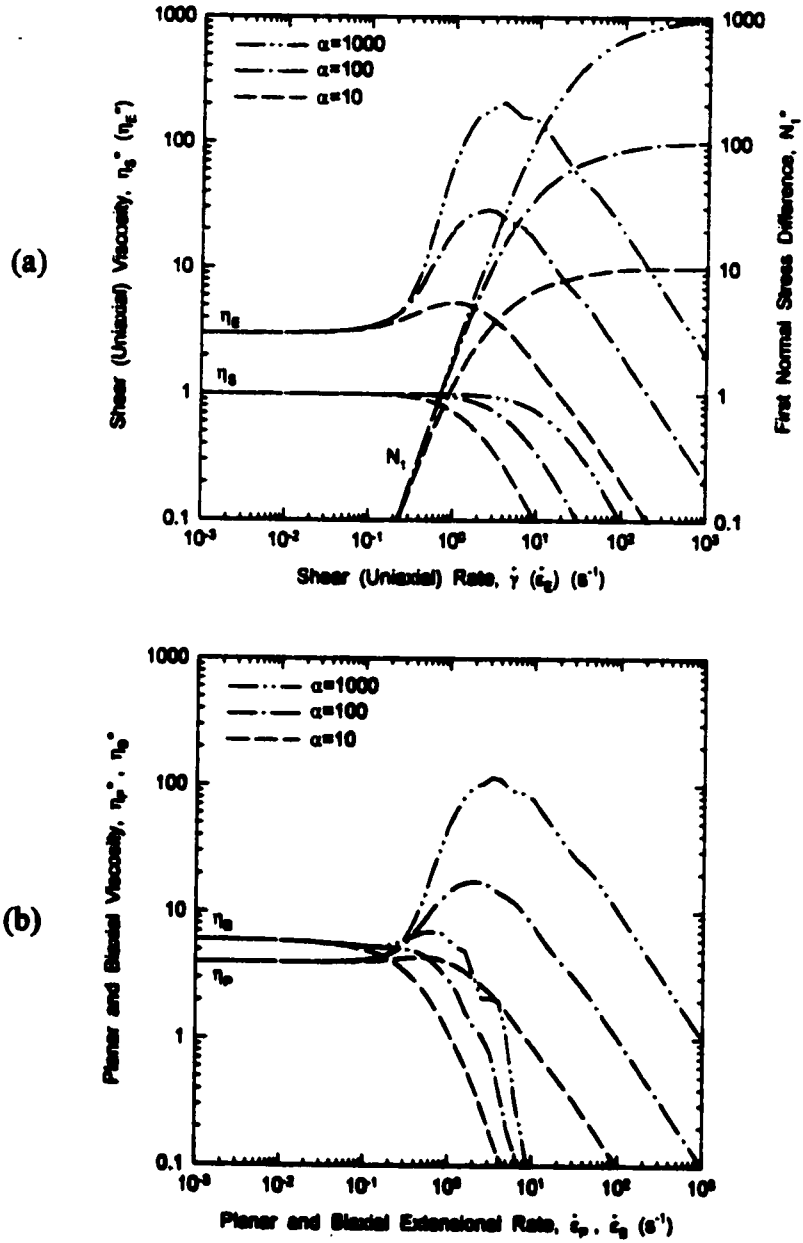


Figure 3.8: (a) Effect of changing the nonlinear parameter, α , in the K-BKZ equation for the shear viscosity (η_s), first normal stress difference (N_1), and the uniaxial extensional viscosity (η_E), and (b) for the planar extensional viscosity (η_p) and the biaxial extensional viscosity (η_b). In each case, $\beta = 0.5$ and $\theta = 0$.

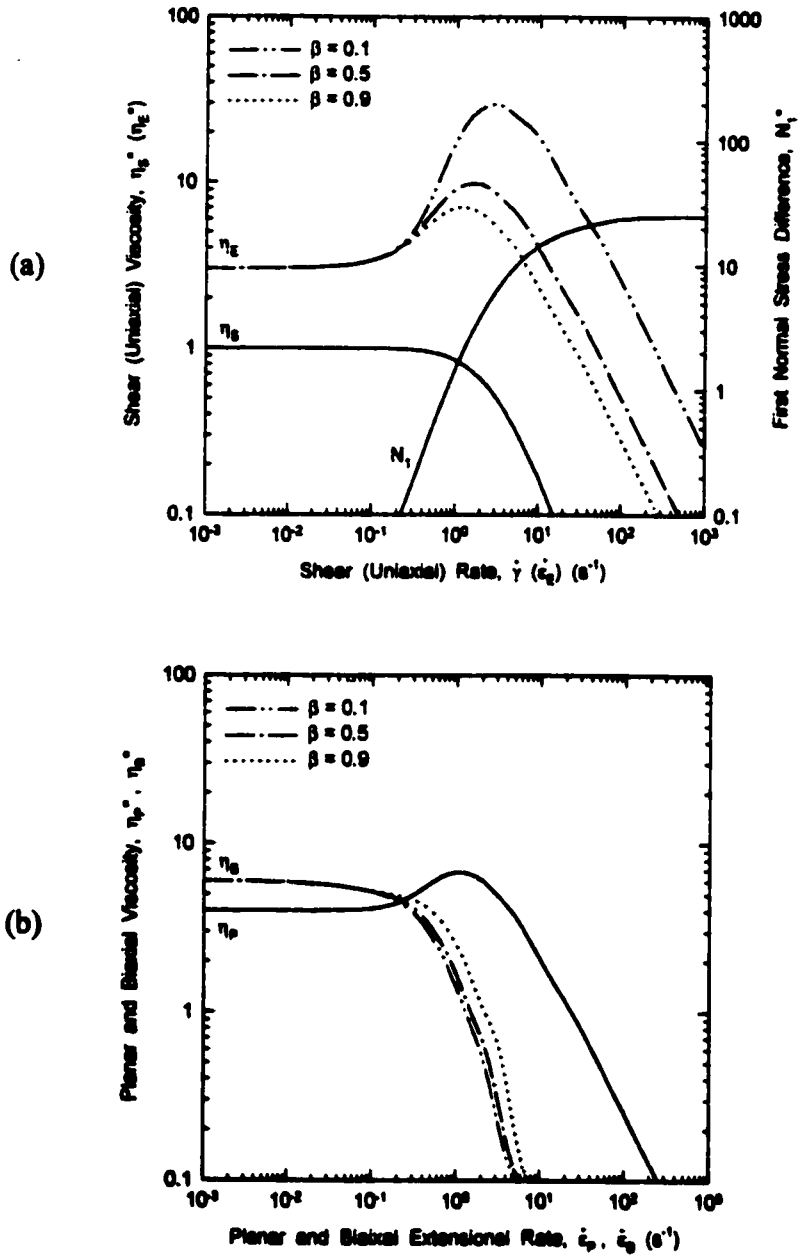


Figure 3.9: (a) Effect of changing the nonlinear parameter, β , in the K-BKZ equation for the shear viscosity (η_s), first normal stress difference (N_1), and the uniaxial extensional viscosity (η_E), and (b) for the planar extensional viscosity (η_p) and the biaxial extensional viscosity (η_b). In each case, $\alpha = 25$ and $\theta = 0$.

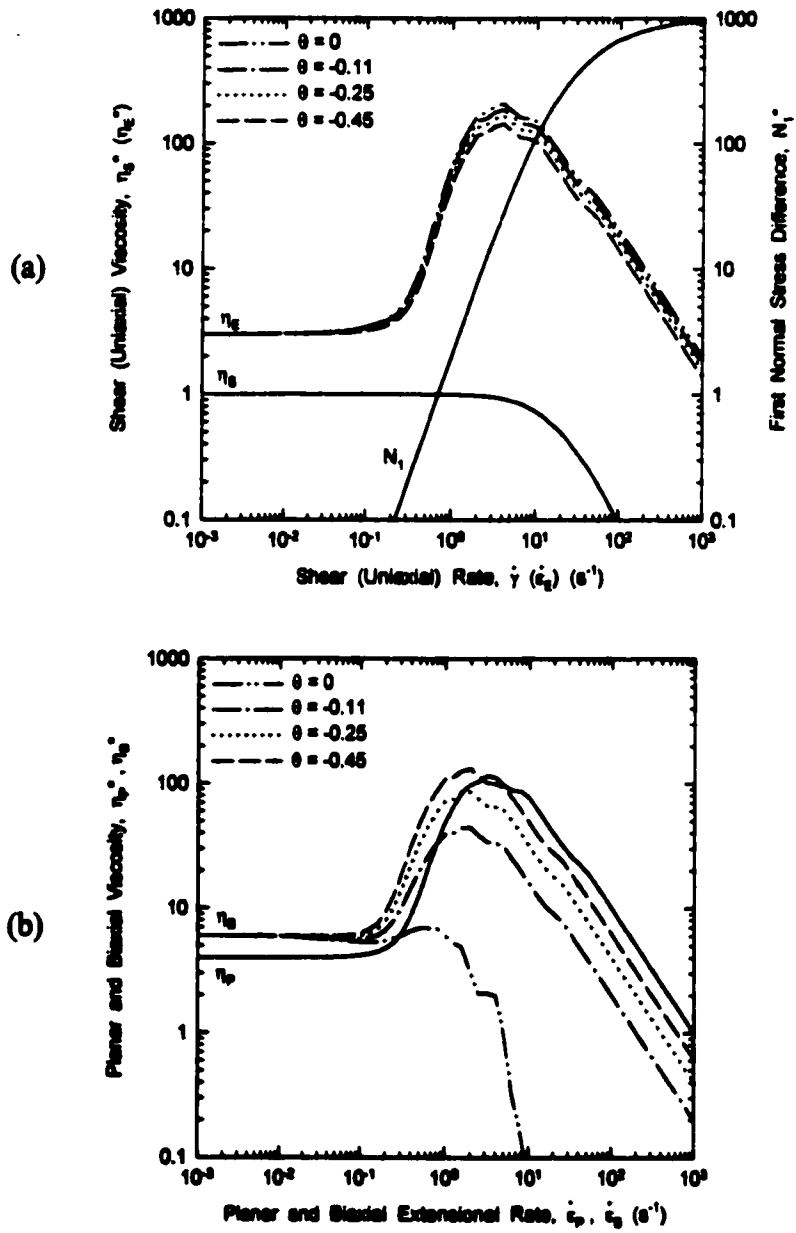


Figure 3.10: (a) Effect of changing the nonlinear parameter, θ , in the K-BKZ equation for the shear viscosity (η_s), first normal stress difference (N_1), and the uniaxial extensional viscosity (η_E), and (b) for the planar extensional viscosity (η_p) and the biaxial extensional viscosity (η_b). In each case, $\alpha = 1000$ and $\beta = 0.5$.

$$\bar{\tau} = \frac{1}{1-\theta} \int_{-\infty}^{\xi(t)} \sum_{k=1}^N \frac{a_k}{\lambda_k} \exp\left(-\frac{\xi - \xi'}{\lambda_k}\right) \frac{\alpha_k}{(\alpha_k - 3) + \beta_k I_C^{-1} + (1 - \beta_k) I_C} \cdot \left[\left\{ \bar{C}_{\alpha(\xi)}^{-1}(t'(\xi')) - \bar{I} \right\} + \theta \left\{ \bar{C}_{\alpha(\xi)}^{-1}(t'(\xi')) - \bar{I} \right\} \right] d\xi' \quad (3.56)$$

The time-temperature shifting factor a_T is obtained from the *Arrhenius equation* given as

$$a_T = \exp\left[\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \quad (3.57)$$

where E is the activation energy, R is the ideal gas constant, and T_{ref} is the reference temperature for the material. Equation (3.57) is the essential factor for non-isothermal constitutive equations since it describes how the fluid will behave with respect to temperature history. Non-isothermal Newtonian and Non-Newtonian constitutive equations typically employ an exponential time-temperature shifting factor of the Arrhenius type (other time-temperature shifting factors exist, such as that of Williams, Landel, and Ferry (1955)). It should be noted that the Arrhenius equation is only valid for temperatures above the glass transition temperature and is not valid when the material solidifies.

3.2.3.4 Prehistory Considerations

Equation (3.48) [and eq. (3.56) for the non-isothermal case] involves a domain of integration from time $t' = -\infty$ to time $t' = t$, where time $t' = t$ refers to the present time and time $t' = 0$ refers to the beginning of the process (i.e., when the material leaves the die). The region from $t' = 0$ to any time $t' = t$, is typically called the *region of history*, and is handled with the differential equations presented above for each process. The region from time $t' = -\infty$ to time $t' = 0$, is typically called the *region of prehistory*, and is not within the region of interest, and thus an assumption is required for the type of deformation there. Two options are available for the deformation within the die (region of prehistory): (a) assume a *purely extensional prehistory*, and (b) assume a *purely shear prehistory*. Previous studies (Chen and Papanastasiou, 1987; Rauschenberger and Laun, 1997) have shown that an extensional prehistory obtained better or similar results compared to a shear prehistory. This work has also studied both types of deformation for

the film-blowing process (see Chapter 7), and similar conclusions were found. The kinematics within the die is such that the material is being deformed extensionally, and obeys the following simple relation

$$u = \exp(cz) \quad (3.58)$$

where the parameter c is found by the requirement that the stresses inside and outside of the die be continuous, i.e.,

$$\left(\frac{\tau_{zz} - \tau_{rr}}{\rho u} \right)_{0+} = \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u} \right)_{0-} \quad (3.59)$$

The parameter c is simultaneously solved for along with the differential equations presented above for each process.

3.3 Concluding Remarks

In this Chapter the governing equations have been given for the three processes under study in this work. An effort has been made to present them with a unified approach, since all of these processes, i.e., fiber spinning, film casting, and film blowing, have common characteristics, mainly the absence of walls, and hence the lack of shear flow. They are dominated by extensional flows, and for their modeling appropriate constitutive equations must be employed. To that effect, three of the most popular rheological models have been used, namely, the Newtonian, the UCM, and the K-BKZ models, under isothermal and non-isothermal conditions. Their predictions for different material functions were presented and commented upon. The solution of the governing equations together with the appropriate boundary conditions and the constitutive equations can only be accomplished with sophisticated numerical techniques. This is the subject of the following Chapter.

Chapter 4

Method of Solution

This chapter presents the numerical methods for solving the governing equations of Chapter 3. In particular, it outlines the finite element method (FEM), and presents special numerical techniques for evaluating integral constitutive equations. Several aspects of numerical solution are also presented, including the Newton-Raphson iterative scheme, the continuation strategy and the convergence criteria. Another numerical method, namely the shooting method, which makes use of the Runge-Kutta scheme and the bisection method, is also presented. Finally, the development of the computer codes used in this thesis is briefly explained.

4.1 Introduction

In recent years, the rapid development of computers has allowed the numerical solution of many complicated problems. Such problems are usually solved with one or more types of numerical methods, and prominent among them is the *finite element method (FEM)*, which is perhaps among the most sophisticated. The main advantages of the FEM is its ability to handle complex geometries and boundary conditions and its flexibility to solve many different types of problems with only slight modifications to the same computer program. One shortcoming of the method seems to be its rather involved formulation, which requires a good understanding of variational principles, matrix algebra, and computer programming skills. However, computer programs can be designed to be user-friendly and data-driven, which greatly simplifies the numerical simulations for a series of parametric studies. In this form, a non-expert on the numerical method and on the governing equations can also use the computer programs without major difficulties.

4.2 The Finite Element Method (FEM)

The numerical method used in this study to solve the differential equations presented in Chapter 3 with the modified K-BKZ model is the FEM. This method was chosen for the reasons stated previously: its ease in implementing slightly different governing equations (as is the case with fiber spinning, film casting, and film blowing) without making major modifications to the computer program. This method was also chosen because of its ease in handling viscoelastic problems using integral constitutive equations, as reported by other researchers (Luo and Tanner, 1987; Luo and Mitsoulis, 1990; Barakos and Mitsoulis, 1996).

The finite element method consists of reducing the continuous boundary value problem, which has an infinite number of *degrees of freedom (DOF)*, to a discrete problem with a finite number of DOF, described by a system of algebraic equations (Gartling, 1991). This is done by dividing the domain of interest into small sections or *finite elements*. The FEM involves the following six steps (Reddy, 1993):

1. Discretize the given domain into finite elements.
2. Form the element equations from the given differential equation(s).
3. Assemble the element equations to obtain the set of global equations.
4. Impose the boundary conditions for the problem.
5. Solve the set of equations.
6. Post-process the results (e.g., compute gradients of primary variables, represent results in graphical form).

Some of the aspects of the FEM will now be discussed.

4.2.1 Discretization of the Domain

The domain of the problem for the three processes under consideration consists of the region between the die exit and the point of solidification or take-up (see Chapter 3). Thus, the material in question is considered to be in a fluid state for the entire domain. The domain, signified as Ω , is divided into a set of elements, and the collection of these elements is called the *finite element mesh* (or *finite element grid*).

The endpoints of each line element, which connect one element to another, are called the *nodes*. Additional nodes may be required within the element, depending on the degree of interpolation used to represent the solution. The nodes play the role of interpolation points used to approximate the solution over the domain. Many previous studies (e.g., Luo and Mitsoulis, 1990; Barakos and Mitsoulis, 1996) have used quadratic interpolation functions with good success. Thus, one-dimensional quadratic interpolation functions are used in this study, and 3 nodes per element (2 nodes at each end of the element with 1 node centered within the element) are required for a quadratic variation. Within each element, the primary variable for which the solution is required, is approximated by

$$a = \sum_{i=1}^3 a_i \psi_i \quad (4.1)$$

where a is the variable in question (e.g., velocity, radius, temperature, etc.) and the subscript i refers to the numbering of nodes within the element. The interpolation functions, ψ_i , are the one-dimensional quadratic interpolation functions given as (Reddy, 1993)

$$\begin{aligned} \psi_1 &= (1 - \xi)(1 - 2\xi) \\ \psi_2 &= 4\xi(1 - \xi) \\ \psi_3 &= -\xi(1 - 2\xi) \end{aligned} \quad (4.2)$$

where ξ is the dimensionless distance within the element. The dimensionless distance ξ is defined as

$$\xi = \frac{l}{l_e} \quad (4.3)$$

where l is the distance from the first node and l_e is the total element length. Figure 4.1(a) illustrates the shape functions plotted against ξ , while Figure 4.1(b) shows a typical element with the variation of a primary variable along the element. Note that the function ψ_i is equal to 1 at node i and zero at the other two nodes. Thus, the approximation of the variable given by eq. (4.1) will always give the value of the variable at the respective node.

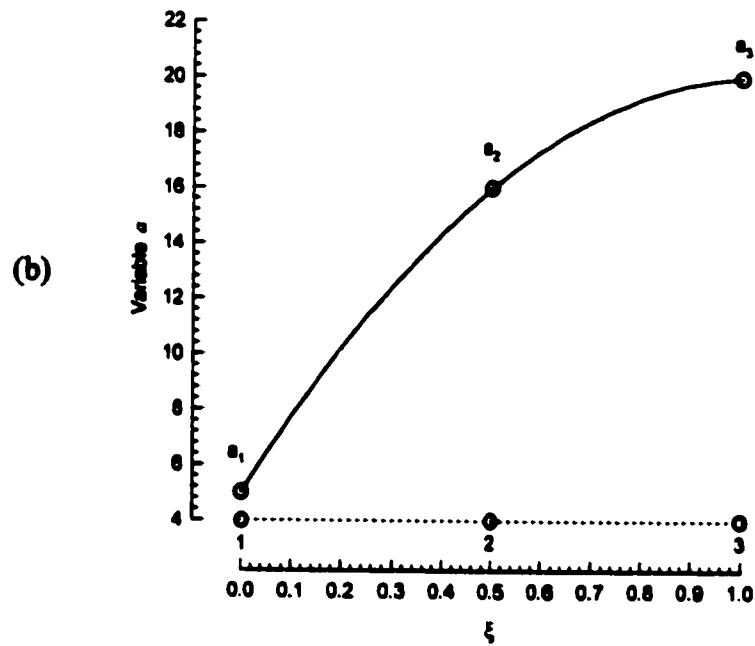
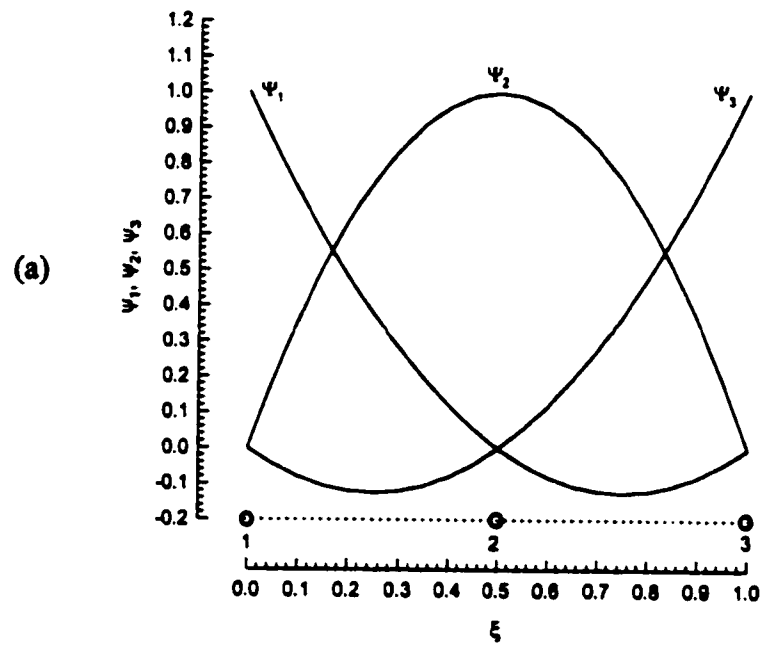


Figure 4.1: (a) Interpolation functions ψ_1 , ψ_2 , and ψ_3 for a typical one-dimensional quadratic element. (b) Approximation of variable and typical element for a quadratic element.

The number of elements used in a problem depends mainly on the geometrical detail desired. However, the solution must also be mesh-independent, whereby the solution does not change (or changes imperceptibly) with a further increase in elements. Figure 4.2 shows a typical solution of one of the problems presented in Chapter 3 for two variables. As can be seen, the solution with 36 quadratic elements is inadequate, and results in small oscillations at the beginning of the solution. The solution with 51 quadratic elements is equivalent with the solution with 104 quadratic elements, thus 51 elements is adequate for the solution of the differential equations presented in Chapter 3. For the remainder of the thesis, the number of elements used is 51.

4.2.2 Formulation and Solution of Equations

The differential equations presented in Chapter 3 are now expressed over the element, and the solution is sought at all the nodes, which make up the domain, as an approximation. In addition to using the interpolation functions for approximating the variable, a , over the element, we also use the interpolation functions to approximate the error in the equation, which eventually will have to go to zero (or a very small number). This is known as the *weighted integral form*. The weighted integral form is necessary in order to obtain the required number of linearly independent algebraic equations in terms of the variable, a . When the same interpolation function, used to approximate the variable, is used to approximate the equation, the method is known as the *Galerkin method* (Reddy, 1993). The differential equations presented in Chapter 3 are then weighted with the same approximation function used for the variables. In integral form, this appears as

$$\{R\} = \int_{\Omega} F(x) \psi_i dx \quad (4.4)$$

where $\{R\}$ is the set of residuals, $F(x)$ is the differential equation defining each one of the three processes under study (see Chapter 3), and Ω is the domain of integration. The boundary conditions are implemented by setting the residual at the appropriate boundaries equal to zero. The residual vector, once the solution is obtained, is equal to

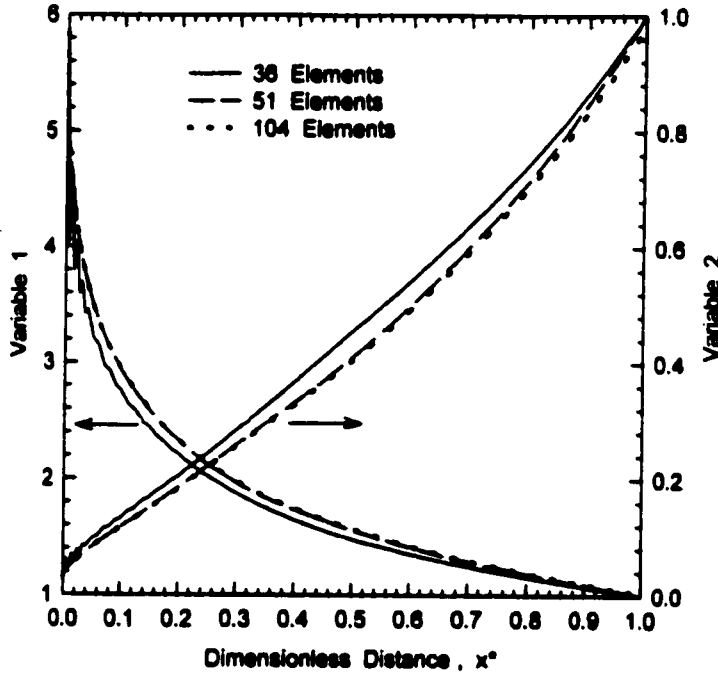


Figure 4.2: Solution to one of the problems presented in Chapter 3 with different numbers of quadratic elements, showing how mesh-independence is achieved with an increase in the number of elements used.

zero. Thus, the solution of the problem is known, when the set of residuals vanishes (i.e., $R_i \approx 0$).

The numerical scheme used to find the unknowns given by eq. (4.1), which cause the set of residuals to vanish, is the *Newton-Raphson* iterative scheme (Reddy, 1993). If $\{S\}$ is the set of unknowns, $\{u_1, u_2, \dots, u_M, \dots, T_1, T_2, \dots, T_M\}$, where M is the total number of nodes, then the Newton-Raphson scheme gives

$$\bar{J}[\{S\}]\{\Delta S\} = -\{R(\{S\})\} \quad (4.5)$$

in which $\{\Delta S\} = \{S\}^{n+1} - \{S\}^n$, and $\bar{J}$ is the Jacobian matrix defined by

$$J_{ij} = \frac{\partial R_i}{\partial S_j} \quad (4.6)$$

Equation (4.5) is then solved, and the updated values of the unknowns are

$$\{S\}^{n+1} = \{S\}^n + \{\Delta S\} \quad (4.7)$$

where n denotes the iteration number. At each iteration step, the resulting linear system of algebraic equations (4.5) is solved by standard Gaussian elimination and a back-substitution scheme (Borse, 1991).

The simulation is considered converged when the root-mean-square (RMS) error falls below a specified value ($\leq 10^{-4}$) (Reddy, 1993). The RMS error is calculated using the following formula:

$$RMS \text{ Error} = \left(\frac{\sum_{i=1}^M \Delta S^2}{M} \right)^{1/2} \quad (4.8)$$

Figure 4.3 shows the solution to one of the problems presented in Chapter 3, demonstrating the typical convergence rate with the Newton-Raphson iterative scheme. As can be seen, the rate of convergence is quadratic (reaching a slope of 2) until machine accuracy is reached, which is in this case around 10^{-14} on a today's typical PC with double precision arithmetic.

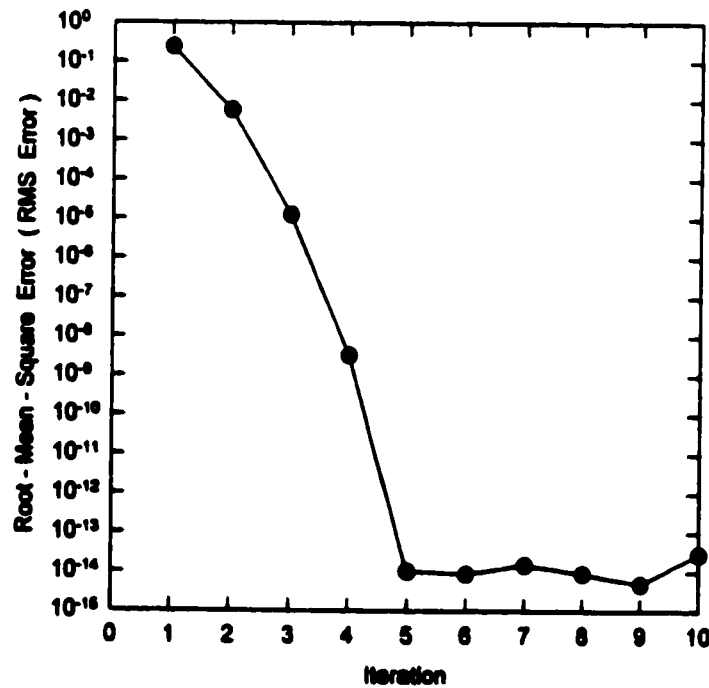


Figure 4.3: Convergence rate for the solution to one of the typical problems presented in Chapter 3 for the Newton-Raphson iterative scheme.

4.2.3 Numerical Integration

The set of residuals, $\{R\}$, in eq. (4.4), does not have an algebraic solution due to the complexity of the differential equations presented in Chapter 3. Therefore, a method known as *numerical integration* or *numerical quadrature* is used to evaluate the integrals within the computer program. This method usually requires the domain of integration to be broken into small intervals. For the FEM, the domain of integration has already been conveniently divided into intervals with the finite element mesh. The integrand in eq. (4.4) is then approximated within each interval with a suitable polynomial, since the integral of a polynomial can be evaluated exactly. Approximating the integrand with a 1st-degree polynomial is popularly known as the *trapezoidal rule*, while approximating the integrand with a 2nd-degree polynomial is known as *Simpson's rule* (Stewart, 1991). However, the most popular numerical integration technique is *Gauss-Legendre quadrature*, due to its accuracy and ease in implementing different degrees of approximating polynomials (Reddy, 1993). In general, numerical integration for a one-dimensional system has the following form

$$I = \int_a^b f(x) dx \approx \sum_{i=1}^L f(x_i) w_i \quad (4.9)$$

where I is the solution of the integral, L depends on the degree of the polynomial, $f(x)$ is the integrand, while x_i are known as the *quadrature points* and w_i are the *quadrature weights*. The Gauss-Legendre quadrature method requires the intervals of integration be cast over the interval $[-1,1]$ or $[0,1]$. This is done with a linear transformation of the form

$$x = c_1 + c_2 \xi \quad (4.10)$$

where c_1 and c_2 are constants to be determined based on the interval of integration, and ξ is the dimensionless distance within the element given by eq. (4.3). Equation (4.9) now takes the form

$$I = \int_a^b f(x) dx = \int_0^1 f(x(\xi)) \frac{dx}{d\xi} d\xi \approx \sum_{i=1}^L f(x(\xi_i)) w_i \quad (4.11)$$

where $x(\xi_i)$ are the transformed quadrature points, while the weights, w_i , are not affected by the transformation. For this study, 5th-degree Legendre polynomials are used, which

results in a very accurate solution of the differential equations presented in Chapter 3. The 5th-order Gauss-Legendre quadrature formula requires 6 points and weights, which are given in Appendix A.

Another type of numerical integration must also be used for the purpose of this study. The K-BKZ integral constitutive equation presented in Chapter 3 must be evaluated in order to solve the governing differential equations, also presented in Chapter 3. In simplified form, the K-BKZ constitutive equation can be written as follows

$$\bar{\tau}(t) = \int_{-\infty}^t \sum_k \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) H(I_C, I_{C^{-1}}) \bar{C}_t^{-1}(t') dt' \quad (4.12)$$

where $H(I_C, I_{C^{-1}})$ is given by eq. (3.50). The K-BKZ integral constitutive equation involves an infinite domain of integration and contains a fading exponential function. Accordingly, a special quadrature method, known as *Gauss-Laguerre quadrature*, exists for the determination of integrals with an infinite domain and a fading exponential function. The Gauss-Laguerre quadrature formula takes the form

$$\int_0^{\infty} e^{-x} f(x) dx \approx \sum_{i=1}^L f(z_i) w_i \quad (4.13)$$

where z_i are the roots of the Laguerre polynomials of order $L+1$ and w_i are the corresponding weights. The K-BKZ equation is then transformed to satisfy the Gauss-Laguerre form with the following substitution

$$S_k = \frac{t-t'}{\lambda_k} \quad (4.14)$$

and the function $f(x)$ in eq. (4.13) is now given as

$$f(x) = \sum_k a_k H(I_C, I_{C^{-1}}) \bar{C}_t^{-1}(t') \quad (4.15)$$

In the present form, a 15-point quadrature is used for evaluation of the stress integral in the K-BKZ constitutive equation, since previous work (Luo and Tanner, 1988) has shown the adequacy of such a number of points for accurate calculations of the integral. The 15-point Gauss-Laguerre quadrature formula, along with the points and weights, are detailed in Appendix A.

4.2.4 Continuation

In the present work, the Newton-Raphson scheme is used in the iterative solution of the governing equations, as described above. Although the Newton-Raphson scheme has the advantage of quadratic convergence, it has the disadvantage of a small radius of convergence (i.e., it requires a good initial guess for convergence) (Stewart, 1991). This is especially true during non-isothermal viscoelastic simulations when the solutions to the processes of fiber spinning, film casting, and film blowing can change drastically. Thus, a strategy for continuation of the solution is required, whereby the solution from a previous converged simulation is used as the initial guess for the next simulation at the new (usually higher) value of a parameter, such as the flow rate or elasticity level.

In the case of a non-isothermal viscoelastic simulation, the following *recipe* is used:

1. The solution for the isothermal Newtonian model is obtained. This is done by using a small flow rate (low elasticity level) and a very large heat capacity (very little or no temperature change).
2. The level of viscoelasticity is slowly raised, by increasing the flow rate to the required value.
3. The non-isothermal solution is obtained by decreasing the heat capacity to the required value.

By using the continuation method, solutions were obtained for a wide variety of non-isothermal viscoelastic simulations.

4.3 The Shooting Method

Another numerical method used in this study to solve the differential equations presented in Chapter 3 is known as the *shooting method*. This method is used to get the solution to the differential equations presented in Chapter 3 with the Newtonian constitutive model. The Newtonian solution can then be used in the continuation method (described above) as the initial guess for the solution to the differential equations with the

modified K-BKZ model. The shooting method is also used in the case of film casting with the upper-convected Maxwell (UCM) model for checking purposes.

The shooting method is used when the boundary conditions for a set of one-dimensional differential equations are specified at *both boundaries*. There also exists at least one unknown parameter, c , within the set of differential equations. Without an unknown parameter, the solution to the set of differential equations is unique, and the second boundary condition over-specifies the solution (i.e., the second boundary condition may never be met). When the boundary conditions are specified at only one boundary, the problem is called an *initial-value problem*. However, when boundary conditions are specified at both boundaries, the problem is called a *boundary-value problem*. Initial-value problems can easily be solved, by starting at one point (initial values) and numerically solving the differential equation progressively until the end point is reached. Boundary-value problems cannot be solved in the same manner, since it is not guaranteed that beginning at one boundary, and numerically solving the differential equation progressively, will result in the other boundary condition being met.

The shooting method consists of the following steps (Borse, 1991):

1. A guess is made for the unknown parameter, c .
2. The set of differential equations is solved, beginning at one boundary, with the first boundary condition.
3. The solution to the set of differential equations is checked to see if the second boundary condition has been met.
4. The unknown parameter, c , is updated using the previous solution. This process continues until a suitable convergence is achieved.

The numerical method used to solve the given set of differential equations is the *Runge-Kutta method*, while the numerical method used to update the unknown parameter, c , is the *bisection method*.

4.3.1 Runge-Kutta Method

The Runge-Kutta method is used to numerically solve one or more differential equations used in conjunction with the shooting method. It consists of using a weighted

average for the slopes (gradients) of the solution, and these gradients are used to progressively solve the set of differential equations. The derivations used to arrive at the final set of Runge-Kutta equations are given elsewhere (Borse, 1991), and only the final set of equations is shown here.

Each differential equation within the given set of differential equations can be represented as

$$\frac{d}{dx}a(x) = g(x, a(x)) \quad (4.16)$$

where $a(x)$ is the variable to which the solution is required, x is the independent variable, and $g(x)$ can be some function of $a(x)$ and its derivatives. Also, the left-hand-side boundary is set at $x = 0$, while the right-hand-side boundary is set at $x = L$, consistent with the problems of Chapter 3 (see Chapter 3). Beginning at the left-hand-side boundary with the boundary condition $a(x=0) = a_0$, the solution of the differential equation with a step of Δx is given as:

$$a_{i+1} = a_i + \frac{1}{6}[k_1 + 2k_2 + 2k_3 + k_4] \quad (4.17)$$

where

$$\begin{aligned} k_1 &= g(x_i, a_i)\Delta x \\ k_2 &= g(x_i + \frac{1}{2}\Delta x, a_i + \frac{1}{2}k_1)\Delta x \\ k_3 &= g(x_i + \frac{1}{2}\Delta x, a_i + \frac{1}{2}k_2)\Delta x \\ k_4 &= g(x_i + \Delta x, a_i + k_3)\Delta x \end{aligned} \quad (4.18)$$

The subscript i refers to the current position x_i where the value of a_i is known, while the subscript $i+1$ refers to the position $x_i + \Delta x$ where the value a_{i+1} is desired. Equations (4.17) and (4.18) represent the 4th-order Runge-Kutta equations (error is of the order $(\Delta x)^4$), and is very popular for solving differential equations.

4.3.2 Bisection method

In addition to the Runge-Kutta method, the bisection method is also used in the shooting method. It is employed as a convergence method for the unknown parameter, c , in the set of differential equations, as described in Section 4.3. For the shooting method, the equation to be solved is

$$h(c) = a(x = L) - a_L = 0 \quad (4.19)$$

where $x = 0$ is the left-hand-side boundary, $x = L$ is the right-hand-side boundary, and a_L is the boundary condition at $x = L$. Thus, we are seeking the value of the unknown parameter, c , which makes $a(x = L)$ equal to the boundary condition a_L within the set of differential equations (i.e., we are seeking the root of eq. (4.19) for c). The bisection method has the following algorithm:

- (a) Two guesses for the parameter c are made such that one value of $c = c_1$ makes $h(c)$ in eq. (4.19) negative and the other $c = c_2$ makes $h(c)$ in eq. (4.19) positive. In other words, the root of eq. (4.19) is bounded by the guesses c_1 and c_2 .
- (b) An updated value of c , given the symbol c_3 , is found at the midpoint between c_1 and c_2 , $c_3 = (c_1 + c_2) / 2$.
- (c) If the root of eq. (4.19) is bounded by c_1 and c_3 , then c_2 is given the value of c_3 .
- (d) If the root of eq. (4.19) is otherwise bounded by c_3 and c_2 , then c_1 is given the value of c_3 .
- (e) This process continues until a suitable convergence is achieved, by continuously reducing the bounded interval by half.

This method has guaranteed convergence as long as the guesses c_1 and c_2 bound the root of $h(c)$ in eq. (4.19).

4.4 Outline of Computer Codes

In this section, a brief history of the computer codes used in the present work is given. The necessary enhancements and changes are presented for the final codes.

4.4.1 History of Codes

The original (parent) code named BLOW was written in the FORTRAN-77 language by Alaie (1993) at the Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan, USA, for the simulation of the film-blowing process using the modified K-BKZ integral constitutive equation. The code, as presented in Alaie's thesis, is apparently a very early version of the final code used for simulations reported by Alaie and Papanastasiou (1993). This assumption is based on the fact that the code was inoperable with many syntax, run-time, and general programming errors. The original program made little use of subroutines and had many GOTO statements, which results in a "*spaghetti*"-like code structure. The original program also did not have any non-isothermal capabilities.

The current film-blowing code named F-BLOW (Film BLOWing) has been totally revamped, overhauled, and further extended, and most parts have been revised with respect to three important points:

- Many subroutines have been implemented such that users will more easily understand the code.
- The code has been enhanced so that computer resources are economized (i.e., the code requires less time for convergence).
- The code is portable and robust by adding such things as '*include*' files, which can be easily altered to handle different systems such as personal computers, workstations, and mainframes.

The following list presents enhancements made to the original code for this work:

- The Newtonian program for the film-blowing process is included in the viscoelastic code and used as the initial guess in the viscoelastic iteration process.
- The non-isothermal counterpart of the film-blowing process has been added to the code (see Chapter 3).

- The method by which the modified K-BKZ integral constitutive equation is integrated has been changed from Gauss-Legendre quadrature to 15-point Gauss-Laguerre quadrature, suitable for infinite domains and exponentially fading functions.
- The particle-tracking scheme has been changed and enhanced giving quicker and more accurate results.
- The prehistory for the modified K-BKZ integral constitutive equation has been changed from a shear-based prehistory, which possesses a singularity point at the die exit, to an extensional-based prehistory, which removes the singularity.
- Effects, such as inertia, gravity, and air drag, have been added to the governing equations, resulting in more realistic results and a better understanding of the process.
- The original code used only a single α - and β -value in eq. (3.48). The current code can handle multiple α_k - and β_k -values.

The original (parent) code, BLOW, was modified into the current code, F-BLOW, which also led to the development of the codes F-SPIN and F-CAST for the simulation of the fiber-spinning and film-casting processes, respectively. The present codes can thus be used as software tools for analysis, design, and understanding of processes in the polymer industry.

4.4.2 Organization of Codes

The standard practice for finite element codes is to separate the code into three sections. These include a *pre-processor*, that deals with the discretization and boundary conditions, a main *processor*, that performs the task of solving the model, and a *post-processor*, that handles any extra requirements and presents the results in a graphical form. In this work, three programs have been used in a slightly different manner. The first codes are named BESTFIT[®] and TIMEFIT[®], and they perform the non-linear regression for the determination of the relaxation spectrum and the parameters α_k and β_k in eq. (3.48). The pre-processor and processor are contained within the codes F-SPIN, F-CAST, and F-BLOW. The post-processor consists of second-party programs, such as Microsoft Excel[®], Jandel Scientific Sigmaplot[®], and Amtec Tecplot[®]. Each code writes

specific output files for each of the above graphical programs. The data exchange between programs is illustrated in Figure 4.4, while the organization of the code F-BLOW, and similarly F-SPIN and F-CAST, is illustrated in Figure 4.5.

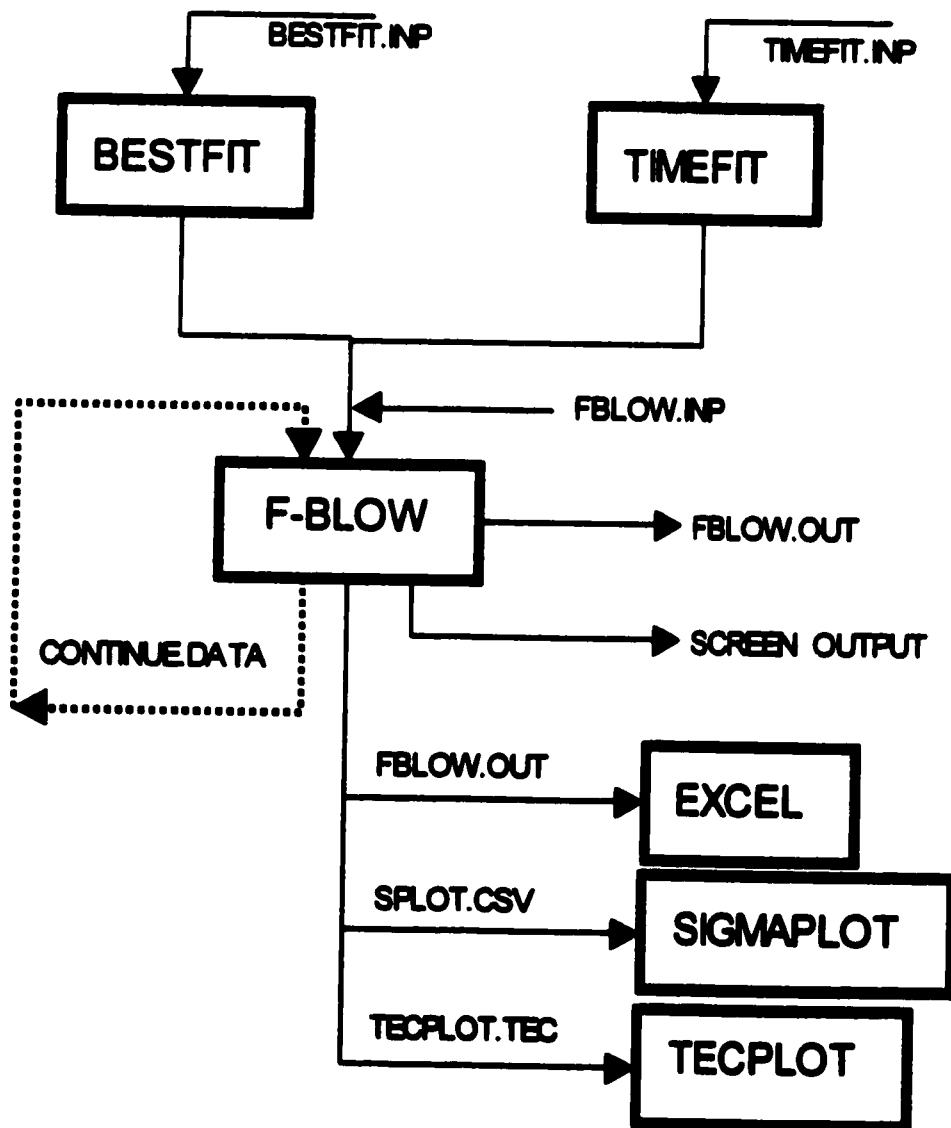


Figure 4.4: Data flow between BESTFIT[®] and TIMEFIT[®] (regression), main processors F-SPIN, F-CAST, and F-BLOW (simulation), and post-processors Excel[®], Sigmaplot[®], and Tecplot[®].

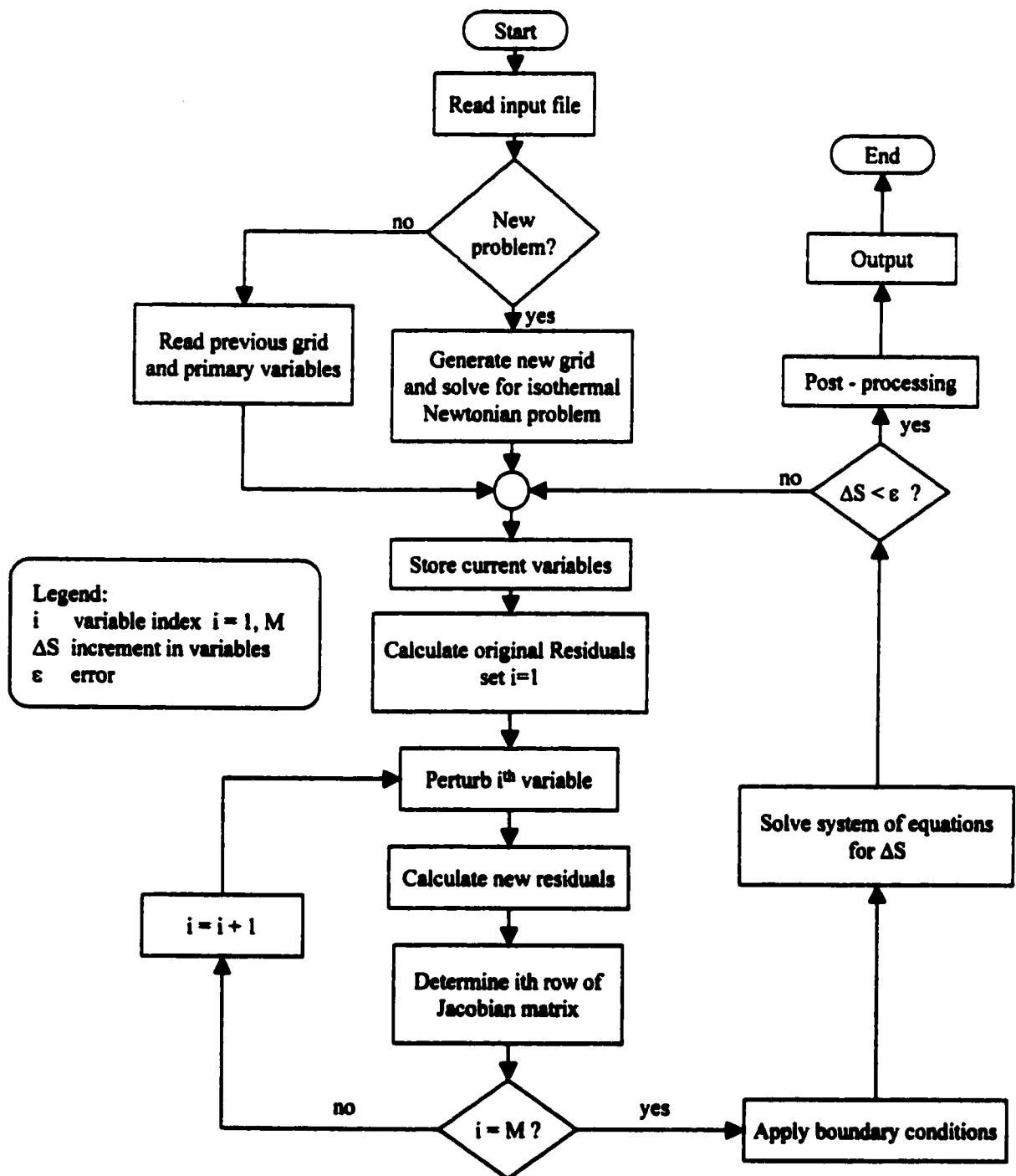


Figure 4.5: General organization of computer code F-BLOW (similarly for F-SPIN and F-CAST).

4.4.3 Efficiency of Codes

With the advancements made to the F-SPIN, F-CAST, and F-BLOW codes (e.g. 15-point Gauss-Laguerre quadrature, improved particle tracking, improved prehistory), the computing time has been considerably reduced, with no decrease in numerical accuracy. Table 4.1 describes the efficiency of the three codes in terms of average number of iterations and average total computing time to reach a final solution for a series of simulations. The computing times calculated in Table 4.1 are based on an Intel® Pentium® 200 MHz central processing unit (CPU). Table 4.1 demonstrates the Newton-Raphson iterative method has the advantage of convergence within only several iterations. However, with the small radius of convergence (Stewart, 1991), a greater number of continuation steps are usually required (see Table 4.1).

Table 4.1: Details of the numerical solution for the three finite-element codes F-SPIN, F-CAST, and F-BLOW, for the processes of fiber spinning, film casting, and film blowing, respectively. The number of elements used for each simulation was 51, which gives a total of 103 nodes. The convergence criterion was $|e| < 10^{-5}$. CPU time is given for simulations with an Intel® Pentium® 200 MHz PC computer. Numbers in parentheses correspond to non-isothermal simulations.

Code	No. of variables	No. of unknowns	Ave. No. of iterations	Ave. No. of continuation steps	Ave. CPU	Total CPU time (min)
					time per iteration (s)	
F-SPIN	1 [2]	102 [204]	5	4	14.0 [28.0]	4.7 [9.3]
F-CAST	2 [3]	204 [306]	5	5	22.7 [34.0]	9.4 [14.2]
F-BLOW	2 [3]	204 [306]	6	16	24.1 [36.2]	38.6 [57.9]

The average total computing time for the F-SPIN code is less than the F-CAST and F-BLOW codes because only one variable (velocity) is required for solution. The F-CAST and F-BLOW codes have two variables that require solution. Also, the F-BLOW code

takes considerably longer than the F-CAST code due to the complexity of the differential equations (see Chapter 3). The complexity of the differential equations in the F-BLOW causes the code to become more sensitive to changes, and thus requires more continuation steps, as shown in Table 4.1.

4.5 Concluding Remarks

This Chapter has presented in some detail the numerical methods used for the solution of the governing equations of Chapter 3 for the three polymer processes studied in this work. Issues related to numerical accuracy, continuation, and convergence have been addressed. A brief history of the computer codes used in the present work was also given together with the necessary enhancements and changes made to the final codes. The time has now come for implementing these numerical methods and computer codes for the three processes under study, i.e., fiber spinning, film casting, and film blowing, each in every subsequent Chapter.

