

AN EXPERIMENTAL AND NUMERICAL ANALYSIS OF THE EXIT FLOW
IN A SLIT DIE FOR POLYMER MELTS

by

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(ABSTRACT)

A slit die has been constructed to use both flow birefringence and direct pressure measurements to study the extrapolated exit pressure (P_x) and the exit pressure theory used to evaluate the magnitude of the primary normal stress difference (N_1) from the value of the exit pressure. Flow birefringence is used to directly assess the principal assumptions in the exit pressure theory and to evaluate the magnitude of P_x from an expression derived from the macroscopic momentum balance equation. The effect of stress field rearrangement upstream of the die exit plane on the value of the exit pressure was then evaluated using flow birefringence data. The effect of stress field rearrangement was also shown to affect the pressure drop $\Delta P/\Delta L$ in the exit region of the die and the pressure distribution from the centerline of the slit to the die wall. To complement the experimental investigation, a mixed penalty method finite element simulation of the die swell problem was performed using the White-Metzner and upper-convected Maxwell constitutive equations.

The flow birefringence experiments were performed for a polystyrene (Styron 678), LDPE (NPE 952), and HDPE (LY600-00) melts for the following shear rate ($\dot{\gamma}$) and wall shear stress (σ_w) $0.05 \leq \dot{\gamma}_w \leq 3.2 \text{ s}^{-1}$ and $4.84 \leq$

$\sigma_w \leq 16.4$ KPa. It was found that the flow in the die exit region is not a unidirectional shear flow, which is direct violation of the assumptions in the exit pressure theory. Normal stresses generated by an elongational flow field were observed along the slit centerline and in the region adjacent to the die walls. Also, shear stress contributions due to stress field rearrangement evaluated using an expression obtained from a macroscopic momentum balance, comprise over 50% of the magnitude of the calculated exit pressure. The numerically calculated stress field was in good agreement with the results of the flow birefringence results. Convergence for the numerical technique was limited to Deborah numbers of 0.61 for the White-Metzner model and 0.75 for the upper-convected Maxwell constitutive equation.

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ORIGINAL CONTRIBUTIONS

Realizing that the results of this investigation represent the collective effort of many individuals, the author regards the following contribution as his own:

1. The design and supervision of the construction of a slit die rheometer capable of obtaining values of P_x from direct pressure measurements and examining the stress field at the die exit from flow birefringence results.
2. The realization that an expression can be derived from the macroscopic momentum balance equation which can be used to provide information on the origin and stress contributions to the magnitude of the exit pressure in a slit or capillary die.
3. The realization that the equation of motion can be used to evaluate the magnitude of the excess pressure drop in a slit die due to stress rearrangement upstream of the die exit.
4. The development and testing of a mixed penalty method finite element code, MAX2D, capable of solving the equation of motion and a generalized Newtonian fluid, upper-convected Maxwell, or White-Metzner constitutive equations for two-dimensional flow with fixed or free surface boundary conditions.

5. The numerical solution of the die swell problem using a White-Metzner constitutive equation with material parameters which approximated the steady shear viscometric properties of Styron 678.

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1.0 CHAPTER ONE - INTRODUCTION

Of major interest in the polymer processing industry is the flow of viscoelastic materials through complex geometries. The study of the rheology of such systems and the resulting knowledge of the flow rates and stress distributions is therefore of great interest to the polymer processing industry. Polymeric fluids exhibit large memory and elastic effects which complicate the analysis using ordinary mathematical methods.

The elastic behavior of fluids is important to the design and operation of plastics processing equipment. Die swell behavior and the stability of polymers in fiber spinning are two examples in which the elastic nature of polymers may strongly influence the processing characteristics of polymeric materials. It is therefore important to predict the elastic behavior of polymers over a wide variety of processing conditions. One technique of measuring fluid elasticity employs the residual stresses at the die exit, also known as the exit pressure. The purpose of this dissertation will be to quantitatively investigate the nature of the exit pressure through both experimental and numerical techniques. The first part of this introduction will discuss the nature of the stress rearrangement and the physical phenomena exhibited by viscoelastic materials in the exit region of a die. The next section will outline various mathematical analyses used to describe the flow in the exit region. A description of the assumptions implicit in the mathematical analyses and their affect on the use of the exit pressure as a characterization method will follow.

1.1 DEFINITION OF FLUID ELASTICITY

This section will deal with more clearly defining the nature of fluid elasticity and its significance for viscoelastic fluids. The concept of viscoelastic fluids is often confusing as it combines the terms viscous and elastic in describing the behavior of materials. In this section, the viscoelastic nature of fluids will be related to simple linear models which represent the behavior of polymer melts and other macromolecular fluids. Also, the advantages of using certain elastic properties as a means of characterization are described.

A viscoelastic material may be considered as a combination of viscous and elastic elements, both of which contribute to the overall materials behavior. A simple linear viscous material obeys Newton's law of viscosity to describe the relationship between the rate of strain imposed on the system and the stress exhibited by the material. Newton's law of viscosity is presented in equation (1.1).

$$\tau = - \eta \dot{\gamma} \quad (1.1)$$

The constant η on the right hand side of equation (1.1) is called the viscosity and relates the rate of deformation to the stress. The simplest elastic model is that of a linear Hookean spring. The mathematical description of this model is given by

$$\sigma = E \gamma \quad (1.2)$$

The Hookean model relates the strain, γ , to the stress imposed on the material, σ . The constant, E Young's modulus, represents the resistance to deformation. A linear spring deforms according to this model. For small deformations, the element will recover to its original length. An elastic material will return to its original dimensions after the imposed force is removed from the system. A viscoelastic material demonstrates behavior composed of both viscous and elastic response: i.e. it flows like a viscous liquid but exhibits strain recovery in response to an imposed deformation.

Polymer molecules are unique as compared with low molecular weight chemicals. Polymer molecules do not have a single molecular weight, but a distribution of molecular weights. Also the architecture or topology of the units within a polymer chain may change. Each of these can affect the final mechanical properties and their behavior during processing. Certain rheological tests can be used to distinguish changes in molecular weight, MW, molecular weight distribution, MWD, and chain architecture. In the next section, fluid elasticity is measured by normal stresses generated in shear flow.