Chapter 5

Fiber Spinning

In this chapter, non-isothermal fiber spinning of viscoelastic polymer melts is analyzed using the K-BKZ integral constitutive equation. The one-dimensional governing equations are restated and specifics concerning the numerical scheme are given. The differential equations are solved using the finite element method (FEM). The resulting code, F-SPIN, is then used for fiber-spinning simulations. The numerical scheme is validated with the Newtonian and upper-convected Maxwell (UCM) solutions. Simulations are then undertaken for *real* polymer solutions and melts with a variant of the K-BKZ integral constitutive model. Isothermal simulations are carried out for the model M1 polymer solution and a polypropylene (PP) melt. Non-isothermal simulations are carried out for a poly(ethylene terephthalate) (PET) melt and the IUPAC-A low-density polyethylene (LDPE) melt. Comparisons are also made with previous simulations when available.

5.1 Introduction

The fiber-spinning process is used throughout the plastics industry to manufacture synthetic fibers. The process is shown schematically in Figure 5.1. The fibers are produced by the extrusion of the polymer through a die, usually of circular cross-section, and taken-up downstream at a higher velocity at the chill roll. The ratio of take-up velocity to extrusion velocity is known as the draw ratio (D_R). The fiber spinning process is a prime example of *uniaxial extension*. In industrial applications, the extrusion occurs through a spinneret plate, containing as many as 5000 small holes, for the simultaneous production of many fibers. The fibers are generally used in the textile industry, but new uses have been identified to produce *reinforced composite plastics*. The fiber-spinning

process consists of two regions. The first is the *extrudate swell region*, where normal forces accumulated during extrusion suddenly relax to cause swelling. The second is the *draw-down region*, where the fiber diameter decreases according to the velocity increase. Usually cross-flow air is used to aid in solidification of the fiber, which occurs between the die and the chill roll. Spinning speeds range from 30 m/min up to 7000 m/min, with fiber diameters ranging from 4 μm to 2 mm. At high spinning speeds (4000 m/min and greater), stress-induced crystallization can become a factor for solidification and hence affect fiber properties (Ziabicki and Kawai, 1985).

Typical industrial goals for the fiber-spinning process are as follows:

- Increase in take-up speeds without increasing instability. This has been accomplished in the past with additives that induce *slip* (non-zero velocity at the walls). With slip, instabilities such as *shark-skin* (rough edges) are reduced.
- Enhanced fiber characteristics such as strength, stretch, and flexibility. This has been accomplished in the past with research into developing new materials, and improved processing (i.e. improved die design).

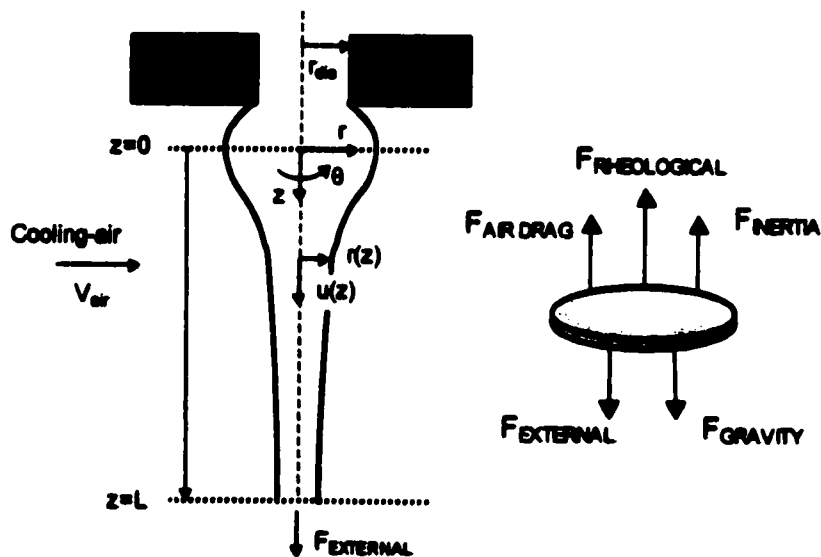


Figure 5.1: Schematic of the fiber-spinning process along with forces acting on the fiber during spinning.

5.2 Literature Review

Numerical simulation of the fiber-spinning process began with the early work of Matovich and Pearson (1969) who analyzed the process for a Newtonian liquid and arrived at an analytical solution. Attempts were then made to analyze the fiber-spinning process with *differential constitutive models*. Denn et al. (1975) performed an analysis of the fiber-spinning process with the UCM model while White and Ide (1978) made use of the White-Metzner model. Fisher and Denn (1977) also performed an analysis with the UCM model but included non-isothermal effects. Phan-Thien (1978) utilized his network model constitutive equation, the Phan-Thien/Tanner (PTT) model, to account for the elasticity of the melt being spun. Later, Gagon and Denn (1981) made use of the PTT model and included non-isothermal effects to simulate experimental data done by George (1982) with PET. Gagon and Denn (1981) also included the extra forces acting on the fiber, namely inertia, gravity, and air drag. Keunings et al. (1983) made use of the UCM, Oldroyd B, and PTT models to simulate short fibers with a two-dimensional FEM.

Attempts were also made to analyze the fiber-spinning process with *integral constitutive models*. Bernstein et al. (1981) made use of the Kaye (1962)/Bernstein-Kearsley-Zapas (1963) (K-BKZ) integral constitutive model with one relaxation time in their analysis. Larson (1983) then made use of the Doi-Edwards model in his analysis. Papanastasiou et al. (1987) used a variant of the K-BKZ model to analyze and simulate experimental data from Zeichner (1973) for polystyrene (PS). Chen and Papanastasiou (1987) performed a similar analysis with the Curtiss-Bird integral model and included non-isothermal effects utilizing the Morland-Lee (1960) hypothesis. Current analyses were performed by Fulchiron et al. (1995) who made use of the Wagner integral model, and Rauschenberger and Laun (1997) who used the K-BKZ model to simulate spinning data with the IUPAC-A LDPE. Papanastasiou et al. (1994) performed non-isothermal simulations for the experimental data of George (1982) with PET, where the effects of inertia, gravity, and air drag, were not properly inserted within their numerical scheme.

Experimental data for the fiber-spinning process is scarce and limited. Zeichner performed spinnability tests with PS. Ishizuka et al. (1980) performed an in-depth study

of the isothermal and non-isothermal spinning of PP. George (1982) performed spinning experiments with PET along with theoretical predictions. Recently, Ferguson and Hudson (1990) performed a variety of spinning experiments with the model polymer solution M1, a solution of polyisobutylene in butene (PIB/PB). Experiments with LDPE were also included in the study by Rauschenberger and Laun (1997).

In each of the aforementioned studies, excluding Rauschenberger and Laun (1997) and Gagon and Denn (1981), proper rheological characterization was not performed and no explanations for the choice of rheological parameters (e.g. relaxation time) were included. Thus, proper rheological characterization has been a focus in this study. Temperature effects have only been included in the studies by Gagon and Denn (1981), Fulchiron et al. (1995), Rauschenberger and Laun (1997), and Papanastasiou et al. (1994). Appropriately, temperature effects are taken into account in this study. Fulchiron et al. (1995) and Gagon and Denn (1981) seem to be the only studies to include properly the effects of inertia, gravity, or air drag. To date, inertia, gravity, and air drag effects have not been introduced properly in the study of fiber spinning with the use of an integral constitutive equation including non-isothermal effects.

5.3 Objectives

This study will present a quick and approximate method of analysis for the fiber-spinning process with the use of an efficient code, F-SPIN. The objectives of this chapter are as follows:

- a) To solve accurately the one-dimensional fiber spinning of a Newtonian fluid. Since the Newtonian model does not possess any elastic response, the model is used here only for checking purposes.
- b) To solve accurately the one-dimensional fiber spinning of a UCM fluid. The UCM model does possess an elastic response, but the predictions for the shear and extensional viscosities are unrealistic, as shown in Chapter 3. The UCM model is also used here only for checking purposes.
- c) To solve accurately the one-dimensional fiber spinning of *real* polymeric fluids. This

is done with the use of the K-BKZ integral constitutive model, which predicts well the nonlinear behaviour of polymeric materials. Thus, the K-BKZ model is used for the following set of simulations:

- A parametric study with the K-BKZ nonlinear parameters to determine the importance of viscoelastic effects in fiber spinning.
- Isothermal simulation of the M1 polymer solution for direct comparison with experiments and determination of the elongational viscosity from spinning experiments.
- Isothermal simulation of a PP polymer melt for direct comparison with previous experimental results in fiber spinning.
- Non-isothermal simulation of a PET polymer melt to determine the importance of including the effects of inertia, gravity, and air drag in industrial fiber spinning, and to compare the present results with previous non-isothermal simulations and experimental data.
- Non-isothermal simulation of the IUPAC-A LDPE melt to compare the present results with previous non-isothermal simulations and experimental data.

5.4 Mathematical Modeling

5.4.1 Governing Equations

The non-isothermal spinning of melts can be described by the equations derived in Chapter 3. Specifically, eqs. (3.19), (3.12), and (3.13), which are restated here for completeness, are

$$\rho(\pi r^2)_{,z} = \rho Q \quad (5.1)$$

$$\frac{d}{dz} \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u} \right) - \frac{du}{dz} + \frac{g}{u} - C_f u \left(\frac{\rho_a}{\rho} \right) \sqrt{\frac{\pi u}{Q}} = 0 \quad (5.2)$$

$$\rho c_p Q \frac{dT}{dz} + 2\pi \sqrt{\frac{Q}{\pi u}} h_c (T - T_\infty) + 2\pi \sqrt{\frac{Q}{\pi u}} \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (5.3)$$

with the following boundary conditions

$$\begin{aligned}
1. \quad & u = u_o \text{ at } z = 0 \\
2. \quad & T = T_o \text{ at } z = 0 \\
3. \quad & u = u_L \text{ at } z = L
\end{aligned} \tag{5.4}$$

where L is the spinline length. Again, eqs. (5.2) and (5.3) are two first-order differential equations which require one boundary condition each. An additional boundary condition is also required for eq. (5.2) to make the solution unique since the stresses are not known *a priori*. Equation (5.1) is simply an algebraic equation solved for in terms of the fiber radius, r , once the fiber velocity, u , is known.

The air drag coefficient, C_f , varies along the spinline due to the increase of the fiber's speed. Matsui and Bogue (1976) derived an equation for C_f based on experiments as

$$C_f = b \left(\frac{\rho_a u D}{\mu_a} \right)^{-0.61} = b \left(2 \frac{\rho_a u}{\mu_a} \sqrt{\frac{Q}{\pi u}} \right)^{-0.61} \tag{5.5}$$

with μ_a as the viscosity of air and ρ_a as the density of air. The parameter b reported by Matsui and Bogue (1976) is 0.6, and is used in this study. The term within brackets is clearly seen as the Reynolds number (Re) for the air surrounding the fiber.

The density of the polymer, ρ , also changes along the spinline according to the temperature of the fiber. A relation for the density as a function of temperature is (Petrie, 1979)

$$\rho(T) = \frac{\rho_o}{1 + \delta(T - T_{ref})} \tag{5.6}$$

where ρ_o is the density of the polymer at a temperature of T_{ref} . The parameter δ is a constant of expansion. Petrie (1979) suggested a value of 0.00069 K^{-1} for the parameter δ that has been previously used by Chen and Papanastasiou (1987) and is also used here. Note that a higher δ value indicates greater expansion as the temperature increases.

The heat capacity also changes along the spinline with changes in temperature of the polymer. According to Haw (1984), the specific heat capacity c_p as a function of temperature is given by

$$c_p(T) = c_p^o \frac{(k_1 + k_2 T)}{k_1 + k_2 T_{ref}} \tag{5.7}$$

where c_p^o is the specific heat capacity at a temperature T_{ref} and k_1 and k_2 are empirical constants. Haw (1984) suggested values of 0.3243 for k_1 and 0.000565 K^{-1} for k_2 .

The heat transfer coefficient, h_c , has been studied experimentally by Kase and Matsuo (1967), who give for it the following expression:

$$\frac{h_c D}{k_a} = \gamma \left(\frac{\rho_a u D}{\mu_a} \right)^{1/3} \left[1 + 8 \left(\frac{\nu_a}{u} \right)^2 \right]^{1/6} \quad (5.8)$$

Here, D is the diameter of the fiber, k_a is the conductivity of air, and ν_a is the velocity of cross flow air. The parameter γ is an empirical constant. Kase and Matsuo (1967) report a value for γ of 0.42, which is also used in this work. The emissivity, ε in eq. (5.3), is given by Gagon and Denn (1981) a value of 0.5, which is also used in this work. A complete list of values used in the non-isothermal simulations is given in Table 5.1. The properties of air are calculated at the film temperature $(0.5 \times T + 0.5 \times T_\infty)$.

Table 5.1: Recurring material parameters used in the fiber spinning simulations.

Property (units)	Value
Coefficient in air drag relation, eq. (5.5), b	0.6
Coefficient of expansion, eq. (5.6), $\delta (\text{K}^{-1})$	6.90×10^{-4}
Empirical constants, eq. (5.7), k_1 and $k_2 (\text{K}^{-1})$	0.324 and 5.65×10^{-4}
Coefficient in heat transfer relation, eq. (5.8), γ	0.42
Emissivity, eq. (5.3), ε	0.5
Stefan-Boltzmann constant, eq. (5.3), $\sigma_{SB} (\text{erg s}^{-1} \text{ cm}^{-2} \text{ K}^{-4})$	5.67×10^{-5}
Ideal gas constant, eq. (3.57), $R (\text{J mol}^{-1} \text{ K}^{-1})$	8.314
Ambient temperature, eq. (7.4), $T_\infty (\text{K}, ^\circ\text{C})$	298 (25)

Equations (5.1), (5.2), and (5.3) are made dimensionless according to the following relations:

$$z^* = \frac{z}{L}, \quad u^* = \frac{u}{u_o}, \quad \rho^* = \frac{\rho}{\rho_o}, \quad T^* = \frac{T}{T_o}, \quad \tau^* = \frac{\tau L}{\eta_o u_o},$$

$$\rho_a^* = \frac{\rho_a}{\rho_o}, \quad T_a^* = \frac{T_a}{T_o} \quad (5.9)$$

in which L is the spinline length, u_o is the die-exit velocity, ρ_o is the die-exit density, T_o is the die-exit temperature, and η_o is the zero-shear-rate viscosity. Combining eq. (5.9) with eqs. (5.1), (5.2), and (5.3) results in the following dimensionless governing equations to be solved in terms of the dimensionless radius, r , dimensionless velocity, u , and dimensionless temperature, T (asterisks are omitted here and hereafter):

$$r^2 u = 1 \quad (5.10)$$

$$\frac{d}{dz} \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u} \right) - \frac{Re}{A} \frac{du}{dz} + \frac{Re}{A^2 Fr} \frac{1}{u} - 2 \frac{Re}{A} C_f \rho_a \sqrt{\frac{u^3}{\rho}} = 0 \quad (5.11)$$

$$\frac{dT}{dz} + \frac{\kappa_1 (T - T_a)}{\sqrt{\rho u}} + \frac{\kappa_2 (T^4 - T_a^4)}{\sqrt{\rho u}} = 0 \quad (5.12)$$

with the following dimensionless quantities

$$Re = \frac{2r_o u_o \rho_o}{\eta_o}, Fr = \frac{u_o^2}{2r_o g}, A = \frac{2r_o}{L}, \kappa_1 = \frac{2Lh_c}{\rho_o r_o u_o c_p}, \kappa_2 = \frac{2L\sigma_{SB}\epsilon T_o^3}{\rho_o r_o u_o c_p} \quad (5.13)$$

where Re is the Reynolds number, Fr is the Froude number, A is an aspect ratio, and κ_1 and κ_2 are non-isothermal coefficients. The boundary conditions, eq. (5.4), are also transformed with the new dimensionless variables, and given as:

1. $u = 1$ at $z = 0$
 2. $T = 1$ at $z = 0$
 3. $u = D_R$ at $z = 1$
- (5.14)

The force required at the take-up position (chill roll) to pull the filament can easily be calculated by integrating eq. (5.8) along the entire length of the spinline. The resulting equation for the dimensionless force is

$$f = \frac{\tau_{zz} - \tau_{rr}}{\rho u} - \frac{Re}{A^2 Fr} \int_z^1 \frac{1}{u} dz + 2 \frac{Re}{A^2} \int_z^1 \rho_a C_f \sqrt{\frac{u^3}{\rho}} dz \quad (5.15)$$

This equation is useful since the force at the take-up is often measured during experiments and can be used to verify the current numerical scheme. It is also useful in calculating the true extensional (uniaxial) viscosity of the polymer melt provided the simulations accurately predict the take-up force.

From eq. (5.11), the coefficient for inertia is Re/A , the coefficient for gravity is

$Re/A^2 \cdot Fr$, and the coefficient for air drag is Re/A^2 . The effects from inertia are considered significant if the coefficient for inertia is greater than 1 ($Re/A > 1$). The effects from gravity are considered significant if the coefficient for gravity is greater than 200 ($Re/A^2 \cdot Fr > 200$). Finally, the effects from air drag are considered significant if the coefficient for air drag is greater than 1 ($Re/A^2 > 1$). For inertial calculations, *upwinding* schemes (see, e.g., Barakos, 1994) could have been applied, but were unnecessary for the series of simulations undertaken here.

5.4.2 Constitutive Equation

The constitutive equation used for the fiber-spinning process is an integral model of the K-BKZ type proposed by Papanastasiou et al. (1983) and further modified by Luo and Tanner (1988). It is restated here for completeness (see Chapter 3) and for showing the specific derivations for the fiber-spinning process:

$$\begin{aligned} \bar{\tau}(t) = \frac{1}{1-\theta} \int_{-\infty}^t \sum_{k=1}^N \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) \frac{\alpha_k}{(\alpha_k - 3) + \beta_k I_{C^{-1}} + (1 - \beta_k) I_C} \\ \times \left[\left\{ \bar{C}_t^{-1}(t') - \bar{I} \right\} + \theta \left\{ \bar{C}_t(t') - \bar{I} \right\} \right] dt' \end{aligned} \quad (5.16)$$

Again, λ_k and a_k are relaxation times and relaxation modulus coefficients at a reference temperature T_{ref} , respectively. The parameters α_k and β_k are material parameters chosen to fit the material's response in high shear and elongation. The parameter θ has been incorporated by Luo and Tanner (1988) to take into account the second normal stress difference, N_2 , and is related to the first normal stress difference, N_1 , via the formula

$$\frac{N_2}{N_1} = \frac{\theta}{1-\theta} \quad (5.17)$$

The value of θ is not zero for polymer melts exhibiting a second normal stress difference. Its usual range is between -0.1 and -0.3 (Tanner, 1985).

The invariants I_C and $I_{C^{-1}}$ are the first invariants of the Cauchy-Green tensor $\bar{C}_t(t')$ and its inverse $\bar{C}_t^{-1}(t')$, the Finger strain tensor. In terms of the deformation gradient tensor, $\bar{F}_t(t') = d\bar{x}'/d\bar{x}$, the Cauchy-Green and Finger strain tensors are

$$\begin{aligned}\bar{C}_t(t') &= \bar{F}_t(t') \cdot \left[\bar{F}_t(t') \right]^T \\ \bar{C}_t^{-1}(t') &= \left[\bar{F}_t^{-1}(t') \right]^T \cdot \bar{F}_t^{-1}(t')\end{aligned}\tag{5.18}$$

For the fiber-spinning process, the deformation gradient tensor can be derived from the equation of continuity, eq. (5.1), and simple geometry. Also, the assumption is made that for free-surface operations, no shear stresses are present and only the left diagonal entries in the deformation gradient tensor are non-zero (i.e. for $i \neq j \rightarrow \bar{F}_i(t') = 0$). Thus, the first term that applies to the z -coordinate is

$$F_z = \frac{u(t)}{u(t')}\tag{5.19}$$

For the second term that applies to the r -coordinate, the radius of the fiber can be expressed in terms of the velocity from the equation of continuity and results in

$$F_{rr} = \frac{r(t)}{r(t')}\tag{5.20}$$

The third term that applies to the θ -coordinate can be found from the condition of incompressibility

$$\text{tr } \bar{F}_t(t') = 1\tag{5.21}$$

where tr is the trace of a tensor. Using eq. (5.21) along with eqs. (5.19) and (5.20), the third term is

$$F_{\theta\theta} = \frac{r(t)}{r(t')}\tag{5.22}$$

From eq. (5.18), with the use of eq. (5.10), the Finger strain tensor can now be obtained and is given as

$$\bar{C}_t^{-1}(t') = \begin{pmatrix} \left(\frac{u(t)}{u(t')}\right)^2 & 0 & 0 \\ 0 & \frac{u(t')}{u(t)} & 0 \\ 0 & 0 & \frac{u(t')}{u(t)} \end{pmatrix} \quad (5.23)$$

The Cauchy-Green tensor $\bar{C}_t(t')$ can be found by simply taking the inverse of the Finger strain tensor. The viscoelasticity of the polymer melt under flowing conditions can be represented by a dimensionless variable known as the *Weissenberg number*, given as

$$W_s = \frac{u_o}{L} \frac{\sum a_k \lambda_k^2}{\sum a_k \lambda_k} = \frac{u_o}{L} \bar{\lambda} \quad (5.24)$$

where $\bar{\lambda}$ is the average relaxation time. The transit times along the fiber can be expressed in terms of the velocity and distance traveled, by

$$t - t' = \int_{z'}^z \frac{dz''}{u(z'')} \quad (5.25)$$

where double prime (") denotes a position between z and z' .

5.4.3 Method of Solution

The numerical method used to solve eqs. (5.11) and (5.12), with the stresses replaced by eq. (5.16), is the FEM explained in Chapter 4. The unknown velocity, u , and temperature, T , are approximated with quadratic finite element interpolation functions, $\psi_i^{(e)}$:

$$\begin{aligned} u^{(e)} &= \sum_{i=1}^3 u_i^{(e)} \psi_i^{(e)} \\ T^{(e)} &= \sum_{i=1}^3 T_i^{(e)} \psi_i^{(e)} \end{aligned} \quad (5.26)$$

where the superscript (e) refers to an element within the domain $\Omega [0, L]$. The differential equations pertaining to the velocity and temperature are then weighted with the same

interpolation functions as those used for the variables, and the resulting Galerkin weighted residuals, on an element basis, are:

$$\begin{aligned}
 R(u)_i^{(e)} = & \left[\left\{ \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u^{(e)}} \right) - \frac{Re}{A} u^{(e)} \right\} \psi_i^{(e)} \right]_{z=0}^{z=1} + \\
 & \int_0^1 \left\{ - \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u^{(e)}} \right) \frac{d\psi_i^{(e)}}{dz} + \frac{Re}{A} u^{(e)} \frac{d\psi_i^{(e)}}{dz} + \right. \\
 & \left. \left[-2C_f \frac{Re}{A^2} \rho_a \sqrt{\frac{u^{(e)^3}}{\rho} + \frac{Re}{A^2 Fr} \frac{1}{u^{(e)}}} \right] \psi_i^{(e)} \right\} dz = 0
 \end{aligned} \quad i = 1, 3 \quad (5.27)$$

$$\begin{aligned}
 R(T)_i^{(e)} = & \left[T^{(e)} \psi_i^{(e)} \right]_{z=0}^{z=1} + \\
 & \int_0^1 \left\{ T^{(e)} \frac{d\psi_i^{(e)}}{dz} + \left[\frac{\kappa_1 (T^{(e)} - T_a)}{\sqrt{\rho u}} + \frac{\kappa_2 (T^{(e)^4} - T_a^4)}{\sqrt{\rho u}} \right] \psi_i^{(e)} \right\} dz = 0
 \end{aligned} \quad i = 1, 3 \quad (5.28)$$

All boundary residuals at the die exit are set to zero in order to impose the velocity and temperature at the die exit. The stresses in the residuals are replaced by the stresses defined by the modified K-BKZ integral constitutive equation, eq. (5.16). The upstream memory resulting from the integral constitutive equation is computed via a 15-point Gauss-Laguerre quadrature suited for exponentially fading functions (see Chapter 4), while the Galerkin residuals are computed with Gauss-Legendre quadrature (see Chapter 4). The residuals, which are required to vanish, result in a system of $2M$ nonlinear equations (where M is the total number of nodes), which are solved by the Newton-Raphson iterative scheme, as explained in Chapter 4.

5.5 Results and Discussion

5.5.1 Fiber Spinning of a Newtonian Fluid

The spinning of a Newtonian fluid was first solved analytically by Matovich and Pearson (1969). In dimensionless form, the velocity of the fiber is given as

$$u = \exp[z \cdot \ln(D_R)] \quad (5.29)$$

As mentioned in Chapter 3, the modified K-BKZ integral constitutive equation reduces to the Newtonian model when $N=1$ and $\lambda_I=0$ (or equivalently a very small number, say $\lambda_I=0.001$). In this case, and by using unit values in eq. (5.24) for the characteristic velocity u_c and length L , the Weissenberg number $Ws=\lambda$, and for the Newtonian fluid $Ws=0$. Thus, the analytical solution to the spinning of a Newtonian fluid can be used to ensure the current numerical scheme is accurate. Since only the numerical scheme is being tested here, the effects of inertia, gravity and air drag are neglected.

Figure 5.2 shows the results of the current simulations for fiber spinning (with $\lambda_I=0.001$) along with the analytical solution for a Newtonian fluid. Agreement with the analytical Newtonian solution is excellent. Another method for ensuring that the current numerical scheme is accurate can be found with the prehistory parameter c . Since it is assumed that the prehistory is purely extensional, and that the stresses are conserved inside and outside of the die, the prehistory parameter c should be equal to $\ln(D_R)$. For a draw ratio of 20 ($\ln(20) = 2.995732$), with $\lambda_I=0.001$, the current simulations gives a value for the prehistory parameter $c=2.995883$ (0.005% error).

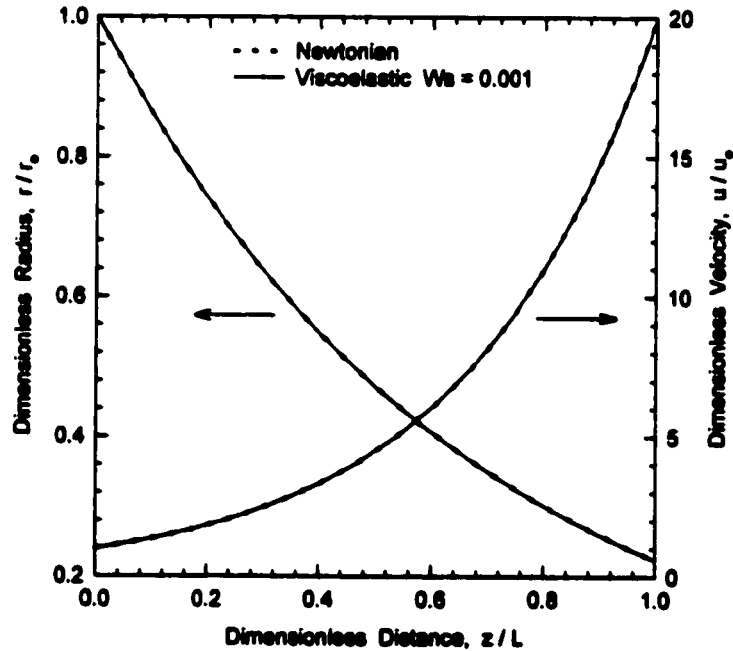


Figure 5.2: Fiber spinning of a Newtonian fluid. Thick dotted lines represent the analytical solution, eq (5.29). Lines represent the current simulations with the modified K-BKZ integral constitutive equation with $N=1$ and $\lambda_I=0.001$ ($Ws=0.001$).

5.5.2 Fiber Spinning of an Upper – Convected Maxwell (UCM) Fluid

The fiber spinning of a UCM fluid was first solved analytically by Denn et al. (1975) for different Weissenberg numbers (Ws) and at different draw ratios (D_R). The modified K-BKZ constitutive model, eq. (5.16), reduces to the UCM model by setting $N = 1$, $\lambda_1 = 1$, and $\alpha \rightarrow \infty$ (or equivalently a very large number, say 10,000). Simulations can then be performed for a UCM fluid and the numerical scheme can be validated for viscoelastic fluids. Again, unit values are used for the tube velocity u_0 and the length L such that $Ws = \lambda$. Since only the numerical scheme is being tested here, the effects of inertia, gravity and air drag are neglected.

Figure 5.3 shows the results of the current simulations for fiber spinning at a draw ratio of $D_R = 20$ for different Weissenberg numbers, along with the results of Denn et al. (1975). Agreement with the results of Denn et al. (1975) is excellent, confirming that the current numerical scheme is accurate for viscoelastic fluids. Analytically, the maximum attainable Weissenberg number for the spinning of a UCM fluid at a given draw ratio is

$$Ws_{\max} = \frac{1}{D_R - 1} \quad (5.30)$$

For a draw ratio of $D_R = 20$, the maximum Weissenberg number is $Ws_{\max} = 0.05263$. The maximum Weissenberg number attained with the current numerical scheme was $Ws_{\max} = 0.052$, with a dimensionless force of $f = 1002.78$ required to pull the fiber.

Figure 5.3 also shows the effect of increasing the Weissenberg number on the fiber velocity and the fiber radius. As the Weissenberg number increases, the more plastic (solid) the material becomes and hence resists deformation. This in turn results in a flatter velocity profile (i.e. uniform deformation). The continuation procedure used in order to reach the final Weissenberg number of $Ws=0.052$, which was the maximum for this numerical scheme, is given in Table 5.2. The continuation procedure of Table 5.2 is similar for subsequent simulations where continuation is required.

Table 5.2: Continuation procedure used in the simulations with the UCM model to reach the maximum Weissenberg number of $Ws = 0.052$.

Continuation step	Weissenberg number, Ws
1	0 (Newtonian)
2	0.02
3	0.04
4	0.045
5	0.048
6	0.05
7	0.051
8	0.0515
9	0.0518
10	0.052

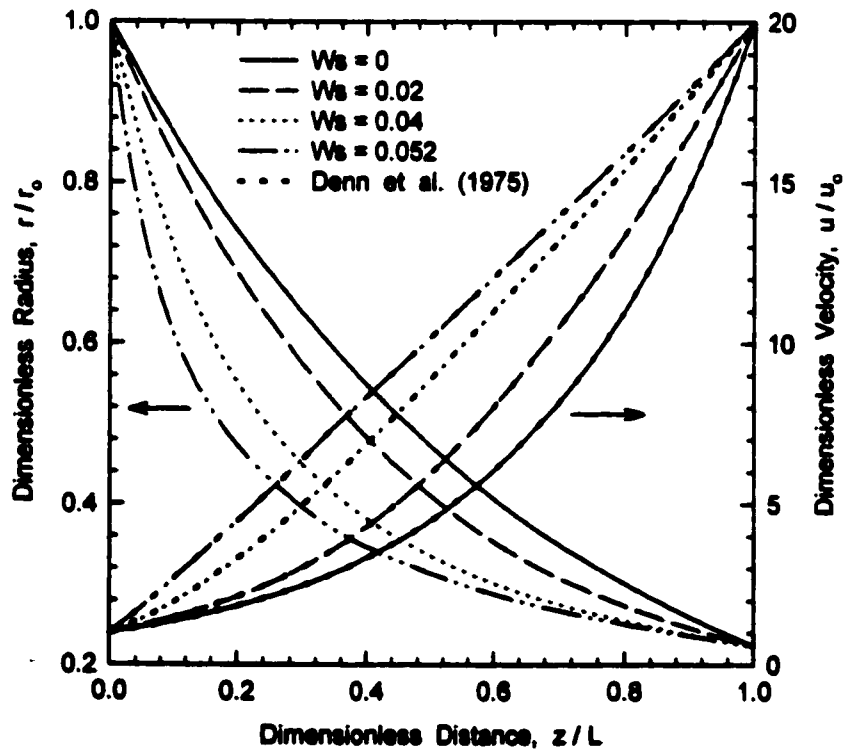


Figure 5.3: Fiber spinning of a UCM fluid for various Weissenberg numbers (Ws). Thick dotted lines represent the solution from Denn et al. (1975) while other lines represent the current simulations with the modified K-BKZ constitutive equation with $N=1$ and $\alpha=10,000$.

5.5.3 Parametric Study with K-BKZ Nonlinear Parameters (α , β , θ)

A parametric study is conducted here, in relation to the nonlinear parameters α , β , and θ in the K-BKZ model (eq. (5.16)), to obtain a better understanding of the rheological effects in the fiber-spinning process. The effects of changing the nonlinear parameters in the K-BKZ model on the rheological functions (e.g. shear viscosity, first normal stress difference, etc.) have already been described in Chapter 3 (see Figures 3.8 through 3.10). The simulations are performed in the same manner as the UCM simulations, i.e., unit values are used for the tube velocity u_o and the length L such that $Ws = \lambda$. The Weissenberg number for the parametric study is $Ws = 0.04$.

Figure 5.4 shows the effect of changing α , the *shear-thinning parameter*, on the fiber velocity and fiber radius. As α increases, so does the uniaxial viscosity at higher extensional rates (decrease in extension-thinning effect), which makes the material more difficult to deform. Therefore, we expect to see a more linear velocity profile in the fiber velocity, with a greater decrease in the radial profile near the tube. This is exactly portrayed in Figure 5.4. It is also interesting to note that at the lowest value of α ($\alpha = 10$), the fiber velocity profile is beyond the Newtonian profile, and similarly for the fiber radius profile.

Figure 5.5 shows the effect of changing β , the *extension-thinning parameter*, on the fiber velocity and radius. As β increases, the uniaxial viscosity at higher extensional rates decreases (increase in extension-thinning effect), which causes the material to be easily deformed. With the material easier to deform, the radial profile will become more linear, and the velocity profile will in turn become more exponential. This is exactly portrayed in Figure 5.5. Once more, a lower extensional viscosity ($\beta = 0.9$) causes the fiber velocity profile to extend beyond the Newtonian profile, and similarly for the fiber radius profile.

Finally, Figure 5.6 shows the effect of changing θ , the *normal stress parameter*, on the fiber velocity and radius. As the value of θ (negative) increases to zero, the uniaxial viscosity at higher extensional rates increases slightly, which makes the material slightly more difficult to deform. Figure 5.6 shows the same trend as Figures 5.4 and 5.5;

increasing the uniaxial viscosity causes the fiber velocity profile to become more linear, with a greater decrease in the radial profile near the tube.

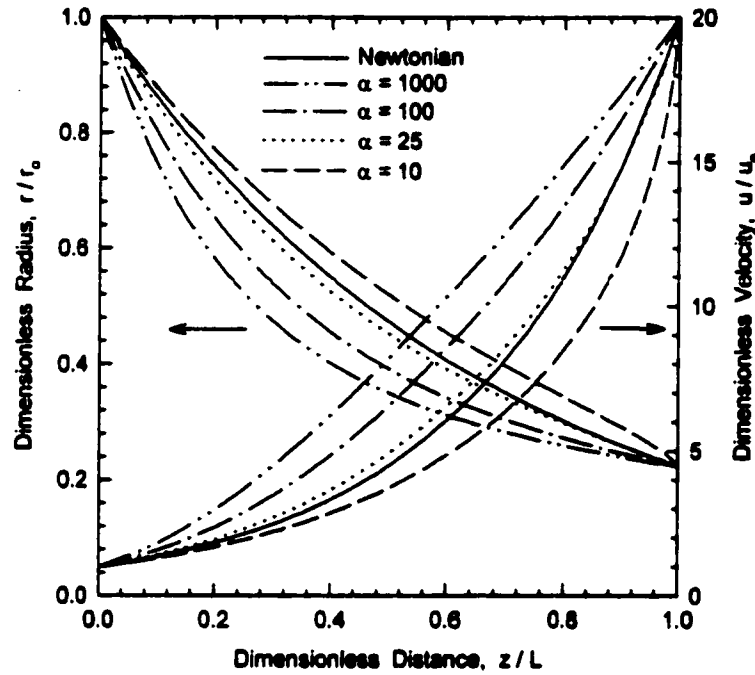


Figure 5.4: Effect of changing the nonlinear parameter α (shear-thinning parameter) in the K-BKZ model on the fiber radius and fiber velocity for $W_s=0.04$. In each case, $\beta=0.5$ and $\theta=0$.

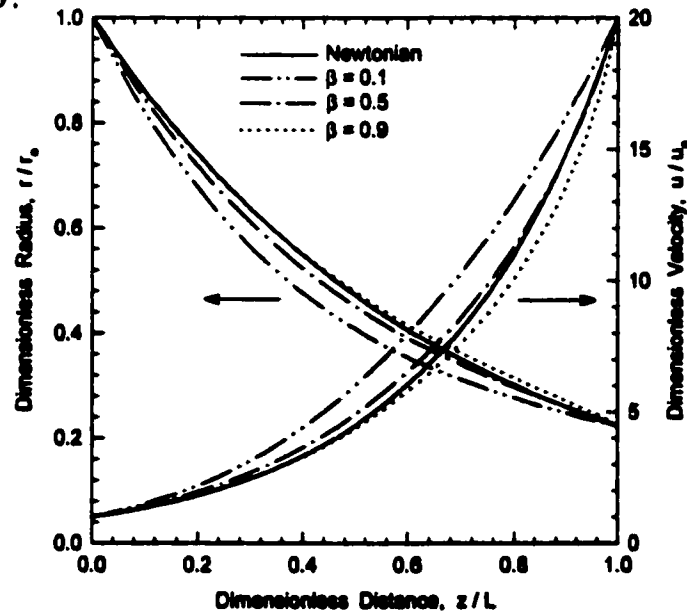


Figure 5.5: Effect of changing the nonlinear parameter β (extension-thinning parameter) in the K-BKZ model on the fiber radius and fiber velocity for $W_s=0.04$. In each case, $\alpha=25$ and $\theta=0$.

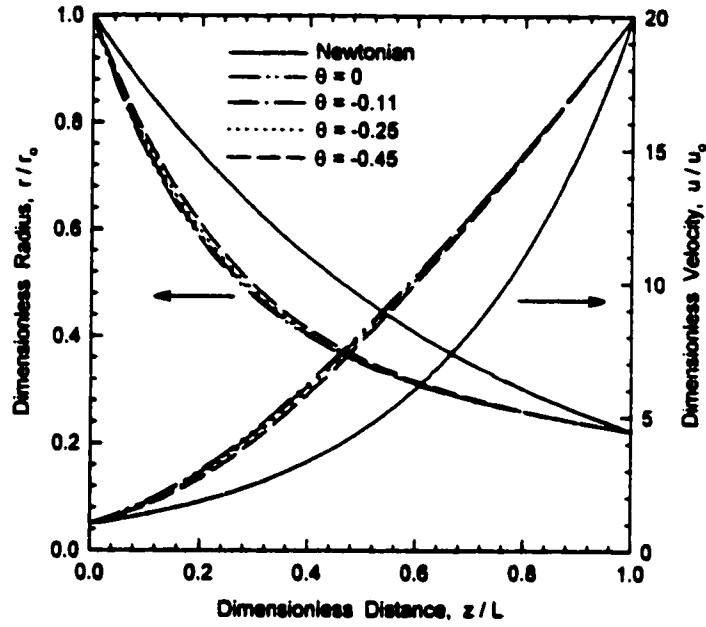


Figure 5.6: Effect of changing the nonlinear parameter θ (normal stress parameter) in the K-BKZ model on the fiber radius and fiber velocity for $Ws=0.04$. In each case, $\alpha=1000$ and $\beta=0.5$.

5.5.4 Isothermal Fiber Spinning of a Polymer Solution

In order to obtain a better understanding of the rheological behaviour of polymer solutions, the M1 project was initiated (Journal of Non-Newtonian Fluid Mechanics, Vol. 35, No. 2-3, 1990). The M1 fluid consisted of 0.244% high-molecular weight polyisobutylene, 7% kerosene, and 93% low-molecular weight polybutene. In a series of “round robin” experiments, different laboratories around the world performed different experiments on the same fluid and the results were compared in literature.

Although measurements for the shear viscosity (η_s) and the first normal stress difference (N_1) agreed quite well from different laboratories, measurements for the extensional viscosity (η_E) diverged considerably. Figure 5.7 (a) shows the results from experiments for the shear viscosity, first normal stress difference, and extensional viscosity. The shear viscosity data and first normal stress difference were extracted from Binding et al. (1990). The extensional viscosity data were extracted from Chai and Yeow

(1990), Binding et al. (1990), and Ferguson and Hudson (1990). The uniaxial viscosity data represent measurements made from spinline rheometers only. Measurements from other types of experiments can be found in Ferguson et al. (1997). Figure 5.7 (b) shows the dynamic data (G' , G'') from Binding et al. (1990). Figures 5.7 (a) and (b) also show the predictions from the modified K-BKZ integral constitutive equation, eq. (5.16), with the relaxation spectrum given in Table 5.3. The predictions from the K-BKZ model fits well the storage modulus (G') but differs slightly with the loss modulus (G''). This was a consequence of not using the solvent viscosity of 1.6 Pa.s in the K-BKZ model, as done by previous studies in simulating the M1 fluid (see e.g., Park et al., 1993). In order to fit the experimental data accurately, multiple α (α_k) and multiple β (β_k) were required in eq. (5.16).

Table 5.3: Original relaxation spectrum and associated parameters for the M1 fluid at 21°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\theta = -0.111$).

k	λ_k (s)	a_k (Pa)	α_k	β_k
1	0.000324	6070	12600	0.99
2	0.101	5.06	1.77×10^6	0.99
3	0.563	0.480	2060	0.000115
4	6.79	0.000213	977	0.000107

Ferguson and Hudson (1990) conducted fiber-spinning experiments with the M1 fluid for a wide range of draw ratios and spinline lengths. A full account of operating conditions for the 13 experiments conducted by Ferguson and Hudson is given in Table 5.4. The effects of inertia, gravity, and air drag are included in these simulations, and the corresponding coefficients are also given in Table 5.4. Initial simulations of the Ferguson and Hudson (1990) experiments done during the course of this work, using the relaxation spectrum of Table 5.3, resulted in good predictions of the take-up force for some experiments but very poor predictions of the take-up force for others. Attempts to use alternate relaxation spectra were also unsuccessful in simulating correctly all of the

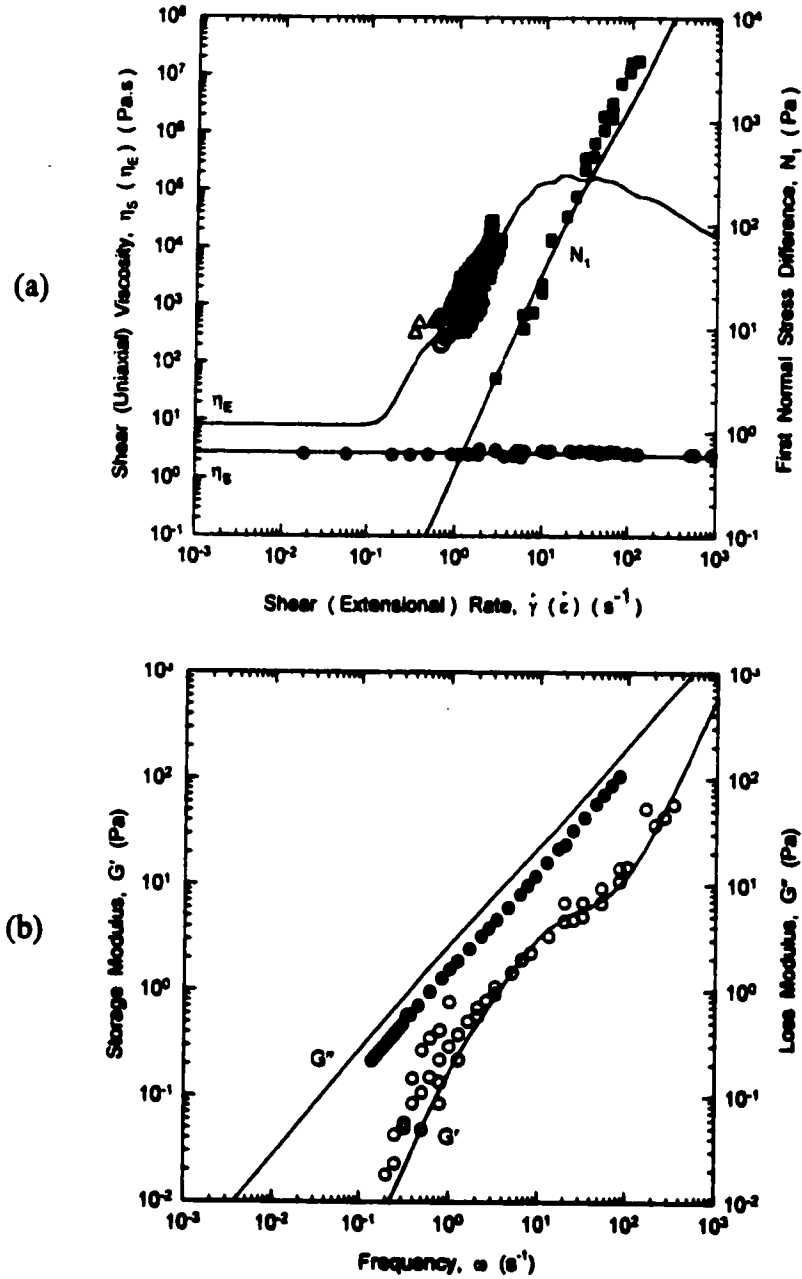


Figure 5.7 (a): Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for the M1 solution at 21°C, and (b) storage and loss moduli (G' , G'') for the M1 solution. Symbols represent experimental measurements while lines represent predictions from the modified K-BKZ constitutive model, eq. (5.16), with the relaxation spectrum of Table 5.3.

take-up forces for each experiment. Recently, Ferguson et al. (1997) have explained why the extensional viscosity from different laboratories have differed. It seems that the M1 fluid does not possess a true steady-state extensional viscosity, but rather a transient extensional viscosity that may differ depending on the time scale of the experiment. This would also explain why the relaxation spectrum of Table 5.3 was only partially successful in the simulations.

Table 5.4: Operating (boundary) conditions used in the simulations for the 13 experiments conducted by Ferguson and Hudson (1990) for the M1 polymer solution at 21°C. The tube radius, r_o , for each experiment is $r_o=0.198$ cm. The density of the M1 polymer solution at 21°C is $\rho=0.9$ g/cm³. The inertia term is Re / A , the gravity term is $Re / A^2 \cdot Fr$, and the drag term is Re / A^2 [for definitions, see eq. (5.13)].

Run #	Length, L (cm)	Tube-exit velocity, u_o (cm / s)	Take-up velocity, u_L (cm / s)	Draw ratio, D_R	Inertia term	Gravity term	Drag term
1	4	0.766	15	19.6	0.100	670	0.218
2	4	0.773	20	25.9	0.101	665	0.220
3	4	0.778	30	38.6	0.102	660	0.222
4	4	0.782	40	51.1	0.102	657	0.223
5	4	0.785	50	63.7	0.103	654	0.224
6	5.05	0.586	20	34.1	0.097	1397	0.266
7	7	0.198	20	101.2	0.045	7945	0.173
8	4.5	0.321	20	62.3	0.047	2025	0.116
9	4.5	0.590	20	33.9	0.087	1102	0.213
10	5.9	0.680	50	73.5	0.131	1644	0.422
11	8	0.682	50	73.3	0.179	3013	0.778
12	7	0.259	50	193.1	0.059	6074	0.226
13	4.5	0.860	50	58.2	0.127	756	0.310

In view of this, a different approach to simulating the experiments by Ferguson and Hudson (1990) was used, called here the *inverse method*. Instead of using one distinct

relaxation spectrum for simulating all of the experiments, the relaxation spectrum and associated parameters were altered slightly such that the simulations would predict the correct force for each experiment (within 2% error). The predicted and measured forces for each run are given in Table 5.5, while the modifications made to relaxation spectrum and associated parameters (Table 5.3) to get the predicted forces are given in Table 5.6. It was also found during the simulations that the predicted force was *hypersensitive* to the extensional viscosity, and hence the relaxation spectrum. The altered relaxation spectra for each experiment mapped a closed region on the extensional viscosity curve, where perhaps the steady-state extensional viscosity would reside. This method was also used by Binding et al. (1990) (see Figure 5.7 (a)) in their experiments, and a region was also mapped where the extensional viscosity would reside.

Table 5.5: Experimentally measured and predicted forces for the series of experiments for the M1 fluid at 21°C.

Run #	Experimental forces from Ferguson and Hudson (1990)	Predicted forces from simulations
	(mN)	(mN)
1	18.9	18.9
2	30.8	30.8
3	44.8	45.1
4	74.3	75.1
5	105.0	104.3
6	19.4	19.3
7	6.8	6.8
8	17.5	17.6
9	16.5	16.8
10	62.2	62.1
11	31.6	32.0
12	28.8	28.5
13	87.3	87.2

Table 5.6: Modifications made to the relaxation spectrum and associated parameters of Table 5.3 to obtain predicted forces of Table 5.5. The uniaxial extensional viscosities from the modified relaxation spectra and associated parameters are shown in Figure 5.8 ($\theta=0.111$).

Run #	Modification
1	$\beta_3=\beta_4=0.00028$
2	$\beta_3=\beta_4=0.00026$
3	$\beta_3=\beta_4=0.000175$
4	$\beta_3=\beta_4=0.000065$
5	$\beta_3=\beta_4=0.00003$
6	$\beta_3=\beta_4=0.000045$
7	$\lambda_3=1.3 \text{ s}, a_3=0.2080 \text{ Pa}, \beta_3=\beta_4=0.000015$
8	$\lambda_3=0.825 \text{ s}, a_3=0.3277 \text{ Pa}, \beta_3=\beta_4=0.000092$
9	$\beta_3=\beta_4=0.00024$
10	$\lambda_3=1.0 \text{ s}, a_3=0.2703 \text{ Pa}, \beta_3=0.00003, \beta_4=0.0001$
11	$\lambda_3=0.9 \text{ s}, a_3=0.3004 \text{ Pa}, \beta_3=0.000065, \beta_4=0.0001$
12	$\lambda_3=1.4 \text{ s}, a_3=0.1931 \text{ Pa}, \beta_3=\beta_4=0.00001$
13	$\lambda_3=1.0 \text{ s}, a_3=0.2703 \text{ Pa}, \beta_3=0.00008, \beta_4=0.0001$

Figure 5.8 shows the results of the mapped extensional viscosity region from simulating the 13 experiments of Ferguson and Hudson (1990). Figure 5.8 shows an overall good agreement with the extensional viscosity measurements of Chai and Yeow (1990), Binding et al. (1990), and Ferguson and Hudson (1990). The region was constructed by plotting the modified fits (Table 5.6) from each experiment for the entire range of applicable extensional rates ($\dot{\epsilon} = dv_z / dz$). The predicted region for the M1 fluid shows an increase in the uniaxial viscosity from an extensional rate of $\dot{\epsilon} = 1 \text{ s}^{-1}$ to $\dot{\epsilon} = 10 \text{ s}^{-1}$, then a gradual decrease in uniaxial viscosity at higher extensional rates. This is reminiscent of the uniaxial behaviour of similar fluids, the A1 and S1 fluids (see e.g., Ferguson et al., 1997).

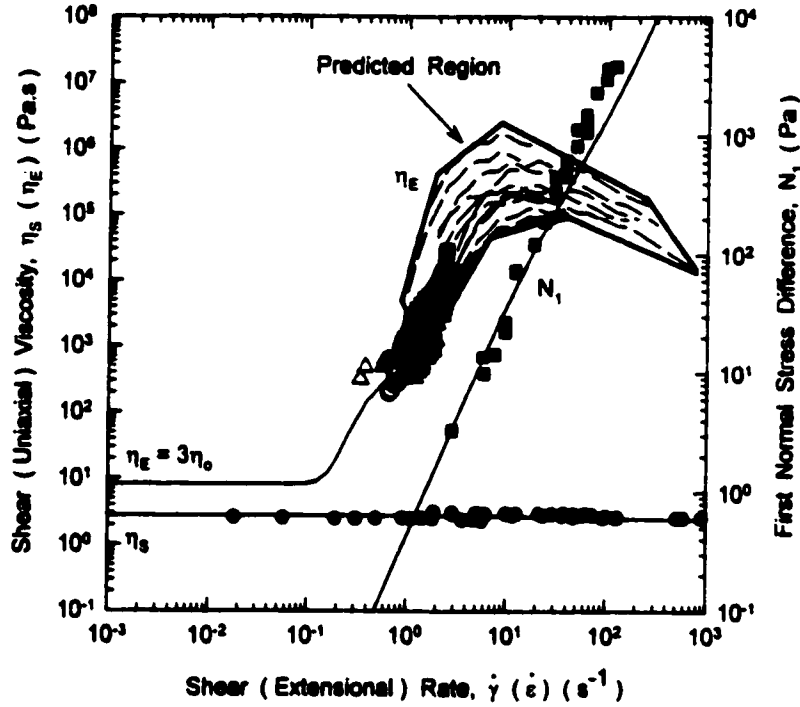


Figure 5.8: Predicted region for the steady state uniaxial viscosity (η_E) from simulating the 13 experiments of Ferguson and Hudson (1990). Also shown are experiments (symbols) and predictions (lines), as in Figure 5.7 (a).

Ferguson and Hudson (1990) also measured the radial profile of the filament for one experiment, #6, and thus also obtained a velocity profile from conservation of mass. Figure 5.9 shows the velocity and radial profiles for the current simulations and that of experiment #6 from Ferguson and Hudson (1990). Overall good agreement is obtained both for the radial and velocity profiles, but subtle differences exist that may have to do either with experimental error (no error estimates were given in the experimental work) or with two-dimensional effects or both. Unsuccessful attempts were made to simulate the experiments with a two-dimensional FEM scheme developed by Luo and Mitsoulis (1990) with the same modified K-BKZ model. Convergence could only be obtained for very low draw ratios ($D_R < 10$). The lowest draw ratio from the experiments of Ferguson and Hudson (1990) is $D_R = 19.6$. Thus, the one-dimensional model is very useful in that convergence is guaranteed for draw ratios as high as $D_R = 193.1$.

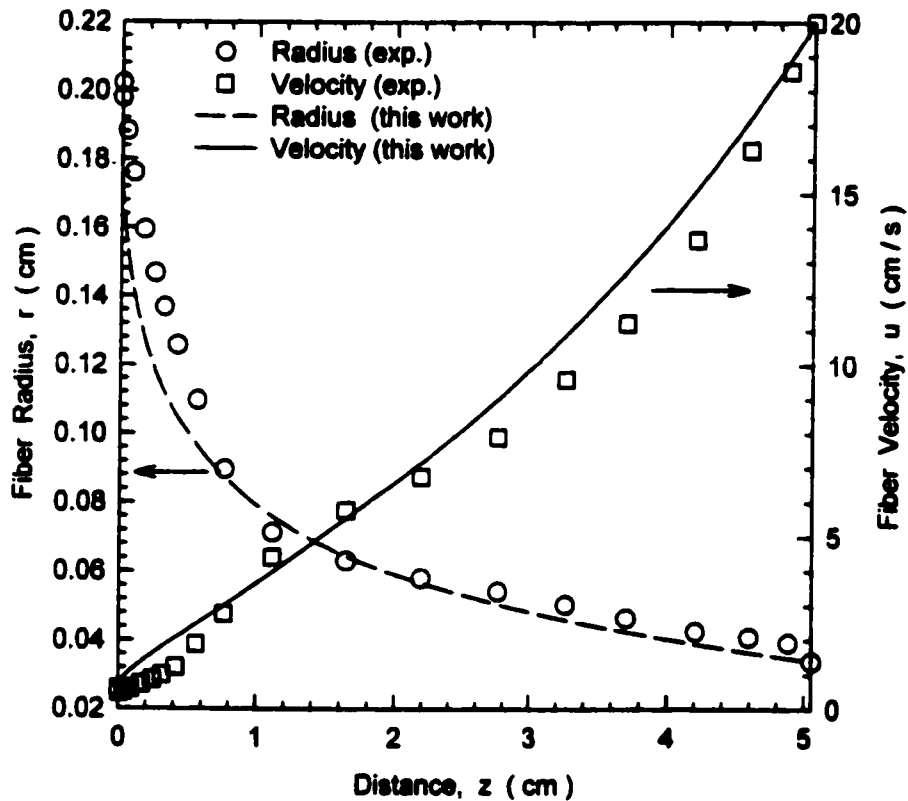


Figure 5.9: Radial and velocity profiles for experiment #6 by Ferguson and Hudson (1990). Symbols represent experimental measurements while lines are predictions from the current simulations.

Figure 5.10 shows the velocity profile from the simulations as a function of distance along the spinline for runs #1 through #5. These runs were conducted at a constant flow rate and constant spinline length, with variations in take-up speed only. Also shown in Figure 5.10 are identical simulations without the effects of inertia, gravity, and air drag. It can be seen that the effects are minimal on the velocity profiles. The effect was also minimal in terms of the predicted forces, where the maximum change was 2.5% for all 13 experiments. It should be emphasized that the effects of inertia, gravity, and air drag are only minimal for this particular set of simulations, and could be very significant for other simulations.

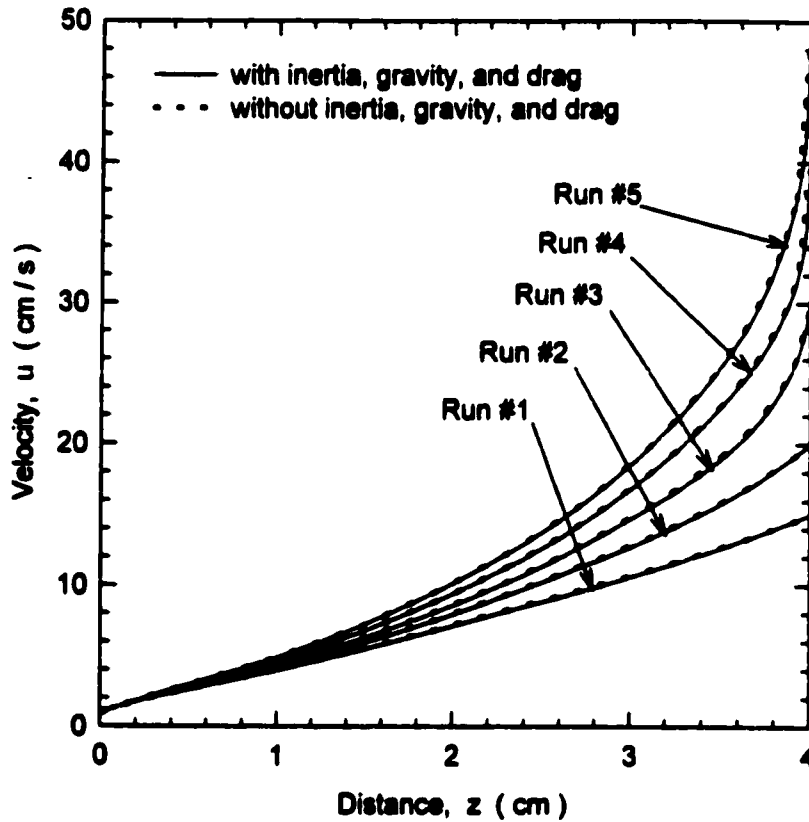


Figure 5.10: Velocity profiles obtained from simulations of runs #1 through #5 (see Table 5.4). Thick dotted lines represent corresponding simulation without the effects of inertia, gravity, and air drag.

5.5.5 Isothermal Fiber Spinning of Polymer Melts

Isothermal fiber-spinning experiments were conducted for a PP melt at 200°C by Ishizuka et al. (1980), who carried out a series of experiments to examine the rheological effects on the fiber-spinning process. The series of experiments included take-up force measurements and velocity profiles for different operating conditions. Disappointingly, Ishizuka et al. (1980) allowed the fiber to solidify past the isothermal zone. This induces a non-isothermal zone past the isothermal zone, resulting in a higher force (due to solidification) and making the experiment ill-conditioned for simulation. Nonetheless, simulations have been carried out for three experiments conducted by Ishizuka et al.

(1980), namely experiments #5, #6, and #7. The effects of inertia, gravity, and air drag are omitted here since the viscosity of the melt is very high, and thus the corresponding coefficients in the governing equation (eq. (5.11)) are small (see Table 5.7). The operating conditions for these three runs are given in Table 5.7.

Table 5.7: Operating (boundary) conditions used in the simulations for the experiments conducted by Ishizuka et al. (1980) for a PP melt at 200°C. Other parameters used in the simulations with the PP melt are also given. The inertia term is Re/A , the gravity term is $Re/A^2 \cdot Fr$, and the drag term is Re/A^2 [for definitions, see eq. (5.13)].

Run #	Length, L (cm)	Initial radius, r_o (cm)	Tube-exit velocity, u_o (cm / s)	Take-up velocity, u_L (cm / s)	Inertia term	Gravity term	Drag term
5	35.4	0.0907	0.394	3.75	6.4×10^{-5}	14.3	0.125
6	35.8	0.0853	0.110	2.95	1.8×10^{-5}	52.4	0.00380
7	70.6	0.0836	0.115	3.30	3.7×10^{-5}	195	0.0157

Reference temperature $T_{ref} = 473 \text{ K}$ (200°C)

Density $\rho_o = 1.0 \text{ g cm}^{-3}$

Activation energy $E = 57500 \text{ J mol}^{-1}$

Specific heat $c_p^o = 2.30 \times 10^7 \text{ erg g}^{-1} \text{ K}^{-1}$

Figure 5.11 shows the predictions of the modified K-BKZ constitutive model along with the rheological data by Ishizuka and Koyama (1980) for the shear viscosity. The relaxation spectrum obtained from nonlinear regression for the PP melt at 200°C is given in Table 5.8. Figures 5.12 (a), (b), and (c) show the simulation results for experiments #5, #6, and #7, respectively, along with the measurements made by Ishizuka et al. (1980) for the radius and velocity. Overall reasonable agreement is obtained for both the radius and velocity for all three experiments. It is not surprising that the velocity is well captured by the simulations, since the velocity measurements were made in the isothermal zone. However, the force measurements reflect the conditions for the entire spinning

length, including the non-isothermal zone. For the sake of comparison, Table 5.9 shows the predicted forces for the three experiments along with the measured forces by Ishizuka et al. (1980). The simulations under-predict the experimental measurements by nearly half for all three experiments, which is again due to the non-isothermal zone.

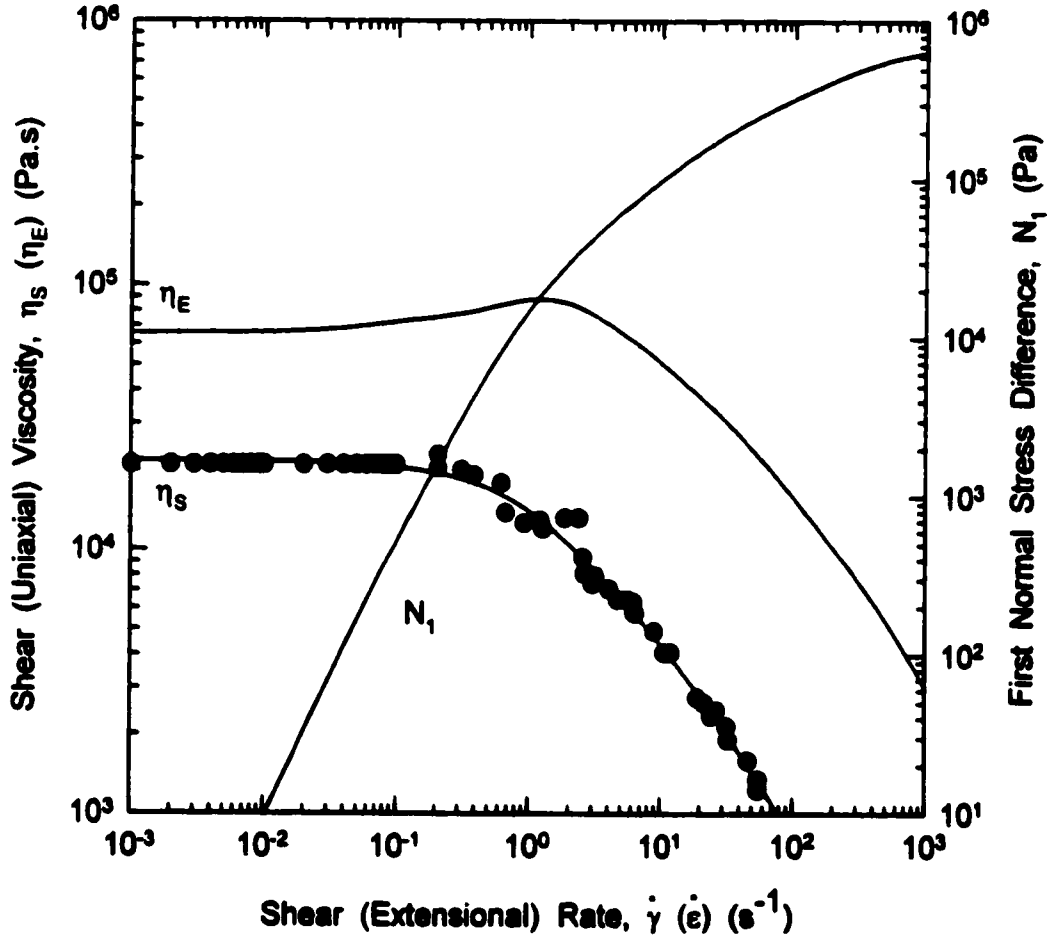


Figure 5.11: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for a PP melt at 200°C. Symbols represent experimental measurements from Ishizuka and Koyama (1980) while lines represent predictions from the modified K-BKZ constitutive model, eq. (5.16), with the relaxation spectrum of Table 5.8.

Table 5.8: Relaxation spectrum and associated parameters for a PP melt at 200°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 5.50$, $\beta = 0.2$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)
1	0.01	82200
2	0.1	42200
3	1	14000
4	10	248
5	100	1.01
6	1000	0.173

Table 5.9: Experimentally measured and predicted forces for the series of experiments for the PP melt at 200°C.

Run #	Experimental forces from Ishizuka et al. (1980) (dynes)	Predicted forces from simulations (dynes)
5	864	415
6	216	149
7	132	77

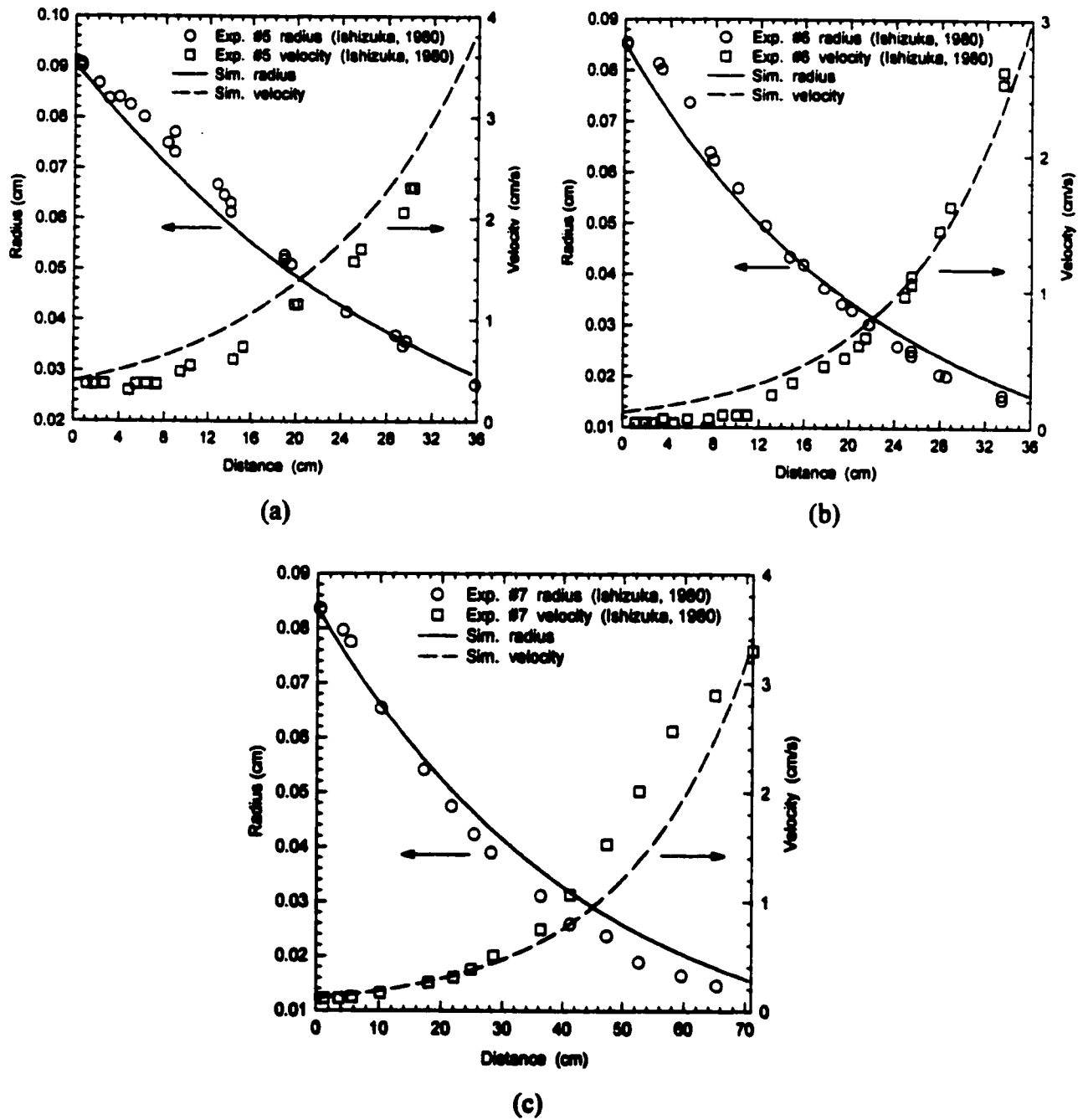


Figure 5.12: Radial and velocity profiles for the spinning of a PP melt at 200°C. Symbols represent experimental measurements by Ishizuka et al. (1980) while lines are predictions from the current simulations for (a) experiment #5, (b) experiment #6, and (c) experiment #7.

5.5.6 Non – Isothermal Fiber Spinning of Polymer Melts

(a) *Poly(Ethylene Terephthalate) (PET) Melt*

Non-isothermal fiber spinning experiments were conducted for a PET melt at 300°C by George (1982), who examined high-speed fiber spinning. Measurements for the fiber velocity and fiber temperature were made for three different experiments. The final velocities for the three experiments were 1000 m/min, 2000 m/min, and 3000 m/min. A full account of the operating conditions is given in Table 5.10, along with the corresponding coefficients for inertia, gravity, and air drag. Although the spinneret hole diameter was 0.25 mm, the initial filament diameter used in the simulations was 0.36 mm, which was based on an estimate of 100% area increase due to extrudate swell (George, 1982). Gagon and Denn (1981) had previously simulated this data for the 1000 m/min and 3000 m/min experiments, and included the effects of inertia, gravity, and air drag. Their simulations made use of the PTT model to account for the viscoelasticity and of the Runge-Kutta numerical method to solve the differential equations. Gagon and Denn (1981) handled the non-isothermal effects by shifting the relaxation times and moduli with appropriate equations of the Arrhenius type.

Current simulations have also been performed for the experiments by George (1982) to compare with those of Gagon and Denn (1981), who have used a very different numerical approach. This comparison can also give insight to the effects of using differential or integral rheological equations in predicting the fiber-spinning process. The effects of inertia, gravity, and air drag have also been included in the current simulations (see Table 5.10). Figure 5.13 shows the rheological data for the shear viscosity (η_s) for PET at 280°C taken from Gregory (1973), along with the predictions from the modified K-BKZ constitutive model, eq. (5.16). The relaxation spectrum used for the predictions is given in Table 5.11, and is the same as that used by Gagon and Denn (1981) for the relaxation times and moduli. The parameters α and β in eq. (5.16) for PET were found by nonlinear regression.

Table 5.10: Operating (boundary) conditions used in the simulations for the experiments conducted by George (1982) for a PET melt solution at 300°C. Other parameters used in the simulations with the PET melt are also given. The inertia term is Re/A , the gravity term is $Re/A^2 \cdot Fr$, and the drag term is Re/A^2 [for definitions, see eq. (5.13)].

Take-up velocity, u_L (m / min)	Take-up velocity, u_L (cm / s)	Initial radius, r_o (cm)	Length, L (cm)	Tube-exit velocity, u_o (cm / s)	Inertia term	Gravity term	Drag term
1000	1667	0.018	100	50	1.82	71.6	5069
2000	3333	0.018	100	50	1.82	71.6	5069
3000	5000	0.018	85	50	1.55	51.7	3662

Reference temperature $T_{ref} = 553 \text{ K}$ (280°C)
Density $\rho_o = 1.0 \text{ g cm}^{-3}$
Activation energy $E = 56535 \text{ J mol}^{-1}$
Specific heat $c_p^o = 2.00 \times 10^7 \text{ erg g}^{-1} \text{ K}^{-1}$

Table 5.11: Relaxation spectrum and associated parameters for the PET melt at 280°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 837$, $\beta = 0.02$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)
1	0.001	1.37×10^{-5}
2	0.005	2.74×10^{-4}

Figure 5.14 shows the current simulation results for the velocity profiles for two experiments, along with the simulation results by Gagon and Denn (1981) and the experimental measurements by George (1982). The current simulation results match very closely with those of Gagon and Denn (1981). The Gagon and Denn (1981) simulations incorporate the PTT model with a Runge-Kutta scheme, while the current simulations

incorporate the K-BKZ model with a FEM scheme. To that effect, two very different approaches to simulating this data result in approximate predictions, which shows the validity of the current numerical scheme to handle well non-isothermal viscoelastic simulations. The agreement also shows that differential and integral models have similar capabilities in viscoelastic modeling, with subtle differences. Also shown in Figure 5.14 are the effects of inertia, gravity, and air drag on the simulation results. It is clear that these effects are very significant and should be included whenever applicable.

Figure 5.15 compares the total filament stress between the current simulations and those of Gagon and Denn (1981), for the 1000 m/min and 3000 m/min experiments. The overall agreement is good with subtle differences. The slight difference between the current simulations and those of Gagon and Denn (1981) can be attributed to either the use of different models (K-BKZ vs. PTT) or the inlet boundary conditions used for the constitutive models. For a differential constitutive model, such as the UCM model, boundary conditions are required for the normal stresses (τ_{xx}, τ_{yy}) in eq. (5.11) at the die exit. For an integral constitutive model, such as the K-BKZ model, no boundary conditions are required for the normal stresses but rather an assumption must be made for the deformation within the die (prehistory). As mentioned in Chapter 3, the deformation within the die is assumed as purely extensional. Previous studies (Chen and Papanastasiou, 1987; Rauschenberger and Laun, 1997) have shown that an extensional prehistory obtained better or similar results compared to a shear prehistory. The current simulations support this claim, and also show that the PTT and K-BKZ models yield similar predictive properties, even though the prehistory for each model is handled differently. Both methods of handling the deformation within the die (prehistory) are accurate. However, it is difficult to know *a priori* the stresses at the die-exit for the PTT model, and thus the method of particle tracking with the K-BKZ model is favored.

Finally, Figure 5.16 compares the current results for the temperature along the fiber for all three take-up speeds against those measured by George (1982), along with the predictions of Gagon and Denn (1981). Agreement with the experimental measurements of George (1982) is quite good. Agreement between the current simulations and those of Gagon and Denn (1981) is also good, again with slight differences. This difference is due

to the inclusion of radiation in the equation of energy, eq. (5.12), causing a more rapid decrease in temperature at the die exit than the simulations by Gagon and Denn (1981).

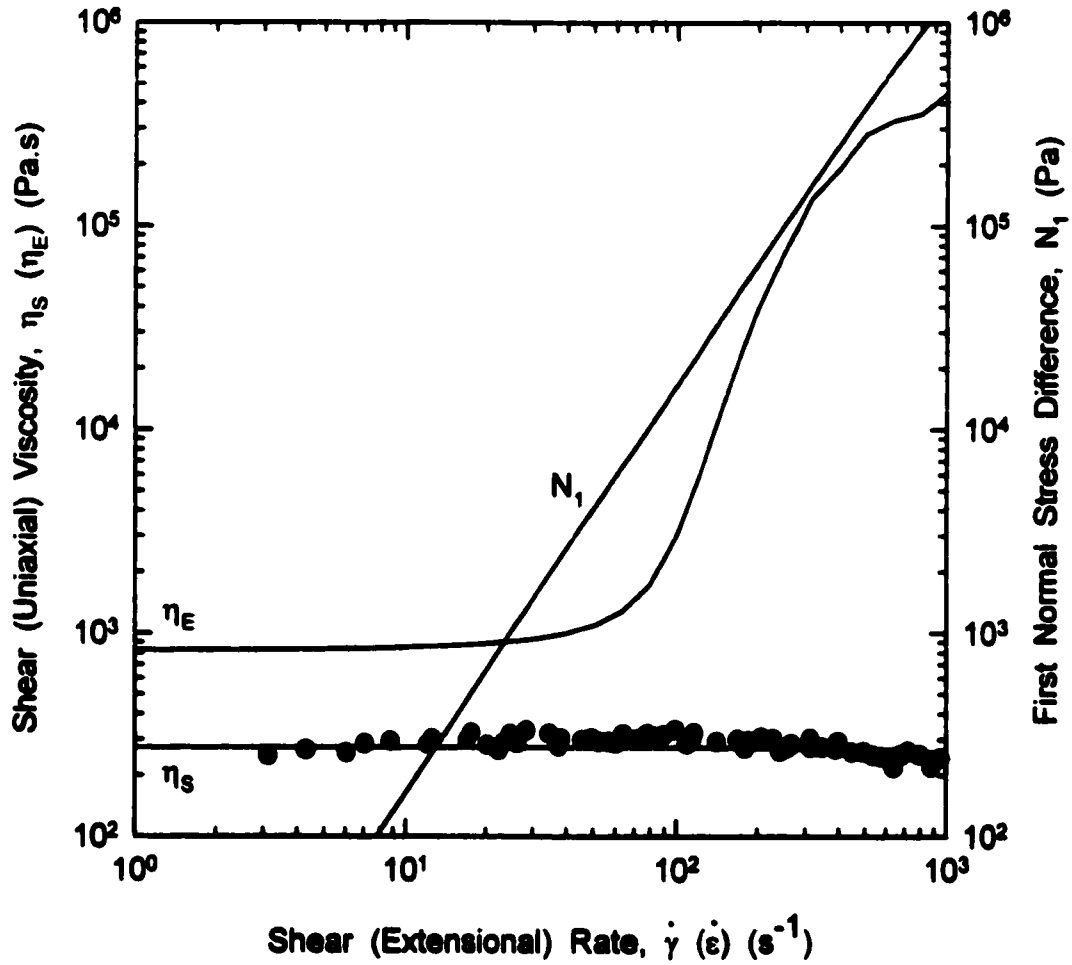


Figure 5.13: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for a PET melt at 280°C. Symbols represent experimental measurements while lines represent predictions from the modified K-BKZ constitutive model, eq. (5.16), with the relaxation spectrum of Table 5.11.

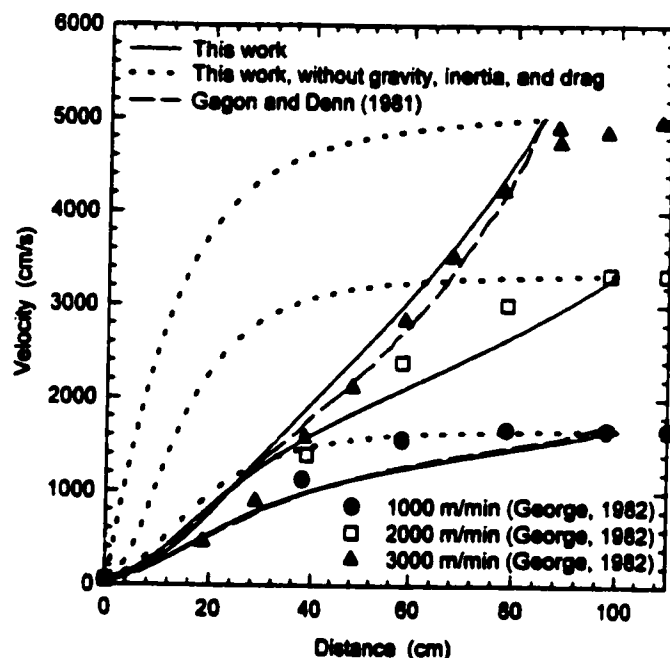


Figure 5.14: Velocity profiles for the spinning of a PET melt at 300°C. Symbols represent experimental measurements by George (1982), dashed lines represent simulations by Gagon and Denn (1981), while full lines are predictions from the current simulations.

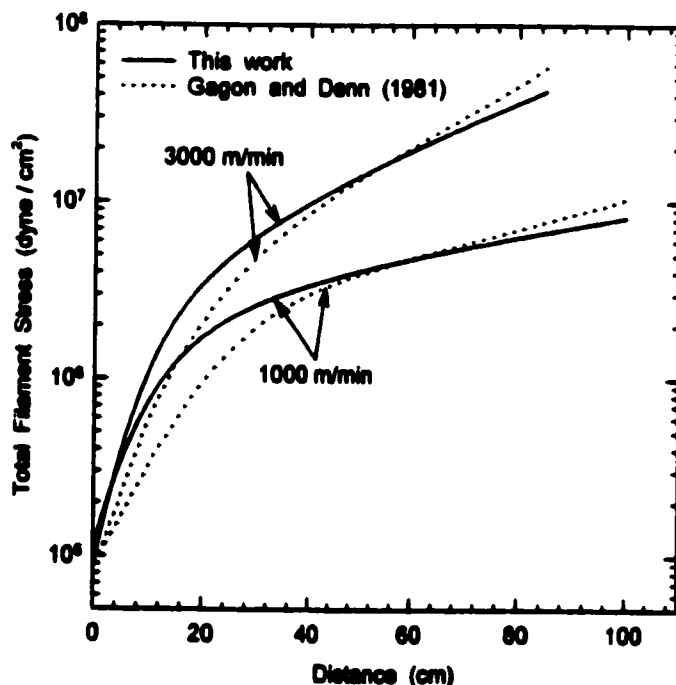


Figure 5.15: Stress profiles for the spinning of a PET melt at 300°C. Dashed lines represent simulations by Gagon and Denn (1981), while lines are predictions from the current simulations.

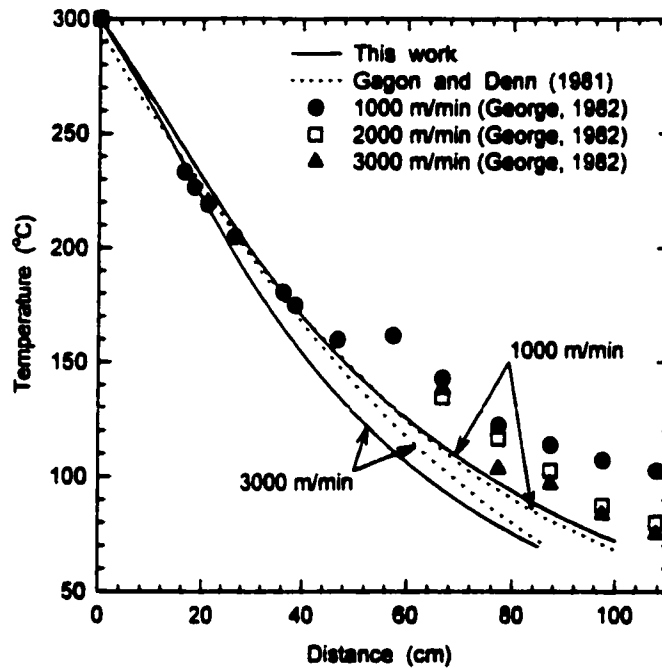


Figure 5.16: Temperature along the fiber for the spinning of a PET melt at 300°C. Symbols represent experimental measurements by George (1982), dashed lines represent simulations by Gagon and Denn (1981), while full lines are predictions from the current simulations.

(b) *IUPAC-A Low-Density Polyethylene (LDPE) Melt*

Non-isothermal fiber spinning experiments were also conducted for the IUPAC-A LDPE at 180°C by Rauschenberger and Laun (1997), along with simulations from a new iterative model. The new model has the capability to account for extrudate swell, given the details of the die geometry, thus giving better predictions for the take-up force. The new model has made use of the same constitutive model, the modified K-BKZ integral constitutive model, eq. (5.16), to account for the viscoelasticity of the material. The new model also uses the Morland-Lee hypothesis to account for non-isothermal effects. Note that Rauschenberger and Laun (1997) made no measurements for the fiber radius or velocity, but rather measurements of the take-up force at different draw ratios.

Figure 5.17 shows the rheological data for the IUPAC-A LDPE at 150°C, along with predictions from the modified K-BKZ model, eq. (5.16). Two predictions are made from

the K-BKZ model, namely parameter set 1 and parameter set 2. The relaxation spectra used for the predictions for both parameter sets are given in Table 5.12, and are the same as those used by Rauschenberger and Laun (1997). The predictions of the steady-state extensional viscosity (η_E), shown in Figure 5.17, do not match with measurements from experiments. Rauschenberger and Laun (1997) have justified the discrepancy by comparing the predictions (with the relaxation spectrum of Table 5.12) with the transient extensional viscosity (η_E^+) of the IUPAC-A LDPE, where agreement was good.

Table 5.12: Relaxation spectrum and associated parameters for the IUPAC-A LDPE melt at 150°C from Rauschenberger and Laun (1997) for Fit 1 and Fit 2 ($\theta = -0.316$).

k	λ_k (s)	a_k (Pa)
1	1.0×10^{-4}	$1.29 \times 10^{+5}$
2	1.0×10^{-3}	$9.48 \times 10^{+4}$
3	1.0×10^{-2}	$5.86 \times 10^{+4}$
4	1.0×10^{-1}	$2.67 \times 10^{+4}$
5	$1.0 \times 10^{+0}$	$9.80 \times 10^{+3}$
6	$1.0 \times 10^{+1}$	$1.89 \times 10^{+3}$
7	$1.0 \times 10^{+2}$	$1.80 \times 10^{+2}$
8	$1.0 \times 10^{+3}$	$1.00 \times 10^{+0}$
Fit 1: $\alpha = 13$, $\beta = 0.011$		
Fit 2: $\alpha = 24$, $\beta = 0.022$		

For the fiber-spinning experiments, two spinline lengths were studied, namely 90 mm and 110 mm, with the details of the operating conditions given in Table 5.13. The effects of inertia, gravity, and air drag are neglected here due to the high viscosity of the melt, and thus the corresponding coefficients for inertia, gravity, and air drag were small (see Table 5.13). Although the draw ratios vary for the individual spinline simulations, the coefficients for inertia, gravity, and air drag do not vary since they are based on tube-exit conditions (for definitions, see eq. (5.13)). As with the simulations of PET, where a

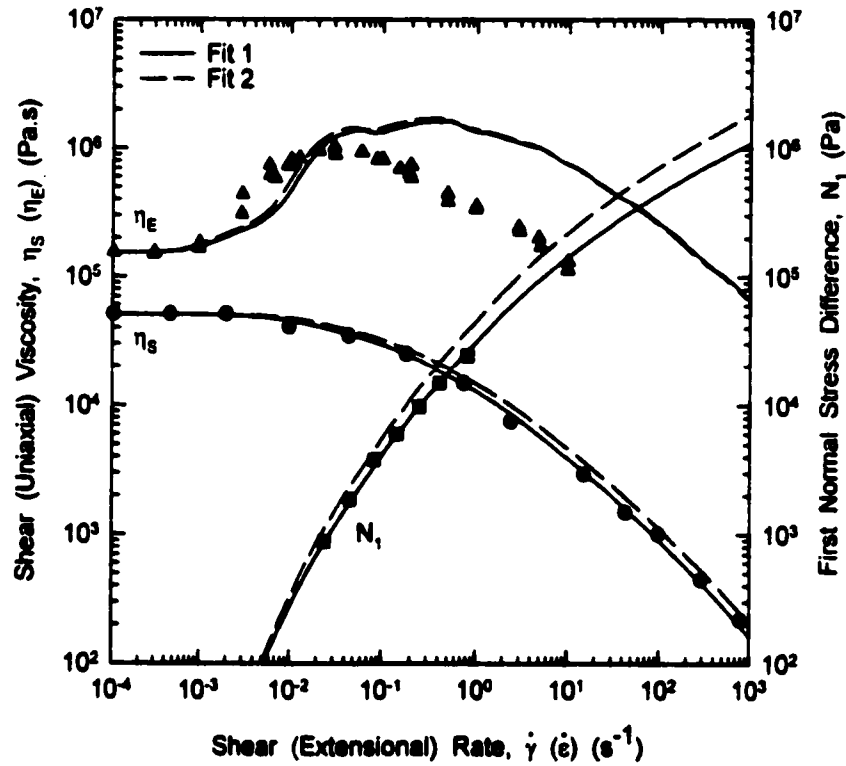


Figure 5.17: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for the IUPAC-A LDPE melt at 150°C for Fit 1 and Fit 2. Symbols represent experimental measurements by Meissner (1975) while lines represent predictions from the modified K-BKZ constitutive model, eq. (5.16), with the relaxation spectra (Fit 1 and 2) of Table 5.12.

100% increase in area was assumed due to extrudate swell, a 50% increase in area was assumed for the simulations of IUPAC-A LDPE, typical of the simulations and experiments of Rauschenberger and Laun (1997). This was done in order to match the predictions of Rauschenberger and Laun (1997), whose new model can account for extrudate swell. It should be noted that the amount of extrudate swell measured from fiber-spinning experiments is less than the amount of extrudate swell measured in simple extrusion experiments. In fiber spinning experiments, the material is drawn resulting in less extrudate swell than if the material is allowed to swell freely (simple extrusion). For simple extrudate swell studies, see Meissner (1975) and Barakos and Mitsoulis (1995).

Table 5.13: Operating (boundary) conditions used in the simulations for the experiments conducted by Rauschenberger and Laun (1997) for the IUPAC-A LDPE melt at 180°C. Other parameters used in the simulations with the IUPAC-A LDPE melt are also given. The inertia term is Re / A , the gravity term is $Re / A^2 \cdot Fr$, and the drag term is Re / A^2 [for definitions, see eq. (5.13)].

Length, L (cm)	Initial radius, r_o (cm)	Tube-exit velocity, u_o (cm / s)	Take-up velocity, u_L (cm / s)	Draw ratio, D_R	Inertia term	Gravity term	Drag term
9	0.16	1.25	2.27→28.4	1.2→15	1.76×10^{-5}	0.100	4.96×10^{-4}
11	0.16	1.25	2.27→28.4	1.2→15	2.15×10^{-5}	0.149	7.40×10^{-4}

Reference temperature $T_{ref} = 423$ K (150°C)
Density $\rho_o = 0.8$ g cm⁻³
Activation energy $E = 57500$ J mol⁻¹
Specific heat $c_p^o = 2.30 \times 10^7$ erg g⁻¹ K⁻¹

Figure 5.18(a) shows the results for both parameter sets (Fit 1 and Fit 2) for the spinline length of 90 mm. Very good agreement is obtained for Fit 1 for the full range of draw ratios compared to the simulations of Rauschenberger and Laun (1997). However, the current simulations for Fit 2 agree with the simulations of Rauschenberger and Laun (1997) only up to a draw ratio of $D_R=5$. Beyond this, the agreement of the simulations of Rauschenberger and Laun (1997) with the experiments is superior than the current simulations. This is due to the ability of the new model of Rauschenberger and Laun (1997) to account for extrudate swell.

Figure 5.18(b) shows the results for both parameter sets (Fit 1 and Fit 2) for the spinline length of 110 mm. Again good agreement is obtained with Fit 1 but not with Fit 2, similar to the simulations for the spinline length of 90 mm. The new model of Rauschenberger and Laun (1997) has the superior ability to predict extrudate swell, which is a function of the draw ratio, and thus can give better predictions for the take-up force. The current numerical scheme cannot account for extrudate swell, but can nevertheless give good predictions for the take-up force if information is given on the extrudate swell

a priori. The amount of extrudate swell for the IUPAC-A LDPE as a function of the draw ratio was not known, and thus a 50% increase in area was assumed for all draw ratios.

The simulations revealed that extrudate swell is significant in the fiber-spinning process. However, the simulations also revealed the importance of viscoelastic effects, from the different predictions of take-up forces from two different viscoelastic fits (see Table 5.12). The modifications made by Rauschenberger and Laun (1997) to the original fit (Fit 1), in order to get the correct forces as a function of draw ratio, lead to speculation about other effects not taken into account (e.g. two-dimensional effects).

5.6 Concluding Remarks

Numerical viscoelastic simulations have been undertaken for the fiber-spinning process with the code F-SPIN. The fiber-spinning process is a prime example of uniaxial extensional flow. The governing equations, first presented in Chapter 3, were made dimensionless. Relations for the air drag, melt density, heat capacity, and heat transfer coefficient as a function of distance along the spinline were presented. Specifics concerning the numerical solution of the governing equations were also presented.

Isothermal Newtonian and UCM results have been successfully reproduced using an integral equation of the K-BKZ type. Consequently, the validity of the numerical scheme was established at low and high Weissenberg (Wi) numbers. However, the Newtonian and UCM models do not predict the behaviour of real polymer melts. The Newtonian model predicts a constant uniaxial viscosity (see Chapter 3) while the UCM model predicts a uniaxial viscosity which eventually reaches infinity (see Chapter 3). Therefore, the K-BKZ model, which predicts adequately the behaviour of real polymer melts, has been used as the workhorse for the simulations.

Simulations were undertaken for the one-dimensional fiber spinning of the polymer solution M1, where two-dimensional simulations could not converge. The simulations were used to predict a region where the steady-state uniaxial viscosity could reside, by

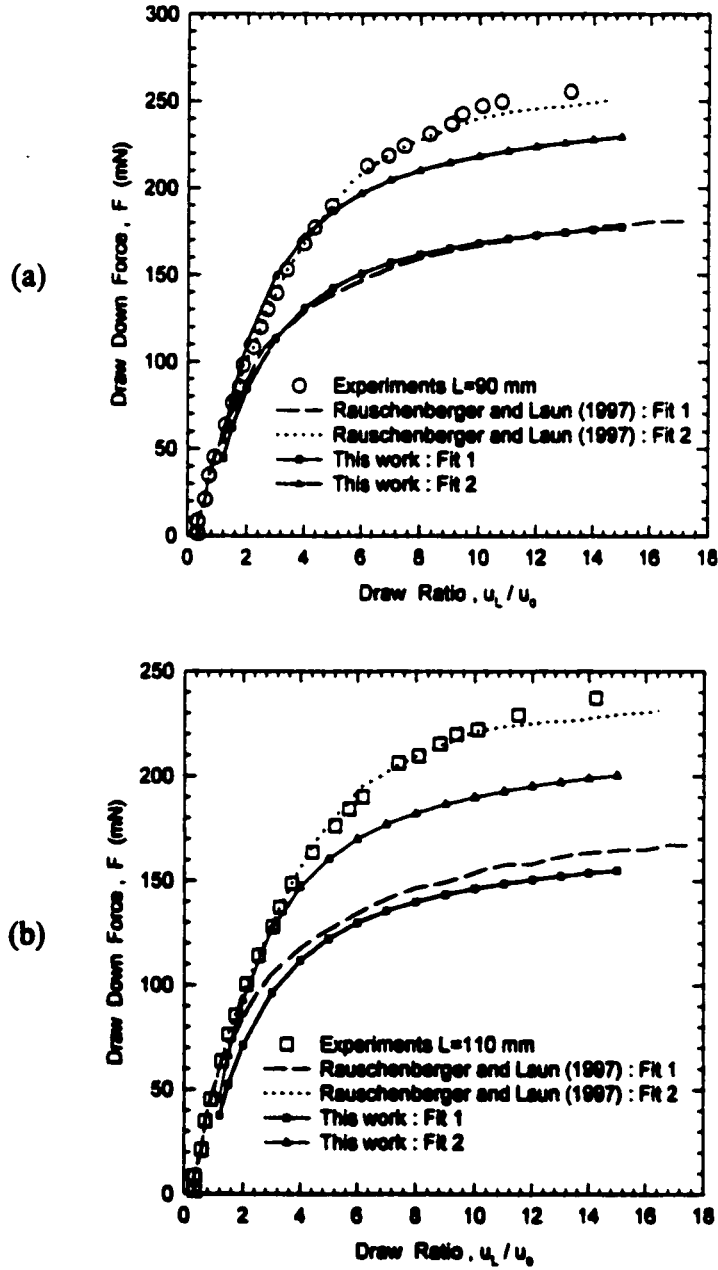


Figure 5.18: Draw forces for the IUPAC-A LDPE melt at 180°C for different draw ratios for a spinline length of (a) $L=90$ mm, and (b) $L=110$ mm. Symbols represent experimental measurements by Rauschenberger and Laun (1997), dashed lines are simulations by Rauschenberger and Laun (1997), while lines are predictions from the current simulations.

changing the relaxation spectrum and associated parameters, called here the *inverse method*. The reason for altering the original relaxation spectrum was due to the transient behaviour of the M1 solution reported by other researchers (Ferguson et al., 1997). The simulations also revealed the contributions from inertia, gravity, and air drag were minor (less than 2.5%) for this particular set of experiments by Ferguson and Hudson (1990). The one-dimensional model was advantageous since it was used to determine the sensitivity of the simulations to viscoelasticity and other external forces (inertia, gravity, and air drag). This information can aid further two- and three-dimensional simulations.

Simulations were also undertaken for the isothermal spinning of a PP melt. The simulations gave good overall agreement in terms of the fiber radius and velocity, but not in terms of the take-up force. This was attributed to non-isothermal effects in the experiments. The melt at a constant temperature was allowed to cool (solidify) beyond the isothermal zone. This resulted in a higher force than would have been measured if the melt was not allowed to cool and solidify. Thus, the experiments were isothermal in terms of fiber radius and velocity in the isothermal zone, but the force had non-isothermal contributions.

The non-isothermal spinning of polymer melts, namely PET and the IUPAC-A LDPE, was also simulated. In the case of the spinning of PET, the simulations revealed that the PTT and K-BKZ have similar predictive capabilities, regardless of the numerical scheme used (Runge-Kutta vs. FEM). The simulations also revealed the importance of inertia, gravity, and air drag in the simulations for PET. In the case of the spinning of the IUPAC-A LDPE, extrudate swell was found to be important in predicting the correct take-up force. However, viscoelastic effects were found to be more significant than the extrudate swell, with different predictions of the take-up force from two different viscoelastic fits (see Table 5.12).

The objective of this study was to develop an efficient code that can give quick and approximate results for the fiber-spinning process. Since two- and three- dimensional simulations take a great deal of effort and time to develop, the one-dimensional formulation for fiber spinning has been used to develop the code F-SPIN. It has the advantages of short computing time with almost guaranteed convergence. It was used to

determine the significance of viscoelastic effects and the sensitivity of the results to the parameters in the K-BKZ constitutive equation. It was also used to find the significance of the effects of inertia, gravity, and air drag. Thus, the F-SPIN code is very useful for an engineer who desires fast information or predictions for the fiber-spinning process.

Chapter 6

Film Casting

Isothermal and non-isothermal viscoelastic simulations are performed for the film-casting process. The one-dimensional governing equations are restated and specifics concerning the numerical scheme are given. The differential equations are solved using the finite element method (FEM). The resulting code, **F-CAST**, is then used for film-casting simulations. The numerical scheme is validated with the Newtonian and upper-convected Maxwell (UCM) solutions. Comparisons are made with previous higher-dimensional simulations and overall reasonable results for viscoelastic materials are obtained. Simulations are then undertaken for *real* polymeric materials. Non-isothermal simulations are carried out for a polypropylene (PP) melt. Parametric studies are undertaken for a poly(ethylene terephthalate) (PET) melt and the IUPAC-A low-density polyethylene (LDPE) melt, where there is a lack of experimental data in the literature.

6.1 Introduction

The film-casting process is used throughout the plastics industry to manufacture thin films or sheets. The process itself is portrayed in Figure 6.1(a). A polymer melt is continuously extruded through a narrow slit or rectangular die and taken up downstream at a higher velocity at the chill roll. The film-casting process, which was thought to be dominated purely by planar extension, is dominated by a *combination of planar extension and uniaxial extension* (Dobroth and Erwin, 1986). The ratio of take-up velocity to extrusion velocity is known as the draw ratio (D_R). Afterwards, the film is subjected to additional processes such as biaxial extension or thermoforming to enhance some of the film properties (e.g. film strength and stretching ability). In industrial practice, cross-flow air is applied to the film to aid in cooling and to reduce instabilities in the film. Cast films are primarily used in the packaging industry for either foodstuffs or other consumer products, but other uses include magnetic strips for audio and video

tapes. A common troublesome effect of creating a film through the film-casting process is known as the *edge-bead effect* or the *bone effect*. It consists of the film being much thicker at the edges than at the center, which is depicted in Figure 6.1(b). This is remedied by trimming the edges of the film before any further processing is undertaken. Another film-casting trait is the *neck-in effect*, where the width of the film recedes due to the increase in film velocity. The neck-in effect is depicted in Figure 6.1(c). For untreated films, the film-casting process has operating speeds ranging from 120 m/min to 400 m/min, whereas if the film undergoes biaxial orientation, speeds range from 280 m/min to 350 m/min. The term *film* is reserved for thicknesses less than 250 μm , while the term *sheet* refers to higher thicknesses. Typical thicknesses range from 10 μm to 2500 μm , whereas lateral dimensions can vary from 40 to 320 cm (Baird and Collias, 1995).

Typical industrial goals for the film-casting process are as follows:

- Reduction of the edge-bead effect to minimize wasted material.
- Increase in take-up speeds without increasing instability. This has been accomplished in the past with what is known as an *air-knife* or a *draw-resonance eliminator*. The air-knife is a high-velocity jet of air, which strikes the film midway between the die and chill roll. This acts as a dampener to reduce any instability in the film.

6.2 Literature Review

In contrast to the fiber-spinning process (Chapter 5), the film-casting process has received less attention in the literature. Kase (1974) conducted early experimental work and presented results on the film casting of a polypropylene melt. Dobroth and Erwin (1986) examined the causes of thick edges or *edge beads* and attributed it to the change from planar extension in the center of the film to uniaxial extension at the edges. Several studies on the film-casting process have been conducted by Co's group (Anturkar and Co, 1988; Vardarajan and Co, 1996; Piz-Lopez and Co, 1996a; Piz-Lopez and Co, 1996b) analyzing the stability of numerous constitutive models (UCM, Carreau, Giesekus). Another major source of studies on the film-casting process has emerged from Agassant's group (Barq et al., 1990; d'Halewyn et al., 1990; Barq et al., 1992;

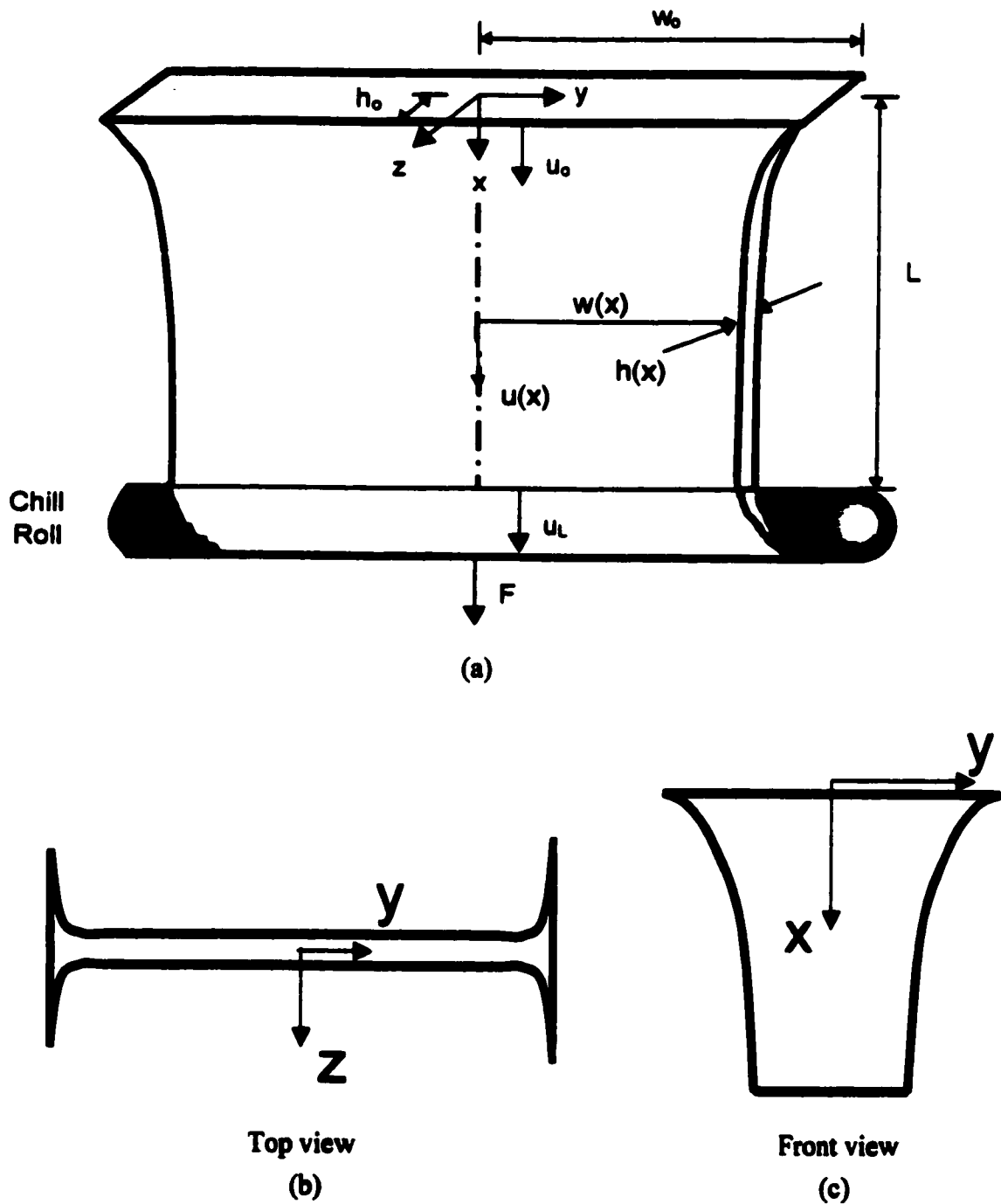


Figure 6.1: (a) Schematic of the film-casting process. (b) The edge-bead effect typically observed during the film-casting process. (c) The neck-in effect typically observed during the film-casting process.