One basic rheological test consists of measuring the viscosity of a material in steady simple shear flow. The viscosity of a material is sensitive to molecular weight due to the effect of entanglements or interaction between polymer chains. The longer the molecule, the greater the probability of interaction with other flexible chain molecules. Above a critical MW most polymer molecules display a characteristic 3.5 molecular weight dependence between the $\log \eta$ and $\log MW$. Viscosity alone, however, is not sensitive enough to distinguish small changes in molecular

structure which can have significant effect on processing performance and final part properties. Fluid elasticity as measured by the primary normal stress difference is much more sensitive to MW, MWD, and chain branching [148]. The molecular weight dependence of fluid elasticity, measured by the primary normal stress coefficient ψ , varies with a 6.8-7.0 dependence on the log MW [137]. The accurate measurement of fluid elasticity may therefore have application to the characterization of materials by its sensitivity to MW and structure.

One important phenomena which may be associated with fluid elasticity is die swell. Die swell, or the die swell ratio, is defined as the ratio of the dimensions of the final extrudate to the dimensions of the die. For a Newtonian or inelastic material, the die sell ratio is 1.1 for low Reynolds numbers and approaches 0.86 for high Reynolds numbers flows. The die swell for a Newtonian fluid is caused by the rearrangement of the velocity field from the parabolic velocity profile within the die to the flat velocity profile in the free surface. Viscoelastic materials can demonstrate very pronounced die swell effects for very low Reynolds numbers. Die swell ratios of 2-3 are not uncommon for some polymer melts [137]. The large dimensional changes in the extrudate from a die must be taken into account in designing parts with specific cross sections. The exact cause of die swell is not well understood, but it is generally accepted to be related to the elasticity of the fluid.

Fluid elasticity is also characterized by additional stresses within a fluid under deformation. These stresses can be described in a steady simple shear experiment. In Figure 1 is shown the coordinate system for a steady shear experiment. The top plate moves with a velocity, V_0 , over

the stationary plate. For inelastic materials, the only stresses generated are shear stresses caused by fluid elements of higher velocity being dragged across fluid of lower velocity or momentum. For elastic materials, in addition to shear stresses, a set of three additional stresses are generated. These are called normal stresses and are demonstrated by a force which tends to push the two plates apart. Under some processing conditions, the normal stresses can be larger than the shear stresses. The elastic stresses generated during deformation are significant in terms of the extra stresses generated during processing. It is therefore desired to measure material parameters related to fluid elasticity. Before the experimental quantities and techniques used to measure fluid elasticity are introduced, the rheological notation used to describe fluid flow is presented.

1.2 RHEOLOGICAL FUNCTIONS OF INTEREST

Before proceeding with a discussion on the techniques used to measure fluid elasticity, it is useful to introduce the rheological quantities of interest and the notation used in describing the state of stress within a fluid.

In this section the definitions of the primary normal stress difference (N_1) and other important stress quantities of unidirectional shear flows are presented. The most simple form of unidirectional shear flow is simple shear flow, in which the shear surfaces are planes and the shear rate $\dot{\gamma}$ is independent of position and time [137]. For flow in a slit, this flow is described by a rectangular Cartesian coordinate system whose axes are oriented with the shear surfaces. These axes are defined by the

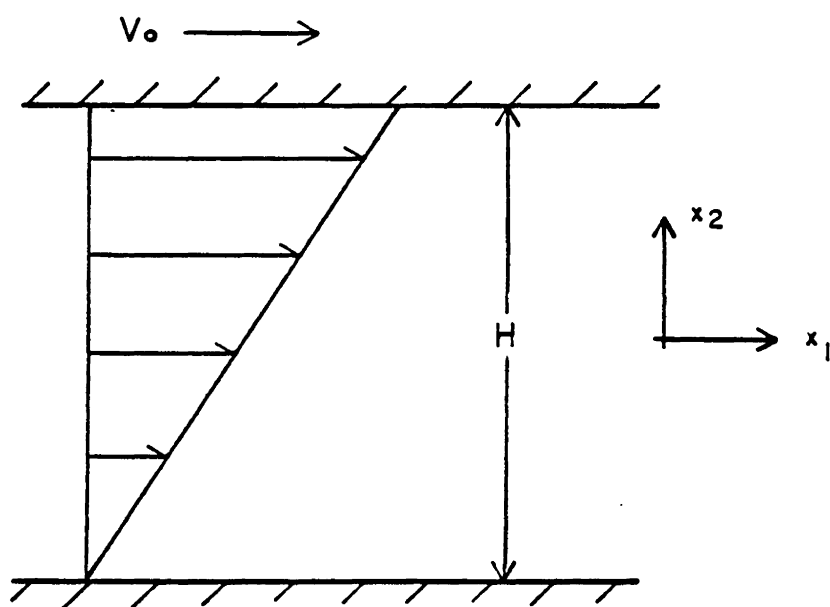


Figure 1. Coordinate System Used in Steady Shear Flow

coordinate system x_i , where $i = 1,2,3$. For this system, x_1 corresponds to the flow direction and represents the tangent to the shear surfaces. The x_2 direction corresponds to the direction of the velocity gradient, and the x_3 axis corresponds to the neutral direction of an orthogonal coordinate system.

The extra stresses σ_{ij} present in a fluid have the following form for simple steady shear flow;

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{21} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix} \quad (1.3)$$

Three stress quantities may be defined which completely describe the state of stress in the system. Equations (1.5) and (1.6) are used to define the normal stress coefficients Ψ_1 and Ψ_2 .

$$\sigma_{12} \quad (1.4)$$

$$N_1 = - \Psi_1 \dot{\gamma}^2 \quad (1.5)$$

$$N_2 = - \Psi_2 \dot{\gamma}^2 \quad (1.6)$$

In the above equations σ_{12} is the shear stress, N_1 is the primary normal stress difference, and N_2 is the secondary normal stress difference. The functions Ψ_1 and Ψ_2 are known as the primary and secondary normal stress coefficients, respectively. It should be emphasized that the quantities on the left hand side of equations (1.5) and (1.6) are only defined for steady shear flow. For flows other than steady shear the combination of stresses on the right side of eqs. (1.5) and (1.6) do not correspond to N_1 or N_2 . The stresses $\sigma_{11} - \sigma_{22}$ and $\sigma_{22} - \sigma_{33}$ may represent combinations

of both shear flow and extensional flow. The sign convention for the normal stresses will consist of tensile stresses as a negative stress and compressive stresses as a positive stress.

An additional class of flows will be introduced known as shear free flows. A shear free flow is defined as a flow for which it is possible to select for every fluid element an orthogonal set of unit vectors fixed in the element so that referred to these axes the rate of strain tensor has a diagonal form [137]:

$$\dot{\gamma}_{ij} = \begin{bmatrix} \dot{\gamma}_{11} & 0 & 0 \\ 0 & \dot{\gamma}_{22} & 0 \\ 0 & 0 & \dot{\gamma}_{33} \end{bmatrix} \quad (1.7)$$

In addition, the incompressibility assumption is used which requires a constant volume element such that $\dot{\gamma}_{11} + \dot{\gamma}_{22} + \dot{\gamma}_{33} = 0$. The shear free flow of interest in the current research is uniaxial extensional flows.

$$\dot{\gamma}_{ij} = \begin{bmatrix} \dot{\epsilon} & 0 & 0 \\ 0 & -\dot{\epsilon}/2 & 0 \\ 0 & 0 & -\dot{\epsilon}/2 \end{bmatrix} \quad (1.8)$$

The material function $\bar{\eta}$ known as the elongational viscosity is used to describe the normal stress difference. The value of $\bar{\eta}$ is given by

$$\tau_{xx} - \tau_{yy} = -\bar{\eta}(\dot{\epsilon}) \dot{\epsilon} \quad (1.9)$$

The zero-elongation-rate elongational viscosity $\bar{\eta}_0$ is approximately three times the zero-shear-rate viscosity η_0 . For Newtonian fluids $\bar{\eta} = 3\eta_0$ for

all shear rates. For polymeric materials, the value of $\bar{\eta}$ may increase or decrease as the elongation rate is increased.

1.3 DEFINITION OF THE EXIT PRESSURE

This section will deal with defining the stress quantities in the exit region of an extrusion die which are currently being used as a means of measuring fluid elasticity. A brief introduction will then be presented to summarize some of the unique flow features associated with extrusion.

One processing variable used in modeling polymer processing is the pressure gradient required to force a material through a channel. This is important in calculating the total energy requirements needed to process a material. In order to measure the pressure gradient in a slit, a series of pressure transducers are mounted flush with the die wall along the flow direction. A schematic diagram of the exit region of a die is shown in Figure 2. If the pressure gradient, as measured by the pressure transducers, is extrapolated to the exit, a residual stress is sometimes seen to exist for viscoelastic fluids. The difference between the residual stress and the atmospheric pressure at the die exit is called the exit pressure (P_x).

In order to explain the origin of the exit pressure, a schematic diagram of the velocity field in the exit region of the die is shown in Figure 3. The flow in this diagram may be divided into three regions which describe the state of the velocity field and stresses. The first region characterizes the fully developed flow found inside the die. Here, the velocity field consists of a parabolic velocity profile for a Newtonian fluid or a non-Newtonian velocity profile for a viscoelastic

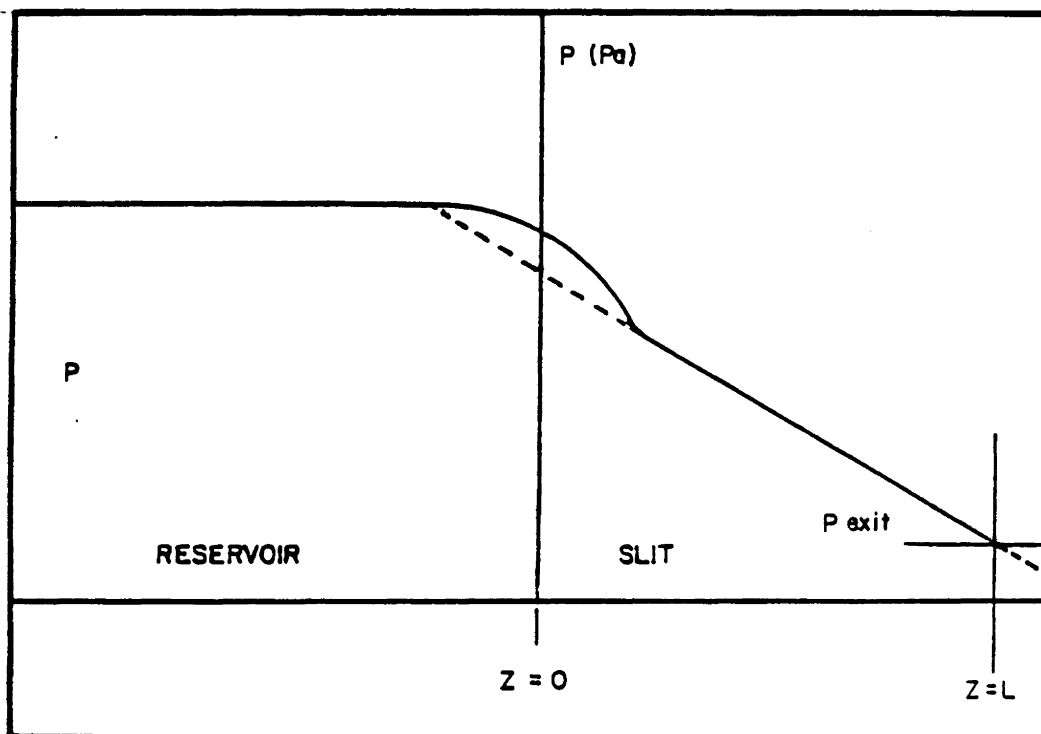


Figure 2. Pressure Profile Measured Inside a Slit

fluid. This flow is characterized as a rectilinear shear flow and has a constant velocity profile along the length of the die. Also, the fluid velocity along the wall is zero. The flow well outside the die consists of a second well defined region. The boundary conditions in this region consist of a free surface boundary and a constant velocity across the extrudate. For low Reynold's number experiments, there are negligible shear forces transmitted from the atmosphere to the extrudate surface.

The last region may be described as a transition region between the fully developed shear flow within the die and the constant velocity jet found in the free surface region. This region is characterized by a rearrangement in the velocity and stress fields. The effect of the rearrangement can be demonstrated by tracing the flow history of two fluid elements; one located along the die wall and another along the centerline of the die. A fluid element along the die wall has a very small velocity within the confines of the die but once outside the die the element must accelerate to the velocity of the free jet. This acceleration creates an extensional gradient within the fluid element. In order to conserve mass in the system, fluid elements along the centerline, however, must decelerate from the maximum velocity found inside the die to the constant velocity of the material in the free jet.