Silagy et al., 1996), who have analyzed stability and performed simulations for the Newtonian and UCM models. An attempt was made by Alaie and Papanastasiou (1991) to simulate the data of Kase (1974), employing a one-dimensional approach using the modified K-BKZ integral constitutive model with no variation of the film width. Debbaut et al. (1995) performed a two-dimensional analysis of the film-casting process with the use of the Newtonian and UCM models. Sakaki et al. (1996) performed a full three-dimensional analysis using the Newtonian model.

The rheology of the polymer melt, with interactions from temperature, will undeniably affect the final characteristics of the film and, in turn, the operating conditions. Thus, rheological characterization of the material to be processed is perhaps the most important aspect in any simulation. A proper rheological constitutive equation, which has the ability to predict well the material's response in extensional flows, is imperative. Previous simulations for the film-casting process have either not used a proper rheological constitutive equation or have not given any explanation as to the choice of rheological parameters (e.g. relaxation time and modulus) used in the constitutive model. In this study, the modified K-BKZ integral constitutive equation is used, which adequately predicts the material's response in both shear and extension.

The effects of temperature have only been studied by Barq et al. (1992) and Alaie and Papanastasiou (1991). The shortcomings of these studies are that Barq et al. (1992) used a Newtonian model, while Alaie and Papanastasiou (1991) used a simple one-dimensional approach with no predictions of the film width. This study uses the Morland-Lee hypothesis (1960) coupled with the modified K-BKZ integral constitutive equation to account for temperature effects on viscoelasticity, and the film width is predicted by using an added differential equation.

There are two previous studies using a two-dimensional approach for the film-casting process (d'Halewyn et al., 1990; Debbaut et al., 1995), and one using a three-dimensional approach (Sakaki et al., 1996). In these studies, the edge-bead effect is predicted. The current study cannot account for the edge-bead effect since either a two-dimensional or three-dimensional approach is required to account for the third coordinate. However, comparisons are made with the previous higher-dimensional approaches and it will be

seen that overall agreement for the film thickness along the centerline and for the film width is obtained.

As mentioned earlier, there is a serious lack of experimental data in the literature for the film-casting process. This may be due to an increased tendency in industry to produce films with better characteristics through the use of the film-blowing process (see Chapter 7). Nonetheless, the film-casting process is widely used today to produce high-quality films.

6.3 Objectives

This study will present a quick and approximate method of analysis for the film-casting process with the use of an efficient code, F-CAST. The objectives of this chapter are as follows:

- a) To solve accurately the one-dimensional film casting of a Newtonian fluid. Since the Newtonian model does not possess any elastic response, the model is used here only for checking purposes. Direct comparisons are also made with a previous three-dimensional simulation.
- b) To solve accurately the one-dimensional film casting of a UCM fluid. The UCM model does possess an elastic response, but the predictions for the shear and extensional viscosities are unrealistic, as shown in Chapter 3. The UCM model is also used here only for checking purposes. Direct comparisons are also made with a previous two-dimensional simulation.
- c) To solve accurately the one-dimensional film casting of *real* polymeric fluids. This is done with the use of the K-BKZ integral constitutive model, which predicts well the nonlinear behaviour of polymeric materials. Thus, the K-BKZ model is used for the following set of simulations:
 - A parametric study with the K-BKZ nonlinear parameters to determine the importance of viscoelastic effects in film casting.
 - Non-isothermal simulation of a PP polymer melt for direct comparison with previous experimental results in film casting.

- Non-isothermal simulation of a PET polymer melt and the IUPAC-A LDPE melt in the form of a parametric study to investigate the viscoelastic effects in film casting with different polymeric materials.

6.4 Mathematical Modeling

6.4.1 Governing Equations

The non-isothermal casting of melts can be described by the equations derived in Chapter 3. Specifically, eqs. (3.18), (3.21), (3.22), and (3.24), which are restated here for completeness, are:

$$\rho(4wh)u = \rho Q \quad (6.1)$$

$$\frac{d}{dx} \left(\frac{\tau_{xx} - \tau_{zz}}{\rho u} \right) = 0 \quad (6.2)$$

$$\left(\frac{dw}{dx} \right)^2 = \frac{\tau_{yy} - \tau_{zz}}{\tau_{xx} - \tau_{zz}} \quad (6.3)$$

$$\rho c_p Q \frac{dT}{dx} + \left(4w + \frac{Q}{4wu} \right) h_c (T - T_\infty) + \left(4w + \frac{Q}{4wu} \right) \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (6.4)$$

with the following boundary conditions:

1. $u = u_o$ at $x = 0$
 2. $T = T_o$ at $x = 0$
 3. $w = w_o$ at $x = 0$
 4. $u = u_L$ at $x = L$
- (6.5)

where L is the length of the cast film from the die exit to the chill roll. It should be noted that the effects of air drag, inertia, and gravity have been neglected in eq. (6.2). The effects from air drag are neglected since no empirical relations exist for the drag coefficient C_f in eq. (3.21). It has also been found that effects of inertia and gravity are negligible due to the geometry of the film (i.e. its thickness is much less than its length and width) and the high viscosity of the melts encountered in the film-casting process (Anturkar and Co, 1988; d'Halewyn and Agassant, 1990; Silagy et al., 1996; Vardarajan and Co, 1996; Pis-Lopez and Co, 1996). Again, eqs. (6.2), (6.3), and (6.4) are three first-

order differential equations that require one boundary condition each. An additional boundary condition is also required for eq. (6.2) to make the solution unique since the stresses are not known *a priori*. Equation (6.1) is simply an algebraic equation solved for in terms of the film thickness, h , once the film velocity and width are known.

The density of the polymer, ρ , also changes along the length of the film according to the temperature of the film. A relation for the density as a function of temperature is used here and is the same as that used for fiber spinning in Chapter 5:

$$\rho(T) = \frac{\rho_o}{1 + \delta(T - T_{ref})} \quad (6.6)$$

where ρ_o is the density of the polymer at a reference temperature of T_{ref} . The parameter δ is a constant of expansion, and is given a value of 0.00069 K^{-1} as in Chapter 5.

The relation for the heat capacity is also the same as that used in Chapter 5 and is given as

$$c_p(T) = c_p^o \frac{(k_1 + k_2 T)}{k_1 + k_2 T_{ref}} \quad (6.7)$$

where c_p^o is the specific heat capacity at the reference temperature T_{ref} . The parameters k_1 and k_2 are empirical constants and are given values of 0.3243 and 0.000565 K^{-1} , respectively, as in Chapter 5.

The heat transfer coefficient, h_c , is given by the relation used for convection from flat plates (Churchill and Chu, 1975), since the film being cast has similar geometry:

$$h_c = \frac{k_a}{L} \left\{ 0.825 + \frac{0.387 Ra^{1/6}}{\left[1 + \left(\frac{0.492}{Pr} \right)^{9/16} \right]^{8/27}} \right\}^2 \quad (6.8)$$

Here, k_a is the conductivity of air and L is the length of the film from the die exit to the chill roll. The Rayleigh number, Ra , is given as

$$Ra = \frac{g(T - T_{air})L^3 c_p^a \rho_a^2}{T_f k_a \mu_a} \quad (6.9)$$

Here, g is the acceleration due to gravity, T_{air} is the ambient temperature, c_p^a is the heat capacity of the air, ρ_a is the density of the air, μ_a is the viscosity of the air, and T_f is the boundary layer temperature given as

$$T_f = \frac{T + T_{air}}{2} \quad (6.10)$$

Finally, the Prandtl number, Pr , is given as

$$Pr = \frac{c_p^a \mu_a}{k_a} \quad (6.11)$$

The emissivity, ϵ in eq. (6.4), is given a value of 0.5, as in Chapter 5. A complete list of values used in the simulations is given in Table 6.1. It should be noted that all of the above relations require that the thermophysical properties of air be computed at the boundary layer temperature, T_f .

Table 6.1: Recurring material parameters used in the film casting simulations.

Property (units)	Value
Coefficient of expansion, eq. (6.6), δ (K ⁻¹)	6.90×10^{-4}
Empirical constants, eq. (6.7), k_1 and k_2 (K ⁻¹)	0.324 and 5.65×10^{-4}
Emissivity, eq. (6.4), ϵ	0.5
Stefan-Boltzmann constant, eq. (6.4), σ_{SB} (erg s ⁻¹ cm ⁻² K ⁻⁴)	5.67×10^{-5}
Ideal gas constant, eq. (3.57), R (J mol ⁻¹ K ⁻¹)	8.314
Ambient temperature, eq. (6.4), T_∞ (K, °C)	298 (25)

Equations (6.1) through (6.4) are made dimensionless using to the following dimensionless variables:

$$x^* = \frac{x}{L}, \quad u^* = \frac{u}{u_o}, \quad w^* = \frac{w}{w_o}, \quad h^* = \frac{h}{h_o}, \quad \rho^* = \frac{\rho}{\rho_o}, \quad \tau^* = \frac{\tau L}{\eta_o u_o}, \quad (6.12)$$

$$T^* = \frac{T}{T_o}, \quad T_a^* = \frac{T_a}{T_o}, \quad f = \frac{FL}{4\eta_o u_o w_o h_o}, \quad D_R = \frac{u_L}{u_o}$$

in which L is the length of the film from the die exit to the chill roll, the subscript o refers to die exit conditions, η_o is the zero-shear-rate viscosity, and f is the dimensionless force.

Combining eq. (6.12) with eqs. (6.1), (6.2), (6.3), and (6.4) results in the following dimensionless governing equations to be solved for in terms of the dimensionless thickness, h , dimensionless width, w , dimensionless velocity, u , and dimensionless temperature, T (asterisks are omitted here):

$$\rho u h w = 1 \quad (6.13)$$

$$\frac{d}{dx} \left(\frac{\tau_{xx} - \tau_{zz}}{\rho u} \right) = 0 \quad (6.14)$$

$$\left(\frac{dw}{dx} \right)^2 = A^2 \left(\frac{\tau_{yy} - \tau_{zz}}{\tau_{xx} - \tau_{zz}} \right) \quad (6.15)$$

$$\frac{dT}{dx} + \kappa_1 \left(\frac{1}{\rho u w} + B w \right) (T - T_a) + \kappa_2 \left(\frac{1}{\rho u w} + B w \right) (T^4 - T_a^4) = 0 \quad (6.16)$$

with the following dimensionless quantities:

$$A = \frac{L}{w_o}, \quad B = \frac{w_o}{h_o}, \quad \kappa_1 = \frac{L h_c}{\rho_o u_o w_o c_p}, \quad \kappa_2 = \frac{L \sigma_{SB} \epsilon T_o^3}{\rho_o u_o w_o c_p} \quad (6.17)$$

Here, A and B are aspect ratios and κ_1 and κ_2 are non-isothermal coefficients. The boundary conditions, eq. (6.5), are also transformed with the new dimensionless variables, and given as:

1. $u = 1$ at $x = 0$
 2. $T = 1$ at $x = 0$
 3. $w = 1$ at $x = 0$
 4. $u = D_R$ at $x = 1$
- (6.18)

The dimensionless force required at the take-up position (chill roll) to pull the film can easily be calculated with the following relation

$$f = \left. \frac{\tau_{xx} - \tau_{zz}}{\rho u} \right|_{x=1} \quad (6.19)$$

This equation arises from a simple force balance at the take-up position (i.e. the force required to pull the film is equal to the stresses within the film at the chill roll).

6.4.2 Constitutive Equations

(a) Isothermal Newtonian Model

The first constitutive equation used for the film-casting process is the Newtonian model. It is restated here for completeness (see Chapter 3) and for showing the specific derivations for the film casting of a Newtonian fluid:

$$\bar{\tau} = \mu \bar{\dot{\gamma}} \quad (6.20)$$

where μ is a constant viscosity and $\bar{\dot{\gamma}}$ is the rate-of-strain tensor given by

$$\bar{\dot{\gamma}} = \bar{\nabla} \bar{u} + \bar{\nabla} \bar{u}^T \quad (6.21)$$

The term $\bar{\nabla} \bar{u}$ is the velocity gradient tensor and is assumed as (Silagy et al., 1996) :

$$\bar{\nabla} \bar{u} = \bar{\dot{\epsilon}} = \begin{bmatrix} \frac{du}{dx} & 0 & 0 \\ 0 & a(x) & 0 \\ 0 & 0 & b(x) \end{bmatrix} \quad (6.22)$$

Here, $a(x)$ and $b(x)$ are functions of the distance x to be determined. The function $b(x)$ can be eliminated through the use of the following relation:

$$\text{tr } \bar{\nabla} \bar{v} = 0 \quad (6.23)$$

where tr is the trace of a tensor. The stresses for the film casting of a Newtonian fluid can now be determined and given as

$$\tau_{xx} = 2\mu \frac{du}{dx} \quad (6.24)$$

$$\tau_{yy} = 2\mu a(x) \quad (6.25)$$

$$\tau_{zz} = -2\mu \frac{du}{dx} - 2\mu a(x) \quad (6.26)$$

At any free surface, no fluid crosses the boundary. This can be expressed mathematically in vector form as

$$\bar{u} \cdot \bar{n} = 0 \quad (6.27)$$

where $\bar{n}$ is the normal to the free surface. When the free surface condition is combined with the equation of continuity, the function $a(x)$ is given as

$$a(x) = \frac{u}{w} \frac{du}{dx} \quad (6.28)$$

After several substitutions and simplifications, with the use of eqs. (6.13), (6.14), and (6.15), the following dimensionless equations arise:

$$\frac{du}{dx} = \left[2 - \frac{1}{A^2} \left(\frac{a(x)w}{u} \right)^2 \right] \frac{uf}{6} \quad (6.29)$$

$$\frac{dw}{dx} = \frac{a(x)w}{u} \quad (6.30)$$

$$a(x)^2 - \frac{3A^2u}{w^2f} a(x) - \frac{u^2A^2}{2w^2} \quad (6.31)$$

Equation (6.31) is a quadratic equation with two possible solutions, but with a physical knowledge of $a(x)$ (i.e. $a(x)$ is a decreasing function), the negative solution is the correct solution.

The boundary equations for the Newtonian differential equations [eqs. (6.29) and (6.30)] are as follows:

1. $u = 1$ at $x = 0$
 2. $w = 1$ at $x = 0$
- (6.32)

The added condition $u = D_R$ at $x = 1$ transforms the problem into a *boundary-value problem* that is solved with the shooting method (see Chapter 4).

(b) Isothermal Upper-Convected Maxwell (UCM) Differential Constitutive Model

The second constitutive equation used for the film-casting process is the UCM differential model. It is restated here for completeness (see Chapter 3) and for showing the specific derivations for the film casting of a UCM fluid:

$$\bar{\tau} + \lambda \left\{ \bar{u} \cdot \bar{\nabla} \bar{\tau} - (\bar{\nabla} \bar{u})^T \cdot \bar{\tau} - \bar{\tau} \cdot \bar{\nabla} \bar{u} \right\} = \mu \bar{\dot{\gamma}} \quad (6.33)$$

where $\bar{\dot{\gamma}}$ is defined as in the Newtonian case. Equation (6.33) along with the governing equations for the film-casting process, eqs. (6.13) through (6.15), are simplified and

manipulated as in the Newtonian case. The resulting dimensionless differential equations are

$$\frac{dw}{dx} = -A \sqrt{\frac{\tau_{yy} - \tau_{xx}}{uf}} \quad (6.34)$$

$$\frac{du}{dx} = \frac{2(u/w)(dw/dx)(\tau_{xx}Ws - ufWs + 1) - uf}{3ufWs - 4\tau_{xx}Ws - 4} \quad (6.35)$$

$$\begin{aligned} \frac{d(\tau_{yy} - \tau_{xx})}{dx} = 2 \frac{du}{dx} \left(\frac{\tau_{xx}}{u} - f + \frac{1}{uWs} \right) \\ + \frac{4}{w} \frac{dw}{dx} \left[\frac{1}{Ws} - uf + \tau_{xx} + \frac{(\tau_{yy} - \tau_{xx})}{2} \right] - \frac{(\tau_{yy} - \tau_{xx})}{uWs} \end{aligned} \quad (6.36)$$

$$\frac{d\tau_{xx}}{dx} = \frac{2(du/dx)(1 + \tau_{xx}Ws) - \tau_{xx}}{uWs} \quad (6.37)$$

where Ws is called the Weissenberg number and has the following form for a UCM fluid

$$Ws = \lambda \frac{u_0}{L} \quad (6.38)$$

The Weissenberg number is a measure of the viscoelasticity of the material under flowing conditions, where $Ws = 0$ is equivalent to a Newtonian fluid and $Ws > 1$ is considered highly elastic. The boundary conditions for the UCM differential equations are as follows:

1. $u = 1$ at $x = 0$
 2. $w = 1$ at $x = 0$
 3. $\tau_{xx} = 0$ at $x = 0$
 4. $(\tau_{yy} - \tau_{xx}) = 0$ at $x = 0$
- (6.39)

The boundary conditions for the stresses τ_{xx} and $(\tau_{yy} - \tau_{xx})$ only moderately affect the final solution, and hence are set to zero (i.e. stresses due to deformation within the die are relaxed). The added condition $u = D_R$ at $x = 1$ transforms the problem into a *boundary-value problem* that is solved with the shooting method (see Chapter 4).

(c) *Modified K-BKZ Integral Constitutive Model*

The final constitutive equation used for the film-casting process is an integral model of the K-BKZ type proposed by Papanastasiou et al. (1983) and further modified by Luo and Tanner (1988). It is restated here for completeness (see Chapter 3) and for showing the specific derivations for the film-casting process:

$$\begin{aligned} \bar{\tau}(t) = \frac{1}{1-\theta} \int_{-\infty}^t \sum_{k=1}^N \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) & \frac{\alpha_k}{(\alpha_k - 3) + \beta_k I_{C^{-1}} + (1 - \beta_k) I_C} \\ & \times \left[\left\{ \bar{C}_t^{-1}(t') - \bar{I} \right\} + \theta \left\{ \bar{C}_t(t') - \bar{I} \right\} \right] dt' \end{aligned} \quad (6.40)$$

Again, λ_k and a_k are relaxation times and relaxation modulus coefficients at a reference temperature T_{ref} , respectively. The parameters α_k and β_k are material parameters chosen to fit the material's response in high shear and elongation. The parameter θ has been incorporated by Luo and Tanner (1988) to take into account the second normal stress difference, N_2 , and is related to the first normal stress difference, N_1 , via the formula

$$\frac{N_2}{N_1} = \frac{\theta}{1-\theta} \quad (6.41)$$

The value of θ is not zero for polymer melts exhibiting a second normal stress difference. Its usual range is between -0.1 and -0.3 (Tanner, 1985).

The invariants I_C and $I_{C^{-1}}$ are the first invariants of the Cauchy-Green tensor $\bar{C}_t(t')$ and its inverse $\bar{C}_t^{-1}(t')$, the Finger strain tensor. In terms of the deformation gradient tensor, $\bar{F}_t(t') = d\bar{x}'/d\bar{x}$, the Cauchy-Green and Finger strain tensors are

$$\begin{aligned} \bar{C}_t(t') &= \bar{F}_t(t') \cdot \left[\bar{F}_t(t') \right]^T \\ \bar{C}_t^{-1}(t') &= \left[\bar{F}_t^{-1}(t') \right]^T \cdot \bar{F}_t^{-1}(t') \end{aligned} \quad (6.42)$$

For the film-casting process, the deformation gradient tensor can be derived from the equation of continuity, eq. (6.1), and simple geometry. Also, the assumption is made that for free-surface operations, no shear stresses are present and only the left diagonal entries in the deformation gradient tensor are non-zero (i.e. for $i \neq j \rightarrow \bar{F}_t(t') = 0$). Thus, the first term that applies to the x -coordinate is

$$F_{xx} = \frac{u(t)}{u(t')} \quad (6.43)$$

For the second term that applies to the y -coordinate, the deformation gradient term is

$$F_{yy} = \frac{w(t)}{w(t')} \quad (6.44)$$

The third term that applies to the z -coordinate can be found from the condition of incompressibility

$$\text{tr } \bar{F}_i(t') = 1 \quad (6.45)$$

where tr is the trace of a tensor. Using eq. (6.45) along with eqs. (6.43) and (6.44), the third term is

$$F_{zz} = \frac{w(t')u(t')}{w(t)u(t)} \quad (6.46)$$

From eq. (6.42), the Finger strain tensor can now be obtained and is given by

$$\bar{C}_i^{-1}(t') = \begin{pmatrix} \left(\frac{u(t)}{u(t')} \right)^2 & 0 & 0 \\ 0 & \left(\frac{w(t)}{w(t')} \right)^2 & 0 \\ 0 & 0 & \left(\frac{w(t')u(t')}{w(t)u(t)} \right)^2 \end{pmatrix} \quad (6.47)$$

The Cauchy-Green tensor $\bar{C}_i(t')$ can be found by simply taking the inverse of the Finger strain tensor. The viscoelasticity of the polymer melt under flowing conditions can be represented by a dimensionless variable known as the Weissenberg number, given by

$$We = \frac{u_o}{L} \frac{\sum a_k \lambda_k^2}{\sum a_k \lambda_k} = \frac{u_o}{L} \bar{\lambda} \quad (6.48)$$

where $\bar{\lambda}$ is the average relaxation time. The transit times along the film can be expressed in terms of the velocity and distance traveled, by

$$t - t' = \int_{x'}^x \frac{dx''}{u(x'')} \quad (6.49)$$

where double prime (") denotes a position between x and x' .

6.4.3 Method of Solution

(a) *Newtonian Model*

The differential equations for the film casting with the Newtonian model, eqs. (6.29) through (6.31), are solved with a 4th-order Runge-Kutta scheme presented in Chapter 4. The convergence method used is the shooting method, which utilizes the bisection method, and is also presented in Chapter 4. The dimensionless force, f , requires two guesses for the shooting method, where the boundary condition $u = D_R$ at $x = 1$ is bounded by both guesses (i.e. one guess produces $u > D_R$ at $x = 1$ while the other guess produces $u < D_R$ at $x = 1$). The bisection method is then used as the convergence method that finds the appropriate dimensionless force, f , that produces $u = D_R$ at $x = 1$. During the iteration process, eqs. (6.29) through (6.31) are solved simultaneously.

(b) *Upper-Convected Maxwell (UCM) Differential Constitutive Model*

The differential equations for the film casting with the UCM model, eqs. (6.34) through (6.37), are also solved with a 4th-order Runge-Kutta scheme as presented in Chapter 4. The convergence method used is the shooting method, which utilizes the bisection method, and is also presented in Chapter 4. The shooting method uses the variable f that satisfies the condition $u = D_R$ at $x = 1$, and is utilized in the same manner as in the Newtonian case (see Section 6.4.3 (a)).

(c) *Modified K-BKZ Integral Constitutive Model*

The numerical method used to solve eqs. (6.14) and (6.16), with the stresses replaced by eq. (6.40), is the finite element method (FEM) explained in Chapter 4. The unknown velocity, u , width, w , and temperature, T , are approximated with quadratic finite element interpolation functions, ψ_i :

$$\begin{aligned}
u^e &= \sum_{i=1}^3 u_i^{(e)} \psi_i^{(e)} \\
w^e &= \sum_{i=1}^3 w_i^{(e)} \psi_i^{(e)} \\
T^e &= \sum_{i=1}^3 T_i^{(e)} \psi_i^{(e)}
\end{aligned} \tag{6.50}$$

The differential equations pertaining to the velocity, width, and temperature are then weighted with the same interpolation functions as those used for the variables, and the resulting Galerkin weighted residuals on an element basis are

$$R(u)_i^{(e)} = \left[\left(\frac{\tau_{xx} - \tau_{zz}}{\rho u^e} \right) \psi_i^{(e)} \right]_{z=0}^{z=1} - \int_0^1 \left(\frac{\tau_{zz} - \tau_{rr}}{\rho u^e} \right) \frac{d\psi_i^{(e)}}{dz} dz = 0 \quad i = 1, 3 \tag{6.51}$$

$$R(w)_i^{(e)} = \int_0^1 \left\{ \left(\frac{dw^e}{dx} \right)^2 - A^2 \left(\frac{\tau_{yy} - \tau_{zz}}{\tau_{xx} - \tau_{zz}} \right) \right\} \psi_i^{(e)} dz = 0 \quad i = 1, 3 \tag{6.52}$$

$$\begin{aligned}
R(T)_i^{(e)} &= \int_0^1 \left\{ \frac{dT^e}{dz} + \kappa_1 \left(\frac{1}{\rho u^e w^e} + B w^e \right) (T^e - T_a) + \right. \\
&\quad \left. \kappa_2 \left(\frac{1}{\rho u^e w^e} + B w^e \right) (T^{e^4} - T_a^4) \right\} \psi_i^{(e)} dz = 0
\end{aligned} \quad i = 1, 3 \tag{6.53}$$

All boundary residuals at the die exit are set to zero in order to impose the velocity, width, and temperature at the die exit. The stresses in the residuals are replaced by the stresses defined by the modified K-BKZ integral constitutive equation, eq. (6.40). The upstream memory resulting from the integral constitutive equation is computed via a 15-point Gauss-Laguerre quadrature suited for exponentially fading functions (see Chapter 4), while the Galerkin residuals are computed with Gauss-Legendre quadrature (see Chapter 4). The residuals, which are required to vanish, result in a system of $3M$ nonlinear equations (where M is the total number of nodes) which are solved by the Newton-Raphson iterative scheme, as explained in Chapter 4.

6.5 Results and Discussion

6.5.1 Film Casting of a Newtonian Fluid

The casting of a Newtonian fluid, with the above governing equations, was first solved numerically by Silagy et al. (1996). As mentioned in Chapter 3, the modified K-BKZ integral constitutive model reduces to the Newtonian model when $N=1$ and $\lambda_1=0$ or respectively a very small number, say $\lambda_1=0.001$. In this case, and by using unit values in eq. (6.48) for the die exit velocity u_0 and length L , the Weissenberg number $Ws=\lambda$, and for the Newtonian fluid $Ws=0$. Thus, the numerical solution to the casting of a Newtonian fluid can be used to ensure the numerical solution with the modified K-BKZ model is accurate.

Figure 6.2 shows the numerical results of the modified K-BKZ model for film casting (with $\lambda_1=0.001$) along with the numerical solution for a Newtonian fluid with an aspect ratio $A=0.8$ and a draw ratio $D_R=10$. Agreement with the numerical Newtonian solution is excellent. Also shown in Figure 6.2 are the results from Silagy et al. (1996) for $A=0.8$ and $D_R=10$. Agreement with the results of Silagy et al. (1996) is also excellent. The agreement with the Newtonian solution and that of Silagy et al. (1996) is proof the numerical scheme with the modified K-BKZ model is accurate at low Weissenberg numbers.

6.5.2 Film Casting of a Newtonian Fluid - Comparisons with Three - Dimensional Simulations

Isothermal three-dimensional simulations have been conducted by Sakaki et al. (1996) for a Newtonian fluid. The three-dimensional analysis can predict the edge-bead effect, which cannot be accounted for with the current one-dimensional formulation. However, Sakaki et al. (1996) have included results for the neck-in effect at different draw ratios (D_R), which can be predicted with the current formulation. Three-dimensional simulations take a great deal of computing time compared to one-dimensional simulations.

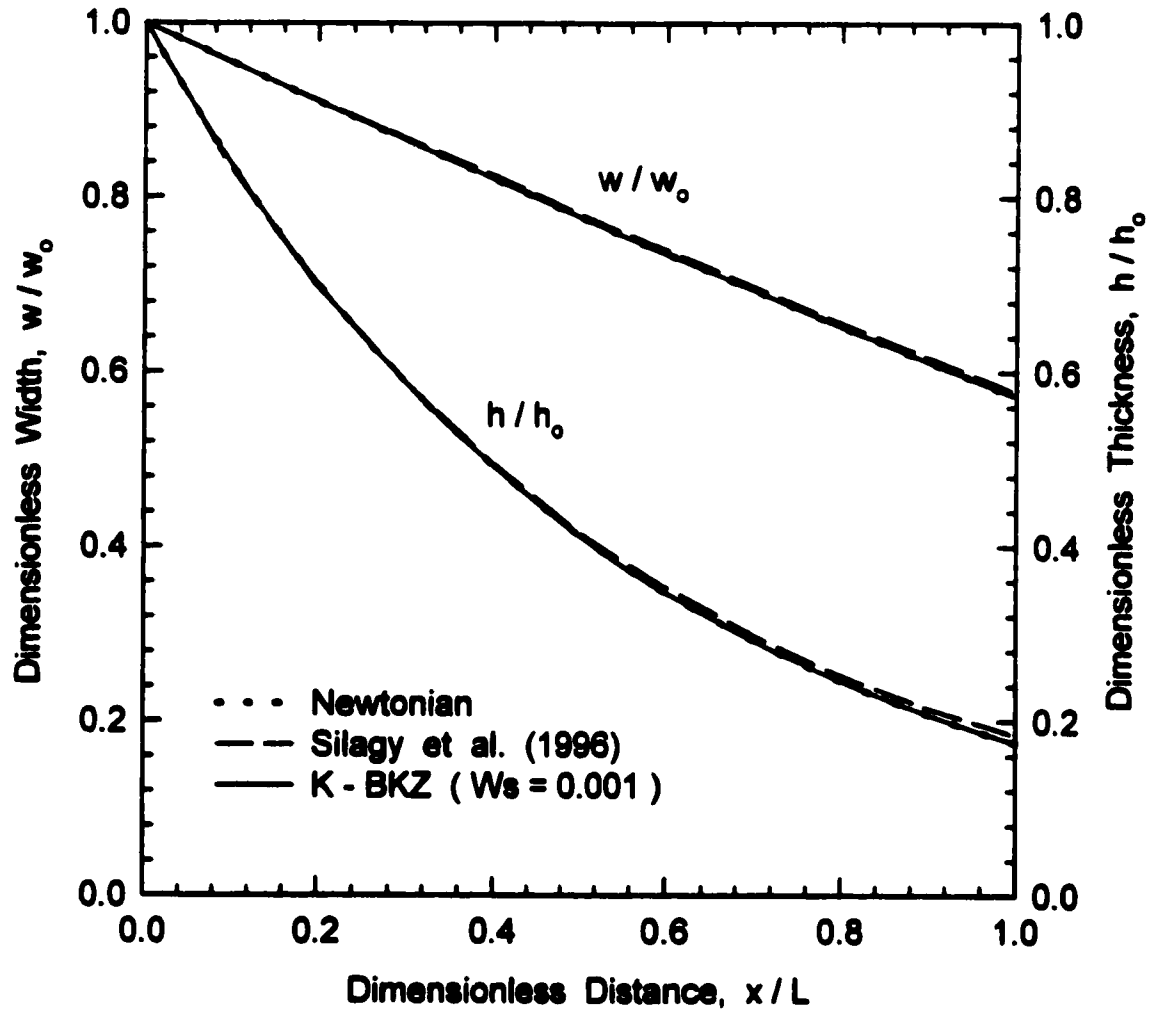


Figure 6.2: Film casting of a Newtonian fluid. Thick dotted lines represent the numerical solution of the Newtonian model with $A=0.8$ and $D_R=10$, dashed lines represent the numerical solution of Silagy et al. (1996), and full lines represent the numerical solution with the modified K-BKZ model with $N=1$ and $\lambda_I=0.001$ ($W_s=0.001$).

The operating conditions used in the simulations by Sakaki et al. (1996) with their results for the neck-in effect are: $w_o=5.0$ cm, $h_o=0.1$ cm, and $u_o=5$ cm/s. Two different lengths from the die exit to the chill roll were used in the simulations: $L=5$ cm and $L=10$ cm. Figure 6.3 shows the results for the final film width (w_L / w_o) as a function of the draw ratio from the current simulations and from the simulations of Sakaki et al. (1996), under the same conditions. The trends for the final film width as a function of draw ratio for the current simulations for both lengths ($L=5$ cm and $L=10$ cm) differ considerably from the simulations of Sakaki et al. (1996). The current simulations predict a smaller final film width at lower draw ratios and a greater final width at higher draw ratios, for both film lengths. Intuitively, the current simulations should predict a greater final width for all draw ratios, due to the ability of the three-dimensional analysis to predict the edge-bead effect. However, the three-dimensional simulations involve 3 velocities in the x -, y -, and z -direction, respectively. This causes the counter-intuitive effects in terms of the final film width.

6.5.3 Film Casting of an Upper – Convected Maxwell (UCM) Fluid

The film casting of a UCM fluid was again first solved by Silagy et al. (1996) at a Weissenberg number $Ws=0.04$ for an aspect ratio $A=0.6$ and a draw ratio $D_R=20$. Since the modified K-BKZ constitutive model can be reduced to the UCM model, simulations for a UCM fluid are possible and the numerical scheme can be validated for viscoelastic fluids at higher Weissenberg numbers. The modified K-BKZ constitutive model reduces to the UCM model when $N=1$ with $\alpha \rightarrow +\infty$, or say a large number ($\alpha=10,000$). Initial simulations were unable to reproduce the results of Silagy et al. (1996) for the UCM model. It was discovered that an error was committed by Silagy et al. (1996) in their formulation with the UCM model. A factor of 2 was missing from the equation of continuity, eq. (6.1), which impacted the dimensionless equations and influenced the final form of the governing equations. Equations (6.34) through (6.37) represent the corrected final form of the governing equations.

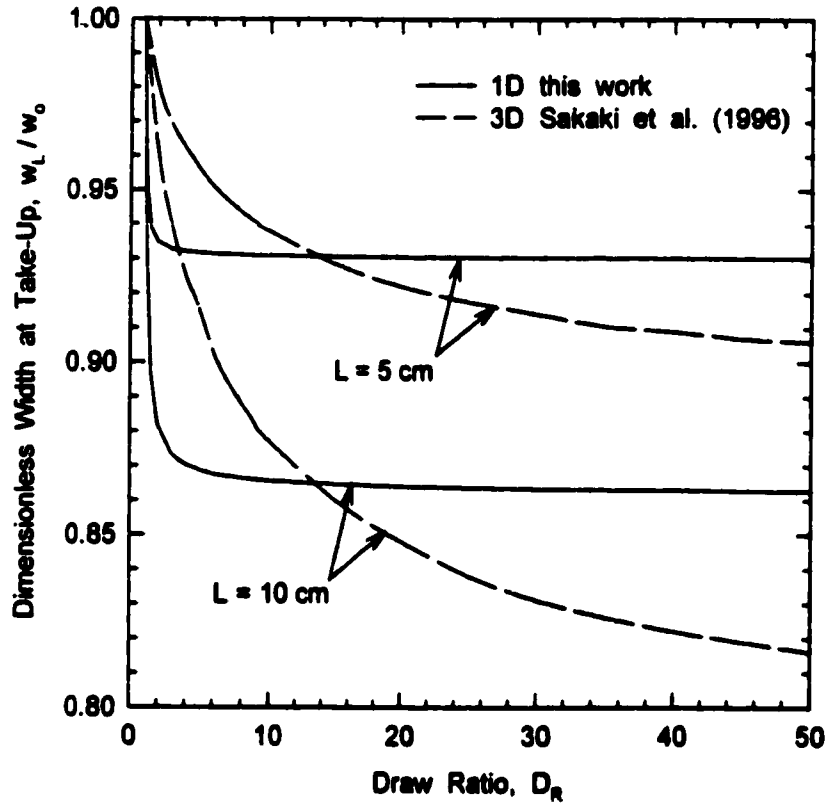


Figure 6.3: Neck-in effect (w_L/w_0) as a function of draw ratio for the film casting of a Newtonian fluid. Dashed lines represent the three-dimensional numerical solution of Sakaki et al. (1996), and full lines represent the current one-dimensional numerical solution.

Figure 6.4 shows the results of the current solution for the UCM model at an aspect ratio $A=0.6$, a draw ratio $D_R=20$, and a Weissenberg number $W_s=0.04$, along with the numerical solution for the modified K-BKZ model reduced to the UCM model, under the same conditions. Unit values were again used for the die exit velocity u_0 and length L , which gives the relation $W_s=\lambda$. The boundary condition for the die exit width was given a value of $w_0=1.667$ which corresponds with $A=0.6$. Agreement of the numerical

solutions for the UCM model and the modified K-BKZ model with $N=1$ and $\alpha=10,000$ is excellent. This confirms that the numerical scheme with the modified K-BKZ model is accurate for viscoelastic fluids of higher Weissenberg numbers. The continuation procedure used in order to reach the final Weissenberg number of $Ws=0.04$, which was the maximum for this numerical scheme, is given in Table 6.2. The continuation procedure of Table 6.2 is similar for subsequent simulations where continuation is required.

Table 6.2: Continuation procedure used in the simulations with the UCM model to reach the maximum Weissenberg number of $Ws = 0.04$.

Continuation step	Weissenberg number, Ws
1	0 (Newtonian)
2	0.02
3	0.03
4	0.035
5	0.038
6	0.039
7	0.04

6.5.4 Film Casting of an Upper – Convected Maxwell (UCM) Fluid - Comparisons with Two – Dimensional Simulations

Isothermal two-dimensional simulations have been conducted by Debbaut et al. (1995) for the Newtonian model and the UCM model. The two-dimensional analysis by Debbaut et al. (1995) also accounts for the edge-bead effect with an additional differential equation, much like the current analysis, which accounts for the neck-in effect. The current one-dimensional analysis cannot predict the edge-bead effect; only two- and three-dimensional formulations can account for the edge-bead effect. However, the one-dimensional approach is much faster than the two- and three-dimensional formulations.

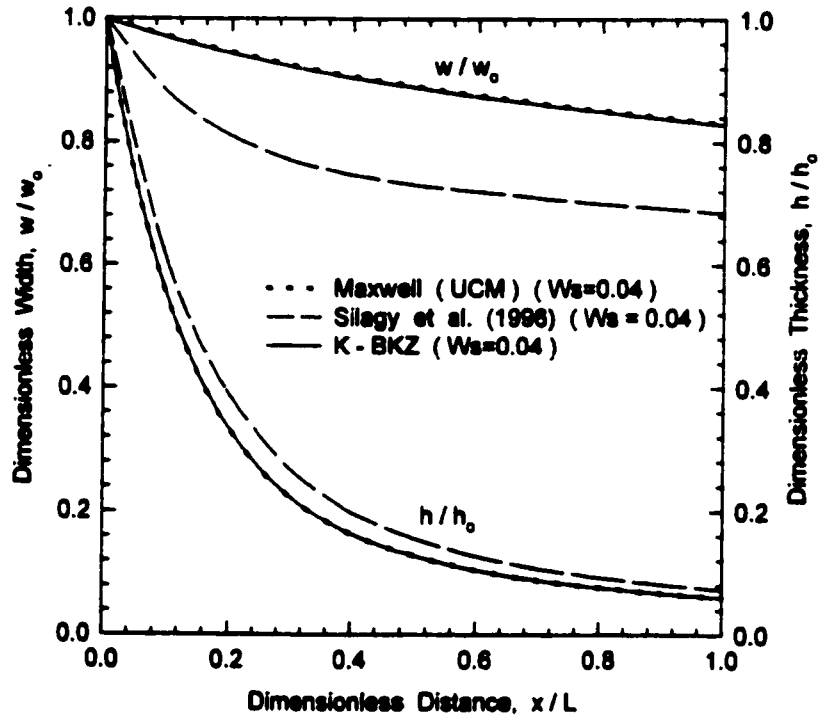


Figure 6.4: Film casting of a UCM fluid. Thick dotted lines represent the numerical solution of the UCM model with $A=0.6$, $D_R=20$, and $Ws=0.04$, while full lines represent the numerical solution with the modified K-BKZ model with $N=1$ and $\alpha=10,000$. Dashed lines represent the UCM solution of Silagy et al. (1996) which contained an error in derivations.

Figure 6.5 shows the current results for the neck-in effect (w_L/w_0) as a function of the draw ratio (D_R) for both the Newtonian model and the UCM model. Also shown are the results of Debbaut et al. (1995) under identical conditions. The operating conditions used in the simulations by Debbaut et al. (1995) are: $w_0=50.0$ cm, $h_0=0.05$ cm, $u_0=10$ cm/s, and $L=50$ cm. With this information, the relaxation time required for a given Weissenberg number (Ws) is $\lambda=5 \cdot Ws$. Agreement between the current results and those of Debbaut et al. (1995) for the Newtonian model is good for small draw ratios ($D_R < 3$) but poor at higher draw ratios ($3 < D_R < 40$). This was not surprising since the three-dimensional comparisons with the Newtonian model were also poor. This is again due to the ability of the two-dimensional analysis to predict the edge-bead effect, where a one-dimensional analysis is incapable of predicting the effect.

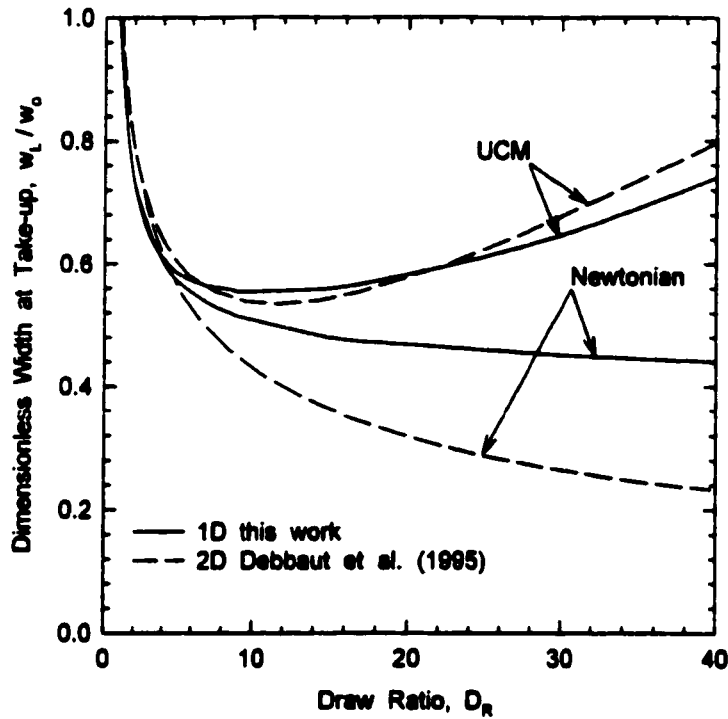


Figure 6.5: Comparison of current simulations with two-dimensional simulations of Debbaut et al. (1995) in terms of final width (neck-in effect) at different draw ratios (D_R). Full lines represent the current simulations and dashed lines represent simulations of Debbaut et al. (1995).

With respect to the UCM model, from Figure 6.5, the current results agree quite well with the results of Debbaut et al. (1995), especially taking into account the differences in each formulation (i.e. two-dimensional approach versus one-dimensional approach). The agreement is due to the *sharp* edge-bead effect resulting from the high elasticity of the UCM model, opposite to the behaviour of Newtonian model. To illustrate this, Figure 6.6 depicts briefly the predicted edge-bead effect from the two-dimensional analysis of Debbaut et al. (1995) for both the Newtonian model and the UCM model. The predicted edge-bead effect from the Newtonian model is greater in cross-sectional area and thus greatly alters the other dimensions (i.e. thickness at the centerline and width). The predicted edge-bead effect from the UCM model is *sharper* (i.e. less cross-sectional area) and lessens the significance on the thickness and width. Thus, for a viscoelastic material such as that encountered with the UCM model, the one-dimensional and two-dimensional analyses give similar predictions for the neck-in effect.

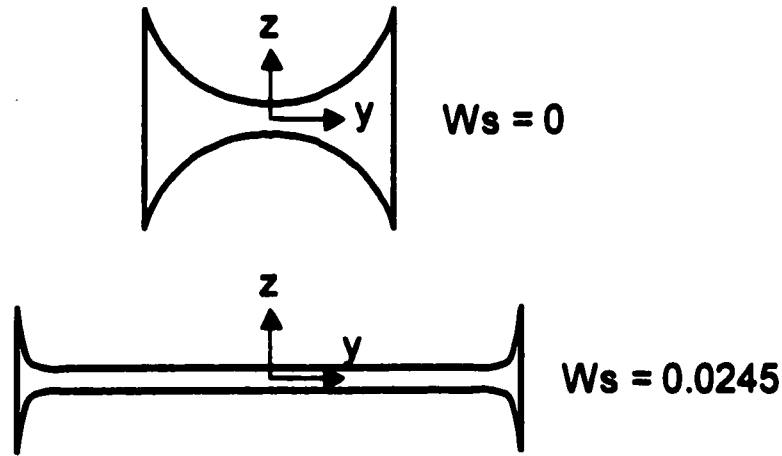


Figure 6.6: Edge-bead effect from simulations of Debbaut et al. (1995) for the Newtonian model and the upper-convected Maxwell (UCM) model. At a given cross-section, the Newtonian edge-bead occupies a larger area while the UCM edge-bead is *sharper*.

Figure 6.7 shows the dimensionless thickness (h/h_0) as a function of dimensionless distance (x/L) along the centerline of the film for different Weissenberg numbers (Ws) at a draw ratio of $D_R=40$. With respect to the current analysis, the thickness of the film at the centerline is the same as that at the edge of the film. With respect to the two-dimensional analysis of Debbaut et al. (1995), the thickness of the film at centerline is different than the thickness at the edge of the film due to the edge-bead effect. In industrial operations, the edge-bead is simply trimmed to produce a film of uniform thickness. Thus, the thickness at the centerline is the final film thickness in industrially produced films and is important in terms of film-casting simulations. The agreement between the current results and those of Debbaut et al. (1995) for the film thickness at the centerline is fair for low Weissenberg numbers ($Ws \approx 0$ and $Ws = 0.01$). However, at higher Weissenberg numbers ($Ws = 0.02$ and $Ws = 0.0245$), agreement between the current results and those of Debbaut et al. (1995) is very good. At the maximum Weissenberg number for these simulations, $Ws = 0.0245$, agreement is excellent. As mentioned earlier, the

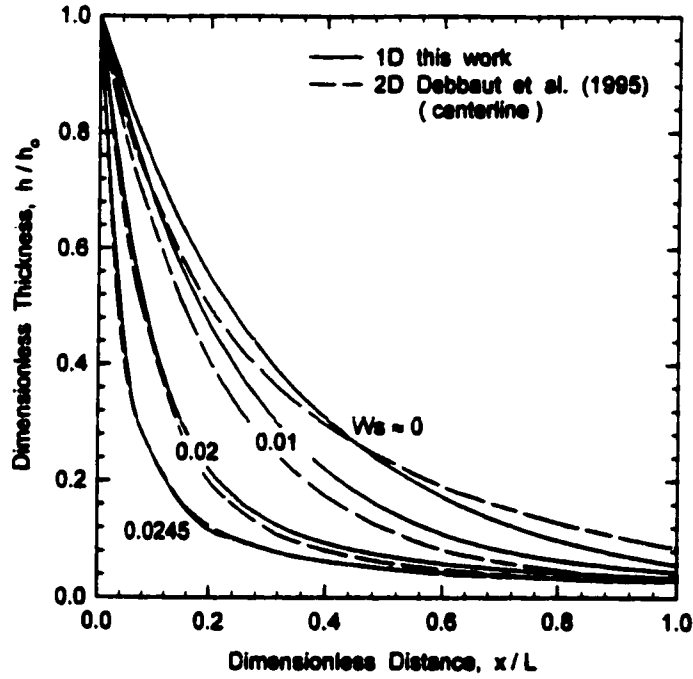


Figure 6.7: Comparison of current simulations with two-dimensional simulations of Debbaut et al. (1995) in terms of thickness profiles at $D_R = 40$ and for different Weissenberg numbers (Ws). Full lines represent the current simulations and dashed lines represent simulations of Debbaut et al. (1995).

edge-bead effect for elastic materials is sharper and has a lesser effect on the thickness and width. Therefore, the one-dimensional and two-dimensional analyses give similar viscoelastic predictions for the neck-in effect *and* the film thickness at the centerline, which are industrially important.

6.5.5 Parametric Study with K-BKZ Nonlinear Parameters (α, β, θ)

A parametric study is conducted here, in relation to the nonlinear parameters α , β , and θ in the K-BKZ model (eq. (5.16)), to obtain a better understanding of the rheological effects in the film-casting process. The effects of changing the nonlinear parameters in the K-BKZ model on the rheological functions (e.g. shear viscosity, first normal stress difference, etc.) have already been described in Chapter 3 (see Figures 3.8 through 3.10). The simulations are performed in the same manner as the UCM simulations, i.e., unit values were used for the die exit velocity u_0 and length L , which gives the relation $Ws = \lambda$. The boundary condition for the die exit width was given a value

of $w_0=1.667$, which corresponds with $A=0.6$. The Weissenberg number for the parametric study is $Ws = 0.03$.

Figure 6.8 shows the effect of changing α , the *shear-thinning parameter*, on the film thickness, width, and velocity. As α increases, so does the uniaxial viscosity at higher extensional rates (decrease in extension-thinning effect), which makes the material more difficult to deform. Therefore, we expect to see a more linear velocity profile in the film velocity, with a greater decrease in the radial profile near the die exit, and a lesser neck-in effect (less deformation). This is exactly portrayed in Figure 6.8. It is also interesting to note that at the lowest value of α ($\alpha = 10$), the film velocity profile is beyond the Newtonian profile, and similarly for the film thickness profile. The width is less affected by the change in α than the film velocity and film thickness.

Figure 6.9 shows the effect of changing β , the *extension-thinning parameter*, on the film thickness, width, and velocity. The film-casting process is only minimally affected by changes in β . Nonetheless, the effects are still visible and some conclusions can be drawn. From Figure 6.9, an increase in β causes the velocity profile to become slightly less linear, which suggests that the deformation is uniaxial due to the decrease in uniaxial viscosity. No change in the film-casting variables would have been noticed with a change in β if the deformation type was planar extension, since β has no effect on the planar extensional viscosity (see Chapter 3). Biaxial extension is ruled out, since stretching in the second or third dimension is required (Larson, 1988). Therefore, the film-casting process, with the differential equations presented in Chapter 3, is dominated by uniaxial extension. In reality, the film-casting process is a combination of uniaxial and planar deformation (see Dobroth and Erwin, 1986).