The origin of the exit pressure in viscoelastic materials may be related to this transition region or rearrangement from rectilinear shear flow within the die to bulk flow in the free jet. Han has suggested that the exit pressure is due to the elasticity of the fluid generated in steady shear flow [4]. If this hypothesis is correct then positive exit pressures should not be generated by inelastic fluids. Comparison between

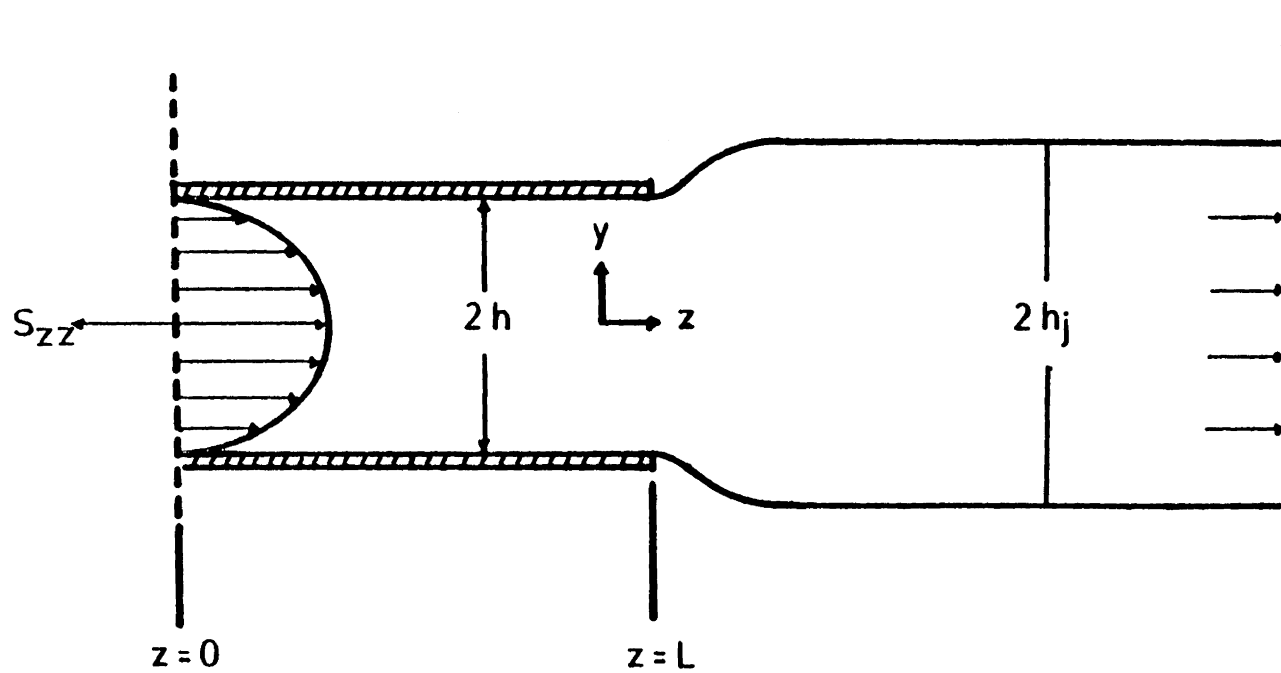


Figure 3. Schematic of the Flow Field at the Exit of a Die

numerical simulations for Newtonian and viscoelastic fluids, however, both demonstrate positive residual stresses at the exit of a die. The disagreement between the numerical simulations and the conclusions by Han may be due to the difference in the nature of the stress field rearrangement between inelastic and viscoelastic fluids.

1.4 SIGNIFICANCE OF THE EXIT PRESSURE

In the previous section, it was shown that residual stresses could be measured at the exit of a die by extrapolating the pressure gradient to the die exit plane. A practical application to this phenomena was generated when it was reported in several theoretical [57,65,66], experimental [1-15], and numerical [101,113] studies that P_x may be simply related to the primary normal stress difference (N_1). The primary normal stress difference is related to fluid elasticity through the magnitude of the ultimate constrained elastic recovery, S_∞ . According to Lodge's rubberlike liquid constitutive equation [64] these are related by the equation

$$S_\infty = N_1 / 2 \sigma \quad (1.10)$$

where N_1 and σ denote the stress values before recovery. The measurement of P_x in capillary or slit die rheometers, therefore, may be used to measure the elasticity in a fluid.

Considerable interest has been generated in the development of slit and capillary rheometers capable of measuring N_1 due to the limitation of currently available techniques. N_1 is most often obtained by means

of a cone-and-plate or plate-plate rotational devices. These devices are limited to low shear rates due to centrifugal forces and edge fracture of the sample in the test fixtures. Furthermore, a single sample rather than a continuous monitoring of polymer processes must be employed. A slit rheometer may be readily adapted for on-line measurement of polymer properties. Thus, a relationship between P_x and N_1 may offer one technique in which to continuously monitor fluid elasticity at shear rates of interest for many industrial processing operations.

There are currently two major difficulties in obtaining N_1 values for viscoelastic fluids from P_x in capillary and slit dies. First, the residual exit pressure, P_x , is a difficult quantity to measure. P_x represents a small quantity compared to the large hydrostatic pressures generated within the die. This makes the exit pressure sensitive to several sources of error [18,20,68] such as nonisothermal flow, pressure dependent viscosity, and extrapolation techniques. Also, previous researchers have reported negative [16,20], zero [16,20,38], and positive values of P_x for polymer melts and solutions [1-21]. In view of the inconsistencies in the data reported in the literature, several questions have been raised as to the existence of a simple relationship between P_x and N_1 .

The second difficulty in obtaining N_1 from P_x involves the use of certain derived equations obtained from the equations of motion or a macroscopic momentum balance over a control volume [60]. The equations proposed by Han [123] which relate N_1 to the exit pressure and the wall shear stress have been criticized [20,60] because several of the assumptions in the derivation may be violated [41-55]. However, several re-

searchers have experimentally [44,45] and numerically shown [101] that the violations in the basic assumptions do not affect the prediction of values of N_1 under certain conditions. The exit pressure relationship is discussed in detail in section 2.1.

Fundamental fluid mechanics research examining the nature of the flow field at the exit of a die may provide insight into the origin of the exit pressure and the relationship between the exit pressure and the rheological behavior of a material. The study of the exit region of an extrusion die, however, is also important to several other significant research problems in the area of polymer processing and rheology. The origin of die swell, profile extrusion, extrusion instabilities, and numerical modeling of free surface problems are all concerned with the exit region of a die. In the case of numerical modeling of viscoelastic fluids, the convergence of non-linear models is effected by the large stress gradients at the die exit lip [83-116,138]. The nature of the stress field associated with the exit pressure studies may offer insight into the poor stability behavior exhibited for non-Newtonian constitutive equations and numerical formulations.

1.5 MATHEMATICAL ANALYSIS OF THE EXIT REGION

Several mathematical analyses have been proposed to describe the relationship between P_x and N_1 in both circular and slit die geometries [57,60,63,65,66,68]. Each of these analyses attempt to relate measurable stress quantities to form a relationship from which N_1 may be obtained. In the next section several different analytical results will be presented

each of which calculates N_1 using different assumptions and analytical approaches.

The original derivation of the exit pressure relationship was published by Han [65] who in the early 1970's conducted an extensive series of experimental investigations which related P_x to N_1 for several polymer melts. For flow in slit dies, with large aspect ratio's, $H/W \ll 0.1$, the equation of motion may be reduced to two dimensions and the following relationship may be obtained

$$N_1 = P_x + \tau_w \frac{\partial P_x}{\partial \tau_w} \quad (1.11)$$

In the above equation, P_x is the extrapolated exit pressure and τ_x is the wall shear stress measured in the fully developed flow region. The above relationship does not depend on the constitutive equation describing the fluid, but does employ the following assumptions.

1. Fully developed flow at the exit
2. Negligible inertial effects.

The assumption which has caused the most controversy is the assumption of fully developed flow at the exit plane. For polymer melts and solutions, flow birefringence [23,44,50,51], flow visualization [45,48,55], laser doppler anemometry [45-47,49,54], and numerical modeling have shown that the velocity field is disturbed before the exit plane.

Boger and Denn [60] used a macroscopic momentum balance to model the exit region of both circular and slit dies. They presented the following equation

$$N_1 = P_x + \tau_w \frac{\partial P_x}{\partial \tau_w} + \frac{1}{h} \frac{\partial}{\partial \tau_w} \left(\int_0^h \rho v_z^2(y, 0) dy - \rho v_j^2 h_j \right) + \frac{\partial}{\partial \tau_w} \tau_w^2 \frac{L}{h} \left(1 - \int_0^1 f(\epsilon) d\epsilon \right) \quad (1.12)$$

The above equation is similar to equation (1.11), but contains two additional terms. The third term on the right hand side of equation contains contributions from the reduced jet thrust, T_1 . This term accounts for fluid inertia. The last term in equation (1.12) accounts for deviation from fully developed flow at the die exit. The function f which represents the deviation from steady flow, was defined by Boger and Denn as a function of the Reynolds number and the wall shear stress. With the assumptions of no inertial forces and fully developed flow at the exit, equation (1.12) reduces to the equation of Han eq. (1.11). In the mathematical analysis of Boger and Denn [60] and Choplin and Carreau [63], both papers emphasize the potential error in ignoring the stress rearrangement terms.

An additional relationship proposed by the author will be used in conjunction with equation (1.11) and (1.12). The macroscopic momentum balance can be used to obtain an expression used to calculate the exit pressure from the stresses in the exit region of a die. This expression permits the evaluation of the relative contributions of the shear stresses and the normal stress differences on the exit pressure. This equation will be employed to evaluate the contribution of flow disturbances on the magnitude of the exit pressure and to assess the contribution of fluid

elasticity on the exit pressure. This expression also provides an independent method to measure the value of the exit pressure in addition to experimentally extrapolated measurements.

In this section the basic mathematical expressions used to evaluate fluid elasticity from experimental measurements have been presented. In the next section numerical modeling of non-Newtonian fluids will be introduced.

1.6 NUMERICAL MODELING OF NON-NEWTONIAN FLUIDS

The numerical modeling of fluid mechanics problems involves the simultaneous solution of the equations of motion, a constitutive equation which relates the deformation to the stresses experienced by a fluid element, and the equation of continuity or the conservation of mass. For classical Newtonian fluid mechanics this involves the solution of the Navier-Stokes equation for a variety of boundary conditions. The modeling of non-Newtonian fluids, which may be defined as any material which does not behave as Newton's law of viscosity, requires the use of highly non-linear constitutive equations in addition to the equation of motion. For these fluids, Newton's law of viscosity is not sufficient to relate the components of the rate of deformation tensor to the state of stress in the fluid. These fluids require more complicated constitutive equations to express the non-linear behavior observed in experimental situations.

A constitutive equation for non-Newtonian fluids must be expected to model a variety of behavior. Shear thinning viscosity, non-zero primary and secondary normal stress differences, secondary flows, elastic recoil, and strain hardening extensional viscosity functions are just a few of

the phenomena which constitutive equations must accurately model. A more complete summary of non-Newtonian behavior may be found in the following texts [64,68,123,137]. Unfortunately, there are no constitutive equations which adequately predict fluid behavior in all flow situations. It is therefore the choice of the researcher to match the expected flow situation to a constitutive equation which most adequately represents that flow.

For most engineering calculations, the most predominant viscoelastic empiricism is the non-Newtonian viscosity or a shear rate dependent viscosity. For some fluids, the viscosity may change several orders of magnitude. These large changes can not be ignored in engineering design calculations. One of the earliest rheological empiricisms was the modification of Newton's law of viscosity to accept a shear rate dependent viscosity. Newton's law of viscosity for steady shear flow was replaced by an empirical viscosity function.

$$\tau_{zy} = - \eta(\dot{\gamma}) \dot{\gamma}_{zy} \quad (1.13)$$

The above expression is known as the generalized Newtonian fluid. This expression may be substituted into the equation of motion in order to directly solve for the velocity. Several different empirical relationships are available to describe experimental non-Newtonian viscosity curves.

The generalized Newtonian fluid (GNF) can be extended to an arbitrary flow. In tensor notation the expression becomes

$$\underline{\underline{\tau}} = - \eta(\dot{\underline{\underline{\gamma}}}) \dot{\underline{\underline{\gamma}}} \quad (1.14)$$

The viscosity function η is usually taken as a function of the magnitude of the rate of deformation tensor, $\dot{\underline{\underline{\gamma}}}$. Some relationships use the stress τ as the independent variable.