Finally, Figure 6.10 shows the effect of changing θ , the *normal stress parameter*, on the film thickness, width, and velocity. As the value of θ (negative) increases to zero, the uniaxial viscosity at higher extensional rates increases slightly, which makes the material slightly more difficult to deform. Figure 6.10 shows the same trend as Figures 6.8 and 6.9; increasing the uniaxial viscosity causes the film velocity to become more linear, with a greater decrease in the thickness profile near the die exit, and a lesser neck-in effect.

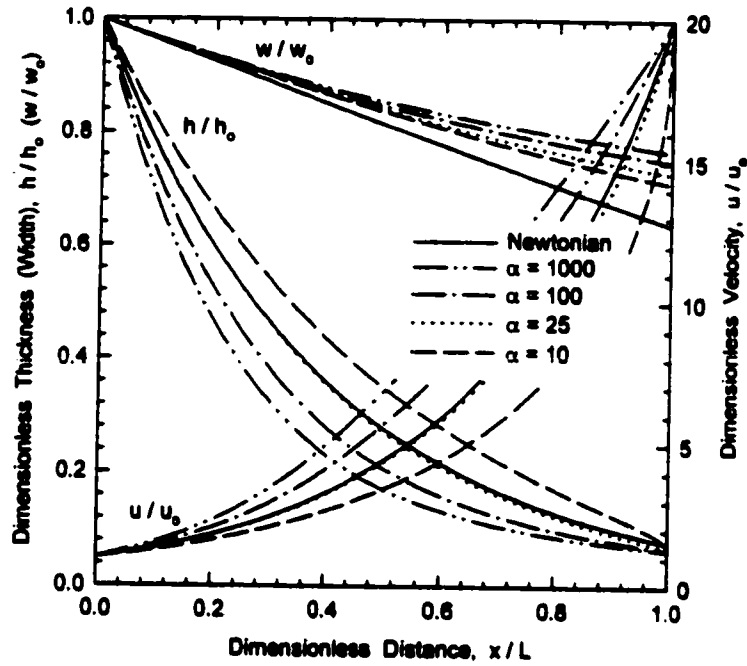


Figure 6.8: Effect of changing the nonlinear parameter α (shear-thinning parameter) in the K-BKZ model on the film thickness, width, and velocity for $A=0.6$ and $Ws=0.03$. In each case, $\beta=0.5$ and $\theta=0$.

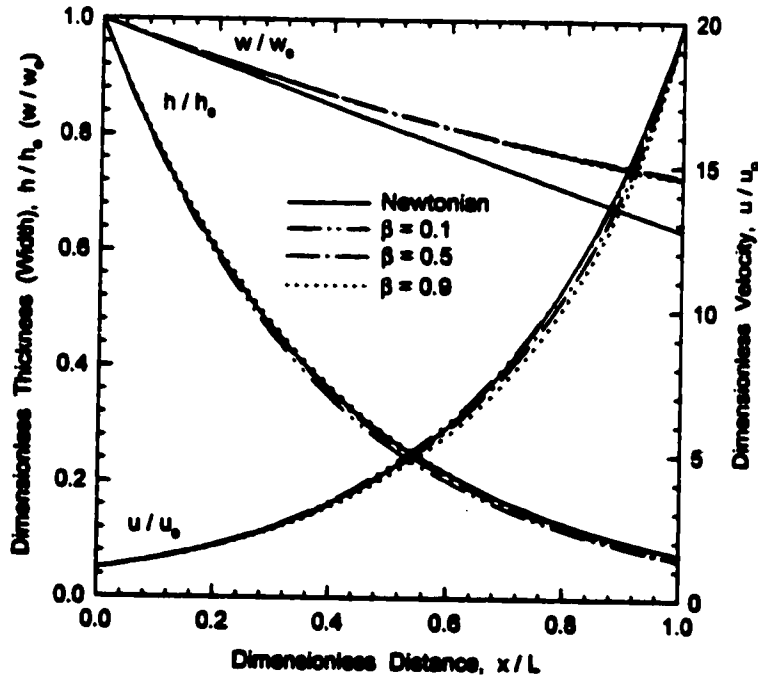


Figure 6.9: Effect of changing the nonlinear parameter β (extension-thinning parameter) in the K-BKZ model on the film thickness, width, and velocity for $A=0.6$ and $Ws=0.03$. In each case, $\alpha=25$ and $\theta=0$.

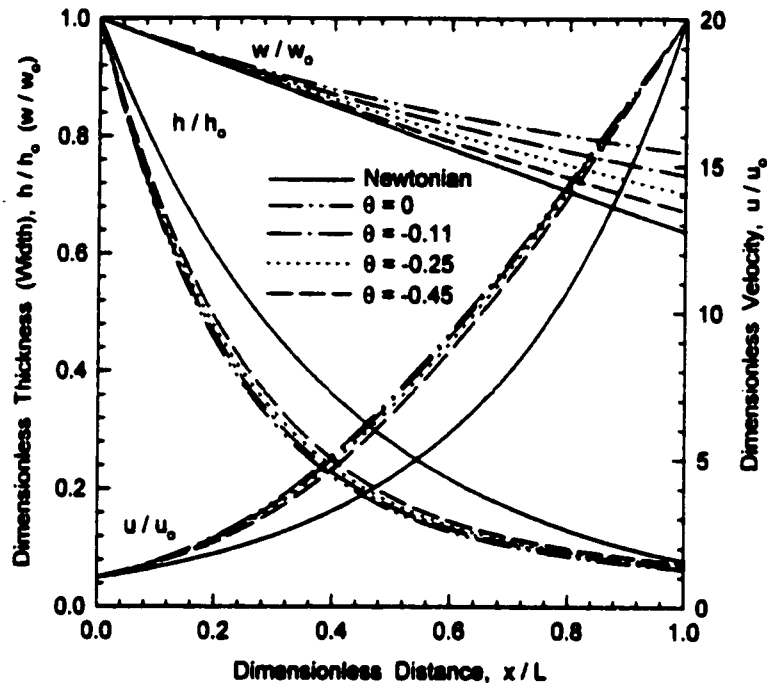


Figure 6.10: Effect of changing the nonlinear parameter θ (normal stress parameter) in the K-BKZ model on the film thickness, width, and velocity for $A = 0.6$ and $Ws = 0.03$. In each case, $\alpha = 1000$ and $\beta = 0.5$.

6.5.6 Non – Isothermal Film Casting of Polymer Melts

Kase (1974) conducted non-isothermal film-casting experiments for a polypropylene (PP) melt at 215°C. Measurements of the film thickness and the film temperature were taken with respect to distance for two draw ratios (D_R). However, due to lack of information in the study by Kase (1974), only the experiment with a draw ratio of $D_R = 33.0$ is simulated. Also, the width is assumed a value of $w_o = 1000$ cm, which is typical in relation to the length of the film ($w_o / L \approx 10 \rightarrow 20$). The operating conditions used in the simulation of the experiment conducted by Kase (1974) are: $w_o = 1000$ cm, $h_o = 0.1$ cm, $u_o = 1.04$ cm/s, $L = 80$ cm, and $D_R = 33$. A full account of operating conditions used for the simulations is given in Table 6.3. Alaie and Papanastasiou (1991) had previously simulated this data with a one-dimensional approach with no variation of

the film width. The experimental data by Kase (1974) is simulated here to examine the predictive qualities of the current numerical scheme with respect to real polymer melts.

Table 6.3: Operating (boundary) conditions used in the simulations for the experiments conducted by Kase (1974) for a PP melt at 215°C. Other parameters used in the simulations with the PP melt are also given.

Die-exit width, $w_o = 1000$ cm
Die-exit thickness, $h_o = 0.1$ cm
Die-exit velocity, $u_o = 1.04$ cm s ⁻¹
Length, $L = 80$ cm
Draw ratio, $D_R = 33.0$
Reference temperature $T_{ref} = 473$ K (200°C)
Density $\rho_o = 1.0$ g cm ⁻³
Activation energy $E = 57500$ J mol ⁻¹
Specific heat $c_p^o = 2.30 \times 10^7$ erg g ⁻¹ K ⁻¹

Figure 6.11 shows the rheological data for the shear viscosity (η_s) for polypropylene (PP) at 200°C taken from Ishizuka and Koyama (1980), along with the predictions from the modified K-BKZ constitutive model, Eq. (61). The relaxation spectrum used for the predictions is given in Table 6.4. The rheological data of Ishizuka and Koyama (1980) was used in this study since the grade of the PP in the study of Kase (1974) was not given. This is the same rheological data that Alaie and Papanastasiou (1991) used in their simulations of the Kase experiments (1974).

Figure 6.12 shows the current simulation results for the thickness profile for the draw ratio of $D_R = 33$ along with the experimental measurements by Kase (1974). Good overall agreement is obtained with the experimental data of Kase (1974) with subtle differences. The prediction for the final thickness of the film (3.16 μm) is only slightly higher than the experimentally observed final thickness of 3.0 μm (5.7% error). As mentioned earlier, the final uniform thickness of the film is industrially important. Figure 6.13 shows the current simulation results for the temperature profile for the draw ratio of

$D_R = 33$ along with the experimental measurements by Kase (1974). Again, good overall agreement is obtained with the experimental data of Kase (1974) in terms of temperature. With the overall agreement between the simulations and experiments by Kase (1974), the current numerical scheme demonstrates itself as a useful tool for quantitative predictions of film thickness and temperature.

Table 6.4: Relaxation spectrum and associated parameters for a PP melt at 200°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 5.50$, $\beta = 0.2$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)
1	0.001	82200
2	0.1	42200
3	1	14000
4	10	248
5	100	1.01
6	1000	0.173

6.5.7 Non – Isothermal Film Casting of Polymer Melts - Parametric Study

A parametric study is undertaken for a PET melt and the IUPAC-A LDPE melt since there is a lack of experimental data in the literature. The operating conditions chosen are the same as those of the two-dimensional analysis of Debbaut et al. (1995) since they reflect the usual operating conditions used in industry. The operating conditions are restated here for ease and completeness: $w_o=50.0$ cm, $h_o=0.05$ cm, $u_o=10$ cm/s, and $L=50$ cm. The inlet temperature for the PET simulations was $T_o=260^\circ\text{C}$ while the inlet temperature for the IUPAC-A LDPE simulations was $T_o=150^\circ\text{C}$. The draw ratio (D_R) ranges from $D_R=1 \rightarrow 40$, as in the analysis of Debbaut et al. (1995). A full account of operating conditions used in the simulations is given in Table 6.5.

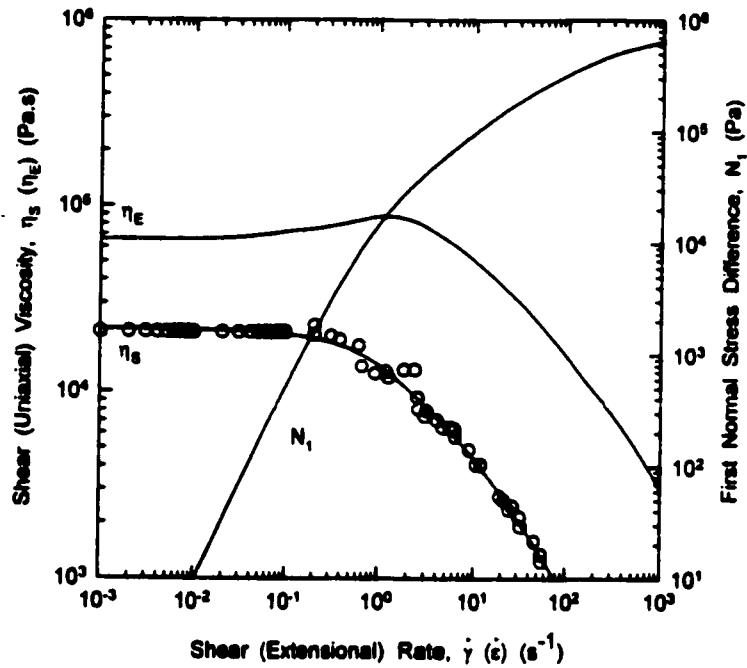


Figure 6.11: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for a PP melt at 200°C. Symbols represent experimental measurements from Ishizuka and Koyama (1980) while lines represent predictions from the modified K-BKZ constitutive model, eq. (6.40), with the relaxation spectrum of Table 6.4.

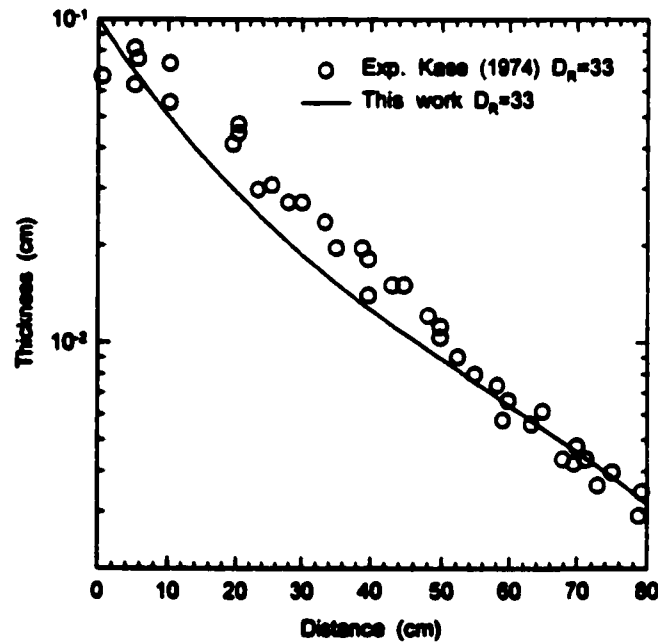


Figure 6.12: Thickness profile for the film casting of a PP melt at 215°C and a draw ratio of $D_R = 33$. Symbols represent measurements by Kase (1974) and lines represent current simulations.

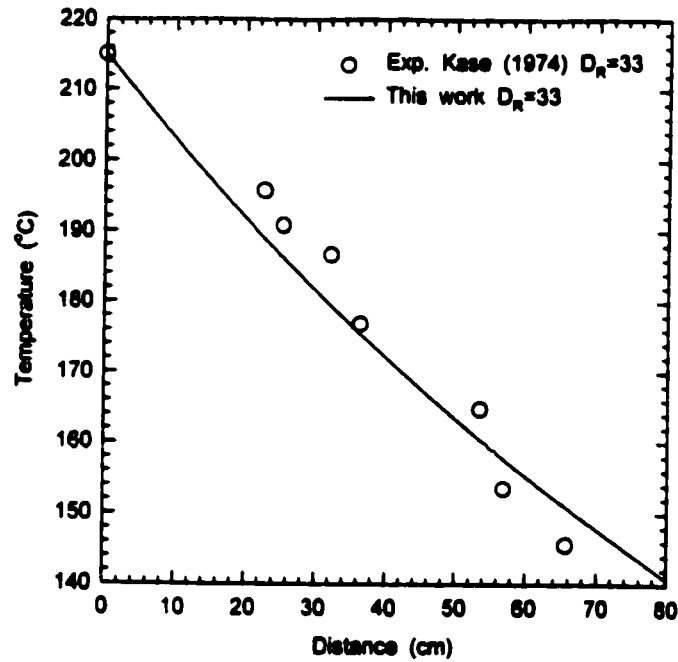


Figure 6.13: Temperature profile for the film casting of a PP melt at 215°C and a draw ratio of $D_R = 33$. Symbols represent measurements by Kase (1974) and lines represent current simulations.

Table 6.5: Operating (boundary) conditions used in the simulations for the parametric study with a PET melt at 260°C and the IUPAC-A LDPE melt at 150°C. Other parameters used in the simulations are also given.

PET	IUPAC-A LDPE
Die-exit width, $w_o = 50$ cm	Die-exit width, $w_o = 50$ cm
Die-exit thickness, $h_o = 0.05$ cm	Die-exit thickness, $h_o = 0.05$ cm
Die-exit velocity, $u_o = 10$ cm s ⁻¹	Die-exit velocity, $u_o = 10$ cm s ⁻¹
Length, $L = 50$ cm	Length, $L = 50$ cm
Draw ratio, $D_R = 1 \rightarrow 40$	Draw ratio, $D_R = 1 \rightarrow 40$
Reference temperature, $T_{ref} = 533$ K	Reference temperature $T_{ref} = 423$ K
Density $\rho_o = 1.0$ g cm ⁻³	Density $\rho_o = 0.95$ g cm ⁻³
Activation energy $E = 48063$ J mol ⁻¹	Activation energy $E = 57500$ J mol ⁻¹
Specific heat $c_p^o = 3.20 \times 10^7$ erg g ⁻¹ K ⁻¹	Specific heat $c_p^o = 2.30 \times 10^7$ erg g ⁻¹ K ⁻¹

Figure 6.14 shows the rheological data for the shear viscosity (η_s) and extensional viscosity (η_E) for PET at 260°C taken from Christodoulou et al. (1997), along with the predictions from the modified K-BKZ constitutive model, eq. (6.40). The discrepancy between the experimental measurements and model predictions at lower shear rates for the extensional viscosity (η_E) is due to the highly Boger fluid behaviour of the PET melt. The relaxation spectrum used for the predictions is given in Table 6.6. Figure 6.15 shows the rheological data for the shear viscosity (η_s), the extensional viscosity (η_E), and the first normal stress difference (N_1) for the IUPAC-A LDPE at 150°C taken from Meissner (1975), along with the predictions from the modified K-BKZ constitutive model, eq. (6.40). The relaxation spectrum used for the predictions is given in Table 6.7.

Table 6.6: Relaxation spectrum and associated parameters for a PET melt at 260°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\theta = -0.111$).

k	λ_k (s)	a_k (Pa)	α_k	β_k
1	0.00140	508000	9.20	0.99
2	0.0187	53400	2.59	0.99
3	0.399	495	30.4	0.0614

Table 6.7: Relaxation spectrum and associated parameters for the IUPAC-A LDPE at 150°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 14.38$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)	β_k
1	1.0×10^{-4}	$1.29 \times 10^{+5}$	0.018
2	1.0×10^{-3}	$9.48 \times 10^{+4}$	0.018
3	1.0×10^{-2}	$5.86 \times 10^{+4}$	0.08
4	1.0×10^{-1}	$2.67 \times 10^{+4}$	0.12
5	$1.0 \times 10^{+0}$	$9.80 \times 10^{+3}$	0.12
6	$1.0 \times 10^{+1}$	$1.89 \times 10^{+3}$	0.16
7	$1.0 \times 10^{+2}$	$1.80 \times 10^{+2}$	0.03
8	$1.0 \times 10^{+3}$	$1.00 \times 10^{+0}$	0.002

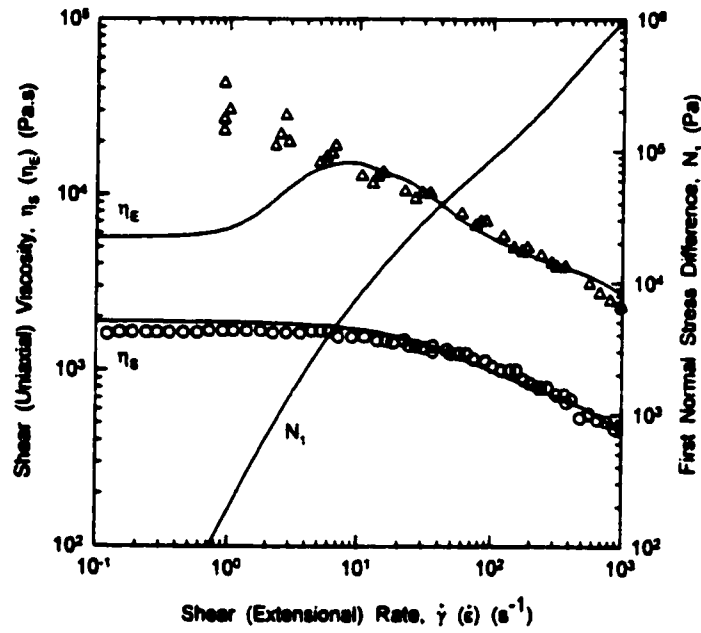


Figure 6.14: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for a PET melt at 260°C. Symbols represent experimental measurements from Christodoulou et al. (1997), while lines represent predictions from the modified K-BKZ constitutive model, eq. (6.40), with the relaxation spectrum of Table 6.6.

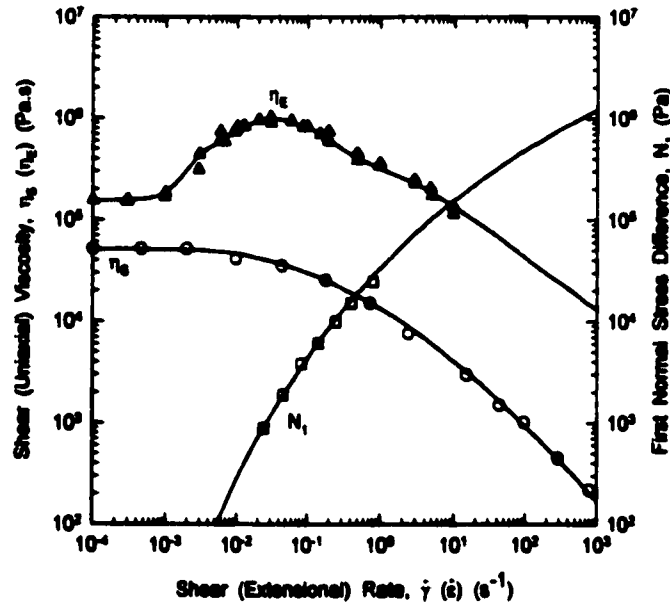


Figure 6.15: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial viscosity (η_E) for the IUPAC-A LDPE melt at 150°C. Symbols represent experimental measurements from Meissner (1975), while lines represent predictions from the modified K-BKZ constitutive model, eq. (6.40), with the relaxation spectrum of Table 6.7.

Figure 6.16 shows the simulation results for the PET melt with $Ws = 0.0104$ and the IUPAC-A LDPE melt with $Ws = 11.7484$ in terms of the neck-in effect (w_l/w_o) as a function of the draw ratio (D_R). Also shown are the current simulation results for the Newtonian model and the upper-convected Maxwell (UCM) model (see section 6.4.4). The neck-in effect for the PET melt behaves much like the results from the Newtonian model, whereas the neck-in effect for the IUPAC-A LDPE behaves like a combination of results from the Newtonian model and the UCM model. The resemblance of the PET results with the Newtonian results can be explained with a useful rheological term known as the Trouton ratio (T_R). The Trouton ratio is a measure of viscoelasticity, and is given as

$$T_R = \frac{\eta_E(\dot{\epsilon})}{\eta_S(\dot{\gamma})} \quad (6.58)$$

A Trouton ratio value of $T_R=3$ signifies Newtonian behaviour while higher values indicate increased elasticity of the material. Figure 6.17 shows the Trouton ratios for both the PET melt and the IUPAC-A LDPE melt at different extensional rates, along with the predictions for the Newtonian model and the UCM model. The Trouton ratio for the PET melt is low and near the Newtonian value of 3 for most extensional rates, whereas the Trouton ratio for the IUPAC-A LDPE is very high and is unlike the Newtonian model. Thus, the PET melt is expected to behave like the Newtonian model, while the IUPAC-A LDPE melt is expected to behave like a combination of the Newtonian model and the UCM model.

6.6 Concluding Remarks

Numerical viscoelastic simulations have been undertaken for the film-casting process with the code F-CAST. The film-casting process, with the governing equations presented in Chapter 3, is another example of uniaxial extensional flow. In reality, the film-casting process is a combination of planar and uniaxial extensional flow. The governing equations, first presented in Chapter 3, were made dimensionless. Relations for the melt density, heat capacity, and heat transfer coefficient as a function of distance along the film were presented. Specifics concerning the numerical solution of the governing

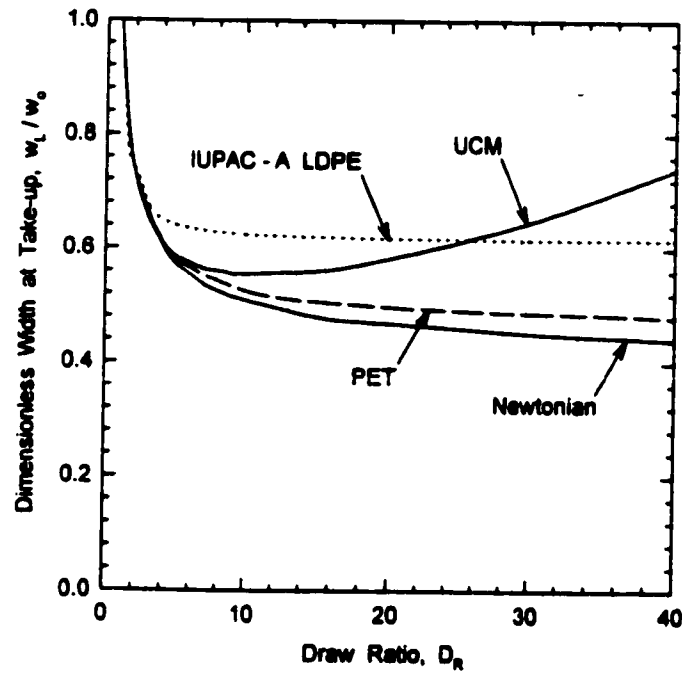


Figure 6.16: Neck-in effect as a function of draw ratio for a PET melt at 260°C and $Ws = 0.0104$, and the IUPAC-A LDPE melt at 150°C and $Ws = 11.7484$ (full lines). Also shown are the current results from the Newtonian model and UCM model (dashed lines).

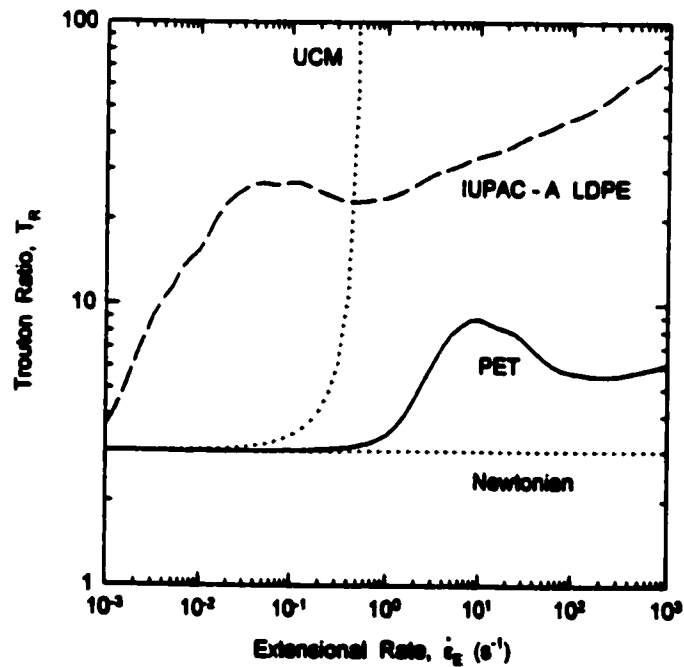


Figure 6.17: Trouton ratio (T_R) as a function of extensional rate for a PET melt at 260°C and the IUPAC-A LDPE melt at 150°C. Also shown are the Trouton ratio values for the Newtonian model and the UCM model.

equations with the Newtonian model, UCM model, and the modified K-BKZ equation were also presented.

The isothermal film casting with the Newtonian model and UCM model were properly solved with a 4th-order Runge-Kutta numerical scheme. The film-casting solutions with the UCM model, first derived from Silagy et al. (1996), contained an error in the calculations, which was rectified with the current formulation. The solutions for the Newtonian and UCM models were used to validate the viscoelastic film casting with the modified K-BKZ integral constitutive model, reduced to the Newtonian and UCM models. Consequently, the validity of the numerical scheme with the modified K-BKZ model was established at low and high Weissenberg (Ws) numbers. However, the Newtonian and UCM models do not predict the behaviour of real polymer melts. The Newtonian model predicts a constant uniaxial viscosity (see Chapter 3) while the UCM model predicts a uniaxial viscosity, which eventually reaches infinity (see Chapter 3). Therefore, the K-BKZ model, which predicts accurately the behaviour of real polymer melts, has been used as the workhorse for the simulations.

Comparisons were also made with previous simulations of higher-dimension, namely two-dimensional (Debbaut et al., 1995) and three-dimensional (Sakaki et al., 1996) solutions. Comparisons were made with the three-dimensional solutions of Sakaki et al. (1996) for the Newtonian model, where agreement was poor. Comparisons with the Newtonian model for the two-dimensional solutions of Debbaut et al. (1995) were also poor. However, good overall agreement was achieved with the UCM model for the two-dimensional solution of Debbaut et al. (1995), with respect to the final width (neck-in effect) and the film thickness at the centerline along the film. The agreement was attributed to the sharp edge-bead effect predicted by the UCM model. Therefore, one-dimensional and two-dimensional viscoelastic film-casting simulations yield approximate results.

The non-isothermal film casting of a PP melt was also simulated for experimental measurements conducted by Kase (1974). Alaie and Papanastasiou (1991) have previously simulated this data with a one-dimensional K-BKZ formulation without predictions for the film width. The work by Alaie and Papanastasiou (1991) lacked proper rheological characterization, without explanation as to the choice of rheological

parameters used in the K-BKZ model. The experimental data by Kase (1974) is simulated here to ensure the current numerical scheme can adequately predict experiments, along with the proper rheological characterization of the PP melt.

Additional non-isothermal film-casting simulations were undertaken for a PET melt and the IUPAC-A LDPE melt in a parametric study. The geometrical boundary conditions were fixed and only the effects of increased draw ratio were examined. In terms of the neck-in effect, the results for the PET melt resembled most the results from the Newtonian model. The results for the IUPAC-A LDPE resembled a combination of results from the Newtonian model and the UCM model, corresponding to viscoelastic behaviour. The film-casting behaviour of both melts was explained in terms of the Trouton ratio (T_R), where a Trouton ratio value of $T_R=3$ signifies Newtonian behaviour and a high Trouton ratio value signifies high viscoelasticity. Corresponding with the Trouton ratio results for both melts, the PET melt is expected to behave like a Newtonian fluid, while the IUPAC-A LDPE is expected to behave like a combination of a Newtonian fluid and a UCM fluid.

The objective of this study was to develop an efficient code that can give quick and approximate results for the film-casting process. Since two- and three- dimensional simulations take a great deal of effort and time to develop, the one-dimensional formulation for film casting has been used to develop the code F-CAST. It has the advantages of short computing time with almost guaranteed convergence. It was used to determine the significance of viscoelastic effects and the sensitivity of the results to the parameters in the K-BKZ constitutive equation. The drawback of using a one-dimensional formulation is a loss of information in simplifying a truly three-dimensional problem into a one-dimensional problem. For the film-casting process, this results in not being able to predict the edge-bead effect. Nonetheless, the F-CAST code is very useful for an engineer who desires fast and approximate information or predictions for the film-casting process.

Chapter 7

Film Blowing

In this chapter, non-isothermal viscoelastic simulations are performed for the film-blowing process. The one-dimensional governing equations are restated and specifics concerning the numerical scheme are given. The differential equations are solved using the finite element method (FEM). The resulting code, **F-BLOW**, is then used for film-blowing simulations. The numerical scheme is validated with the Newtonian and upper-convected Maxwell (UCM) solutions. Simulations are then undertaken for a real polymeric material, namely the Stamylan L8 low-density polyethylene (LDPE) melt. Comparisons are also made to previous simulations. Suggestions are made for improving the film-blowing governing equations. A review of the study by Alaie and Papanastasiou (1993) is performed.

7.1 Introduction

The film-blowing process is used throughout the plastics industry to manufacture plastic bags or films that are biaxially oriented. Many attempts have been made to predict and model this complex but important process, which continues to mystify rheologists and polymer processing engineers worldwide. The process is shown schematically in Figure 7.1, where a polymer melt is extruded through an annular die, and biaxial extension is effected by slight internal pressurization (blow-up pressure) and axial drawing (take-up force). Air ring jets surrounding the mid- to upper-portion of the bubble supply cooling air. The height above the die at which solidification occurs, also known as the *freeze line*, can be controlled by the cooling air. The deformation of the bubble, as well as changes in the velocity and temperature, are negligible above the freeze line due to solidification. The bubble dimensions are measured in terms of the *blow-up ratio* and the *draw ratio*. The blow-up ratio (**BUR**) is the ratio of the bubble

radius at the freeze line to the inner die radius, and is typically in the range of 1 to 5. The draw ratio (D_R) is the ratio of the velocity at the freeze line to that of the velocity at the die, and is typically in the range of 5 to 40. The distance from the die to the freeze line ranges from 25 cm to 5 m. The pressure difference across the film is near or about 50 Pa (i.e. pressure inside bubble is 50 Pa higher than atmospheric pressure) (Baird and Collias, 1995). After the freeze line, the bubble is collapsed by a set of guide rolls and taken up by a set of nip rolls that form an airtight seal. Finally, the collapsed tube is wound onto a reel and sold as plastic bags or trimmed at the edges and wound into two reels of film. While the film is being drawn and blown, it undergoes non-uniform *biaxial extension*. The biaxial extension of the film is the primary attraction of the film-blowing process, which increases the strength of the film in two directions and allows for precise control over the mechanical and optical properties of the final product.

Typical industrial goals for the film-blowing process are as follows:

- Increase in take-up speeds without increasing instability. This has been done in the past with improvements in the annular die, leading to such specific designs as the *spider die* and the *spiral mandrel die*.
- A simulation package that can give process engineers an insight into the process. This can also help in design and control of the film-blowing process. Until now, there have not been any successful simulations of the film-blowing process.
- A comprehensive automation system for stable production, consistent efficiency, and higher product quality.

7.2 Literature Review

The analysis of the film-blowing process began with the approach proposed by Pearson and Petrie (1970a,b) by regarding the molten polymer as a thin membrane shell in tension with the use of the Newtonian model. Since the classical analysis of Pearson and Petrie (1970a,b), various simulation studies have emerged for a wide number of rheological models: the power-law model by Han and Park (1975), a crystallization model by Kanai and White (1984), the UCM model by Luo and Tanner (1985) and by Cain and Denn (1988), the Leonov model by Luo and Tanner (1985), the Marrucci model

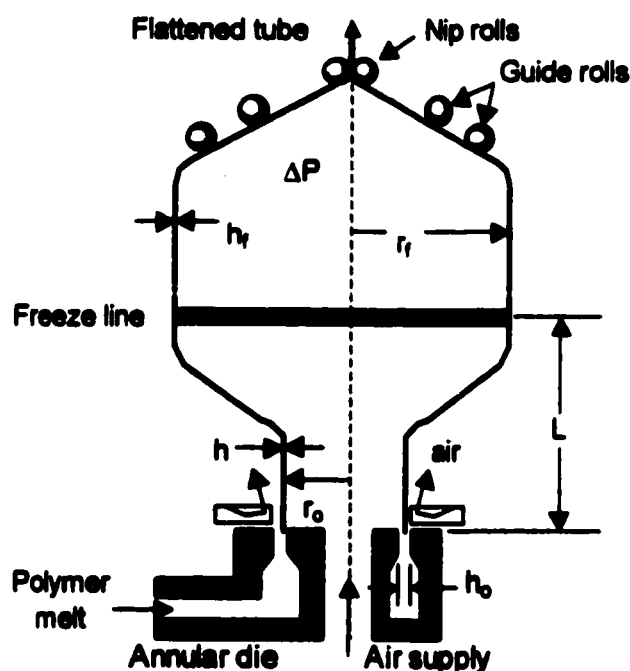


Figure 7.1: Schematic diagram of the film blowing process (from Baird and Collias, 1995).

by Cain and Denn (1988), a viscoplastic-elastic model by Cao and Campbell (1990), and the modified K-BKZ model by Alaie and Papanastasiou (1993). Recently, Sidiropoulos et al. (1996) studied the predictive capabilities of a non-isothermal Newtonian model. The majority of the simulation studies have included non-isothermal effects on the material during film blowing. Kurtz (1995) conducted an investigation of the stresses of the film-blowing process and discovered an error in the work of Alaie and Papanastasiou (1993). Liu et al. (1995a,b) have conducted experiments with different polyethylene melts and proposed a new model without the use of the thin-shell theory proposed by Pearson and Petrie (1970a,b).

Han and Park (1975) conducted isothermal film-blowing experiments. Kanai and White (1984) and Minoshima and White (1986) reported flow instabilities in film-blowing experiments. Film-blowing experiments were conducted by Gupta (1980) for a

polystyrene (PS) melt, and by Tas (1994) for three different grades of LDPE melts. Numerous studies were performed by Ghaneh-Fard et al. (1996a,b, 1997a,b) dealing with birefringence (stress) measurements and flow stability of the film-blowing process.

In each of the aforementioned simulation studies, excluding Alaie and Papanastasiou (1993), proper rheological characterization was not performed and no explanations for the choice of rheological parameters (e.g. relaxation time) were included. The constitutive models used by these studies do not predict the rheological behaviour of *real* polymer melts. In all of the simulation studies, only quantitative agreement was achieved between the simulations and experiments, in terms of the bubble radius, bubble velocity, bubble temperature, take-up force, and blow-up pressure.

7.3 Objectives

This study will present a quick and approximate method of analysis for the film-blowing process with the use of an efficient code, F-BLOW. The objectives of this chapter are as follows:

- a) To solve accurately the one-dimensional film blowing of a Newtonian fluid. Since the Newtonian model does not possess any elastic response, the model is used here only for checking purposes.
- b) To solve accurately the one-dimensional film blowing of a UCM fluid. The UCM model does possess an elastic response, but the predictions for the shear and extensional viscosities are unrealistic, as shown in Chapter 3. The UCM model is used here for checking purposes and to investigate two non-isothermal approaches: the Morland-Lee hypothesis and the shifting of relaxation times.
- c) To solve accurately the one-dimensional film blowing of *real* polymeric fluids. This is done with the use of the K-BKZ integral constitutive model, which predicts well the nonlinear behaviour of polymeric materials. Thus, the K-BKZ model is used for the following set of simulations:
 - A parametric study with the K-BKZ nonlinear parameters to determine the importance of viscoelastic effects in film blowing.

- Non-isothermal simulation of the L8-Stamylan LDPE polymer melt for direct comparison with previous non-isothermal simulations and experimental data.
- Non-isothermal simulation of the Styron 666 PS polymer melt for testing of a previous non-isothermal simulation carried out by Alaie and Papanastasiou (1993).

7.4 Mathematical Modeling

7.4.1 Governing Equations

The non-isothermal film blowing of melts can be described by the equations derived in Chapter 3. Specifically, eqs. (3.31), (3.36), (3.37), and (3.39), which are restated here for completeness, are

$$\rho(2\pi h)u = \rho Q \quad (7.1)$$

$$\frac{\sigma_{ss}}{r} \left[1 + \left(\frac{dr}{dz} \right)^2 \right]^{1/2} - \frac{d^2 r}{dz^2} \sigma_{ss} \left[1 + \left(\frac{dr}{dz} \right)^2 \right]^{3/2} - \frac{2\pi u \Delta P}{Q} = 0 \quad (7.2)$$

$$\frac{Q}{u} \sigma_{ss} \left[1 + \left(\frac{dr}{dz} \right)^2 \right]^{1/2} + \pi r^2 \Delta P \left(\frac{r_L^2}{r^2} - 1 \right) - F = 0 \quad (7.3)$$

$$\rho c_p Q \cos \phi \frac{dT}{dz} + 2\pi r h_c (T - T_\infty) + 2\pi r \sigma_{SB} \epsilon (T^4 - T_\infty^4) = 0 \quad (7.4)$$

with the following boundary conditions

1. $r = r_o$ at $z = 0$
 2. $\frac{dr}{dz} = 0$ at $z = L$
 3. $u = u_o$ at $z = 0$
 4. $T = T_o$ at $z = 0$
- (7.5)

where L is the length between the die and freeze line.

The density of the polymer, ρ , also changes along the length of the film according to the temperature of the film. A relation for the density as a function of temperature is used here and is the same as that used for fiber spinning in Chapter 5:

$$\rho(T) = \frac{\rho_o}{1 + \delta(T - T_{ref})} \quad (7.6)$$

where ρ_o is the density of the polymer at a reference temperature of T_{ref} . The parameter δ is a constant of expansion, and is given a value of 0.00069 K^{-1} as in Chapter 5.

The relation for the heat capacity is also the same as that used in Chapter 5 and is given as

$$c_p(T) = c_p^o \frac{(k_1 + k_2 T)}{k_1 + k_2 T_{ref}} \quad (7.7)$$

where c_p^o is the specific heat capacity at the reference temperature T_{ref} . The parameters k_1 and k_2 are empirical constants and are given values of 0.3243 and 0.000565 K^{-1} , respectively, as in Chapter 5.

Unlike the cases of fiber spinning and film casting, no empirical relation yet exists to the best of knowledge for the heat transfer coefficient, h_c , for film blowing. Therefore, the heat transfer coefficient is assumed constant over the length of the bubble and becomes an adjustable parameter. This method is the same as those used in previous studies (see, e.g., Alaie and Papanastasiou, 1993; Luo and Tanner, 1985). A complete list of values used in the simulations is given in Table 7.1. The properties of air are calculated at the film temperature ($0.5 \times T + 0.5 \times T_\infty$).

Table 7.1: Recurring material parameters used in the film-blowing simulations.

Property (units)	Value
Coefficient of expansion, eq. (7.6), $\delta (\text{K}^{-1})$	6.90×10^{-4}
Empirical constants, eq. (7.7), k_1 and $k_2 (\text{K}^{-1})$	0.324 and 5.65×10^{-4}
Emissivity, eq. (7.4), ϵ	0.5
Stefan-Boltzmann constant, eq. (7.4), $\sigma_{SB} (\text{erg s}^{-1} \text{ cm}^{-2} \text{ K}^{-4})$	5.67×10^{-5}
Ideal gas constant, eq. (3.57), $R (\text{J mol}^{-1} \text{ K}^{-1})$	8.314
Ambient temperature, eq. (7.4), $T_\infty (\text{K}, ^\circ\text{C})$	298 (25)

Equations (7.1) through (7.4) are made dimensionless according to the following dimensionless variables:

$$\begin{aligned}
z^* &= \frac{z}{r_o}, \quad r^* = \frac{r}{r_o}, \quad u^* = \frac{u}{u_o}, \quad h^* = \frac{h}{h_o}, \quad \rho^* = \frac{\rho}{\rho_o}, \quad \tau^* = \frac{\tau r_o}{\eta_o u_o}, \\
T^* &= \frac{T}{T_o}, \quad T_a^* = \frac{T_a}{T_o}, \quad B = \frac{\pi \Delta P r_o^3}{\eta_o Q}, \quad A = \frac{F r_o}{\eta_o Q} - B \left(\frac{r_L}{r_o} \right)^2
\end{aligned} \tag{7.8}$$

Here, the subscript o refers to die-exit conditions, the subscript L refers to freeze-line conditions, η_o is the zero-shear-rate viscosity, B is a dimensionless pressure, and A is a dimensionless force. It should be noted that r_o refers to the inner die radius. Combining eq. (7.8) with eqs. (7.1), (7.2), (7.3), and (7.4) results in the following dimensionless governing equations to be solved for in terms of the dimensionless thickness, h , dimensionless radius, r , dimensionless velocity, u , and dimensionless temperature, T (asterisks are omitted here and hereafter):

$$\rho r h u = 1 \tag{7.9}$$

$$\left(A + r^2 B \right) \frac{d^2 r}{dz^2} + 2rB \left[1 + \left(\frac{dr}{dz} \right)^2 \right] - \frac{(\tau_u - \tau_m)}{ur} \left[1 + \left(\frac{dr}{dz} \right)^2 \right]^{1/2} = 0 \tag{7.10}$$

$$(\tau_{ss} - \tau_m) - u \left(A + r^2 B \right) \left[1 + \left(\frac{dr}{dz} \right)^2 \right]^{1/2} \tag{7.11}$$

$$\frac{dT}{dz} + r \left[\kappa_1 (T - T_a) + \kappa_2 (T^4 - T_a^4) \right] \tag{7.12}$$

with the following non-isothermal coefficients:

$$\kappa_1 = \frac{2\pi r_o^2 h_c}{\rho c_p Q_o \cos \phi}, \quad \kappa_2 = \frac{2\pi r_o^2 \epsilon \sigma_{SB} T_o^3}{\rho c_p Q_o \cos \phi} \tag{7.13}$$

where $\cos \phi$ is defined as in Chapter 3. The boundary conditions, eq. (7.5), are also transformed with the new dimensionless variables, and are given as:

1. $r = 1$ at $z = 0$
 2. $\frac{dr}{dz} = 0$ at $z = L / r_o$
 3. $u = 1$ at $z = 0$
 4. $T = 1$ at $z = 0$
- (7.14)

7.4.2 Constitutive Equations

(a) *Isothermal Newtonian Model*

The Newtonian model is used here for the film-blowing process as the initial guess for the modified K-BKZ model, as described in Chapter 4. It is restated here for completeness (see Chapter 3) and for showing the specific derivations for the film blowing of a Newtonian fluid:

$$\bar{\tau} = \mu \bar{\dot{\gamma}} \quad (7.15)$$

where μ is a constant viscosity and $\bar{\dot{\gamma}}$ is the rate-of-strain tensor given by

$$\bar{\dot{\gamma}} = \bar{\nabla} \bar{u} + \bar{\nabla} \bar{u}^T \quad (7.16)$$

where $\bar{\nabla} \bar{u}$ is the velocity gradient tensor given as (Pearson and Petrie, 1970a)

$$\bar{\nabla} \bar{u} = \bar{\dot{\epsilon}} = 2u \cos \phi \begin{bmatrix} \frac{1}{r} \frac{dr}{dz} & 0 & 0 \\ 0 & \frac{1}{u} \frac{du}{dz} & 0 \\ 0 & 0 & \frac{1}{h} \frac{dh}{dz} \end{bmatrix} \quad (7.17)$$

which leads to the following normal stress differences in eqs. (7.10) and (7.11)

$$(\tau_{zz} - \tau_{rr}) = -\frac{2 \cos \phi}{rh} \left[\frac{2}{h} \frac{dh}{dz} + \frac{1}{r} \frac{dr}{dz} \right] \quad (7.18)$$

$$(\tau_{zz} - \tau_{\theta\theta}) = \frac{2 \cos \phi}{rh} \left[\frac{1}{r} \frac{dr}{dz} - \frac{1}{h} \frac{dh}{dz} \right] \quad (7.19)$$

Equations (7.18) and (7.19), when combined with eqs. (7.10) and (7.11), give the well-known dimensionless governing equations for the isothermal film blowing of a Newtonian fluid:

$$2r^2(A + r^2B) \frac{d^2r}{dz^2} = 6 \frac{dr}{dz} + r \left[1 + \left(\frac{dr}{dz} \right)^2 \right] (A - 3r^2B) \quad (7.20)$$

$$\frac{dh}{dz} = -h \left[\frac{dr}{dz} \frac{1}{2r} + \frac{\left[1 + \left(\frac{dr}{dz} \right)^2 \right] (A + r^2 B)}{4} \right] \quad (7.21)$$

The velocity of the film is easily found, once the thickness and radius is found, from the continuity equation, eq. (7.9). The boundary conditions for the Newtonian film-blowing equations are as follows:

1. $r = 1$ at $z = 0$
 2. $\frac{dr}{dz} = 0$ at $z = L/r_0$
 3. $h = 1$ at $z = 0$
- (7.22)

The boundary condition at $z = L/r_0$ transforms the problem into a boundary-value problem that is solved with the shooting method (see Chapter 4).

(b) Modified K-BKZ Integral Constitutive Model

The final constitutive equation used for the film-blowing process is an integral model of the K-BKZ type proposed by Papanastasiou et al. (1983) and further modified by Luo and Tanner (1988). It is restated here for completeness (see Chapter 3) and for showing the specific derivations for the film-blowing process:

$$\begin{aligned} \bar{\tau}(t) = \frac{1}{1-\theta} \int_{-\infty}^t \sum_{k=1}^N \frac{a_k}{\lambda_k} \exp\left(-\frac{t-t'}{\lambda_k}\right) & \frac{\alpha_k}{(\alpha_k - 3) + \beta_k I_{C^{-1}} + (1 - \beta_k) I_C} \\ & \times \left[\left\{ \bar{C}_t^{-1}(t') - \bar{I} \right\} + \theta \left\{ \bar{C}_t(t') - \bar{I} \right\} \right] dt' \end{aligned} \quad (7.23)$$

Again, λ_k and a_k are relaxation times and relaxation modulus coefficients at a reference temperature T_{ref} , respectively. The parameters α_k and β_k are material parameters chosen to fit the material's response in high shear and elongation. The parameter θ has been incorporated by Luo and Tanner (1988) to take into account the second normal stress difference, N_2 , and is related to the first normal stress difference, N_1 , via the formula

$$\frac{N_2}{N_1} = \frac{\theta}{1-\theta} \quad (7.24)$$

The value of θ is not zero for polymer melts exhibiting a second normal stress difference. Its usual range is between -0.1 and -0.3 (Tanner, 1985).

The invariants I_C and $I_{C^{-1}}$ are the first invariants of the Cauchy-Green tensor $\bar{C}_t(t')$ and its inverse $\bar{C}_t^{-1}(t')$, the Finger strain tensor. In terms of the deformation gradient tensor, $\bar{F}_t(t') = d\bar{x}'/d\bar{x}$, the Cauchy-Green and Finger strain tensors are

$$\begin{aligned}\bar{C}_t(t') &= \bar{F}_t(t') \cdot \left[\bar{F}_t(t') \right]^T \\ \bar{C}_t^{-1}(t') &= \left[\bar{F}_t^{-1}(t') \right]^T \cdot \bar{F}_t^{-1}(t')\end{aligned}\tag{7.25}$$

For the film-blowing process, the deformation gradient tensor can be derived from the equation of continuity, eq. (7.1), and simple geometry. Also, the assumption is made that for free-surface operations, no shear stresses are present and only the left diagonal entries in the deformation gradient tensor are non-zero (i.e. for $i \neq j \rightarrow \bar{F}_i(t') = 0$). Thus, the first term that applies to the modified t -coordinate is

$$F_{tt} = \frac{r(t)}{r(t')}\tag{7.26}$$

For the second term that applies to the modified s -coordinate, the deformation gradient term is

$$F_{ss} = \frac{u(t)}{u(t')}\tag{7.27}$$

The third term that applies to the modified n -coordinate can be found from the condition of incompressibility

$$\text{tr } \bar{F}_t(t') = 1\tag{7.28}$$

where tr is the trace of a tensor. Using eq. (7.28) along with eqs. (7.26) and (7.27), the third term is

$$F_{nn} = \frac{r(t')u(t')}{r(t)u(t)}\tag{7.29}$$

From eq. (7.25), the Finger strain tensor can now be obtained and is given as

$$\bar{C}_i^{-1}(t') = \begin{pmatrix} \left(\frac{r(t)}{r(t')}\right)^2 & 0 & 0 \\ 0 & \left(\frac{u(t)}{u(t')}\right)^2 & 0 \\ 0 & 0 & \left(\frac{r(t')u(t')}{r(t)u(t)}\right)^2 \end{pmatrix} \quad (7.30)$$

The Cauchy-Green tensor $\bar{C}_i(t')$ can be found by simply taking the inverse of the Finger strain tensor. The viscoelasticity of the polymer melt under flowing conditions can be represented by a dimensionless variable known as the Weissenberg number, given as

$$We = \frac{u_o}{r_o} \frac{\sum a_k \lambda_k^2}{\sum a_k \lambda_k} = \frac{u_o}{r_o} \bar{\lambda} \quad (7.31)$$

where $\bar{\lambda}$ is the average relaxation time. The transit times along the film can be expressed in terms of the velocity and distance traveled, by

$$t - t' = \int_{s'}^s \frac{ds''}{u(s'')} \quad (7.32)$$

where double prime (") denotes a position between s and s' .

7.4.3 Method of Solution

(a) Newtonian Model

The differential equations for the film-blowing process with the Newtonian model, eqs. (7.20) and (7.21), are solved with a shooting method, utilizing the 4th-order Runge-Kutta scheme and the bisection method, as presented in Chapter 4. The dimensionless blow-up pressure, B , and the dimensionless take-up force, A , are fixed. The unknown dimensionless final radius, $r_L / r_o = BUR$, and the unknown draw ratio, D_R , require two guesses each for the shooting method, and the differential equations are solved in the reverse z -direction, beginning with the boundary condition at $z = L / r_o$ from eq. (7.22). Thus, the boundary conditions at $z = 0$ from eq. (7.22) are the target equations to be

solved for in the shooting method (see Chapter 4). Once the radius and thickness are known, the velocity is easily solved for from the equation of continuity, eq. (7.9).