The generalized Newtonian fluid model provides a fairly accurate representation of the shear rate dependent viscosity function. The numerical solution of GNF models consists of the solution of the equation of motion and the continuity equation. The stresses predicted by this model will be similar to those predicted by Newton's law of viscosity. For modeling viscoelastic fluids, prediction of the stresses as well as velocity fields are important for design purposes. The generalized Newtonian fluid model, however, cannot describe normal-force phenomena, time dependent flows, or flows other than steady shear flows. Thus, the model is severely limited in describing stresses for viscoelastic materials. An alternative to the generalized Newtonian fluid model that contains both viscous and elastic contributions are a class of general linear viscoelastic fluids. This class of fluids contains a viscous term described by Newton's law and a elastic term described by a Hookean spring.

A viscoelastic constitutive equation should relate the stresses observed in the fluid to strain or shear history of the fluid. The constitutive equations are usually expressed in two general forms [137]: differential and integral. A differential constitutive equation consists of a series of differential equations relating the stress tensor and its derivatives to the rate of deformation tensor and its derivatives. In

general, no explicit form of the stress tensor as a function of $\dot{\gamma}$ and its derivatives exists. A numerical solution of a flow problem therefore requires simultaneous solution of the equation of motion and the constitutive equation with velocities, stresses, and pressures as the unknowns.

An integral constitutive equation consists of a class of constitutive equations in which the stress tensor is expressed explicitly as an integral function of some functions of the rate of deformation tensor and its derivatives. The limits of the integral expression consist of the deformation history of each particle in the fluid in all past times until the current time. The solution of this type of system eliminates the stresses as primary unknown variables, but requires knowledge (or guess) of each particles streamlines over the entire flow history. An iterative procedure is usually implemented which uses an initial solution to estimate particle streamlines. The streamlines are then used to evaluate the integral in the constitutive equation. The iteration procedure continues until some convergence criteria is met. The predictions of integral type models are, in general, better than differential models, but are more difficult to use.

Several molecular theories are used currently, which simulate the motion of macromolecules during flow using analogies such as the simple dumbbell model [137] to the more complicated non-affine network theories [144]. By writing the constitutive equation using corotational and codeformational coordinate systems objectivity is obtained. Thus molecular theories or empirically derived constitutive equations are written which predict the extra components of the stress tensor and estimate the

memory effects. However, no one rheological equation of state is sufficient to predict the behavior of all viscoelastic fluids. A single constitutive equation is appropriate only for certain flow fields such as steady shear flow or elongational flow fields. The solution of the associated boundary value problems describing fluid flow consists, first, of choosing the appropriate constitutive equation based on the type of flow being considered and the difficulty in obtaining a numerical solution.

In the several flow problems for which non-Newtonian models have been used [83-116], the success of the numerical simulation is limited to flows where the elastic or non-Newtonian nature of the flow is not the dominant factor. The main parameters used to characterize the magnitude of the elastic effects are the Deborah number (De) and the Weissenberg number (We). The Deborah number is defined as the ratio of the characteristic fluid relaxation time, λ , to the characteristic time scale on the flow, T . The Weissenberg number is defined as the ratio of the primary normal stress difference over twice the shear stress, usually measured at the wall. As both De and We increase, the elastic nature of the fluid increases. Most of the previous numerical investigations report a failure of the numerical methods to converge at a Deborah number at or below one. This failure of convergence at very low elasticity levels presents the greatest hurdle in modeling viscoelastic fluids.

The final check on a numerical simulation on non-Newtonian flow requires the comparison between predictions and experimental data. If the agreement is not satisfactory, the numerical technique and the original choice of the constitutive equation must be critically examined. By

comparison of the experimental results to the numerical technique some insight may be obtained into the nature of the divergence in the numerical simulation.

1.7 FINITE ELEMENT ANALYSIS

The finite element method consists of representing a given irregular domain by geometrically simple shapes over which a set of approximation functions can be derived. In the method the domain of the problem is subdivided into an assembly of sub-domains called elements. These elements are interconnected at specific spatial coordinates or nodes, which usually lie on the element boundaries. The field variables are approximated as a linear combination by simple functions (usually polynomials). The approximating functions have specific properties which are discussed in a latter section. The field equations are rewritten for each element using the interpolating function. The equations over all elements in the domain are then assembled using the continuity of the primary variables. The resulting system of equations can then be solved, once the proper boundary conditions are imposed. A continuous global solution at any point in the domain can then be found by using the approximation polynomials.

1.8 SUMMARY

The purpose of the chapter has been to introduce the basic concepts of fluid elasticity exhibited by viscoelastic materials flowing through a die. In the following chapter a detailed review of the literature associated with direct measurement of the exit pressure, studies examining the flow field at the die exit, and numerical simulations modeling the

flow of a fluid exiting an extrusion die will be given. The objectives of the current investigation will then be presented in light of the previous studies outlined in the literature review.

2.0 CHAPTER TWO - LITERATURE REVIEW

2.1 EXPERIMENTAL MEASUREMENT OF THE EXIT PRESSURE

In this chapter, experimental studies which attempt to measure directly the exit pressure are reviewed. The objective of this section will be to critically examine studies of P_x for both Newtonian and non-Newtonian fluids. The review will also serve to point out the contribution of processing variables to the magnitude of P_x . The next section will review the experimental difficulties in obtaining accurate measurements of the exit pressure. The last part of the review will examine numerical modeling of viscoelastic fluids. The finite element numerical technique will be highlighted. The review will examine numerical studies which yield information on the magnitude of P_x or provide information as to the nature of the stress rearrangement found in the exit region of a die.

2.1.1 SCOPE

In chapter one, it was shown that at the exit of an extrusion die there may exist residual stresses above atmospheric pressure known as the exit pressure. It was stated that previously published experimental values of the magnitude of the exit pressure varied widely for similar systems. Also, precise and reproducible results were difficult to obtain due to the experimental errors present. In this study, the magnitude of the exit pressure for a polystyrene and a low-density polyethylene melt will be investigated. These systems were chosen due to their highly viscoelastic character and since these resins may be studied by the flow birefringence

technique. The review of direct measurements will therefore concentrate on the behavior of viscoelastic materials. This includes both polymer solutions and polymer melts. For comparison, results of P_x measurements for Newtonian fluids are presented. The review is structured in the following manner. Direct measurement studies on Newtonian fluids are presented first. This forms the basis of comparison with the behavior of non-Newtonian or viscoelastic fluids. Following this, direct measurement studies for polymer solutions and polymer melts are reviewed. The effect of processing variables on the exit pressure is then discussed. Finally, experimental errors affecting the measurement of the exit pressure are reviewed.

2.1.2 EXIT PRESSURE FOR NEWTONIAN FLUIDS

In this section the experimental studies reporting exit pressure values for Newtonian fluids are reviewed. The stresses generated by an incompressible Newtonian fluid are due only to viscous forces. A Newtonian fluid can therefore be used as a basis of comparison to determine the effect of fluid elasticity on the magnitude of the exit pressure.

Han et al. [4] proposed that the exit pressure is an elastic phenomena and therefore the exit pressure of a Newtonian fluid should be zero. Han measured the axial pressure profiles for Indopol H-1900 which is a low molecular weight polyisobutylene. The values of the exit pressure were, to within experimental error, zero. Based on these results, Han concluded that P_x is an elastic and not a viscous phenomena. A similar experiment was conducted by Blum, Yerushalmi, and Williams [13] using a 100000 cs silicone oil. A zero exit pressure was obtained over a shear rate range

of 5-1000 $\bar{s}^{-1}$. Blum et al. concluded that this was due to the materials inelastic nature.

Only one published study presented non-zero values of the exit pressure. Ybarra has reported values of exit pressures equal to twenty times the wall shear stress for a Newtonian fluid (glycerine) [39]. No explanation for the large positive values of this material was available. Viscous dissipation effects have been shown to significantly change the viscosity of a material in a die. The presence of temperature non-uniformities near the die exit may account for the positive values of P_x in this study.

The value of the exit pressure was reported as zero by the experimental investigations by Han and Blum et al. The positive exit pressure values reported for glycerine may be subject to viscous dissipation effects which may significantly influence the results. The results reported by Han confirm the hypothesis that the exit pressure is an elastic and not a viscous phenomena. Numerical results, however, for inelastic fluids demonstrate excess pressure losses at the exit of a die which increase with shear stress. The disparity between the numerical and experimental results may be due to the difficulty in numerical models to simulate the abrupt change in boundary conditions found at the exit of a die. The review of numerical simulations is presented in section 2.5.

2.1.3 EXIT PRESSURE FOR VISCOELASTIC FLUIDS

If the hypothesis that the exit pressure is an elastic phenomena is correct, then all viscoelastic materials should exhibit a positive value of P_x . Values of the exit pressure have been reported by a number of

investigators [1-35]. A summary of investigations on polymer solutions is presented in Table 2.1. The results of exit pressure studies for polymer melt systems are shown in Table 2.2. In the tables above, column 1 shows the composition of the systems studied. The range of shear rates employed is shown in column 2 and 3. The next two columns show the geometry of the experimental apparatus, and the magnitude of the exit pressure reported. The last two columns comments on additional information contained within the paper and finally the reference is given in the last column.

One of the difficulties in the use of P_x in determining the primary normal stress difference is the lack of agreement between the various studies reporting values of P_x in polymer solutions and melts. In Tables 2.1 and 2.2 are presented a summary of the experimental investigations reporting the magnitude of P_x . A comparison of the results presented in Table 2.2 shows negative, zero, and positive values for the magnitude of the exit pressure. The wide variation in the value of P_x reported in the literature may be due to the large number of possible sources of experimental errors present in the experimental determination of P_x . In the next section the geometric variables affecting the magnitude of P_x are discussed. Experimental errors influencing P_x are then presented in section 2.2.

2.1.4 DEPENDENCE OF P_x ON ENTRANCE LENGTH

The use of P_x as a measure of N_1 is based on a macroscopic momentum balance analysis which assumes the presence of a steady viscometric flow field inside the die. To satisfy the condition of steady viscometric

Table 2.1

Summary of Experimental Studies Reporting Px Values for
Polymer Solutions

System	Shear Rate [s ⁻¹]	Geometry	Px values	Ref.
Polyvinyl alcohol- H ₂ O	30-300	Capillary	Positive	[1]
Cellosize HE(WP4400) H ₂ O	30-1100	Capillary	+	[24]
Polyisobutane - Varsol	4-1E4	Slit & Tube	+	[13]
Separan/H ₂ O	200-7000	Capillary	+	[28]
Separan/H ₂ O	10-2000	Slit	+	[12]
ET597/H ₂ O	1E3-1E5	Capillary	+ & -	[30]
PEO/H ₂ O	500-1E4	Slit	+	[34]
Maltose Syrup	1E2-1E4	Capillary	+	[117]
Polyisobutylene/ decaline	10-1E4	Slit & Capillary	+	[14]
CMC/H ₂ O				
Polyacrylamide/H ₂ O				

Table 2.2

Summary of Experimental Studies Reporting P_x Values For
Polymer Melts

System	Shear Rate [s ⁻¹]	Geometry	P_x	Comments	Reference
LDPE	50-400	Capillary & Slit	Positive	Pressure holes	[37]
HDPE PS	100-500	Capillary	+	L/D=4 Pressure holes	[3]
HDPE	10-100	Capillary	+	Pressure holes	[22]
PP PE	10-100	Capillary	+	Birefringence	[23]
HDPE PP	300-700	Capillary	+	Pressure taps	[31]
HDPE PP	300-700	Capillary	+	Pressure taps	[4]
PS	175-600	Capillary	+	Pressure taps	[70]
HDPE PP	100-900	Capillary	+	Pressure taps	[56]
HDPE LDPE	100-700	Capillary	+	MW effects	[6]
PS/PP Blends	150-1000	Capillary	+	Pressure holes	[7]
PS/PE Blends					
HDPE PP	1-50	Duct (Rectangular)	+	Taps (2x1 aspect ratio)	[25]
PS HDPE LDPE	100-900	Capillary	+	Pressure taps	[27]
HDPE	100-500	Capillary	+	Reservoir Dia.	[8]
HDPE PP LDPE	10-400	Slit die	+	Aspect ratio	[9]
PE Blends	20-400	Slit die	+	Blends	[10]
PS/PP Blends					
PP PS					
HIPS ABS	30-200	Slit die	+	Two-phase	[11]
HDPE PP	100-400	Slit die	+	HP Test	[66]
HDPE LDPE PS	10-1000	Slit & Capillary	+	Cap(tap holes)	[14]
PMMA PP					
PS	20-1000	Slit die	+		[15]
Butadiene-PS Block Copolymer	0.1-4	Slit die	≈0 to Negative	Aspect ratio	[16]
LDPE	100-1000	Capillary	+	Pressure taps	[103]
HDPE		Capillary	+	Pressure taps	[71]
HDPE LDPE	0.1-10	Slit die	0	Error analysis	[20]
PS	0.1-10	Slit die	+	Comparison to RMS	[19]
LDPE	0.1-1E4	Slit die	+	n(P)	[18]
HDPE	200-1000	Slit die	+		[21]