(b) *Modified K-BKZ Integral Constitutive Model*

The numerical method used to solve eqs. (7.10) and (7.12), with the stresses replaced by eq. (7.23), is the finite element method (FEM) explained in Chapter 4. The unknown radius, r , velocity, u , and temperature, T , are approximated with quadratic finite element interpolation functions, ψ_i :

$$\begin{aligned} r^e &= \sum_{i=1}^3 u_i^{(e)} \psi_i^{(e)} \\ u^e &= \sum_{i=1}^3 u_i^{(e)} \psi_i^{(e)} \\ T^e &= \sum_{i=1}^3 T_i^{(e)} \psi_i^{(e)} \end{aligned} \quad (7.33)$$

The differential equations pertaining to the radius, velocity, and temperature are then weighted with the same interpolation functions as those used for the variables, and the resulting Galerkin weighted residuals on an element basis are

$$\begin{aligned} R(r)_i^{(e)} &= \left[\frac{dr^e}{dz} \psi_i^{(e)} \right]_{z=0}^{z=1} - \int_0^1 \left[\frac{dr^e}{dz} \frac{d\psi_i^{(e)}}{dz} + \right. \\ &\quad \left. \frac{\psi_i^{(e)}}{A + r^{e2} B} \left[2r^e B \left[1 + \left(\frac{dr^e}{dz} \right)^2 \right] - \frac{(\tau_u - \tau_m)}{u^e r^e} \left[1 + \left(\frac{dr^e}{dz} \right)^2 \right]^{1/2} \right] \right] dz = 0 \quad i = 1, 3 \quad (7.34) \end{aligned}$$

$$R(u)_i^{(e)} = \int_0^1 \left\{ (\tau_{ss} - \tau_m) - u^e \left(A + r^{e2} B \right) \left[1 + \left(\frac{dr^e}{dz} \right)^2 \right]^{1/2} \right\} \psi_i^{(e)} dz = 0 \quad i = 1, 3 \quad (7.35)$$

$$R(T)_i^{(e)} = \int_0^1 \left\{ \frac{dT^e}{dz} - r^e \left[\kappa_1 (T^e - T_a) + \kappa_2 (T^{e4} - T_a^4) \right] \right\} \psi_i^{(e)} dz = 0 \quad i = 1, 3 \quad (7.36)$$

All boundary residuals at the die exit are set to zero in order to impose the radius, velocity, and temperature at the die exit. The stresses in the residuals are replaced by the stresses defined by the modified K-BKZ integral constitutive equation, eq. (7.23). The

upstream memory resulting from the integral constitutive equation is computed via a 15-point Gauss-Laguerre quadrature suited for exponentially fading functions (see Chapter 4), while the Galerkin residuals are computed with Gauss-Legendre quadrature (see Chapter 4). The residuals, which are required to vanish, result in a system of $3M$ nonlinear equations (where M is the total number of nodes), which are solved by the Newton-Raphson iterative scheme, as explained in Chapter 4.

7.5 Results and Discussion

7.5.1 Film Blowing of a Newtonian Fluid

The film blowing of a Newtonian fluid was first solved numerically by Pearson and Petrie (1970b). As mentioned in Chapter 3, the modified K-BKZ integral constitutive model reduces to the Newtonian model when $N = 1$ and $\lambda_1 = 0$ or respectively a small number, say $\lambda_1 = 0.001$. In this case, and by using unit values in eq. (7.31) for the die exit velocity u_0 and inner die radius r_0 , the Weissenberg number $Ws = \lambda$, and for the Newtonian fluid $Ws = 0$. Thus, the numerical solution to the blowing of a Newtonian fluid can be used to ensure the numerical solution with the K-BKZ model is accurate.

Figure 7.2 shows the numerical results of the modified K-BKZ model for film blowing (with $\lambda_1 = 0.001$) along with the numerical solution for a Newtonian fluid with a dimensionless blow-up pressure of $B = 0.2$ and a dimensionless take-up force of $A = 2.9$. The dimensionless length is $L/r_0 = 5$. Agreement with the numerical Newtonian solution is excellent. Also shown in Figure 7.2 are the numerical results from Luo and Tanner (1985) under the same blowing conditions. Agreement with the results of Luo and Tanner (1985) is also excellent. The agreement with the Newtonian solution and that of Luo and Tanner (1985) is proof the numerical scheme with the modified K-BKZ model is accurate at low Weissenberg numbers.

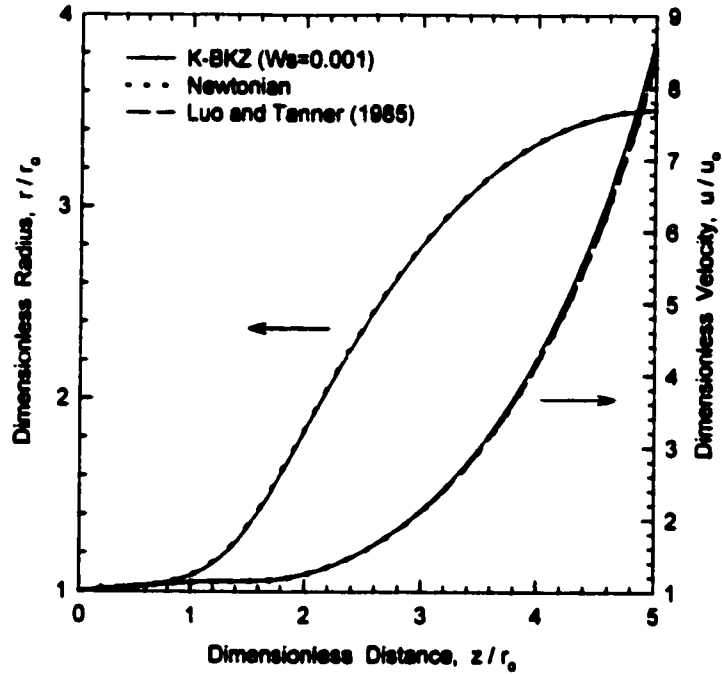


Figure 7.2: Film blowing of a Newtonian fluid. Thick dotted lines represent the numerical solution of the Newtonian model with $B = 0.2$, $A = 2.9$, and $L/r_0 = 5$. Dashed lines represent the numerical solution of Luo and Tanner (1985). Full lines represent the numerical solution with the modified K-BKZ model with $N = 1$ and $\lambda_1 = 0.001$ ($Ws = 0.001$).

7.5.2 Film Blowing of an Upper-Convected Maxwell (UCM) Fluid

The film blowing of a UCM fluid was first solved by Luo and Tanner (1985) at varying Weissenberg numbers. Since the modified K-BKZ model can be reduced to the UCM model, simulations for a UCM fluid are possible and the numerical scheme can be validated for viscoelastic fluids at higher Weissenberg numbers. The modified K-BKZ model reduces to the UCM model when $N = 1$ and $\alpha \rightarrow +\infty$, or say a large number ($\alpha = 10,000$). Again, unit values are used for the die-exit velocity u_0 and inner die radius r_0 , such that $Ws = \lambda$.

Figure 7.3 shows the numerical results of the modified K-BKZ model for film blowing (with $\alpha = 10,000$), along with the numerical results of Luo and Tanner (1985), for different Weissenberg numbers ($Ws = 0, 0.1, 0.15, 0.2, 0.25$). The blowing conditions for these simulations are $B = 0.2$, $A = 2.9$, and $L/r_o = 5$, the same as in the Newtonian case. Agreement with the results of Luo and Tanner (1985) is excellent for each corresponding Weissenberg number, confirming the numerical scheme is accurate for viscoelastic fluids of higher Weissenberg numbers. The maximum attainable Weissenberg number for the current numerical scheme was $Ws = 0.272$, higher than the maximum attained by Luo and Tanner (1985) which was $Ws = 0.25$. The continuation procedure used in order to reach the maximum Weissenberg number of $Ws = 0.272$ is given in Table 7.2. The continuation procedure of Table 7.2 is similar for subsequent simulations where continuation is required.

Table 7.2: Continuation procedure used in the simulations with the UCM model to reach the maximum Weissenberg number of $Ws = 0.272$.

Continuation step	Weissenberg number, Ws
1	0 (Newtonian)
2	0.1
3	0.2
4	0.25
5	0.26
6	0.265
7	0.268
8	0.270
9	0.271
10	0.272

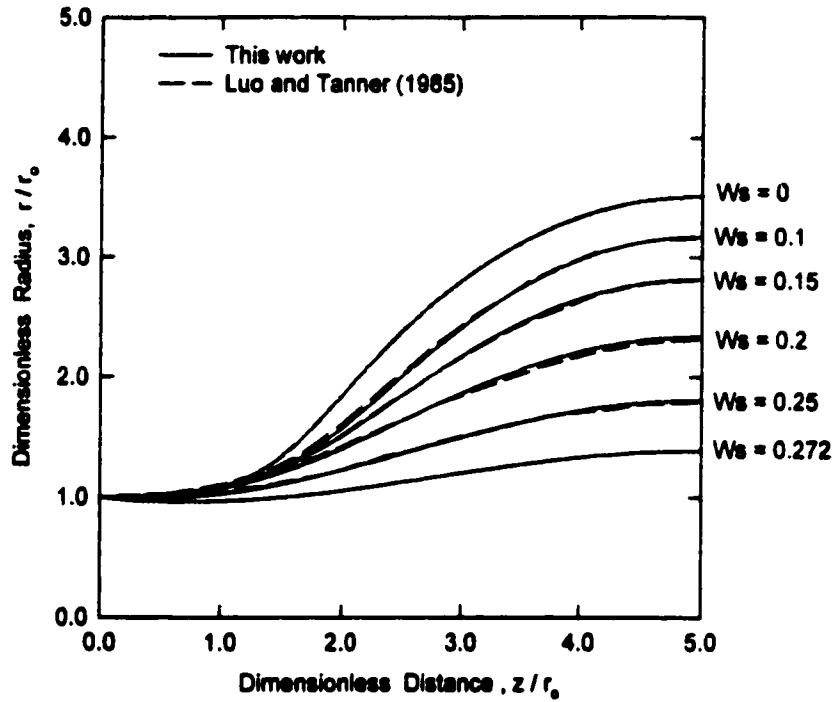


Figure 7.3: Film blowing of a UCM fluid for various Weissenberg numbers (Ws). Dashed lines represent the numerical solution of Luo and Tanner (1985) with $B = 0.2$, $A = 2.9$, and $L/r_0 = 5$. Full lines represent the current simulations with the modified K-BKZ model with $N = 1$ and $\alpha = 10,000$.

Figure 7.3 also shows the effect of increasing the Weissenberg number on the final radius, r_L . Increasing the relaxation time of the material increases the Weissenberg number, and the process operates in the region of very high extensional uniaxial viscosity (see Figure 3.5). Thus, the material deforms as an elastic solid and resists deformation, explaining the reduced bubble radius. The limiting case for the UCM model at higher Weissenberg numbers would result in a completely flat radial profile and a linear velocity profile (drawing of an elastic solid tube).

It is interesting to note that two very dissimilar approaches to solving the film-blowing governing equations with the UCM model gave identical results. Luo and Tanner (1985) used a 4th-order Runge-Kutta procedure with the UCM differential constitutive equation to solve the film-blowing problem. This study uses the FEM with

the integral equivalent of the UCM model, and the integral constitutive equation was solved via a 15-point Gauss-Laguerre quadrature.

7.5.3 Non – Isothermal Film Blowing of an Upper – Convected Maxwell (UCM) Fluid

In order to perform non-isothermal simulations of viscoelastic fluids, a method for deriving the non-isothermal constitutive equation from the isothermal constitutive equation must be chosen. The method of choice, reported by previous studies (see e.g., Barakos and Mitsoulis, 1996; Rauschenberger and Laun, 1997) when using integral constitutive equations, is the Morland-Lee hypothesis (Tanner, 1985), as described in Chapter 3. However, the opportunity is offered here to compare the Morland-Lee hypothesis with a method of *shifting the relaxation times* as methods to evaluate non-isothermal stresses. Only the UCM model will be considered in this comparison.

The method of shifting the relaxation times is based on the time-temperature superposition principle where the temperature history within the material's time scale is taken into account (Luo and Tanner, 1987). The equation used to shift the relaxation times in the material's history is given as (Luo and Tanner, 1987)

$$\lambda(T(t')) = \lambda(T_{ref}) \cdot a_T(T(t')) \quad (7.37)$$

where $\lambda(T(t'))$ is the relaxation time used in eq. (7.23) at the temperature T at time t' , $\lambda(T_{ref})$ is the relaxation time at the reference temperature T_{ref} , and $a_T(T(t'))$ is the corresponding shift factor at the temperature T at time t' . The shift factor used in the method of shifting relaxation times is the same shift factor used in the Morland-Lee hypothesis (see Chapter 3).

To properly evaluate the two different techniques described above, different temperature profiles are examined for each case. This is accomplished by using different heat capacities in the equation of energy, eq. (7.12). One heat capacity gives a temperature drop of only about 7°C along the length of the bubble, while the other gives a temperature drop of about 27°C along the length of the bubble. The latter temperature

drop is more typical of real film-blowing experiments. The complete list of operating conditions for each case is given in Table 7.3.

Table 7.3: Material parameters used in the non-isothermal simulations of the Maxwell test cases for the Morland-Lee hypothesis against the shifting of relaxation times.

Property	Value
Reference temperature, T_{ref} (K, °C)	458 (185)
Density, ρ_o (g cm ⁻³)	1.0
Activation energy, E (J mol ⁻¹)	70000.0
Specific heat (7°C drop), c_p^o (erg g ⁻¹ K ⁻¹)	2.00×10^7
Specific heat (27°C drop), c_p^o (erg g ⁻¹ K ⁻¹)	7.00×10^6
Relaxation time, λ (s)	0.3
Zero-shear-rate viscosity, η_o (Pa·s)	90000.0
Heat transfer coefficient, h_c (erg cm ⁻² K ⁻¹)	6000.0
Die-exit radius, r_l (cm)	1.0
Die-exit velocity, u_o (cm s ⁻¹)	1.0
Die-exit thickness, h_o (cm)	0.1
Dimensionless length, L / r_o	5.0
Inlet temperature, T_o (°C, K)	185 (458)
Dimensionless force, A	2.9
Dimensionless pressure, B	0.2

Figure 7.4 shows the film variables (radius, velocity, and temperature) for the first case where the temperature drops only about 7°C for both methods. It can be seen that the Morland-Lee hypothesis and the shifting of relaxation times give very similar predictions for each variable along the length of the bubble, with only slight differences. Therefore, the method of shifting relaxation times does not differ significantly compared to the Morland-Lee hypothesis for small temperature changes.

Figure 7.5 shows again the film variables (radius, velocity, and temperature) for the second case where the temperature drops 27°C . It can be seen that the Morland-Lee hypothesis and the shifting of relaxation times differ more than the case where the temperature dropped 7°C . However, the difference is only slight between the predictions for both methods and the trend is conserved. Thus, the method of shifting relaxation times does not differ considerably compared to the Morland-Lee hypothesis, but the differences will amplify for very large temperature drops.

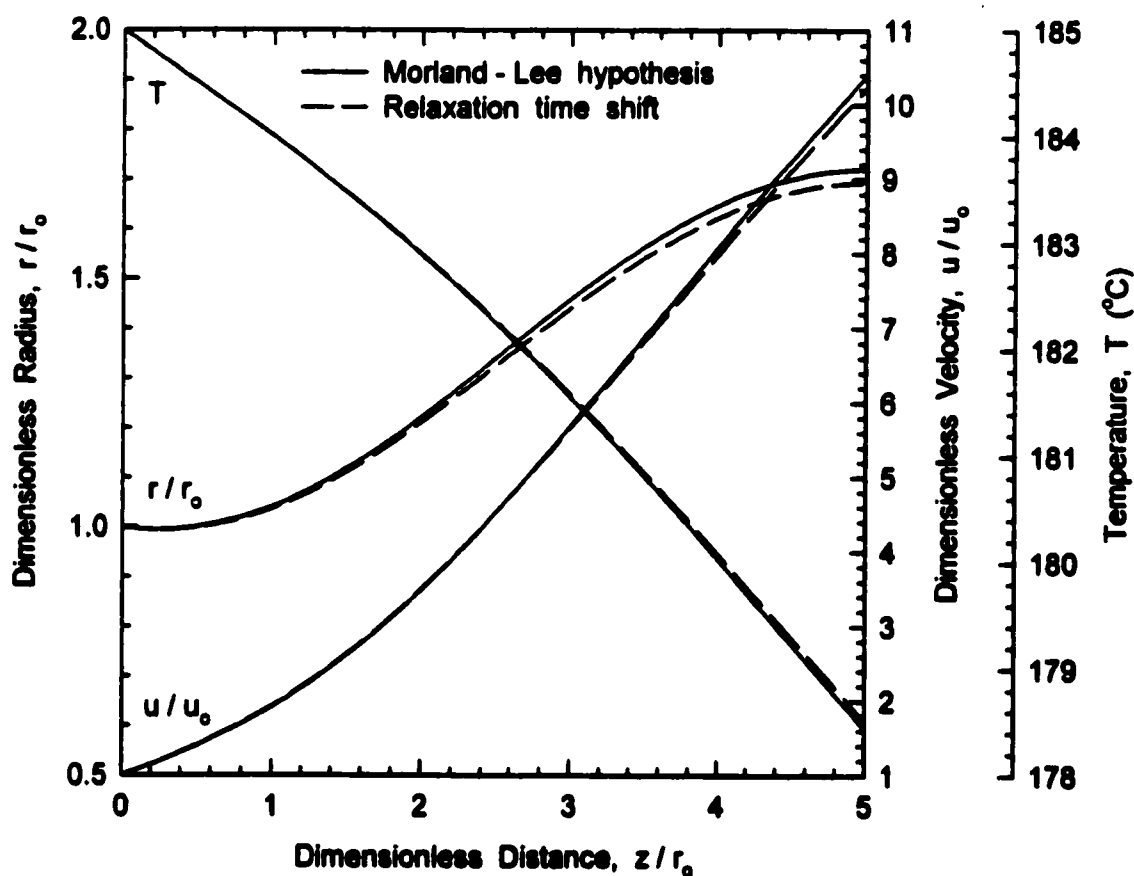


Figure 7.4: Predictions of the film variables (radius, velocity, and temperature) from non-isothermal simulations with the UCM model for a temperature drop of 7°C along the bubble. Full lines represent simulations with the use of the Morland-Lee hypothesis (Tanner, 1985). Dashed lines represent simulations with the method of shifting relaxation times (Luo and Tanner, 1987).

Both methods, the shifting of relaxation times and the Morland-Lee hypothesis, are capable of handling non-isothermal conditions when using integral constitutive equations. However, the Morland-Lee hypothesis has been chosen in this study because of its ease of implementation in the current numerical scheme, its speed, and accuracy. This advantage occurs because the Morland-Lee hypothesis allows the use of Gauss-Laguerre quadrature, which is well suited for exponentially fading functions and requires only 15 positions in the particle's deformation history for the computation of the stresses given by the integral constitutive equation.

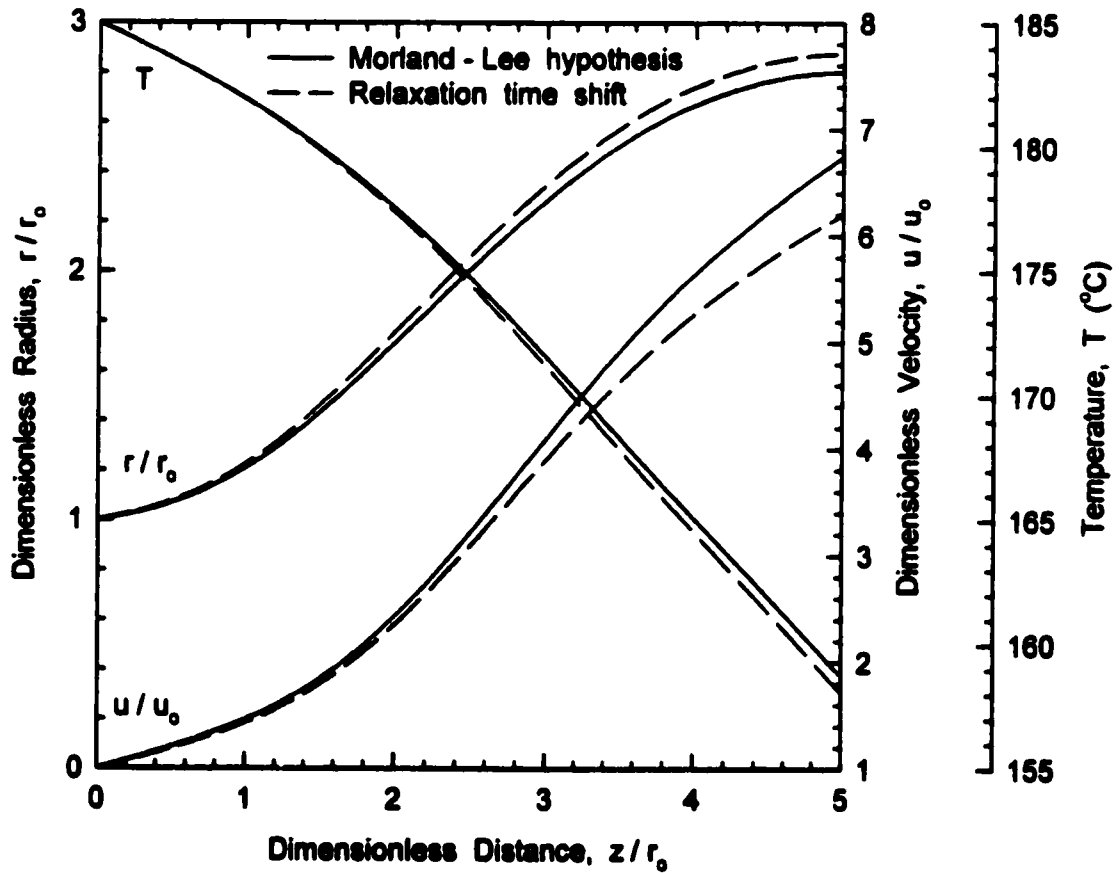


Figure 7.5: Predictions of the film variables (radius, velocity, and temperature) from non-isothermal simulations with the UCM model for a temperature drop of 27°C along the bubble. Full lines represent simulations with the use of the Morland-Lee hypothesis (Tanner, 1985). Dashed lines represent simulations with the method of shifting relaxation times (Luo and Tanner, 1987).

7.5.4 Parametric Study with K-BKZ Nonlinear Parameters (α , β , θ)

A parametric study is conducted here, in relation to the nonlinear parameters α , β , and θ in the K-BKZ model (eq. (7.23)), to obtain a better understanding of the rheological effects in the film-blowing process. The effects of changing the nonlinear parameters in the K-BKZ model on the rheological functions (e.g. shear viscosity, first normal stress difference, etc.) have already been described in Chapter 3 (see Figures 3.8 through 3.10). The simulations are performed in the same manner for the UCM simulations, i.e., unit values are used for the die-exit velocity u_o and inner die radius r_o , such that $Ws = \lambda$. The operating conditions used for the parametric study are the same as the UCM simulations ($B = 0.2$, $A = 2.9$, and $L/r_o = 5$), while the Weissenberg number is $Ws = 0.1$.

Figure 7.6 shows the effect of changing α , the *shear-thinning parameter*, on the bubble radius, film thickness, and film velocity. Lowering α has little effect on the bubble radius and film thickness. However, lowering α has a substantial effect on the final film velocity, which doubles when α goes from $\alpha = 1000$ to $\alpha = 35$. This is expected since the extent of biaxial viscosity thinning increases from $\alpha = 1000$ to $\alpha = 35$. The lowest α value attainable for this parametric study was $\alpha = 35$, after which the solution diverges.

Figure 7.7 shows the effect of changing β , the *extension-thinning parameter*, on the bubble radius, film thickness, and film velocity. The film-blowing process is only minimally affected by changes in β . Nonetheless, the effects are still visible and some conclusions can be drawn. An increase in β causes the final film velocity profile to slightly decrease, with very little effect on the bubble radius and film thickness. This is anticipated because as β increases, the biaxial viscosity increases at higher extensional rates (decrease in extension-thinning effect), which makes the material more difficult to deform. This effect is opposite to the uniaxial extensional viscosity (see Chapter 3).

Finally, Figure 7.8 shows the effect of changing θ , the *normal stress parameter*, on the bubble radius, film thickness, and film velocity. As θ increases, the bubble radius decreases, the film velocity increases, and the film thickness also decreases. This is expected because as the value of θ increases to zero, the biaxial viscosity decreases significantly, which makes the material easier to deform.

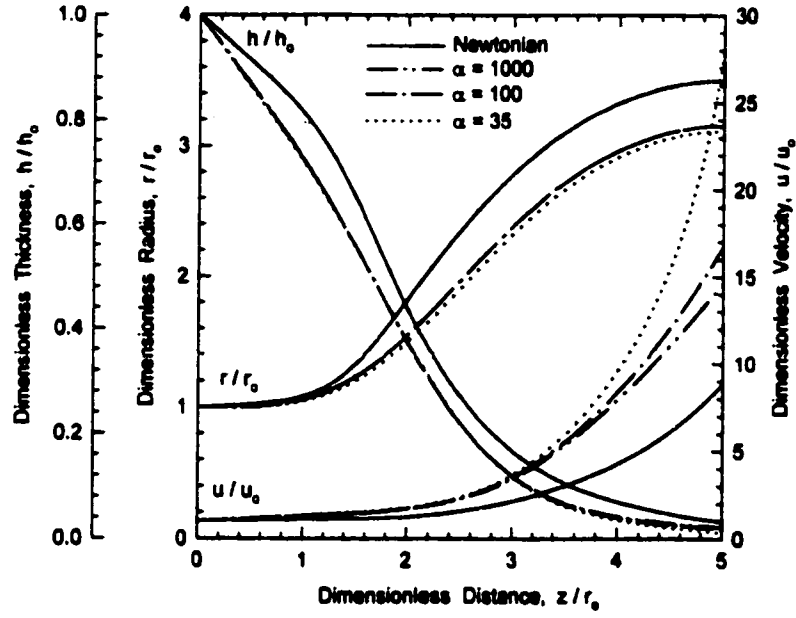


Figure 7.6: Effect of changing the nonlinear parameter α (shear-thinning parameter) in the K-BKZ model on the bubble radius, film thickness, and film velocity for $B = 0.2$, $A = 2.9$, $L/r_0 = 5.0$, and $Ws = 0.1$. In each case, $\beta = 0.5$ and $\theta = 0$.

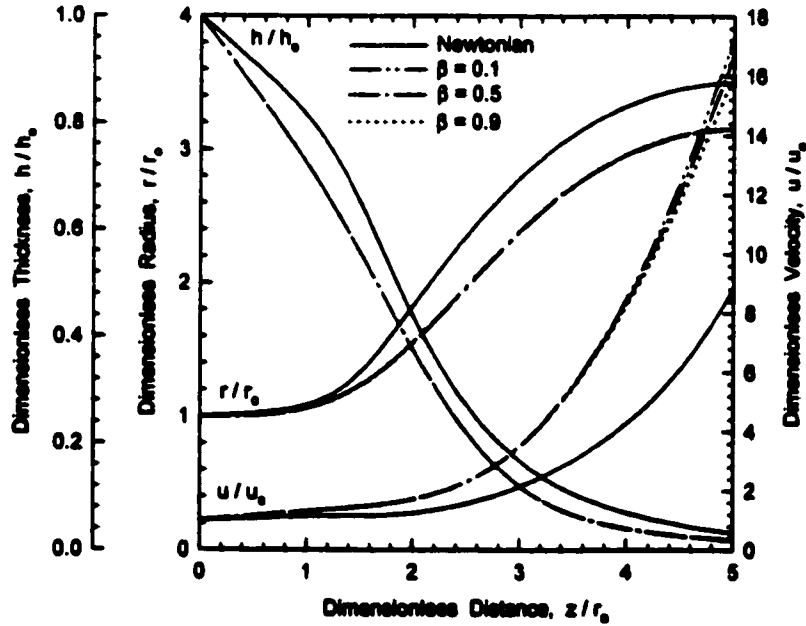


Figure 7.7: Effect of changing the nonlinear parameter β (extension-thinning parameter) in the K-BKZ model on the bubble radius, film thickness, and film velocity for $B = 0.2$, $A = 2.9$, $L/r_0 = 5.0$, and $Ws = 0.1$. In each case, $\alpha = 100$ and $\theta = 0$.

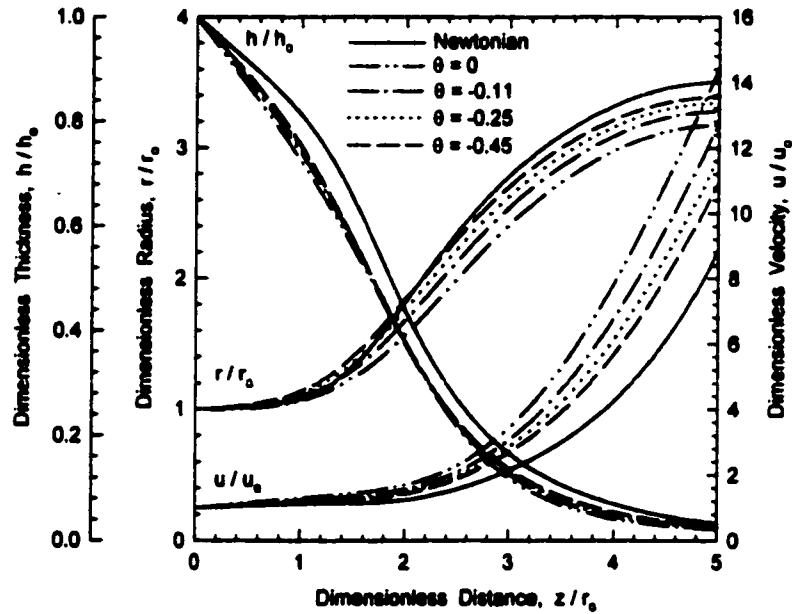


Figure 7.8: Effect of changing the nonlinear parameter θ (normal stress parameter) in the K-BKZ model on the bubble radius, film thickness, and film velocity for $B = 0.2$, $A = 2.9$, $L/r_0 = 5.0$, and $Ws = 0.1$. In each case, $\alpha = 1000$ and $\beta = 0.5$.

7.5.5 Non – Isothermal Film Blowing of Polymer Melts

Tas (1994) conducted non-isothermal film blowing experiments for three different grades of LDPE. Measurements of the film velocity, bubble radius, and film temperature were made for a wide variety of different operating conditions, in an attempt to relate operating conditions to film characteristics. In this study, the film blowing of the L8-Stamylan LDPE is simulated and compared to experiments #23 and #29 from Tas (1994) under the same operating conditions. The operating conditions used for the simulations are given in Table 7.4. Experiment #23 and #29 have identical operating conditions apart from the take-up force and the blow-up pressure. This data has also been simulated by Sidiropoulos et al. (1996), with the use of a non-isothermal Newtonian model. Comparisons are made between the current simulations and those of Sidiropoulos et al. (1996).

Table 7.4: Operating (boundary) conditions used in the simulations for the experiments conducted by Tas (1994) for the Stamylan L8 LDPE melt at 145°C. Other parameters used in the simulations are also given.

Die-exit radius, $r_i = 1.78$ cm
Die-exit velocity, $u_o = 0.42$ cm s ⁻¹
Die-exit thickness, $h_o = 0.22$ cm
Dimensionless length, $L / r_o = 10$
Heat transfer coefficient, $h_c = 40000$ erg cm ⁻² K ⁻¹
Reference temperature $T_{ref} = 463$ K (190°C)
Density $\rho_o = 0.92$ g cm ⁻³
Activation energy $E = 57500$ J mol ⁻¹
Specific heat $c_p^o = 2.00 \times 10^7$ erg g ⁻¹ K ⁻¹

Figure 7.9 shows the experimental data from Tas (1994) for the shear viscosity (η_s) and the first normal stress difference (N_I) for the L8-Stamylan LDPE at 190°C. Also shown are the respective model predictions from the modified K-BKZ model, as well as predictions of the uniaxial viscosity (η_E) and the biaxial viscosity (η_B). The relaxation spectrum used for the predictions is given in Table 7.5. Figure 7.10 shows the experimental data from Tas (1994) for the storage and loss modulus, G' and G'' respectively, for the L8-Stamylan LDPE at 190°C. Also shown are the predictions from the modified K-BKZ model, with the relaxation spectrum given in Table 7.5.

Figure 7.11 shows the experimental measurements for the bubble radius for experiments #23 and #29, along with the current simulation predictions and the predictions of Sidiropoulos et al. (1996). It can be seen that the current simulations and those of Sidiropoulos et al. (1996) both have difficulty in predicting the correct bubble shape. The reason may be due to external forces not taken into account in the film-blowing governing equations presented in Chapter 3. Such forces are the aerodynamic forces coming from the turbulent jet of air used in cooling the bubble surface, air drag, and gravity. Surface tension and inertia can be assumed to be negligible in most polymer melt operations (Pearson and Petrie, 1970a). Figure 7.11 also shows that the current

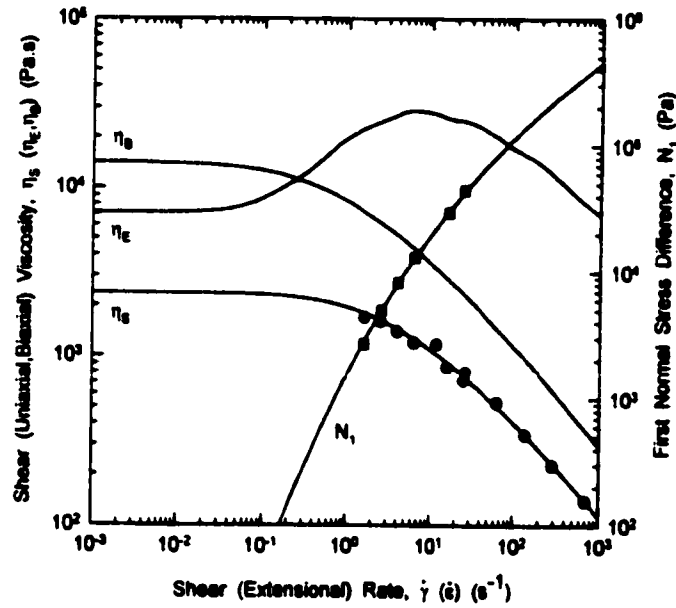


Figure 7.9: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial and biaxial viscosities (η_E , η_B) for the L8-Stamylan LDPE at 190°C. Symbols represent experimental measurements by Tas (1994) while lines represent predictions from the K-BKZ constitutive model, eq. (7.23), with the relaxation spectrum of Table 7.5.

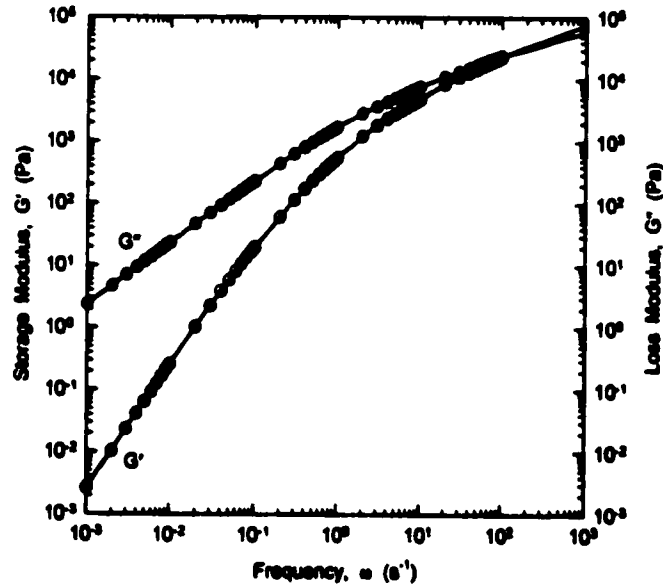


Figure 7.10: Storage and loss moduli (G' , G'') for the L8-Stamylan LDPE at 190°C. Symbols represent experimental measurements by Tas (1994) while lines represent predictions from the K-BKZ constitutive model, eq. (7.23), with the relaxation spectrum of Table 7.5.

simulation predictions and the predictions from Sidiropoulos et al. (1996) differ only slightly, although different constitutive equations are used. This again suggests that the model proposed by Pearson and Petrie (1970b) is inadequate for simulating real film-blowing experiments. Another reason for the discrepancy between simulations and experiments is the problem of multiple solutions, a characteristic of the film-blowing governing equations introduced in Chapter 3. Other studies (Luo and Tanner, 1985; Cain and Denn, 1988; Petrie, 1973) have also encountered difficulties in using these governing equations, including multiplicities and instabilities.

Table 7.5: Relaxation spectrum and associated parameters for the L8 Stamylan LDPE melt at 190°C found from nonlinear regression for the modified K-BKZ integral constitutive equation ($\alpha = 12.82$, $\beta = 0.058$, $\theta = -0.111$).

k	λ_k (s)	a_k (Pa)
1	4.28×10^{-5}	$2.17 \times 10^{+5}$
2	2.07×10^{-4}	$9.18 \times 10^{+4}$
3	1.34×10^{-3}	$5.75 \times 10^{+4}$
4	9.02×10^{-3}	$2.43 \times 10^{+4}$
5	5.69×10^{-2}	$8.91 \times 10^{+3}$
6	3.44×10^{-1}	$2.34 \times 10^{+3}$
7	$1.82 \times 10^{+0}$	$3.21 \times 10^{+2}$
8	$9.94 \times 10^{+0}$	$1.24 \times 10^{+1}$

The method used in this study to predict the experiments by Tas (1994) is to manually change the dimensionless take-up force, A , and the dimensionless blow-up pressure, B , until the predicted final radius, r_L , and final velocity, u_L , match that of the experiments. Table 7.6 shows the results from the simulations for the take-up force and blow-up pressure compared to the experiments. The simulations under-predict the force and over-predict the pressure compared to the experiments, for experiments #23 and #29. The current simulations with the K-BKZ model predict forces closer to the experiments than that of Sidiropoulos et al. (1996) with the non-isothermal Newtonian model. However,

the current simulations predict pressures further from the experiments than that of Sidiropoulos et al. (1996). Once more, this is due to the inability of the governing equations to capture all of the forces exerted on the blown film.

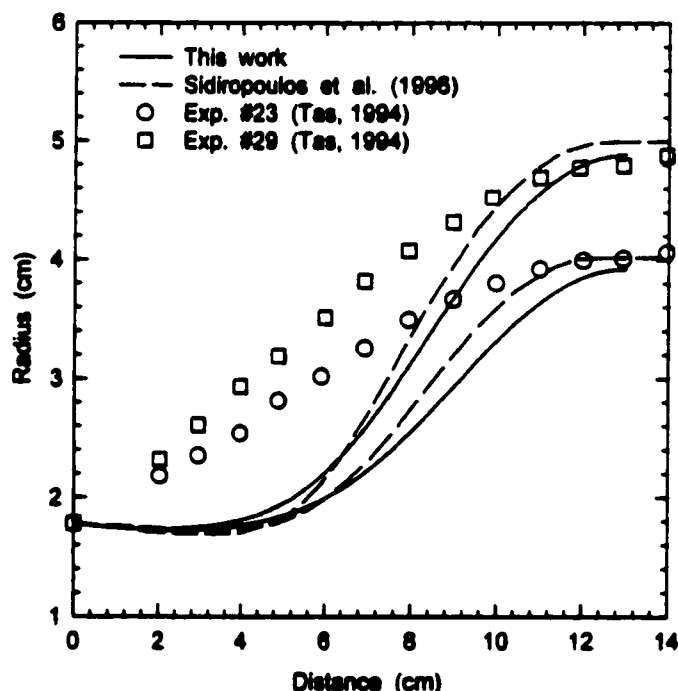


Figure 7.11: Comparison of current simulations with those of Sidiropoulos et al. (1996) and experiments conducted by Tas (1994) with the L8-Stamylan LDPE for the bubble radius. Operating conditions are given in Table 7.4.

Table 7.6: Comparison between experimental and predicted take-up forces and blow-up pressures for the experiments with the L8 Stamylan LDPE by Tas (1994) and simulations by Sidiropoulos et al. (1996).

Run #	Experiments		Simulations		Simulations	
	Tas (1994)		This work		Sidiropoulos et al. (1996)	
	Force	Pressure	Force	Pressure	Force	Pressure
	(N)	drop (Pa)	(N)	drop (Pa)	(N)	drop (Pa)
23	4.30	85	1.86	186	1.20	150
29	3.50	70	2.13	168	1.30	120

Figure 7.12 shows the experimental measurements for the film velocity for experiments #23 and #29, along with the current simulation predictions and the predictions of Sidiropoulos et al. (1996). It can be seen that the current simulations and those of Sidiropoulos et al. (1996) both have difficulty in predicting the correct film velocity. Figure 7.12 shows that the current simulation predictions and the predictions from Sidiropoulos et al. (1996) also differ.

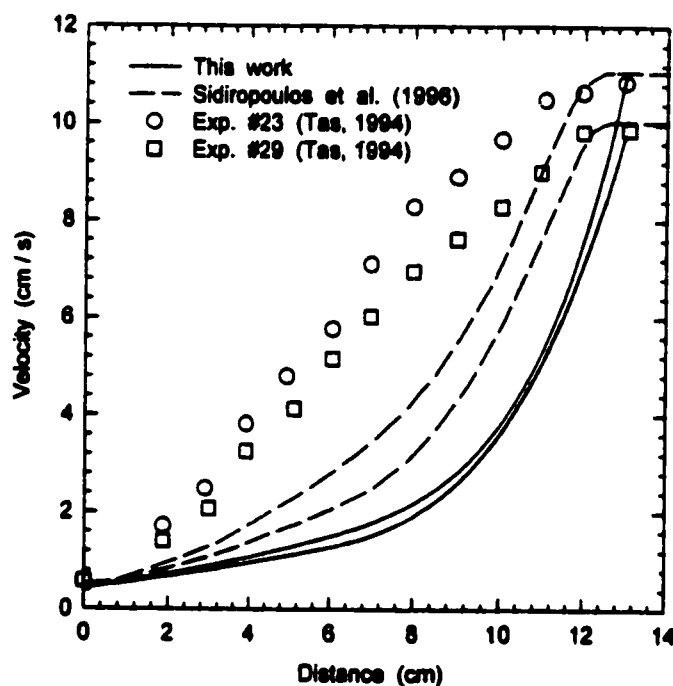


Figure 7.12: Comparison of current simulations with those of Sidiropoulos et al. (1996) and experiments conducted by Tas (1994) with the L8-Stamylan LDPE for the film velocity. Operating conditions are given in Table 7.4.

Finally, Figure 7.13 shows the experimental measurements for the film temperature for experiments #23 and #29, along with the current simulation predictions and the predictions of Sidiropoulos et al. (1996). The simulated temperature profiles agree in general with the experimental temperature profiles for both cases. However, from Table 7.4, the heat transfer coefficient, h_c , required in the simulations to obtain the proper temperature profile is 10 times that used in other reported simulations (Luo and Tanner, 1985; Cain and Denn, 1988). This may be due to the poor predictions of the bubble

radius and film velocity, as seen in Figures 7.11 and 7.12. It is also possible that Tas (1994) used higher velocities of cooling air to solidify the bubble for the discrepancies. The principal reason for the discrepancy is more likely due to the use of a constant heat transfer coefficient. A better relation is required to relate the heat transfer coefficient, h_c , to the bubble conditions and turbulent air surrounding the bubble. Such relations exist for cross-flow air with cylinders and plates (as in the fiber-spinning and film-casting simulations, see Chapters 5 and 6), but do not exist to the best of knowledge for complicated situations such as this one (impinging turbulent air with changing bubble radius).

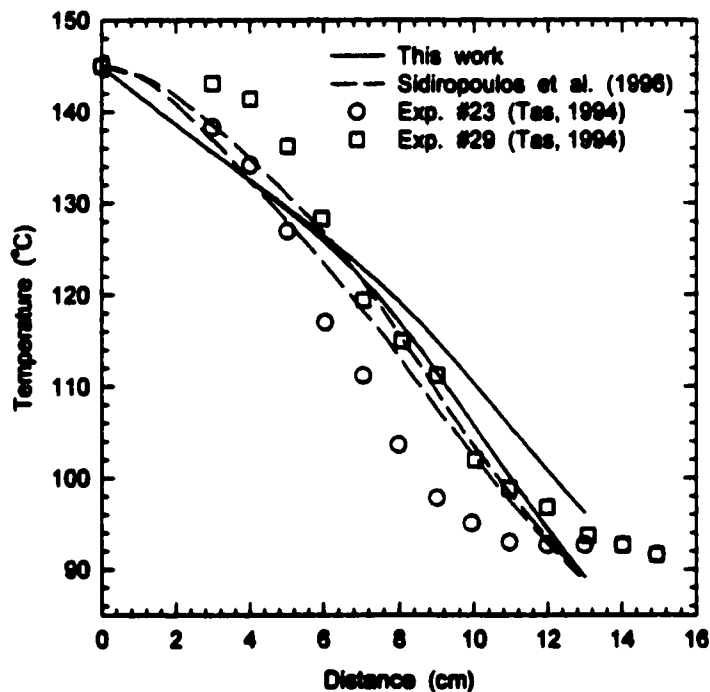


Figure 7.13: Comparison of current simulations with those of Sidiropoulos et al. (1996) and experiments conducted by Tas (1994) with the L8-Stamylan LDPE for the film temperature. Operating conditions are given in Table 7.4.

7.5.6 Comments on the Study by Alaie and Papanastasiou (1993)

The simulation of the film-blowing process conducted by Alaie and Papanastasiou (1993) made use of the modified K-BKZ constitutive model with non-isothermal effects, and assumed a shear prehistory. Simulations were reported for a polypropylene (PP) melt and the Styron 666 polystyrene (PS) melt. The Styron 666 PS melt was chosen in an

attempt to simulate the experiments performed by Gupta et al. (1982), namely experiment #20. The results for the Styron 666 PS melt simulation showed a surprisingly good agreement with the experiment, in terms of the bubble radius, film velocity, and film temperature. It was the good agreement between the simulations of Alaie and Papanastasiou (1993) and the experiments that incited the current study of the film-blowing process, and similarly the studies of the fiber-spinning and film-casting processes.

The current study for the film-blowing process made use of the modified K-BKZ constitutive model with non-isothermal effects, much like the study of Alaie and Papanastasiou (1993). However, where Alaie and Papanastasiou (1993) assumed a shear prehistory, the current study assumed an extensional prehistory (see Chapter 3). Previous studies (Chen and Papanastasiou, 1987; Rauschenberger and Laun, 1997) have demonstrated that an extensional prehistory gives equivalent or improved results compared to a shear prehistory. Initially, the current study made use of a shear prehistory like that of Alaie and Papanastasiou (1993). However, after numerous simulations with the Newtonian and UCM models, it was discovered that a shear prehistory gave spurious stresses and inaccurate radius and velocity profiles when compared to previous simulations. The problem was found to be in the averaging of the shear stresses, a method used by Alaie and Papanastasiou (1993). The averaging procedure used by Alaie and Papanastasiou (1993) consisted of determining the velocity profile within the annulus and averaging the resulting stresses (see Alaie and Papanastasiou, 1993). To visualize this problem, the results of the UCM model at a Weissenberg number of $Ws = 0.25$ are given for two cases, i.e., with shear prehistory using shear averaging and extensional prehistory. The operating conditions are the same as those used in the study of the film blowing of a UCM fluid, Section 7.5.2. Figure 7.14 shows the dimensionless stresses, $\sigma_{ss}^{\circ} = \tau_{ss}^{\circ} - \tau_{nm}^{\circ}$ (machine-direction stress) and $\sigma_{tt}^{\circ} = \tau_{tt}^{\circ} - \tau_{nm}^{\circ}$ (transverse-direction stress), for the shear prehistory using shear averaging and extensional prehistory, respectively. It can be seen that the shear averaging procedure used by Alaie and Papanastasiou (1993) results in incorrect stresses with oscillations. The method of shear averaging was corrected by Tas (1994), who used an unknown shear rate, $\dot{\gamma}_o$, which was used to balance the stresses inside and outside of the die (see Tas, 1994). This new method is

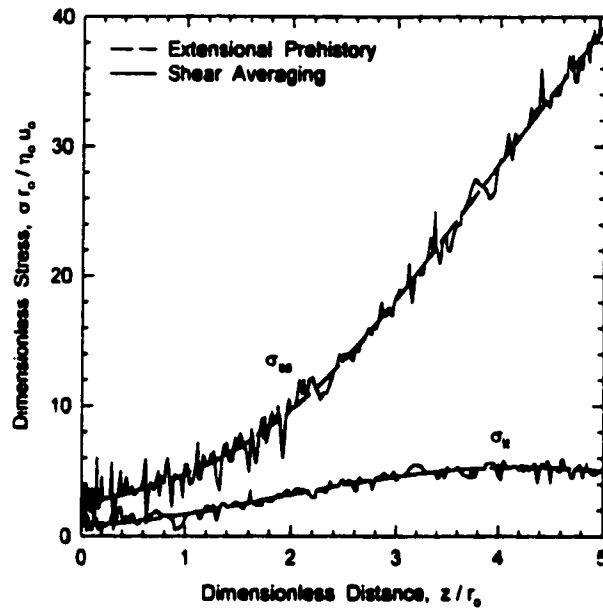


Figure 7.14: Predictions of the machine-direction stress, σ_{xx}^* , and the transverse-direction stress, σ_{zz}^* , for the UCM model at $Ws = 0.25$. Full lines represent the shear prehistory with stress averaging used by Alaie and Papanastasiou (1993). Dashed lines represent the extensional prehistory used in the current study.

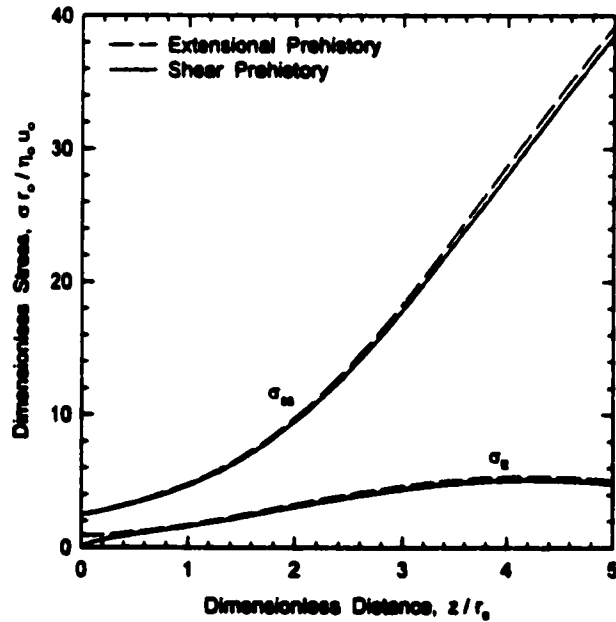


Figure 7.15: Predictions of the machine-direction stress, σ_{xx}^* , and the transverse-direction stress, σ_{zz}^* , for the UCM model at $Ws = 0.25$. Full lines represent the corrected shear prehistory proposed by Tas (1994). Dashed lines represent the extensional prehistory used in the current study.

similar to the extensional prehistory used in this study, where the unknown parameter, c , is used to balance the stresses inside and outside of the die (see Chapter 3). Figure 7.15 shows the results using the shear prehistory improved by Tas (1994), along with the current extensional prehistory. It can be seen that even at high Weissenberg numbers with the UCM model, the corrected shear prehistory and the extensional prehistory give almost identical stresses.

It was found during the testing of the Newtonian solution that an error is present in the study of Alaie and Papanastasiou (1993). In validating their numerical scheme against the Newtonian solution, Alaie and Papanastasiou (1993) used a dimensionless force of $A = 2.3$, dimensionless pressure of $B = 0.2$, and dimensionless length of $L/r_0 = 7$. Under these conditions, the correct Newtonian solution is for the final dimensionless radius $r^* = 3.015$, with a final dimensionless velocity of $u^* = 6.593$. Alaie and Papanastasiou (1993) report that their viscoelastic case at $Ws = 0.001$, which gave a final dimensionless radius of $r^* = 3.12$ and a final dimensionless velocity of $u^* = 11.8$, matched the Newtonian solution (see Fig. 8 in Alaie and Papanastasiou, 1993). This is a false claim and their numerical scheme validation is incorrect. Therefore, the results from Alaie and Papanastasiou (1993) for viscoelastic cases are questionable.

Attempts were also made to simulate the film-blowing experiment #20 from Gupta et al. (1982) with the Styron 666 PS melt. The final Weissenberg number for this experiment was $Ws = 1.82$. Unfortunately, the highest attainable Weissenberg number for the current film-blowing simulation of the Styron 666 PS melt from Gupta et al. (1982) was $Ws = 0.90$. Simulations from Alaie and Papanastasiou (1993) showed convergence at $Ws = 1.82$ for experiment #20 from Gupta et al. (1982), with very good agreement for the bubble radius, film velocity, and film temperature. Alaie and Papanastasiou (1993) also predicted very successfully the take-up force and blow-up pressure from the experiments. Figures 7.16 through 7.18 show the experimental measurements from Gupta et al. (1982) along with the predictions from Alaie and Papanastasiou (1993), for the bubble radius, film velocity, and film temperature, respectively. It can be seen that the predictions from Alaie and Papanastasiou (1993) are surprisingly good for all three variables. The rheological characterization and the operating conditions used by Alaie and Papanastasiou (1993) in the simulations of

experiment #20 are given in Table 7.7. Again, Alaie and Papanastasiou (1993) achieved very good predictions for the take-up force and blow-up pressure. Figures 7.19 and 7.20 show the predictions from the K-BKZ model with the relaxation spectrum from Alaie and Papanastasiou (1993) for the Styron 666 PS melt from Gupta et al. (1982) (see Table 7.7). It is obvious that Alaie and Papanastasiou did not perform a proper rheological characterization of the Styron 666 PS melt, and thus did not simulate experiment #20 from Gupta et al. (1982) properly.

Table 7.7: Relaxation spectrum and associated parameters for the Styron 666 PS melt at 170°C from Alaie and Papanastasiou (1993) ($\alpha = 10.57$, $\beta = 0.02$). Also shown are the operating conditions from Alaie and Papanastasiou (1993) for the simulation of experiment #20 from Gupta et al. (1982). The take-up force and blow-up pressure were $F = 2.13 \times 10^5$ dynes and $\Delta P = 2160$ dynes cm⁻², respectively.

k	λ_k (s)	a_k (Pa)
1	$1.77 \times 10^{+2}$	$9.78 \times 10^{+1}$
2	$2.09 \times 10^{+1}$	$3.46 \times 10^{+3}$
3	3.93×10^0	$6.78 \times 10^{+3}$
4	4.39×10^{-1}	$1.01 \times 10^{+4}$
5	5.05×10^{-2}	$1.26 \times 10^{+4}$
6	7.55×10^{-3}	$1.45 \times 10^{+4}$
7	4.55×10^{-4}	$1.47 \times 10^{+4}$

Die-exit radius, $r_i = 1.27$ cm

Die-exit velocity, $u_o = 0.42$ cm s⁻¹

Die-exit thickness, $h_o = 0.1$ cm

Die-exit temperature, $T_o = 458$ K (185°C)

Dimensionless length, $L/r_o = 10$

Heat transfer coefficient, $h_c = 5400$ erg cm⁻² K⁻¹

Reference temperature $T_{ref} = 443$ K (170°C)

Density $\rho_o = 1.05$ g cm⁻³

Activation energy $E = 157168$ J mol⁻¹

Specific heat $c_p^o = 1.710 \times 10^7$ erg g⁻¹ K⁻¹

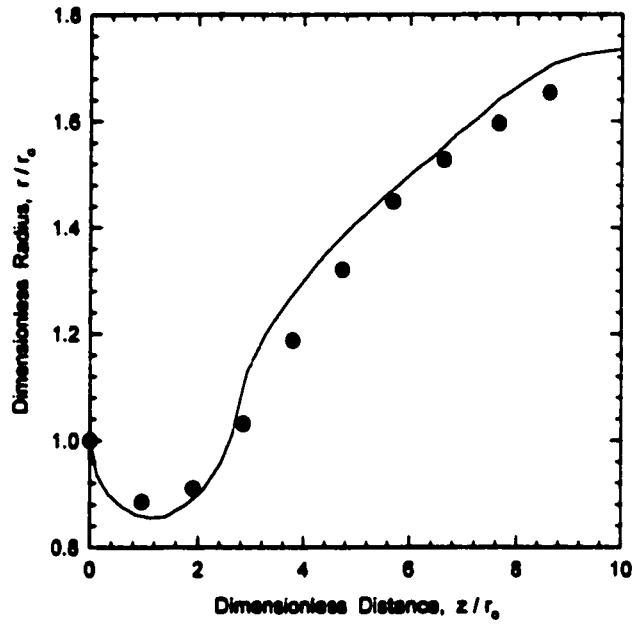


Figure 7.16: Comparison of the simulations of Alaie and Papanastasiou (1993) with experiments conducted by Gupta et al. (1982) for the Styron 666 PS melt in terms of the bubble radius. Operating conditions are given in Table 7.7.

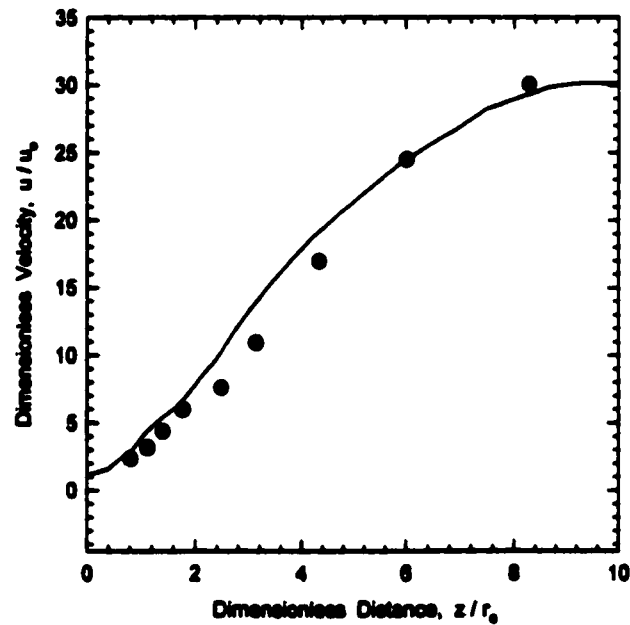


Figure 7.17: Comparison of the simulations of Alaie and Papanastasiou (1993) with experiments conducted by Gupta et al. (1982) for the Styron 666 PS melt in terms of the film velocity. Operating conditions are given in Table 7.7.

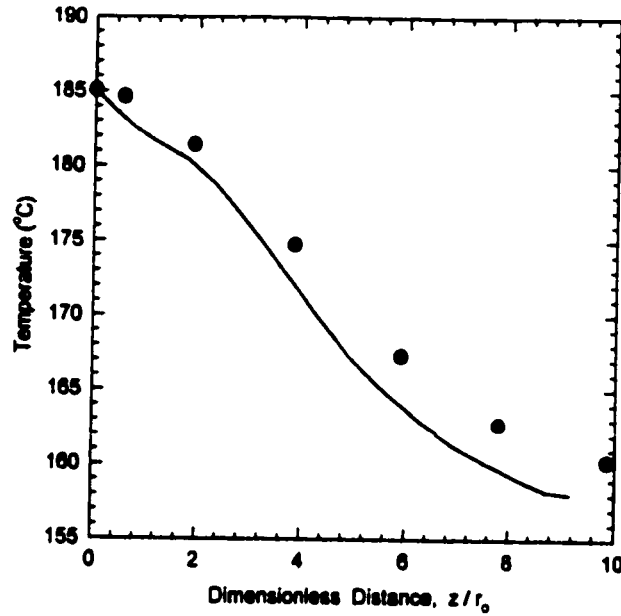


Figure 7.18: Comparison of the simulations of Alaie and Papanastasiou (1993) with experiments conducted by Gupta et al. (1982) for the Styron 666 PS melt in terms of the film temperature. Operating conditions are given in Table 7.7.

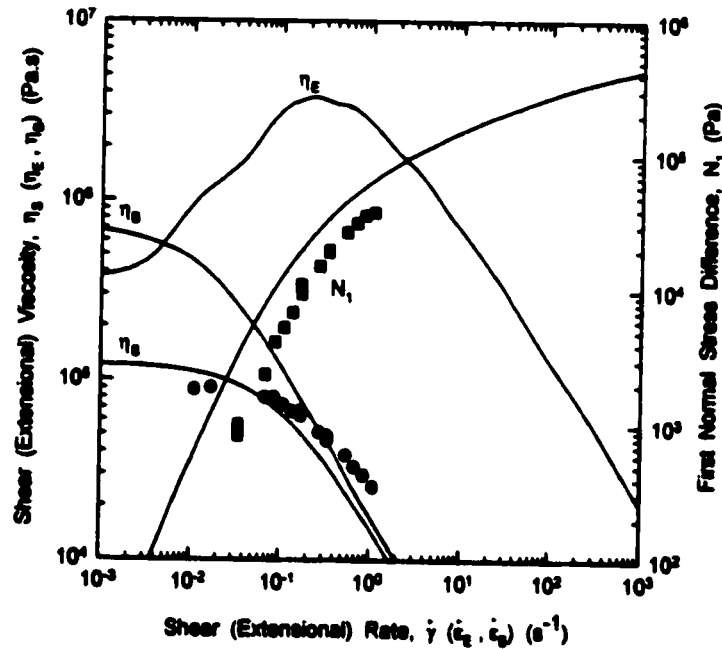


Figure 7.19: Shear viscosity (η_s), first normal stress difference (N_1), and uniaxial and biaxial viscosities (η_E , η_B) for the Styron 666 PS at 170°C. Symbols represent experimental measurements by Gupta (1980) while lines represent predictions from the K-BKZ constitutive model, eq. (7.23), with the relaxation spectrum from Alaie and Papanastasiou (1993) (see Table 7.7).

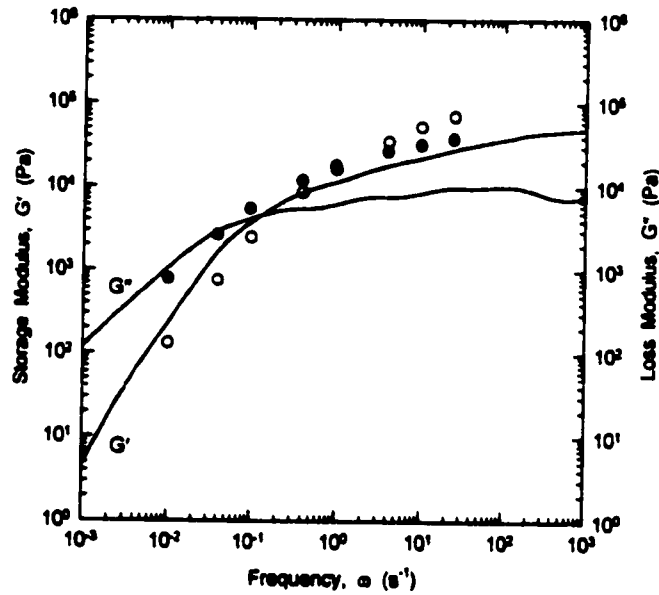


Figure 7.20: Storage and loss moduli (G' , G'') for the Styron 666 PS at 170°C. Symbols represent experimental measurements by Gupta (1980) while lines represent predictions from the K-BKZ constitutive model, eq. (7.23), with the relaxation spectrum from Alaie and Papanastasiou (1993) (see Table 7.7).

Another study performed by Kurtz (1995) has also raised questions concerning the study by Alaie and Papanastasiou (1993) with regard to the simulation of the experiments by Gupta et al. (1982). The governing equations proposed by Pearson and Petrie (1970a,b) can be rearranged to give the stress ratio, $\sigma_{ss}^* / \sigma_n^*$, for any bubble shape. Kurtz (1995) showed that the stress ratio should always be greater than 1 (i.e. σ_{ss}^* should always be greater than σ_n^*). Kurtz (1995) also pointed out that the study by Gupta et al. (1982) contained a small error in conversion of units, and Gupta et al. (1982) calculated a stress ratio less than 1. Alaie and Papanastasiou (1993) reproduced the error made by Gupta et al. (1982), which should have been uncovered in the simulations. The simulations of experiment #20 from Gupta et al. (1982) for the Styron 666 PS melt conducted by Alaie and Papanastasiou (1993) should have reported the stress ratio to be greater than 1, since it is impossible to predict otherwise with the governing equations from Pearson and Petrie (1970a,b). The current simulations have always given results for the stress ratio in agreement with the statement by Kurtz (1995).

Therefore, the study by Alaie and Papanastasiou (1993) raises the following questions:

- How could the numerical scheme be validated with an incorrect Newtonian solution?
- How could convergence be reached at $Ws = 1.82$ (experiment #20 from Gupta et al. (1982) for the Styron 666 PS melt) with the stress averaging procedure, which has been shown to give oscillatory stresses?
- How could such good predictions be obtained for all film-blowing variables (bubble radius, film velocity, film temperature, take-up force, blow-up pressure) when the current simulations, with improved stress calculations, cannot accurately predict film-blowing variables for other experiments (see Section 7.5.4)?
- How could the simulations predict an impossible stress ratio, which was reported by experiments that contained an error in conversion of units?

It appears at present that the experimental data by Gupta et al. (1982) have not been successfully simulated in the open literature with a fully non-isothermal viscoelastic model.

7.6 Concluding Remarks

Numerical viscoelastic simulations have been undertaken for the film-blowing process with the code F-BLOW. The film-blowing process is a prime example of biaxial extensional flow. The governing equations, first presented in Chapter 3, were made dimensionless. Relations for the melt density and heat capacity as a function of distance along the film were presented. Specifics concerning the numerical solution of the governing equations were also presented.

Isothermal Newtonian and UCM results have been successfully reproduced using an integral equation of the K-BKZ type. Consequently, the validity of the numerical scheme was established at low and high Weissenberg (Ws) numbers. However, the Newtonian and UCM models do not predict the behaviour of real polymer melts. The Newtonian model predicts a constant uniaxial viscosity (see Chapter 3) while the UCM model predicts a uniaxial viscosity which eventually reaches infinity (see Chapter 3). Therefore,

the K-BKZ model, which predicts adequately the behaviour of real polymer melts, has been used as the workhorse for the simulations.

Simulations were then undertaken for a non-isothermal UCM fluid, utilizing the Morland-Lee hypothesis (Tanner, 1985) and a method of shifting the relaxation times (Luo and Tanner, 1987). Both methods are capable of handling non-isothermal conditions when using integral constitutive equations, and were found to give similar results for low to moderate temperature drops. However, at higher temperature drops, the two methods gave different predictions. The non-isothermal behaviour of viscoelastic fluids is an active area of research, both experimentally and theoretically, and much work needs to be done.

Simulations were also undertaken for the experiments conducted by Tas (1994) for the L8-Stamylan LDPE. Experiments #23 and #29 from Tas (1994) were simulated and predictions were compared to experimental measurements and previous simulations conducted by Sidiropoulos et al. (1996). The simulations were performed in hope that a viscoelastic model, such as the modified K-BKZ constitutive model, would give better predictions for the experiments than the non-isothermal Newtonian model used by Sidiropoulos et al. (1996). The current simulations gave no better predictions than those of Sidiropoulos et al. (1996). Surprisingly, the current simulations gave very similar predictions to those of Sidiropoulos et al. (1996). This suggests that the governing equations are much more important in predicting the correct film-blowing behaviour than the constitutive equations. It also suggests that the governing equations proposed by Pearson and Petrie (1970a,b) do not take into account all of the external forces acting on the bubble.

Finally, comments were made and questions were raised concerning the study conducted by Alaie and Papanastasiou (1993). It was found that the stress-averaging procedure used by Alaie and Papanastasiou (1993) for a shear prehistory results in oscillatory stresses. The corrected shear prehistory proposed by Tas (1994) was tested and was found to give identical results compared to the extensional prehistory used in the current study. The very good agreement that was reported by Alaie and Papanastasiou (1993) for the simulations of experiment #20 by Gupta et al. (1982) raised many questions concerning the validity of their study. Therefore, experiment #20 for the

Styron 666 PS melt performed by Gupta et al. (1982) has still not been successfully simulated in the open literature.

The objective of this study was to develop an efficient code that can give quick and approximate results for the film-blowing process. Since two- and three-dimensional simulations take a great deal of effort and time to develop, the one-dimensional formulation for film blowing has been used to develop the code F-BLOW. Two- and three-dimensional simulations for this process have not yet been developed in the open literature due to the inherent complexity of this process. The F-BLOW code was used to determine the significance of viscoelastic effects and the sensitivity of the results to the parameters in the K-BKZ constitutive equation. It was also used to determine the deficiencies of the one-dimensional formulation in predicting correctly the film-blowing process. The use of the complex K-BKZ rheological model, with non-linear material functions, did not produce improved predictions compared to previous simulations. The effects of temperature were also included, which also did not improve predictions. Thus, the governing equations, first presented in Chapter 3, dictate the quality of the predictions. Improvements in the film-blowing simulations could be obtained by including other dominant forces, such as the aerodynamic effects of cooling air, or by discarding the thin-shell approximation (see Chapter 3) by performing two-dimensional simulations.

Chapter 8

Conclusions and Recommendations

In this work, rheological characterization of complex materials was performed and numerical simulations of shear-free flows with such materials were undertaken. The modified K-BKZ integral constitutive model was used to predict the viscoelastic behaviour of these materials. Rheological characterization was conducted for two polymer solutions at room temperature and a polymer melt at a high temperature. Characterization was also performed under steady-state and transient conditions. Non-linear regression with the Levenberg-Marquardt method was used to find the parameters within the modified K-BKZ model, and these are used in the shear-free flow simulations.

Viscoelastic simulations were undertaken for the shear-free flows of fiber spinning, film casting, and film blowing. The finite element method (FEM) was used to solve the governing one-dimensional differential equations, which originated from the equations of conservation of mass, momentum, and energy. The Newton-Raphson method is used as the iterative method for the resulting system of equations. Non-isothermal effects on the viscoelasticity of the material are taken into account with the use of the Morland-Lee hypothesis (Tanner, 1985). The modified K-BKZ integral constitutive equation is solved with a 15-point Gauss-Laguerre quadrature, well suited for exponentially fading functions. An assumption is required for the deformation within the die for integral models, and the assumption is made in this study of a purely extensional prehistory. The resulting numerical schemes are used in the simulation of fiber spinning, film casting, and film blowing of *real* polymer melts.

In this chapter, conclusions are drawn concerning the methods used and the results obtained in this study. The sections are conveniently divided according to the key chapters of this study. Recommendations are also given for future work.

8.1 Rheological Characterization

8.1.1 Conclusions

A cone-and-plate rheometer was used to measure the shear-viscosity, η_s , and first normal stress difference, N_1 , at a wide range of shear rates for two polymer solutions at room temperature, namely a poly(ethylene oxide) resin (Union Carbide, Inc.) and a polyacrylamide resin (Polysciences, Inc.). Modifications were made to the existing equipment to test materials at high temperatures, and measurements were made for a polypropylene (PP) melt (Shell Canada, Inc.) at 230°C. Previous measurements for the PP melt agreed with current measurements, thus validating the experimental procedure and equipment.

A computer code (TIMEFIT[®]) was developed for the nonlinear regression of the modified K-BKZ integral constitutive equation with respect to transient material functions (e.g. shear viscosity growth, η_s^+ , first normal stress difference growth, N_1^+ , etc.). The program was tested against a typical low-density polyethylene (LDPE) melt with transient measurements, and good predictions for the transient functions were obtained.

8.1.2 Recommendations

In terms of the cone-and-plate rheometer, the following modifications could be made to the existing equipment to facilitate rheological measurements:

- One of the analog meters failed during testing. This was corrected by routing the signal to a functional meter. The analog signal for all measurements could be converted to a digital signal, which can then be interpreted on a PC with a DAC card.
- An extra 1500 hp motor could be purchased such that dynamic measurements for the storage modulus, G' , and the loss modulus, G'' , could be made. This would require the analog signal to be converted to a digital signal, as mentioned above.
- A controller is required for better stability of the temperature during non-isothermal measurements. The current method requires constant supervision and adjustment of the rheostats for temperature control.

- A capillary rheometer should be developed or purchased, which produces shear viscosity measurements at higher shear rates.

In terms of transient nonlinear regression, the only recommendation is that a substantial amount of transient data is required, at a wide range of shear rates, in order to predict accurately the steady-state material functions.

8.2 Fiber Spinning

8.2.1 Conclusions

New results were obtained for the one-dimensional fiber-spinning simulation of viscoelastic melts. In particular, the M1 polymer solution was characterized and simulated for the series of spinning experiments conducted by Ferguson and Hudson (1990). The simulations were used to predict a region where the steady-state uniaxial viscosity could reside. The simulations also revealed that the contributions from inertia, gravity, and drag were minimal for this set of experiments. Isothermal spinning simulations for the experiments with a PP melt from Ishizuka et al. (1980) showed that the radius and velocity could be captured within the isothermal zone, however the force could not be predicted accurately due to non-isothermal effects. Non-isothermal spinning simulations were also conducted for the set of experiments with a poly(ethylene terephthalate) (PET) melt from George (1982) and the experiments with the IUPAC-A LDPE melt from Rauschenberger and Laun (1997). The simulations with the PET melt revealed that inertia, gravity, and drag do have significant effects for industrial operations. The simulations with the PET melt were also compared to a previous set of simulations performed by Gagon and Denn (1981), where the K-BKZ model used in the current study and the PTT model used by Gagon and Denn (1981) gave similar results. The simulations with the IUPAC-A LDPE melt revealed that the extrudate swell effect is important for accurate predictions of the take-up force.

The one-dimensional model for fiber spinning possessed the advantages of short computing time with almost guaranteed convergence. The significance of viscoelastic

effects were determined for the fiber-spinning process, as well as other effects, such as inertia, gravity, and air drag. The one-dimensional model was useful for exploring the importance of viscoelastic effects and gave valuable information in comparisons to experiments and previous simulations.

8.2.2 Recommendations

Some recommendations for future work in the understanding of the fiber-spinning process include:

- An increased amount of extensional rheological experiments in the open literature to help determine the uniaxial viscosity of viscoelastic materials, which would lead to better experimental procedures. It is not yet known how to produce a purely uniaxial extensional flow in experiments.
- Two-dimensional simulations to determine if there are any two-dimensional effects not taken into account with the current one-dimensional analysis. The simulations should be performed with the M1 solution especially since nonlinear observations in the velocity field were made during the experiments of Ferguson and Hudson (1990). Two-dimensional simulations could also be performed for the non-isothermal spinning experiments with the IUPAC-A LDPE from Rauschenberger and Laun (1997). The IUPAC-A LDPE melt is a well characterized melt, and the two-dimensional simulations would establish the effects of extrudate swell. Two-dimensional simulations could also be performed for the set of experiments with the PET melt by George (1982) to determine if there is any shearing along the surface of the fiber, since these experiments were conducted at industrial speeds (> 1000 m/min).

8.3 Film Casting

8.3.1 Conclusions

New results were obtained for the one-dimensional film-casting simulation of viscoelastic melts. In particular, comparisons were made with previous two- and three-dimensional studies, by Debbaut et al. (1995) and by Sakaki et al. (1996), respectively. The current one-dimensional analysis could not predict the same film-casting behaviour of the higher-dimensional analyses with Newtonian fluids. However, the current one-dimensional analysis was shown to give matching results with the two-dimensional analysis in terms of film thickness and the neck-in effect with viscoelastic fluids. Simulations were also carried out for the experiment conducted by Kase (1974) with a PP melt. Due to lack of film-casting experimental data in the open literature, parametric studies were performed for a PET melt and the IUPAC-A LDPE melt. The geometrical boundary conditions were fixed, and only the effects of increased take-up speeds were examined. The PET melt was shown to behave like a Newtonian fluid, while the IUPAC-A LDPE melt behaved like a combination of a Newtonian and UCM fluid.

The one-dimensional model for film casting possessed the advantages of short computing time with almost guaranteed convergence. The one-dimensional film-casting analysis gave similar predictions compared to the two-dimensional analysis in terms of the film thickness and the neck-in effect, which are industrially important. The significance of viscoelastic effects was determined for the film-casting process with the use of a parametric study. The one-dimensional model was useful for exploring the importance of viscoelastic effects and gave valuable information in comparisons to experiments and previous simulations.

8.3.2 Recommendations

Some recommendations for future work in the understanding of the film-casting process include:

- An increase in the amount of film-casting experiments in the open literature, at bench-scale and industrial speeds, which could help relate operating conditions with some of the problems encountered in industry (e.g. instability). The experiments could also be used for simulation purposes, which can greatly help in the understanding of this process.

- Three-dimensional viscoelastic simulations could be performed for the film-casting process. The three-dimensional results could then be compared to the one-dimensional results, to see if they match as they did in the two-dimensional case.

8.4 Film Blowing

8.4.1 Conclusions

New results were obtained for the one-dimensional film-blowing simulation of viscoelastic melts. In particular, simulations for the L8-Stamylan LDPE were undertaken for experiments #23 and #29 performed by Tas (1994). Comparisons were also made with previous simulations conducted by Sidiropoulos et al. (1996). The simulations revealed that the governing equations proposed by Pearson and Petrie (1970a,b) do not take into account all of the external forces acting on the bubble (e.g. impinging cooling jets). Nonetheless, simulations were also conducted for a non-isothermal UCM fluid, where the Morland-Lee hypothesis (Tanner, 1985) and a method of shifting relaxation times (Luo and Tanner, 1987) yielded approximate results for low to moderate temperature drops. Finally, comments were made questioning the validity of the study conducted by Alaie and Papanastasiou (1993).

8.4.2 Recommendations

Some recommendations for future work in the understanding of the film-blowing process include:

- Film-blowing experiments should be conducted with new techniques to help understand the overall process. New techniques, such as birefringence measurements, are only now being conducted by a select group of researchers (Ghaneh-Fard et al., 1996a,b; 1997a,b).
- A two-dimensional simulation technique should be devised to simulate the film blowing process, as was done with the two-dimensional simulation of the film-casting

process (see e.g., Debbaut et al., 1995). All significant forces must also be taken into account, especially the effects of the surrounding turbulent air from impinging jets.

- A new relation for the heat transfer coefficient, h_c in eq. (7.4), as function of the distance along the bubble is required. The new relation should also take into account the effect of the impinging jets.
- Since the free-flow of the material continues until the material has completely solidified, the crystallinity of the material may also have significant contributions to the behaviour of the film-blowing process. Studies should investigate the significance of crystallinity on the process by some appropriate crystallinity model.

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Appendices

A. Gaussian Quadrature

B. F-BLOW Code for Film Blowing

Appendix A

Gaussian Quadrature

Legendre polynomials are of the following form:

$$P_{-1}(x) = 0 \quad (\text{A-1})$$

$$P_0(x) = 1 \quad (\text{A-2})$$

$$P_1(x) = x \quad (\text{A-3})$$

$$P_2(x) = \frac{3x^2 - 1}{2} \quad (\text{A-4})$$

while the following general recursive relation (A-5) can be used along with the first two members (given by A-1 and A-2) to generate a Legendre polynomial of any given order, i.e.

$$P_j(x) = \frac{(2j+1)xP_{j-1}(x) - jP_{j-2}(x)}{j+1} \quad (\text{A-5})$$

This family of polynomials can be used to generate a Gaussian quadrature formula to evaluate integrals of the form:

$$\int_{-1}^1 F(x) dx \doteq \sum_{i=0}^j w_i F(x_i) \quad (\text{A-6})$$

In the above formula, x_i are the roots of the Legendre polynomials of $j+1$ order, w_i are the corresponding weight factors (given by A-7), and for $F(x)$ being a polynomial it is exact up to a degree less than $2j+1$.

$$w_i = \frac{j! \Gamma(j+1) x_i}{[P_{j+1}(x_i)]^2} \quad (\text{A-7})$$

In the present work, a 6-point quadrature is used for evaluation of the governing differential equations in relation to the finite element method. Table A-1 gives the Legendre polynomial roots and weighting factors in double-precision arithmetic.

Table A-1: Roots and weighting factors for the 6-point Legendre quadrature.

6-Point Legendre Quadrature		
Roots and Weighting Factors		
i	x_i	w_i
0	-0.932469514203152	0.171324492379170
1	-0.661209386466265	0.360761573048139
2	-0.238619186083197	0.467913934572691
3	0.238619186083197	0.467913934572691
4	0.661209386466265	0.360761573048139
5	0.932469514203152	0.171324492379170

Laguerre polynomials are of the following form:

$$L_{-1}(x) = 0 \quad (\text{A-8})$$

$$L_0(x) = 1 \quad (\text{A-9})$$

$$L_1(x) = -x + 1 \quad (\text{A-10})$$

$$L_2(x) = \frac{x^2 - 4x + 1}{2} \quad (\text{A-11})$$

while the following general recursive relation (A-12) can be used along with the first two members (given by A-8 and A-9) to generate a Laguerre polynomial of any given order, i.e.

$$L_j(x) = \frac{(-x + 2j + 1)L_{j-1}(x) - jL_{j-2}(x)}{j + 1} \quad (\text{A-12})$$

This family of polynomials can be used to generate a Gaussian quadrature formula to evaluate integrals of the form:

$$\int_0^\infty e^{-x} F(x) dx \doteq \sum_{i=0}^j w_i F(z_i) \quad (\text{A-13})$$

In the above formula, z_i are the roots of the Laguerre polynomials of $j+1$ order, w_i are the corresponding weight factors (given by A-14), and for $F(x)$ being a polynomial it is exact up to a degree less than $j+1$.

$$w_i = \frac{j! \Gamma(j+1) z_i}{[P_{j+1}(z_i)]^2} \quad (\text{A-14})$$

In the present work, a 15-point quadrature is used for evaluation of the stress integral in the K-BKZ constitutive equation. Table A-2 gives the Legendre polynomial roots and weighting factors.

Table A-2: Roots and weighting factors for the 15-point Laguerre quadrature.

15-Point Laguerre Quadrature		
Roots and Weighting Factors		
i	z_i	w_i
0	$9.330781201700 \times 10^{-2}$	0.218234885940
1	0.492691740302	0.342210177923
2	1.215595412071	0.263027577942
3	2.269949526204	0.126425818106
4	3.667622721751	$4.020686492100 \times 10^{-2}$
5	5.425336627414	$8.563877803610 \times 10^{-3}$
6	7.565916226613	$1.212436147210 \times 10^{-3}$
7	10.120228568019	$1.116743923440 \times 10^{-4}$
8	13.130282482176	$6.459926762020 \times 10^{-6}$
9	16.654407708330	$2.226316907100 \times 10^{-7}$
10	20.776478899449	$4.227430384980 \times 10^{-9}$
11	25.623894226729	$3.921897267040 \times 10^{-11}$
12	31.407519169754	$1.456515264070 \times 10^{-13}$
13	38.530683306486	$1.483027051110 \times 10^{-16}$
14	48.026085572686	$1.600594906210 \times 10^{-20}$

Appendix B

F-BLOW Code for Film Blowing

(a) FORTRAN Source Code "fblow.f"

```
C
C .....
C *   program name: FBLOW
C *
C *   ver 1.0 : 22 Feb. 1997   First Working Version
C *   ver 1.1 : 14 Mar. 1997   Quadratic Elements
C *   ver 1.2 : 21 Mar. 1997   Gauss-Laguerre
C *   ver 2.0 : 14 Jul. 1997   New "TIMES" Algorithm
C *
C *   (c) 1997 Michel Beaulne
C *
C .....
C
C   PROGRAM FBLOW
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C   INTEGER*2 HRS,MINS,SECS,HSECS
C   INTEGER*2 YEAR,MONTH,DAY
C   CHARACTER*8 ADATE,ATIME,ATIME0,date,clock_
C   CHARACTER*512 BUFFER
C
C   SAVE ATIME0
C
C   INCLUDE 'malloc.inc'
C   INCLUDE 'common.inc'
C
C   DIMENSION DREL(10),DCOEF(10),PHIX(3)
C   DIMENSION SZZ(MAXE*6),STAUSS(MAXE*6),STAUTT(MAXE*6)
C   DIMENSION SSRATE(MAXE*6)
C   DIMENSION EZ(MAXN),E11(MAXN),E22(MAXN),E33(MAXN),EE(MAXN)
C   DIMENSION ET(MAXN)
C
C   OPEN INPUT AND OUTPUT FILES
C
C   IN=10
C   IO=11
C   ITEC=12
C   ICON=13
C   ISP=14
C   ISURF=15
C   IRATE=16
C   IFBVIS=17
C   OPEN (IN,FILE='fblow.inp')
C   OPEN (IO,FILE='fblow.out')
C   OPEN (ITEC,FILE='tecplot.tec')
C   OPEN (ICON,FILE='continue.data')
C   OPEN (ISP,FILE='splot.csv')
C   OPEN (ISURF,FILE='surface.tec')
C   OPEN (IRATE,FILE='erate.csv')
C   OPEN (IFBVIS,FILE='fbvis.add')
C
C .....
C *
C *   P R E - P R O C E S S I N G
C *
```

```

C *****
C
C GET TIME AND DATE
C
C   INCLUDE 'system.inc'
C   ATIME0=ATIME
C
C WELCOME MESSAGE
C
C   WRITE (*,1000) ADATE,ATIME
C   WRITE (IO,1000) ADATE,ATIME
C
C START THE CLOCK
C
C   CALL CPTIME(1)
C
C READ IN PROGRAM PARAMETERS
C
C   READ (IN,*)
C   READ (IN,*)
C   READ (IN,*) NELE,EPS,IMAX,UNREL
C
C READ IN CONTROL FLAGS
C
C   READ (IN,*)
C   READ (IN,*) ITEMP,ICONT,ICONS,IFORCE,IPRESS
C
C READ IN PROBLEM SPECIFICATIONS
C
C   READ (IN,*)
C   READ (IN,*) CONS,FORCE,PRESS
C   READ (IN,*)
C   READ (IN,*) U0,RAD0,H0,DL,DR,RADF
C   READ (IN,*)
C   READ (IN,*) fDrL,fDrR,BrfL,BrfR
C
C GUESS FOR CONTINUOUS STRESS CONSTANT AND FORCE
C
C   IF (ICONS.EQ.0) CONS=1.D0
C   IF (IFORCE.EQ.0) FORCE=3.D0
C
C READ IN NON-ISOTHERMAL PARAMETERS
C
C   READ (IN,*)
C   READ (IN,*)
C   READ (IN,*) T0,TREF,RHO0,EACT,HEATC
C   READ (IN,*)
C   READ (IN,*) GC,CP0,CK1,CK2,XPANC
C   READ (IN,*)
C   READ (IN,*) TAIR,EMIS,SB
C
C READ IN VISCOELASTIC PARAMETERS
C
C   READ (IN,*)
C   READ (IN,*)
C   READ (IN,*) NREL,THETA
C
C READ IN RELAXATION SPECTRUM
C
C   READ (IN,*)
C   READ (IN,*)
C   READ (IN,*) (DREL(I),DCOEF(I),ALPHA(I),BETA(I),I=1,NREL)
C
C MESH CONSTANTS
C
C   NNODE=NELE+1
C   NE2=2*NELE
C   NNQ=2*NNODE-1
C   NNQ2=2*NNQ
C   NNQ3=3*NNQ
C

```

```

C READ IN MESH FROM INPUT FILE
C
C READ (IN,*)
C READ (IN,*) (Z(I),I=1,NNQ,2)
C
C IF ICONT.EQ.0 FIND INTERIOR NODAL VALUES
C AND FIND NEWTONIAN PROFILES
C
C IF (ICONT.EQ.0) THEN
C DO 5 I=2,NE2,2
C Z(I)=0.5DO*(Z(I+1)+Z(I-1))
5 CONTINUE
C DO 6 I=1,NNQ
C Z(I)=Z(I)*DL
C T(I)=1.DO
6 CONTINUE
C CALL FBNEW
C ENDF
C
C IF ICONT.EQ.1 READ IN GUESSES FROM CONTINUATION FILE
C (QUADRATIC VALUES ALSO)
C
C IF (ICONT.EQ.1) THEN
C READ (ICON,*) DCONS,DFORCE,DPRESS
C READ (ICON,*) (Z(I),R(I),U(I),H(I),T(I),I=1,NNQ)
C IF (ICONS.EQ.0) CONSD=DCONS
C IF (IFORCE.EQ.0) FORCE=DFORCE
C IF (IPRESS.EQ.0) PRESS=DPRESS
C ENDF
C
C GETTING TIME
C
C CALL CPTIME(2)
C
C CALCULATE ZERO-SHEAR VISCOSITY
C
C VIS0=0.DO
C DO 10 I=1,NREL
C VIS0=VIS0+DREL(I)*DCOEF(I)
10 CONTINUE
C
C DIMENSIONLESS RELAXATION TIME AND MODULUS
C
C DO 20 I=1,NREL
C REL(I)=DREL(I)*U0/RAD0
C COEF(I)=DCOEF(I)*RAD0/(VIS0*U0)
20 CONTINUE
C
C DETERMINE AVERAGE RELAXATION TIME
C
C AN=0.DO
C DEN=0.DO
C DO 30 IR=1,NREL
C AN=AN+REL(IR)**2.DO*COEF(IR)
C DEN=DEN+REL(IR)*COEF(IR)
30 CONTINUE
C AVREL=AN/DEN
C WRITE (*,1010) VIS0,AVREL
C WRITE (IO,1010) VIS0,AVREL
C
C CONSTANTS USED THROUGHOUT THE PROGRAM
C
C PI=4.DO*ATAN(1.DO)
C Q=2.DO*PI*RAD0*U0*H0
C
C *****
C *
C * P R O C E S S I N G *
C *
C *****
C

```

```

C CALLING "DRIVER" WHICH DRIVES THE PROGRAM
C AND ITERATION PROCESS
C
C CALL DRIVER
C
C .....
C *
C * P O S T - P R O C E S S I N G *
C *
C .....
C
C GETTING TIME
C
C CALL CPTIME(4)
C
C DO 40 I=1,NNQ
C H(I)=1.D0/U(I)/R(I)
40 CONTINUE
C
C CALCULATING LOCATIONS OF GAUSS POINTS
C AS Z COORDINATE AND STRAIN RATES
C
C DO 50 I=1,NELE
C I2=I*2
C DZ=Z(I2+1)-Z(I2-1)
C DO 50 J=1,6
C ZZ(I,J)=Z(I2-1)+DZ*GP(J)
C C=GP(J)
C SRATE(I,J)=0.D0
C PHIX(1)=(4.D0*C-3.D0)/DZ
C PHIX(2)=(4.D0-8.D0*C)/DZ
C PHIX(3)=(4.D0*C-1.D0)/DZ
C DO 50 L=1,3
C SRATE(I,J)=SRATE(I,J)+PHIX(L)*U(I2-2+L)*U0/RAD0
50 CONTINUE
C
C USING CENTRAL-DIFFERENCES
C FOR BETTER EXTENSIONAL RATES
C DETERMINATION
C
C DO 55 I=1,NELE
C I2=I*2
C DZ=Z(I2+1)-Z(I2-1)
C DR=(R(I2+1)-R(I2-1))/DZ
C DU=(U(I2+1)-U(I2-1))/DZ*U0/RAD0
C CTHETA=1.D0/DSQRT(1.D0+DR**2.D0)
C E11(I)=2.D0*CTHETA*DU
C E22(I)=2.D0*CTHETA*U(I2)/R(I2)*DR
C E33(I)=-E11(I)-E22(I)
C EE(I)=DSQRT(0.5D0*(E11(I)**2.D0+E22(I)**2.D0+E33(I)**2.D0))
C EZ(I)=Z(I2)
C ET(I)=T(I2)*T0-273.
55 CONTINUE
C
C OUTPUT FILE
C
C WRITE (IO,1020)
C WRITE (IO,1100) (Z(I),R(I),U(I),H(I),T(I),I=1,NNQ)
C WRITE (IO,1030)
C WRITE (IO,1110) ((ZZ(I,J),TAUSS(I,J),TAUTT(I,J), !CHECK
C & TAUSS(I,J)/TAUTT(I,J),J=1,6),I=1,NELE)
C
C CONTINUATION FILE
C
C REWIND (ICON)
C WRITE (ICON,2000) CONS, FORCE, PRESS
C WRITE (ICON,2010) (Z(I),R(I),U(I),H(I),T(I),I=1,NNQ)
C
C TECPLOT FILE
C
C ZERO=0.D0

```

```

WRITE (ITEC,3000) NNQ
WRITE (ITEC,3060) (R(I)*RADO,Z(I)*RADO,U(I)*UO,H(I)*HO,
6 T(I)*T0-273.,ZERO,ZERO,ZERO,I=1,NNQ)
WRITE (ITEC,3010) NNQ
WRITE (ITEC,3060) (-R(I)*RADO,Z(I)*RADO,U(I)*UO,H(I)*HO,
6 T(I)*T0-273.,ZERO,ZERO,ZERO,I=1,NNQ)
WRITE (ITEC,3020) NNQ
WRITE (ITEC,3060) (R(I)*RADO+H(I)*HO,Z(I)*RADO,U(I)*UO,H(I)*HO,
6 T(I)*T0-273.,ZERO,ZERO,ZERO,I=1,NNQ)
WRITE (ITEC,3030) NNQ
WRITE (ITEC,3060) (-R(I)*RADO-H(I)*HO,Z(I)*RADO,U(I)*UO,H(I)*HO,
6 T(I)*T0-273.,ZERO,ZERO,ZERO,I=1,NNQ)
WRITE (ITEC,3040) NNQ
WRITE (ITEC,3060) (R(I),Z(I),U(I),H(I),T(I),
6 ZERO,ZERO,ZERO,I=1,NNQ)
WRITE (ITEC,3050) NELE*6
WRITE (ITEC,3060) ((DRDZ(I,J),ZZ(I,J),SRATE(I,J),ZERO,ZERO,
6 TAUSS(I,J),TAUTT(I,J),
6 TAUSS(I,J)/TAUTT(I,J),J=1,6),I=1,NELE)
C
C TECPLOT 3-D SURFACE PLOT ID=1
C
ID=1
IMAX=37
WRITE (ISURF,6000) ID,IMAX,NNQ
DO 61 J=1,NNQ
ANGLE=0.DO
DO 61 I=1,IMAX
RAD=R(J)*RADO
XX=RAD*COS(ANGLE)
YY=(RAD**2.DO-XX**2.DO)**0.5DO
IF (ANGLE.GE.PI) YY=-YY
IF (I.EQ.1.OR.I.EQ.19.OR.I.EQ.37) YY=0.DO
WRITE (ISURF,6010) -Z(J)*RADO,XX,YY,U(J)*UO,T(J)*T0-273.
ANGLE=ANGLE+PI/18.DO
61 CONTINUE
C
C TECPLOT 3-D SURFACE PLOT ID=2
C
ID=2
IMAX=37
WRITE (ISURF,6020) ID,IMAX,NNQ
DO 62 J=1,NNQ
ANGLE=0.DO
DO 62 I=1,IMAX
RAD=R(J)*RADO+H(J)*HO
XX=RAD*COS(ANGLE)
YY=(RAD**2.DO-XX**2.DO)**0.5DO
IF (ANGLE.GE.PI) YY=-YY
IF (I.EQ.1.OR.I.EQ.19.OR.I.EQ.37) YY=0.DO
WRITE (ISURF,6010) -Z(J)*RADO,XX,YY,U(J)*UO,T(J)*T0-273.
ANGLE=ANGLE+PI/18.DO
62 CONTINUE
C
C SIGMAPLOT FILE
C
NC=0
DO 70 I=1,NELE
DO 70 J=1,6
NC=NC+1
S22(NC)=22(I,J)
STAUSS(NC)=TAUSS(I,J)
STAUTT(NC)=TAUTT(I,J)
SSRATE(NC)=SRATE(I,J)
70 CONTINUE
C
WRITE (ISP,4000)
C
DO 80 I=1,NNQ
WRITE (BUFFER,4010) Z(I)*RADO,-Z(I)*RADO,R(I)*RADO,-R(I)*RADO,
6 R(I)*RADO+H(I)*HO,-R(I)*RADO-H(I)*HO,

```

```

      U(I)*UO,T(I)*TO-273.,
      Z(I),R(I),U(I),H(I),T(I),
      SZZ(I),SSRATE(I),STAUSS(I),STAUTT(I),
      STAUSS(I)/STAUTT(I)
      WRITE (ISP,4020) BUFFER
80    CONTINUE
C
      DO 90 I=NNQ+1,NC
        WRITE (BUFFER,4030) SZZ(I),SSRATE(I),STAUSS(I),STAUTT(I),
          STAUSS(I)/STAUTT(I)
        WRITE (ISP,4020) BUFFER
90    CONTINUE
C
C    ADDITIONAL FILE FOR BETTER EXTENSIONAL RATES
C
      WRITE (IRATE,4040)
      WRITE (IRATE,4050) (EZ(I),EZ(I)*RADO,E11(I),E22(I),E33(I),
        EE(I),ET(I),I=1,NELE)
      WRITE (IFBVIS,4060) (EZ(I),EZ(I)*RADO,EE(I),ET(I)+273.,I=1,NELE)
C
C    STOP THE CLOCK
C
      CALL CPTIME(9)
      INCLUDE 'system.inc'
      WRITE (IO,1200) ATIME0,ATIME
C
C    *** FORMAT STATEMENTS ***
C
C    OUTPUT FILE
C
1000  FORMAT (/ ,6X,'.....',/,
      6      6X,'*
      6      6X,'*      FFFFF BBBB L      OOO W W      *',/,
      6      6X,'*      F      B B L      O O W W W      *',/,
      6      6X,'*      FFF --- BBBB L      O O W W W      *',/,
      6      6X,'*      F      B B L      O O W W W      *',/,
      6      6X,'*      F      BBBB LLLLL OOO W W      *',/,
      6      6X,'*
      6      6X,'*',21X,A8,2X,A8,5X,'*',/,
      6      6X,'.....',/)
1010  FORMAT (/ ,9X,'*** Viscoelastic Problem Being Solved ***',/,
      6      6X,'Zero-Shear-Rate Viscosity      : ',G12.4,/,
      6      6X,'Weissenberg Number              : ',F10.4,/)
C
1020  FORMAT (/ ,7X,'Distance',11X,'Radius',9X,'Velocity',
      6      8X,'Thickness',6X,'Temperature')
1030  FORMAT (/ ,7X,'Distance',10X,'Tau(ss)',
      6      10X,'Tau(tt)',2X,'Tau(ss)/Tau(tt)')
1100  FORMAT (5X,G14.7,3X,G14.7,3X,G14.7,3X,G14.7,3X,G14.7)
1110  FORMAT (5X,G14.7,3X,G14.7,3X,G14.7,3X,G14.7)
1200  FORMAT (/ ,2X,'*** CLOCK TIME AT START OF PROGRAM      : ',2X,A8,/,
      6      2X,'*** CLOCK TIME AT END OF PROGRAM          : ',2X,A8,/)
C
C    CONTINUATION FILE
C
2000  FORMAT (2(3X,E18.12))
2010  FORMAT (5(3X,E18.12))
C
C    TECPLOT FILE
C
3000  FORMAT ('TITLE="FilmBlow"',/,'VARIABLES="radius","z",',
      6      'vel","thick","temp","Tss","Ttt","ratio"',/,'
      6      'ZONE T="Film1",I=',I3)
3010  FORMAT ('ZONE T="Film2",I=',I3)
3020  FORMAT ('ZONE T="Film3",I=',I3)
3030  FORMAT ('ZONE T="Film4",I=',I3)
3040  FORMAT ('ZONE T="DimZone1",I=',I3)
3050  FORMAT ('ZONE T="DimZone2",I=',I3)
3060  FORMAT (8(3X,G18.12))
C
C    SURFACE PLOT

```

```

C
6000  FORMAT ('TITLE="Surface"',/, 'VARIABLES="axial","xx"',,
        &      '"yy","vel","temp"',/,
        &      'ZONE T="Surface', I2, '"', I=' , I3, ', J=' , I3)
6010  FORMAT (5(3X,G18.12))
6020  FORMAT ('ZONE T="Surface', I2, '"', I=' , I3, ', J=' , I3)
C
C   SIGMAPLOT FILE
C
4000  FORMAT ('z(i)*rad0', 5x, ', -z(i)*rad0', 4x, ', r(i)*rad0', 5x,
        &      ', -r(i)*rad0', 4x, ', r+h(i)*h0', 5x, ', -r-h(i)*h0', 4x,
        &      ', u(i)*u0', 7x,
        &      ', T(i)*T0', 7x, ', z(i)', 10x, ', r(i)', 10x, ', u(i)', 10x,
        &      ', h(i)', 10x, ', T(i)', 10x, ', z(i:j)', 8x, ', erate(i:j)', 4x,
        &      ', tss(i:j)', 6x, ', ttt(i:j)', 6x, ', tss/ttt')
4010  FORMAT (17(G14.7, ', '), G14.7)
4020  FORMAT (A350)
4030  FORMAT (13(14X, ', '), 4(G14.7, ', '), G14.7)
4040  FORMAT ('z(i)', 10x, ', z(i)*r0', 7x, ', ell(i)', 8x, ', e22(i)', 8x,
        &      ', e33(i)', 8x, ', lel', 11x, ', T(i)*T0-273')
4050  FORMAT (6(G14.7, ', '), G14.7)
4060  FORMAT (4(G14.7))
C
C   USED FOR CLOCK
C
5000  FORMAT (I2.2, ': ', I2.2, ': ', I2.2)
5010  FORMAT (I2.2, '/ ', I2.2, '/ ', I2.2)
C
      STOP
      END
C
C*****
C
      SUBROUTINE DRIVER
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      INCLUDE 'malloc.inc'
      INCLUDE 'common.inc'
C
      BEGIN ITERATIONS
C
      DO 999 K=1,IMAX
C
      STORING OLD VALUES
C
      DO 10 I=1,NNQ
          OV(I)=R(I)
          OV(I+NNQ)=U(I)
          OV(I+NNQ2+3)=T(I)
10      CONTINUE
          OV(NNQ2+1)=CONS
          OV(NNQ2+2)=FORCE
          OV(NNQ2+3)=PRESS
C
      CALLING "JACOB" TO CALCULATE THE JACOBIANS
C
      CALL JACOB
C
      CALLING "GAUSS" TO SOLVE SYSTEM OF EQUATIONS
C
      CALL GAUSS
C
      UPDATE VALUES
C
      DO 20 I=1,NNQ
          R(I)=OV(I)+UNREL*SF(I)
          U(I)=OV(I+NNQ)+UNREL*SF(I+NNQ)
          IF (ITEMP.EQ.1) T(I)=OV(I+NNQ2+3)+UNREL*SF(I+NNQ2+3)
20      CONTINUE
          CONS=OV(NNQ2+1)+UNREL*SF(NNQ2+1)

```

```

      FORCE=OV(NNQ2+2)+UNREL*SF(NNQ2+2)
      PRESS=OV(NNQ2+3)+UNREL*SF(NNQ2+3)
C
C   CALCULATE ROOT-MEAN SQUARE OF THE ERROR
C
      IF (ITEMP.EQ.0) NVAR=NNQ2+3
      IF (ITEMP.EQ.1) NVAR=NNQ3+3
      RMS=0.D0
      DO 30 I=1,NVAR
        RMS=RMS+SF(I)**2.D0
30    CONTINUE
C
C   CALCULATE ROOM-MEAN-SQUARE ERROR
C
      RMS=DSQRT(RMS/NVAR)
C
C   FIND OSCILLATIONS IN VARIABLES
C
      NOR=0
      NOU=0
      NOT=0
      DO 35 I=2,NNQ-1
        IF (R(I).LT.R(I-1).AND.R(I).LT.R(I+1)) NOR=NOR+1
        IF (R(I).GT.R(I-1).AND.R(I).GT.R(I+1)) NOR=NOR+1
        IF (U(I).LT.U(I-1).AND.U(I).LT.U(I+1)) NOU=NOU+1
        IF (U(I).GT.U(I-1).AND.U(I).GT.U(I+1)) NOU=NOU+1
        IF (T(I).LT.T(I-1).AND.T(I).LT.T(I+1)) NOT=NOT+1
        IF (T(I).GT.T(I-1).AND.T(I).GT.T(I+1)) NOT=NOT+1
35    CONTINUE
C
C   ITERATION RESULTS TO OUTPUT FILE
C
      WRITE (IO,1000) K
      WRITE (IO,1010) RMS
      WRITE (IO,1020) R(NNQ),U(NNQ),T(NNQ),CONS,FORCE,PRESS
      WRITE (IO,1030) NOR,NOU,NOT
C
C   ITERATION RESULTS TO SCREEN
C
      WRITE (*,1000) K
      WRITE (*,1010) RMS
      WRITE (*,1020) R(NNQ),U(NNQ),T(NNQ),CONS,FORCE,PRESS
      WRITE (*,1030) NOR,NOU,NOT
C
C   CONVERGENCE
C
      IF (DABS(RMS).LT.EPS) RETURN
C
C   BLOW-UP
C
      IF (DABS(RMS).GT.1.D+4) THEN
        WRITE (*,1040)
        WRITE (IO,1040)
        STOP
      ENDIF
C
C   CHECK FOR NEGATIVE VALUES FOR RADIUS, VELOCITY, AND TEMPERATURE
C
      DO 40 I=1,NNQ
        IF (R(I).LT.0.D0) R(I)=-1.D0*R(I)
        IF (U(I).LT.0.D0) U(I)=-1.D0*U(I)
        IF (T(I).LT.0.D0) T(I)=-1.D0*T(I)
40    CONTINUE
      IF (CONS.LT.0.D0) CONS=-1.D0*CONS
      IF (FORCE.LT.0.D0) FORCE=-1.D0*FORCE
      IF (PRESS.LT.0.D0) PRESS=-1.D0*PRESS
C
C   GETTING TIME
C
      CALL CPTIME (3)
C

```

```

999  CONTINUE
C
C *** FORMAT STATEMENTS ***
C
1000 FORMAT (/,10X,'Iteration = ',I3)
1010 FORMAT (10X,'RMS Error = ',E10.4,/)
1020 FORMAT (6x,'Dimensionless radius at take-up      : ',F12.6,/,
&        6x,'Dimensionless velocity at take-up      : ',F12.6,/,
&        6x,'Dimensionless temperature at take-up   : ',F12.6,/,
&        6x,'Conservation of stress constant        : ',F12.6,/,
&        6x,'Dimensionless force at take-up         : ',F12.6,/,
&        6x,'Dimensionless pressure at take-up      : ',F12.6)
1030 FORMAT (6x,'Oscillations in variables (r:u:T)   : ',
&        I3,1X,':',I3,1X,':',I3,/)
1040 FORMAT (4X,'RMS error greater than 10,000: FCAST ENDED!')
C
      END
C
C*****
C
      SUBROUTINE JACOB
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      INCLUDE 'malloc.inc'
      INCLUDE 'common.inc'
C
      CALLING "RESID" TO CALCULATE INITIAL RESIDUALS
C
      CALL RESID
C
      DETERMINING NUMBER OF PERTURBATIONS
C
      IF (ITEMP.EQ.0) NPER=NNQ2+3
      IF (ITEMP.EQ.1) NPER=NNQ3+3
C
      STORING ORIGINAL RESIDUALS IS "RSO"
C
      DO 5 I=1,NPER
        RSO(I)=RS(I)
5      CONTINUE
C
      STORING INITIAL VALUES OF WIDTH, VELOCITY AND TEMPERATURE
C
      DO 10 I=1,NNQ
        UTO(I)=R(I)
        UTO(I+NNQ)=U(I)
        UTO(I+NNQ2+3)=T(I)
10     CONTINUE
        UTO(NNQ2+1)=CONS
        UTO(NNQ2+2)=FORCE
        UTO(NNQ2+3)=PRESS
C
      DO 20 I=1,NNQ
        UT(I)=R(I)
        UT(I+NNQ)=U(I)
        UT(I+NNQ2+3)=T(I)
20     CONTINUE
        UT(NNQ2+1)=CONS
        UT(NNQ2+2)=FORCE
        UT(NNQ2+3)=PRESS
C
      INITIALIZE JACOBIAN MATRIX AND RHS VECTOR
C
      DO 40 I=1,NPER
        SF(I)=0.00
        DO 40 J=1,NPER
          SK(I,J)=0.00
40     CONTINUE
C
      LOOP FOR JACOBIAN

```

```

C      DO 50 K=1,NPER
C
C      PERTURB ONE VARIABLE
C
C      UT(K)=UTO(K)+0.0000001D0*UTO(K)
C
C      UPDATE VALUES [FOR JACOBIAN PURPOSES]
C
C      DO 60 I=1,NNQ
C        R(I)=UT(I)
C        U(I)=UT(I+NNQ)
C        T(I)=UT(I+NNQ2+3)
60    CONTINUE
C      CONS=UT(NNQ2+1)
C      FORCE=UT(NNQ2+2)
C      PRESS=UT(NNQ2+3)
C
C      CALLING "RESID" TO CALCULATE RESIDUALS FOR PERTURBED VARIABLE
C
C      CALL RESID
C
C      *** JACOBIAN ***
C
C      DO 80 J=1,NPER
C        SK(J,K)=(RS(J)-RSO(J))/(0.0000001D0*UTO(K))
80    CONTINUE
C
C      RESTORE PERTURBED VARIABLE
C
C      UT(K)=UTO(K)
C
C      END OF LOOP FOR JACOBIAN
C
50  CONTINUE
C
C      RESIDUAL BOUNDARY CONDITIONS
C
C      RSO(1)=0.D0      ! INLET RADIUS
C      IF (IPRESS.EQ.0) RSO(NNQ)=0.D0      ! EXIT RADIUS
C      RSO(NNQ+1)=0.D0   ! INLET VELOCITY
C      IF (IFORCE.EQ.0) RSO(NNQ2)=0.D0      ! EXIT VELOCITY
C      IF (ICONS.EQ.1) RSO(NNQ2+1)=0.D0     ! STRESS CONSTANT
C      IF (IFORCE.EQ.1) RSO(NNQ2+2)=0.D0    ! FORCE
C      IF (IPRESS.EQ.1) RSO(NNQ2+3)=0.D0    ! PRESSURE
C      RSO(NNQ2+4)=0.D0      ! INLET TEMPERATURE
C
C      JACOBIAN BOUNDARY CONDITIONS
C
C      DO 90 I=1,NPER
C        SK(1,I)=0.D0      ! INLET RADIUS
C        IF (IPRESS.EQ.0) SK(NNQ,I)=0.D0    ! EXIT RADIUS
C        SK(NNQ+1,I)=0.D0   ! INLET VELOCITY
C        IF (IFORCE.EQ.0) SK(NNQ2,I)=0.D0    ! EXIT VELOCITY
C        IF (ICONS.EQ.1) SK(NNQ2+1,I)=0.D0   ! STRESS CONSTANT
C        IF (IFORCE.EQ.1) SK(NNQ2+2,I)=0.D0  ! FORCE
C        IF (IPRESS.EQ.1) SK(NNQ2+3,I)=0.D0  ! PRESSURE
C        SK(NNQ2+4,I)=0.D0      ! INLET TEMPERATURE
90    CONTINUE
C
C      SK(1,1)=1.D0      ! INLET RADIUS
C      IF (IPRESS.EQ.0) SK(NNQ,NNQ)=1.D0    ! EXIT RADIUS
C      SK(NNQ+1,NNQ+1)=1.D0   ! INLET VELOCITY
C      IF (IFORCE.EQ.0) SK(NNQ2,NNQ2)=1.D0   ! EXIT VELOCITY
C      IF (ICONS.EQ.1) SK(NNQ2+1,NNQ2+1)=1.D0 ! FORCE
C      IF (IFORCE.EQ.1) SK(NNQ2+2,NNQ2+2)=1.D0 ! PRESSURE
C      IF (IPRESS.EQ.1) SK(NNQ2+3,NNQ2+3)=1.D0 ! INLET TEMPERATURE
C      SK(NNQ2+4,NNQ2+4)=1.D0
C
C      FOR NEWTON-RAPHSON
C

```

```

      DO 100 I=1,NPER
        SF(I)=-1.D0*RSO(I)
100    CONTINUE
      C
      RETURN
      END
      C
      C.....
      C
      SUBROUTINE RESID
      C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      C
      INCLUDE 'malloc.inc'
      INCLUDE 'common.inc'
      C
      DIMENSION PHI(3),PHIX(3)
      DIMENSION RR(MAXN+3),RU(MAXN),RT(MAXN)
      C
      C INITIALIZE RESIDUALS
      C
      DO 5 I=1,NNQ
        RR(I)=0.D0
        RU(I)=0.D0
        RT(I)=0.D0
      5    CONTINUE
        RU(NNQ+1)=0.D0
        RU(NNQ+2)=0.D0
        RU(NNQ+3)=0.D0
      C
      C CALLING "TIMES" TO CALCULATE TRAVELLING TIME
      C OF PARTICLE AT EACH GAUSS POINT
      C
      CALL TIMES
      C
      C CALLING "STRESS" TO DETERMINE STRESSES
      C DUE TO HISTORY AND PREHISTORY IN THE FILM
      C
      CALL STRESS
      C
      C NOW CALCULATING THE RESIDUALS
      C
      DO 10 I=1,NELE
        I2=I*2
        DZ=Z(I2+1)-Z(I2-1)
        DO 20 J=1,6
          C=GP(J)
          ZZ(I,J)=Z(I2-1)+DZ*C
          RAD=0.D0
          VEL=0.D0
          TEMP=0.D0
          DTEMP=0.D0
          DRDZ(I,J)=0.D0
        20 CONTINUE
      10 CONTINUE
      C
      C SHAPE FUNCTIONS
      C
      PHI(1)=(1.D0-C)*(1.D0-2.D0*C)
      PHI(2)=4.D0*C*(1.D0-C)
      PHI(3)=-1.D0*C*(1.D0-2.D0*C)
      PHIX(1)=(4.D0*C-3.D0)/DZ
      PHIX(2)=(4.D0-8.D0*C)/DZ
      PHIX(3)=(4.D0*C-1.D0)/DZ
      C
      C VARIABLE VALUES AT GAUSS POINTS
      C
      DO 30 L=1,3
        RAD=RAD+PHI(L)*R(I2-2+L)
        VEL=VEL+PHI(L)*U(I2-2+L)
        TEMP=TEMP+PHI(L)*T(I2-2+L)
        DTEMP=DTEMP+PHIX(L)*T(I2-2+L)
        DRDZ(I,J)=DRDZ(I,J)+PHIX(L)*R(I2-2+L)
      30 CONTINUE

```

```

30      CONTINUE
C
C      CONSTANTS
C
      BUR=R(NNQ)
      AF=FORCE-PRESS*(BUR)**2.DO
      BF=PRESS
C
C      NON-ISOTHERMAL DENSITY
C
      RHO=RHO0/(1.DO+XPANC*(TEMP*T0-TREF))
      IF (ITEMP.EQ.0) RHO=RHO0
C
C      NON-ISOTHERMAL HEAT CAPACITY
C
      CP=CP0*(CK1+CK2*TEMP*T0)/(CK1+CK2*TREF)
C
C      CONSTANTS FOR HEAT TRANSFER RESIDUALS
C
      G1=2.DO*PI*RADO**2.DO*HEATC/CTHT(I,J)/(RHO*CP*Q)
      G2=2.DO*PI*RADO**2.DO*EMIS*SB*T0**3.DO/CTHT(I,J)/(RHO*CP*Q)
C
C      SECANT OF ANGLE THETA
C
      STHT=DSQRT(1.DO+DRDZ(I,J)**2.DO)
C
C      ASSEMBLING RESIDUALS
C
      DO 40 L=1,3
C
C      *** RESIDUAL FOR RADIUS ***
C
      RR(I2-2+L)=RR(I2-2+L)+DZ*WG(J)*(-1.DO*DRDZ(I,J)*PHIX(L)+
&      1.DO/(AF+BF*RAD**2.DO)*(2.DO*BF*RAD*STHT**2.DO-
&      TAUTT(I,J)/RAD/VEL*STHT)*PHI(L))
C
C      *** RESIDUAL FOR VELOCITY ***
C
      RU(I2-2+L)=RU(I2-2+L)+DZ*WG(J)*(TAUSS(I,J)-
&      (AF+BF*RAD**2.DO)*STHT*VEL)*PHI(L)
C
C      *** RESIDUAL FOR TEMPERATURE ***
C
      RT(I2-2+L)=RT(I2-2+L)+DZ*WG(J)*(DTEMP*RAD*(
&      G1*(TEMP-TAIR/T0)+
&      G2*(TEMP**4.DO-(TAIR/T0)**4.DO))*PHI(L)
C
40      CONTINUE
20      CONTINUE
10      CONTINUE
C
      C=GP(1)
      PHI(1)=(1.DO-C)*(1.DO-2.DO*C)
      PHI(2)=4.DO*C*(1.DO-C)
      PHI(3)=-1.DO*C*(1.DO-2.DO*C)
      VEL1=PHI(1)*U(1)+PHI(2)*U(2)+PHI(3)*U(3)
C
      C=GP(6)
      PHI(1)=(1.DO-C)*(1.DO-2.DO*C)
      PHI(2)=4.DO*C*(1.DO-C)
      PHI(3)=-1.DO*C*(1.DO-2.DO*C)
      VELN=PHI(1)*U(NNQ-2)+PHI(2)*U(NNQ-1)+PHI(3)*U(NNQ)
C
C      *** RESIDUAL FOR CONTINUOUS STRESS CONSTANT ***
C
      RU(NNQ+1)=TAUSSC/U(1)-TAUSS(1,1)/VEL1
C
C      RESIDUAL FOR FORCE AT TAKE-UP END
C
      RU(NNQ+2)=TAUSS(NELE,6)-(AF+BF*R(NNQ)**2.DO)*U(NNQ)
C

```

```

C   RESIDUAL FOR PRESSURE
C
C       RU(NNQ+3)=TAUTT(NELE,6)-2.D0*U(NNQ)*BF*R(NNQ)**2.D0
C
C   STORE RESIDUALS IN ONE COLUMN ARRAY
C
C       DO 50 I=1,NNQ
C           RS(I)=RR(I)
C           RS(I+NNQ)=RU(I)
C           RS(I+NNQ2+3)=RT(I)
50  CONTINUE
C       RS(NNQ2+1)=RU(NNQ+1)
C       RS(NNQ2+2)=RU(NNQ+2)
C       RS(NNQ2+3)=RU(NNQ+3)
C
C       RETURN
C       END
C
C .....
C
C   SUBROUTINE STRESS
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C   INTEGER ELEM,ELEM2
C
C   INCLUDE 'malloc.inc'
C   INCLUDE 'common.inc'
C
C   DIMENSION PHI(3)
C
C   FACTOR OF THETA
C
C       FACTHT=1.D0/(1.D0-THETA)
C
C .....
C *
C *       H I S T O R Y
C *
C .....
C
C       DO 10 I=NELE,1,-1
C           I2=2*I
C
C       DO 20 J=6,1,-1
C           C=GP(J)
C
C           PHI(1)=(1.D0-C)*(1.D0-2.D0*C)
C           PHI(2)=4.D0*C*(1.D0-C)
C           PHI(3)=-C*(1.D0-2.D0*C)
C
C       RAD=0.D0
C       VEL=0.D0
C       DO 25 M=1,3
C           RAD=RAD+PHI(M)*R(I2-2+M)
C           VEL=VEL+PHI(M)*U(I2-2+M)
25  CONTINUE
C
C   INITIALIZE PRINCIPAL STRESSES
C
C       TAU11(I,J)=0.D0
C       TAU22(I,J)=0.D0
C       TAU33(I,J)=0.D0
C
C   LOOP FOR EACH RELAXATION TIME
C
C       DO 30 K=1,NREL
C
C   LOOP FOR EACH GAUSS-LAGUERRE POINT
C
C       DO 40 L=1,15

```

```

C  CALCULATE t' FROM GAUSS-LAGUERRE POINT XO(L) AND REL(K)
C
C      TPRIME=TIME(I,J)-XO(L)*REL(K)
C
C  PREHISTORY CHECK (JUMP TO 99 IF WITHIN PREHISTORY)
C
C      IF (TPRIME.LT.0.D0) GOTO 99
C
C  FINDING ELEMENT WHICH CONTAINS t'
C
C      DO 50 M=1,NNODE-1
C          TRM=TNODE(M+1) ! RIGHTMOST TIME
C          IF (TPRIME.LT.TRM) THEN
C              ELEM=M
C              GOTO 33
C          ENDIF
50      CONTINUE
C
C      ELEM2=ELEM*2
C
C      DO 55 M=1,7
C
C          IF (M.EQ.1) THEN
C              TLM=TNODE(ELEM)
C              ZLM=0.D0
C          ELSE
C              TLM=TIME(ELEM,M-1)
C              ZLM=GP(M-1)
C          ENDIF
C
C          IF (M.EQ.7) THEN
C              TRM=TNODE(ELEM+1)
C              ZRM=1.D0
C          ELSE
C              TRM=TIME(ELEM,M)
C              ZRM=GP(M)
C          ENDIF
C
C          IF (TPRIME.LT.TRM) THEN
C              GPZ=ZLM+(TPRIME-TLM)/(TRM-TLM)*(ZRM-ZLM)
C              GOTO 66
C          ENDIF
55      CONTINUE
C
C      C=GPZ
C
C      PHI(1)=(1.D0-C)*(1.D0-2.D0*C)
C      PHI(2)=4.D0*C*(1.D0-C)
C      PHI(3)=-C*(1.D0-2.D0*C)
C      RPRIME=0.D0
C      VPRIME=0.D0
C      DO 90 M=1,3
C          RPRIME=RPRIME+PHI(M)*R(ELEM2-2+M)
C          VPRIME=VPRIME+PHI(M)*U(ELEM2-2+M)
90      CONTINUE
C
C  CALCULATING FINGER AND CAUCHY-GREEN TENSORS
C
C      FINGER1=(VEL/VPRIME)**2.D0
C      FINGER2=(VPRIME*RPRIME/VEL/RAD)**2.D0
C      FINGER3=(RAD/RPRIME)**2.D0
C      FINV1=(VPRIME/VEL)**2.D0
C      FINV2=(VEL*RAD/VPRIME/RPRIME)**2.D0
C      FINV3=(RPRIME/RAD)**2.D0
C
C  CALCULATING FIRST AND SECOND INVARIANTS
C
C      VAR1=FINGER1+FINGER2+FINGER3
C      VAR2=FINV1+FINV2+FINV3
C
C  STRAIN MEMORY FUNCTION

```

```

C      FACT=ALPHA(K) / (ALPHA(K)-3.DO+BETA(K)*VAR1+
      &      (1.DO-BETA(K))*VAR2)
C
C      CALCULATING PRINCIPAL STRESSES
C
      TAU11(I,J)=TAU11(I,J)+COEF(K)*CO(L)*FACTHT*FACT*
      &      ((FINGER1-1.DO)+THETA*(FINV1-1.DO))
      TAU22(I,J)=TAU22(I,J)+COEF(K)*CO(L)*FACTHT*FACT*
      &      ((FINGER2-1.DO)+THETA*(FINV2-1.DO))
      TAU33(I,J)=TAU33(I,J)+COEF(K)*CO(L)*FACTHT*FACT*
      &      ((FINGER3-1.DO)+THETA*(FINV3-1.DO))
C
      GOTO 40
C
C      DONE WITH HISTORY
C
C      *****
C      *          P R E H I S T O R Y          *
C      *          *          *          *
C      *****
C
C      USING INTEGRAL FORMULA TO FIND LOCATION OF  $\epsilon'$ 
C
99      TERM=1.DO-CONS*TPRIME
      IF (TERM.LE.0.DO) TERM=1.D-40
      PZPRIME=DLOG(TERM)/(-1.DO*CONS)
      VPRIME=EXP(CONS*PZPRIME)
C
C      NOW CALCULATING FINGER AND CAUCHY-GREEN TENSORS
C
      FINGER1=(VEL/VPRIME)**2.DO
      FINGER2=(VPRIME/VEL/RAD)**2.DO
      FINGER3=(RAD)**2.DO
      FINV1=(VPRIME/VEL)**2.DO
      FINV2=(VEL*RAD/VPRIME)**2.DO
      FINV3=(1.DO/RAD)**2.DO
C
C      CALCULATING FIRST AND SECOND INVARIANTS
C
      VAR1=FINGER1+FINGER2+FINGER3
      VAR2=FINV1+FINV2+FINV3
C
C      STRAIN MEMORY FUNCTION
C
      FACT=ALPHA(K) / (ALPHA(K)-3.DO+BETA(K)*VAR1+
      &      (1.DO-BETA(K))*VAR2)
C
C      CALCULATING PRINCIPAL STRESSES
C
      TAU11(I,J)=TAU11(I,J)+COEF(K)*CO(L)*FACTHT*FACT*
      &      ((FINGER1-1.DO)+THETA*(FINV1-1.DO))
      TAU22(I,J)=TAU22(I,J)+COEF(K)*CO(L)*FACTHT*FACT*
      &      ((FINGER2-1.DO)+THETA*(FINV2-1.DO))
      TAU33(I,J)=TAU33(I,J)+COEF(K)*CO(L)*FACTHT*FACT*
      &      ((FINGER3-1.DO)+THETA*(FINV3-1.DO))
C
C      DONE WITH PREHISTORY
C
40      CONTINUE ! LOOP FOR EACH GAUSS-LAGUERRE POINT
30      CONTINUE ! LOOP FOR RELAXATION TIMES
20      CONTINUE ! LOOP FOR EACH GAUSS-LEGENDRE LOCATION
10      CONTINUE ! LOOP FOR EACH ELEMENT
C
C      STRESSES IN MACHINE AND TRANSVERSE DIRECTIONS
C
      DO 200 I=1,NELE
      DO 200 J=1,6
      TAUSS(I,J)=TAU11(I,J)-TAU22(I,J)
      TAUTT(I,J)=TAU33(I,J)-TAU22(I,J)

```

```

200  CONTINUE
C
C *****
C *
C * SECTION FOR PREHISTORY PARAMETER C *
C *
C *****
C
      TAU11C=0.D0
      TAU22C=0.D0
      TAU33C=0.D0
      VEL=1.D0
      RAD=1.D0
C
      DO 100 K=1,NREL
C
C      LOOP FOR EACH GAUSS-LAGUERRE POINT
C
C        DO 110 L=1,15
C
C        CALCULATE t' FROM GAUSS-LAGUERRE POINT XO(L) AND REL(K)
C
C          TPRIME=-XO(L)*REL(K)
C
C        USING INTEGRAL FORMULA TO FIND LOCATION OF t'
C
C          TERM=1.D0-CONS*TPRIME
C          IF (TERM.LE.0.D0) TERM=1.D-40
C          PZPRIME=DLOG(TERM)/(-1.D0*CONS)
C          VPRIME=EXP(CONS*PZPRIME)
C
C        CALCULATING FINGER AND CAUCHY-GREEN TENSORS
C
C          FINGER1=(VEL/VPRIME)**2.D0
C          FINGER2=(VPRIME/VEL/RAD)**2.D0
C          FINGER3=(RAD)**2.D0
C          FINV1=(VPRIME/VEL)**2.D0
C          FINV2=(VEL*RAD/VPRIME)**2.D0
C          FINV3=(1.D0/RAD)**2.D0
C
C        CALCULATING FIRST AND SECOND INVARIANTS
C
C          VAR1=FINGER1+FINGER2+FINGER3
C          VAR2=FINV1+FINV2+FINV3
C
C        STRAIN MEMORY FUNCTION
C
C          FACT=ALPHA(K)/(ALPHA(K)-3.D0+BETA(K)*VAR1+
C            & (1.D0-BETA(K))*VAR2)
C
C        CALCULATING PRINCIPAL STRESSES
C
C          TAU11C=TAU11C+COEF(K)*CO(L)*FACTHT*FACT*
C            & ((FINGER1-1.D0)+THETA*(FINV1-1.D0))
C          TAU22C=TAU22C+COEF(K)*CO(L)*FACTHT*FACT*
C            & ((FINGER2-1.D0)+THETA*(FINV2-1.D0))
C          TAU33C=TAU33C+COEF(K)*CO(L)*FACTHT*FACT*
C            & ((FINGER3-1.D0)+THETA*(FINV3-1.D0))
110  CONTINUE
100  CONTINUE
C
      TAUSSC=TAU11C-TAU22C
      TAUTTC=TAU33C-TAU22C
C
      RETURN
      END
C
C *****
C
C THIS SUBROUTINE DETERMINES THE TRAVELLING TIME
C FROM THE DIE EXIT TO ANY GAUSS POINT IN EACH ELEMENT

```

```

C      SUBROUTINE TIMES
C
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C      INCLUDE 'malloc.inc'
C      INCLUDE 'common.inc'
C
C      DIMENSION DTIME(MAXN,7)
C      DIMENSION PHIX(3)
C
C      FINDING COSINES
C
C      DO 10 I=1,NELE
C          I2=2*I
C          DZ=Z(I2+1)-Z(I2-1)
C          DO 11 J=1,6
C              C=GP(J)
C              DRDZ(I,J)=0.D0
C              PHIX(1)=(4.D0*C-3.D0)/DZ
C              PHIX(2)=(4.D0-8.D0*C)/DZ
C              PHIX(3)=(4.D0*C-1.D0)/DZ
C              DO 12 L=1,3
C                  DRDZ(I,J)=DRDZ(I,J)+PHIX(L)*R(I2-2+L)
C              CONTINUE
C              CTHT(I,J)=1.D0/DSQRT(1.D0+DRDZ(I,J)**2.D0)
C          CONTINUE
C      CONTINUE
C
C      NOW FINDING SURFACE LOCATIONS
C      CORRESPONDING TO Z COORDINATE
C
C      S(1)=0.D0
C      DO 15 I=1,NELE
C          I2=2*I
C          DZ=Z(I2+1)-Z(I2-1)
C          S(I2)=S(I2-1)+DZ/2.D0/CTHT(I,3)
C          S(I2+1)=S(I2)+DZ/2.D0/CTHT(I,3)
C      CONTINUE
C
C      TRAVELLING TIMES
C
C      DO 1 I=1,NELE
C          DO 1 J=1,7
C              DTIME(I,J)=0.D0
C          CONTINUE
C
C      DO 20 I=1,NELE
C          I2=2*I
C          DS=S(I2+1)-S(I2-1)
C          DO 20 J=1,7
C              IF (J.EQ.1) ASL=S(I2-1)
C              IF (J.NE.1) ASL=DS*GP(J-1)+S(I2-1)
C              IF (J.EQ.7) ASR=S(I2+1)
C              IF (J.NE.7) ASR=DS*GP(J)+S(I2-1)
C              ADS=ASR-ASL
C
C          DO 20 K=1,6
C
C      FINDING GAUSS POINT LOCATION BETWEEN SEGMENT AZL AND AZR
C
C          ASG=ASL+ADS*GP(K)
C          AGP=(ASG-S(I2-1))/DS
C
C      SHAPE FUNCTIONS FOR VELOCITY
C
C      C=AGP
C
C      FI1=(1.D0-C)*(1.D0-2.D0*C)
C      FI2=4.D0*C*(1.D0-C)
C      FI3=-C*(1.D0-2.D0*C)

```

```

C
C VELOCITY AT AGP
C
      UABS=U(I2-1)*FI1+U(I2)*FI2+U(I2+1)*FI3
      TEMP=T(I2-1)*FI1+T(I2)*FI2+T(I2+1)*FI3
      AT=DEXP(EACT/GC*(1.DO/(T0*TEMP)-1.DO/TREF))
      IF (ITEMP.EQ.0) AT=1.DO
C
C CALCULATING TIME LAPSE BETWEEN EACH GAUSS POINT
C
      DTIME(I,J)=DTIME(I,J)+ADS*WG(K)/UABS/AT
C
20  CONTINUE
C
C ASSEMBLING TIME LAPSES TO FIND TRAVELLING TIMES
C AT EACH GAUSS POINT
C
      TIME(1,1)=DTIME(1,1)
      DO 30 J=2,6
        TIME(1,J)=DTIME(1,J)+TIME(1,J-1)
30  CONTINUE
C
      DO 40 I=2,NELE
        DO 40 J=1,6
          IF (J.EQ.1) TIME(I,J)=TIME(I-1,6)+DTIME(I,J)+DTIME(I-1,7)
          IF (J.NE.1) TIME(I,J)=TIME(I,J-1)+DTIME(I,J)
40  CONTINUE
C
C FINDING NODAL TIMES
C
      TNODE(1)=0.0
      DO 50 I=2,NNODE
        TNODE(I)=TIME(I-1,6)+DTIME(I-1,7)
50  CONTINUE
C
      RETURN
      END
C
C.....
C
C THIS SUBROUTINE PERFORMS GAUSSIAN ELIMINATION
C FOR THE SYSTEM {SK}{dU}={-R}
C
      SUBROUTINE GAUSS
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      INCLUDE 'malloc.inc'
      INCLUDE 'common.inc'
C
      N=NNQ2+3
      IF (ITEMP.EQ.1) N=NNQ3+3
      NM=N-1
C
C START PIVOTING AND SCALING PROCESS
C
      DO 10 K=1,NM
        C=0.0
C
        DO 2 I=K,N
          IF (DABS(SK(I,K)).LE.DABS(C)) GO TO 2
          C=SK(I,K)
          IO=I
2        CONTINUE
C
          IF (DABS(C).GE.EPS) GO TO 3
C
          WRITE (IO,8000)      ! SINGULAR MATRIX
C
          IF (IO .EQ. K) GO TO 6
C

```

```

      DO 4 J=K,N
        TMP=SK(K,J)
        SK(K,J)=SK(I0,J)
4      SK(I0,J)=TMP
      C
        TMP=SF(K)
        SF(K)=SF(I0)
        SF(I0)=TMP
6      KPl=K+1
        C=1.0/C
        SF(K)=SF(K)*C
      C
        DO 10 J=KPl,N
          SK(K,J)=SK(K,J)*C
          DO 20 I=KPl,N
20          SK(I,J)=SK(I,J)-SK(I,K)*SK(K,J)
10      SF(J)=SF(J)-SK(J,K)*SF(K)
      C
        SF(N)=SF(N)/SK(N,N)
      C
      C      BACK SUBSTITUTION
      C
        DO 40 K=1,NM
          I=N-K
          C=0.D0
          IPl=I+1
          DO 50 J=IPl,N
50          C=C+SK(I,J)*SF(J)
40      SF(I)=SF(I)-C
      C
      C      FORMAT STATEMENTS
      C
8000      FORMAT (//,10X,'MATRIX IS SINGULAR')
      C
      C      RETURN
      C      END
C.....
C
C      THIS SUBROUTINE GIVES ALL THE GAUSS POINTS AND WEIGHTS
C      REQUIRED BY THE PROGRAM
C
      C      BLOCK DATA INIT
      C
      C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      C
      C      INCLUDE 'malloc.inc'
      C      INCLUDE 'common.inc'
      C
      C      GAUSS-LEGENDRE (6-POINT FORMULA) POINTS (GP) AND WEIGHTS (WG)
      C
      DATA GP /0.033765242898424,0.169395306766867,0.380690406958402,
6      0.619309593041598,0.830604693233133,0.966234757101576/
      C
      DATA WG /0.085662246189585,0.180380786524069,0.233956967286345,
6      0.233956967286345,0.180380786524069,0.085662246189585/
      C
      C      GAUSS-LAGUERRE (15-POINT FORMULA) POINTS (XO) AND WEIGHTS (CO)
      C
      DATA XO /9.33078120170D-2,4.926917403020D-1,1.2155954120710D+0,
6      2.2699495262040D+0,3.6676227217510D+0,5.4253366274140D+0,
6      7.5659162266130D+0,1.0120228568019D+1,1.3130282482176D+1,
6      1.6654407708330D+1,2.0776478899449D+1,2.5623894226729D+1,
6      3.1407519169754D+1,3.8530683306486D+1,4.8026085572686D+1/
      C
      DATA CO /2.18234885940D-1,3.42210177923D-1,2.63027577942D-1,
6      1.26425818106D-1,4.02068649210D-2,8.56387780361D-3,
6      1.21243614721D-3,1.11674392344D-4,6.45992676202D-6,
6      2.22631690710D-7,4.22743038498D-9,3.92189726704D-11,
6      1.45651526407D-13,1.48302705111D-16,1.60059490621D-20/
      C
      C      END

```

```

C
C*****
C
C   THIS PROGRAM TIMES THE PROGRAM
C
C   SUBROUTINE CPTIME (IREQ)
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C   INCLUDE 'malloc.inc'
C   INCLUDE 'common.inc'
C
C   INTEGER*2 I HOUR, I MIN, I SEC, I HUND
C   SAVE CPUTO, CPUT1
C
C   INCLUDE 'clock.inc'
C
C   START THE CLOCK
C
C   IF (IREQ.EQ.1) CPUTO=CPUT
C   IF (IREQ.EQ.1) CPUT1=CPUT
C   IF (IREQ.EQ.1) WRITE (IO,1)
C
C   TIME TO READ INPUT DATA
C
C   IF (IREQ.EQ.2) WRITE (IO,2) CPUT-CPUTO
C
C   TIME BETWEEN ITERATIONS
C
C   IF (IREQ.EQ.3) WRITE (IO,3) CPUT-CPUT1
C   IF (IREQ.EQ.3) CPUT1=CPUT
C
C   TIME AT POST-PROCESSING
C
C   IF (IREQ.EQ.4) WRITE (IO,4) CPUT-CPUTO
C
C   TIME AT END OF PROGRAM
C
C   IF (IREQ.EQ.9) WRITE (IO,9) CPUT-CPUTO
C
C   FORMAT STATEMENTS
C
1   FORMAT (/,2X,'!!! TIMER SET TO ZERO',/)
2   FORMAT (/,2X,'!!! INPUT DATA READ          CPU TIME:',F10.4,/)
3   FORMAT (/,2X,'!!! TIME BETWEEN ITERATIONS      : ',F10.4,/)
4   FORMAT (/,2X,'!!! POST-PROCESSING REACHED      CPU TIME:',F10.4,/)
9   FORMAT (/,2X,'!!! END OF PROGRAM REACHED      CPU TIME:',F10.4,/)
C
C   RETURN
C   END
C
C*****
C
C   THE FOLLOWING SUBROUTINE IS USED TO FIND
C   THE NEWTONIAN PROFILES OF RADIUS AND VELOCITY
C   FOR A GIVEN BLOW-UP-RATIO 'BUR' AND DRAW RATIO 'DR'
C
C   SUBROUTINE FBNEWT
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C   INCLUDE 'MALLOC.INC'
C   INCLUDE 'COMMON.INC'
C
C   PARAMETER (NP=499,NNP=500)
C   COMMON /FBN/ ZN(NNP),UN(NNP),RN(NNP),HN(NNP),YN(NNP)
C
C   SAVE X1,X2,X3,FX1,FX2,FX3
C   SAVE Y1,Y2,Y3,FY1,FY2,FY3
C   SAVE DX,DX0,DY,DY0
C   SAVE RELAX

```

```

C      WRITE (*,1000)
C      WRITE (IO,1000)
C
C      YN(NNP)=0.D0
C
C      X1=FDRL
C      X3=FDRL
C      Y1=BRFL
C      Y3=BRFR
C
C      CALCULATE LEFT RADIUS AND VELOCITY PROFILES
C
C      CALL RK3 (X1,Y1,UI,RI)
C
C      FX1=UI-1.D0
C      FY1=RI-1.D0
C
C      CALCULATE RIGHT RADIUS AND VELOCITY PROFILES
C
C      CALL RK3 (X3,Y3,UI,RI)
C
C      FX3=UI-1.D0
C      FY3=RI-1.D0
C
C      CHECK TO SEE IF ROOT IS BOUNDED BY LEFT AND RIGHT GUESSES
C
C      IF (FX1*FX3.GT.0.D0) THEN
C        WRITE (*,1010)
C        STOP
C      ENDIF
C
C      IF (FY1*FY3.GT.0.D0) THEN
C        WRITE (*,1020)
C        STOP
C      ENDIF
C
C      SOME CONSTANTS
C
C      RELAX=0.9D0
C      DX0=DABS(X3-X1)
C      DY0=DABS(Y3-Y1)
C
C      START REGULA-FALSI LOOP
C
C      DO 30 I=1,IMAX
C        DX=(X3-X1)/DX0
C        DY=(Y3-Y1)/DY0
C
C        X2=X1-DX*DX0*FX1/(FX3-FX1)
C        Y2=Y1-DY*DY0*FY1/(FY3-FY1)
C
C        CALL RK3 (X2,Y2,UI,RI)
C
C        FX2=UI-1.D0
C        FY2=RI-1.D0
C
C        IF (DX.GT.DY) ERR=ABS(DX)
C        IF (DY.GE.DX) ERR=ABS(DY)
C
C        IF (ERR.LT.EPS) GOTO 99
C
C      CONDITIONS FOR FORCE-VELOCITY
C
C      IF (FX1*FX2.LE.0.D0) THEN
C        FX3=FX2
C        X3=X2
C        FX1=RELAX*FX1
C      ELSE
C        FX1=FX2
C        X1=X2

```

```

        FX3=RELAX*FX3
    ENDIF
C
C   CONDITIONS FOR PRESSURE-RADIUS
C
        IF (FY1*FY2.LE.0.D0) THEN
            FY3=FY2
            Y3=Y2
            FY1=RELAX*FY1
        ELSE
            FY1=FY2
            Y1=Y2
            FY3=RELAX*FY3
        ENDIF
30    CONTINUE
C
C   END OF REGULA-FALSI LOOP
C
C   NO SOLUTION AFTER IMAX ITERATIONS
C
        WRITE (*,1030)
        STOP
C
C   CONVERGED SOLUTION
C
99    IF (IFORCE.EQ.0) FORCE=X2
    IF (IPRESS.EQ.0) PRESS=Y2
C
        WRITE (*,1040) PRESS, FORCE, RN(NNP), UN(NNP)
C
        UN(1)=1.D0
        RN(1)=1.D0
        ZN(1)=0.D0
C
C   CALCULATE DISTANCES AND THICKNESSES
C
        DZ=DL/NP
        DO 40 I=1,NP
            ZN(I+1)=ZN(I)+DZ
40    CONTINUE
        ZN(NNP)=DL
C
        DO 50 I=1,NNP
            HN(I)=1.D0/UN(I)/RN(I)
50    CONTINUE
C
C   NOW LOCATING VALUES FOR FE MESH
C
        U(1)=1.D0
        R(1)=1.D0
        DO 60 I=2,NNQ
            DO 61 J=1,NNP-1
                IF (Z(I).GT.ZN(J).AND.Z(I).LE.ZN(J+1)) THEN
                    R(I)=(Z(I)-ZN(J))/(ZN(J+1)-ZN(J))*(RN(J+1)-RN(J))+RN(J)
                    U(I)=(Z(I)-ZN(J))/(ZN(J+1)-ZN(J))*(UN(J+1)-UN(J))+UN(J)
                    H(I)=(Z(I)-ZN(J))/(ZN(J+1)-ZN(J))*(HN(J+1)-HN(J))+HN(J)
                    GOTO 60
                ENDIF
            CONTINUE
61        CONTINUE
60    CONTINUE
C
C   *** FORMAT STATEMENTS ***
C
1000  FORMAT (/ ,10X, '*** NEWTONIAN PROBLEM BEING SOLVED ***')
1010  FORMAT (/ ,1X, 'NO ROOT IN FORCE-VELOCITY INTERVAL [FDRR,FDRL]')
1020  FORMAT (/ ,1X, 'NO ROOT IN PRESSURE-RADIUS INTERVAL [BRFR,BRFL]')
1030  FORMAT (/ ,1X, 'MAXIMUM # OF ITERATIONS REACHED')
1040  FORMAT (/ ,6X, 'NEWTONIAN RESULTS:', /,
&      10X, 'DIMENSIONLESS PRESSURE      : ', F12.6, /,
&      10X, 'DIMENSIONLESS FORCE         : ', F12.6, /,
&      10X, 'RADIUS AT TAKE-UP           : ', F12.6, /,

```

```

C      10X,'VELOCITY AT TAKE-UP      : ',F12.6)
C      RETURN
C      END
C.....
C      SUBROUTINE RK3 (XC,YC,UI,RI)
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C      INCLUDE 'MALLOC.INC'
C      INCLUDE 'COMMON.INC'
C
C      PARAMETER (NP=499,NNP=500)
C      COMMON /FBN/ ZN(NNP),UN(NNP),RN(NNP),HN(NNP),YN(NNP)
C
C      IF (IFORCE.EQ.0) THEN
C        UN(NNP)=DR
C        F=XC
C      ELSE
C        F=FORCE
C        UN(NNP)=XC
C      ENDIF
C
C      IF (IPRESS.EQ.0) THEN
C        RN(NNP)=RADF
C        B=YC
C      ELSE
C        B=PRESS
C        RN(NNP)=YC
C      ENDIF
C
C      DZ=-DL/NP
C
C      DO 1 I=NNP,2,-1
C        UU=UN(I)
C        RR=RN(I)
C        YY=YN(I)
C
C        DU0=FFU(F,B,UU,RR,YY)*DZ
C        DR0=FFR(YY)*DZ
C        DY0=FFY(F,B,RR,YY)*DZ
C
C        DU1=FFU(F,B,UU+0.5D0*DU0,RR+0.5D0*DR0,YY+0.5D0*DY0)*DZ
C        DR1=FFR(YY+0.5D0*DY0)*DZ
C        DY1=FFY(F,B,RR+0.5D0*DR0,YY+0.5D0*DY0)*DZ
C
C        DU2=FFU(F,B,UU+0.5D0*DU1,RR+0.5D0*DR1,YY+0.5D0*DY1)*DZ
C        DR2=FFR(YY+0.5D0*DY1)*DZ
C        DY2=FFY(F,B,RR+0.5D0*DR1,YY+0.5D0*DY1)*DZ
C
C        DU3=FFU(F,B,UU+DU2,RR+DR2,YY+DY2)*DZ
C        DR3=FFR(YY+DY2)*DZ
C        DY3=FFY(F,B,RR+DR2,YY+DY2)*DZ
C
C        DDU=(DU0+2.D0*DU1+2.D0*DU2+DU3)/6.D0
C        DDR=(DR0+2.D0*DR1+2.D0*DR2+DR3)/6.D0
C        DDY=(DY0+2.D0*DY1+2.D0*DY2+DY3)/6.D0
C
C        UN(I-1)=UN(I)+DDU
C        RN(I-1)=RN(I)+DDR
C        YN(I-1)=YN(I)+DDY
C
C      1 CONTINUE
C
C      UI=UN(1)
C      RI=RN(1)
C      RETURN
C      END
C.....

```

```

C      DOUBLE PRECISION FUNCTION FFU(F,B,UU,RR,YY)
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C      INCLUDE 'MALLOC.INC'
C      INCLUDE 'COMMON.INC'
C
C      PARAMETER (NNP=500)
C      COMMON /FBN/ ZN(NNP),UN(NNP),RN(NNP),HN(NNP),YN(NNP)
C
C      A=F-B*RN(NNP)**2.DO
C
C      FFU=UU/4.DO*(A+B*RR**2.DO)*(1.DO+YY**2.DO)-UU/2.DO/RR*YY
C
C      RETURN
C      END
C
C*****
C
C      DOUBLE PRECISION FUNCTION FFR(YY)
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C      INCLUDE 'MALLOC.INC'
C      INCLUDE 'COMMON.INC'
C
C      PARAMETER (NNP=500)
C      COMMON /FBN/ ZN(NNP),UN(NNP),RN(NNP),HN(NNP),YN(NNP)
C
C      FFR=YY
C
C      RETURN
C      END
C
C*****
C
C      DOUBLE PRECISION FUNCTION FFY(F,B,RR,YY)
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C      INCLUDE 'MALLOC.INC'
C      INCLUDE 'COMMON.INC'
C
C      PARAMETER (NNP=500)
C      COMMON /FBN/ ZN(NNP),UN(NNP),RN(NNP),HN(NNP),YN(NNP)
C
C      A=F-B*RN(NNP)**2.DO
C
C      FFY=(1.DO+YY**2.DO)/2.DO/RR+
C      6 (3.DO*YY/RR**2.DO-2.DO*RR*B*(1.DO+YY**2.DO))/(A+B*RR**2.DO)
C
C      RETURN
C      END
C
C*****
C

```

(b) FORTRAN Source Code "malloc.inc"

```

C
C      MEMORY ALLOCATION PARAMETERS
C
C      PARAMETER (MAXE=201, ! MAX NUMBER OF ELEMENTS
C      1      MAXN=2*MAXE+1, ! MAX NUMBER OF NODES FOR QUAD.ELEM.
C      2      MAXV=3*MAXN) ! MAX NUMBER OF VARIABLES - 3 VARIABLES PER NODE
C
C      DONE
C

```

(c) FORTRAN Source Code "common.inc"

```

C
C.....
C
C   COMMON BLOCKS USED IN PROGRAM FSPIN ver. 3.0
C
C.....
C
COMMON /LIMS/ EPS,UNREL
COMMON /INTS/ IMAX,NREL
COMMON /MESH/ NELE,NNODE,NNQ,NNQ2,NNQ3
COMMON /INOUT/ IN,IO,ITEC,ISP
COMMON /FLAGS/ ITEMP,ICONT,ICONS,IFORCE,IPRESS
COMMON /PARM/ CONS,FORCE,PRESS
COMMON /RHEO/ ALPHA(10),BETA(10),
+             THETA,REL(10),COEF(10),
+             VISQ
COMMON /PROB/ RAD0,U0,H0,DL,RADF,DR,
+             PI,Q,fDrL,fDrR,BrfL,BrfR
COMMON /THERM/ T0,TREF,RHO0,EACT,HEATC,
+             GC,CP0,CK1,CK2,XPANC,
+             TAIR,VISA,EMIS,SB
COMMON /GALE/ GP(6),WG(6),XO(15),CO(15)
COMMON /VARS/ Z(MAXN),R(MAXN),U(MAXN),H(MAXN),T(MAXN),
+             S(MAXN),ZZ(MAXN,6),SRATE(MAXN,6),DRDZ(MAXN,6),
+             CHTT(MAXN,6)
COMMON /TRACK/ TIME(MAXN,6),TNODE(MAXN)
COMMON /MATRX/ SK(MAXV,MAXV),SF(MAXV)
COMMON /STRS/ TAU11(MAXN,6),TAU22(MAXN,6),TAU33(MAXN,6),
+             TAUSS(MAXN,6),TAUTT(MAXN,6),TAUSSC,TAUTC
COMMON /STORE/ OV(MAXV),UT(MAXV),UTO(MAXV),
+             RS(MAXV),RSO(MAXV)
C
C.....
C

```

(d) FORTRAN Source Code "clock.inc"

```

C
C.....
C
C   THIS IS USED FOR SYSTEM CLOCK
C
C   [WINDOWS NT]  WATCOM F77
C
C       call gettim (ihour,imin,isec,ihund)
C       cput=float(ihour)*3600.+float(imin*60+isec)+float(ihund)*.01
C
C   [UNIX]  AIX COMPILER
C
C       cput=mclock()/100.0
C
C.....
C

```

(e) FORTRAN Source Code "system.inc"

```

C
C .....
C
C [Windows NT]  WATCOM F77
C
  CALL GETTIM (HRS,MINS,SECS,HSECS)
  CALL GETDAT (YEAR,MONTH,DAY)
  YEAR=YEAR-1900
  WRITE (ATIME,5000) HRS,MINS,SECS
  WRITE (ADATE,5010) MONTH,DAY,YEAR
  clock_=' '
  date_=' '
C
C [UNIX]  AIX IBM XL Fortran
C
  ATIME=clock_()
  ADATE=date()
C
C .....
C

```

(f) ASCII Input File for an Isothermal UCM simulation ($B=0.2$, $A=2.9$, $L/r_s=5.0$, $W_s=0.01$)

```

*****----- INPUT FILE FOR FBLow -----*****
NELE      EPS      IMAX      UNREL
51         1.0e-05   200       1.0
ITEMP     ICONT     ICONS     IFORCE    IPRESS
0          0        0         1          1
CONS      FORCE      PRESS
1.0        2.9      0.2
U0         RAD0     H0        DL         DR         RADF
1.0        1.0      1.0      5.0        8.379      3.51
fDrL       fDrR     BrfL      BrfR
5.0        10.0     3.0       3.6
----- NON-ISOTHERMAL INPUT -----
T0         TREF     RHOO      EACT       HEATC
533.0      533.0    1.00     48063.2  3600.0
GC         CP0      CK1       CK2       XPANC
8.314      1.302e+7 0.3243  5.65e-4  3.7e-4
TAIR       EMIS     SB
303.0      0.5      5.67e-5
----- VISCOELASTIC INPUT -----
NREL       THETA
1          0.0
RELAXATION SPECTRUM (REL(I),COEF(I),ALPHA(I),BETA(I),I=1,NREL)
relk(k)    ak(k)    alpha(k)    beta(k)
0.01       1.0     1.e+6       0.02
##### M E S H #####
0.0        0.001    0.003    0.005    0.008    0.01    0.015
0.02       0.03    0.04    0.06    0.08    0.1
0.125      0.15    0.175    0.2     0.225    0.25    0.275    0.3
0.325      0.35    0.375    0.4     0.425    0.45    0.475    0.5
0.525      0.55    0.575    0.6     0.625    0.65    0.675    0.7
0.725      0.75    0.775    0.8     0.825    0.85    0.875    0.9
0.92       0.94    0.96    0.97    0.98    0.99    1.0
*****

```

(g) ASCII Output File for an Isothermal UCM Simulation
($B=0.2, A=2.9, L/r_e=5.0, W_s=0.01$)

```

*****
*                                     *
*      FFFFF BBBB L      OOO W W   *
*      F      B B L      O O W W   *
*      FFF --- BBBB L      O O W W W *
*      F      B B L      O O W W W   *
*      F      BBBB LLLLL OOO W W   *
*                                     *
*                                05/12/98 20:52:24 *
*                                     *
*****

```

*** TIMER SET TO ZERO

*** Newtonian Problem Being Solved ***

*** INPUT DATA READ CPU TIME: 0.2200

*** Viscoelastic Problem Being Solved ***

Zero-Shear-Rate Viscosity : 0.1000E-01
Weissenberg Number : 0.0100

Iteration = 1
RMS Error = 0.2131E+00

Dimensionless radius at take-up : 3.491333
Dimensionless velocity at take-up : 9.223474
Dimensionless temperature at take-up : 1.000000

Conservation of stress constant : 0.158580
Dimensionless force at take-up : 2.900000
Dimensionless pressure at take-up : 0.200000
Oscillations in variables (r:u:T) : 0 : 0 : 0

*** TIME BETWEEN ITERATIONS : 15.4400

Iteration = 2
RMS Error = 0.2674E-02

Dimensionless radius at take-up : 3.490543
Dimensionless velocity at take-up : 9.234202
Dimensionless temperature at take-up : 1.000000

Conservation of stress constant : 0.166158
Dimensionless force at take-up : 2.900000
Dimensionless pressure at take-up : 0.200000
Oscillations in variables (r:u:T) : 0 : 0 : 0

*** TIME BETWEEN ITERATIONS : 15.1500

Iteration = 3
RMS Error = 0.6458E-05

Dimensionless radius at take-up : 3.490541

Dimensionless velocity at take-up : 9.234227
Dimensionless temperature at take-up : 1.000000

Conservation of stress constant : 0.166159
Dimensionless force at take-up : 2.900000
Dimensionless pressure at take-up : 0.200000
Oscillations in variables (r:u:T) : 0 : 0 : 0

*** POST-PROCESSING REACHED CPU TIME: 45.7500

*** END OF PROGRAM REACHED CPU TIME: 45.9700

*** CLOCK TIME AT START OF PROGRAM : 20:52:24

*** CLOCK TIME AT END OF PROGRAM : 20:53:10