flow, the flow in the capillary or slit must be fully developed which assumes the velocity and stress field does not change with axial position along the die. One definition of fully developed flow is a constant axial pressure gradient as measured by a series of pressure transducers. The total pressure drop in a capillary or slit may be divided into contributions due to the different flow regions in a die as shown in equation (2.1).

$$\Delta P_{tot} = \Delta P_{ent} + \Delta P_{vis} + \Delta P_{exit} \quad (2.1)$$

The total pressure drop is comprised of ΔP_{ent} , an entrance region pressure drop, ΔP_{vis} , the pressure drop due to viscometric flow, and ΔP_{exit} the pressure drop at the exit region of the die. The analysis of the exit pressure is based on the measurement of the pressure drop found in the viscometric flow region, ΔP_{vis} . The geometry of the experimental apparatus must be chosen so the entrance and exit effects are negligible.

The geometric variable affecting the location of a fully developed flow region in a capillary or slit is the entrance length. Pressure transducers should be located beyond this entrance length to insure a constant pressure gradient. Han, Charles, and Philippoff [4] presented the most complete investigation on the effect of L/D ratio on elastic properties, specifically the exit pressure. The effect of entrance length of P_x was examined by varying the total length of the die by changing the L/D ratio for each capillary. Five capillaries having a range of L/D ratios of 4 to 20 were used with high density polyethylene and

polypropylene melts. In Figure 4 are shown the results of exit pressure versus the L/D ratio for a polyethylene melts.

The figure shows that the exit pressure is a function of the L/D ratio and in all cases a L/D ratio of 20 was sufficient for constant values of P_x . Han suggested that the functional dependence of P_x on L/D was consistent with the origin of P_x as an elastic phenomena. This was similar to observations on the effect of L/D ratio on die swell measurements [69,118]. Constant pressure gradients for this polypropylene, however, were obtained for L/D ratios larger than one. The conclusion of Han concerning fully developed flow must therefore be based on two conditions, a constant pressure gradient and constancy of an elastic property such as die swell or the exit pressure. However, a L/D ratio greater than twenty will not insure constant values of P_x for all polymer melts [4] but will vary with different polymer systems. The same results of Han et al. [4] were also presented in a note [2]. Additional confirmation of the effect of L/D ratio for polyethylene and polypropylene is found in [14,56].

A similar study investigating the effect of L/D ratio for Styron 686 polystyrene melt was published by Han & Yu [70]. For L/D ratios greater than 20 consistent values of P_x were obtained.

The entrance length for viscoelastic solutions vary between 15 and 150 [4,14,28,69,118,119] as determined by die swell measurements. The effect of L/D on the exit pressure was discussed by Han [14,28]. He concluded that an entrance length greater than 200 L/H for a slit die was sufficient to insure consistent exit pressure results. The L/D ratio of 200 was based on the previous results from die swell measurements.

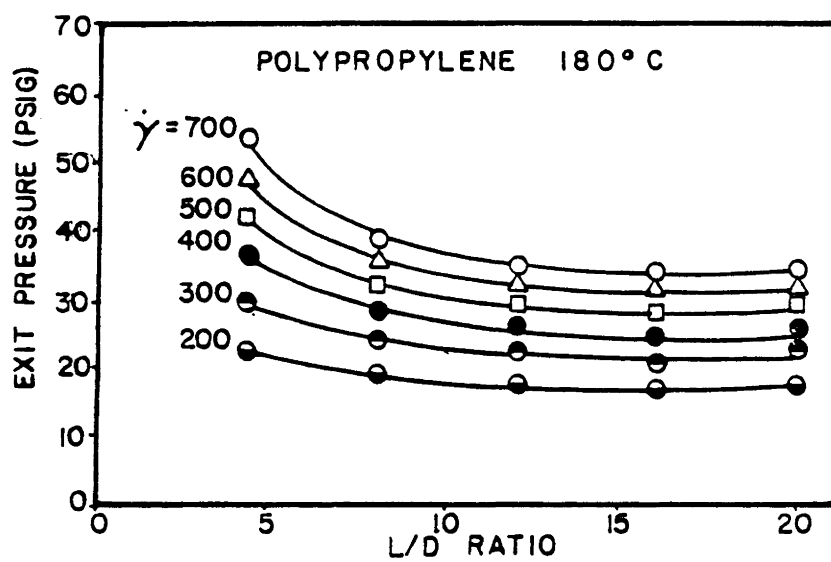


Figure 4. The Effect of L/D Ratio of the Value of P_x [123]

The technique of flow birefringence can be used to test for fully developed flow by examining the birefringence patterns as a function of the entrance length in a capillary or slit. Wales [125] measured birefringence with a long slit ($L/D = 100$) as a function of the entry length. For low density polyethylene, steady flow, as characterized by constant birefringence, was not found for any shear rate. This cast doubts on the use of capillary or slit rheometry to measure "constant" viscometric properties. Comparison of the same experiment with polystyrene melts, however, found constant birefringence within two die heights. Han and Drexler [120] have also used birefringence measurements for high density polyethylene melts in the entrance region of a slit die. Han, Mori [23], and Vinogradov [51] reported parallel fringe patterns within 1-4 times the slit thickness.

The entrance length reported by flow birefringence results were shorter than those reported through the direct measurement of die swell or exit pressure values. Constant birefringence measurements and pressure profiles were obtained within 1-2 die heights of the die entrance. These techniques establish the presence of a constant stress field after the initial entry region. The discrepancies between the birefringence results and the constancy of the exit pressure suggest that the exit pressure measurements depend on the strain history of the sample. A longer entrance length was required for die swell and P_x measurements before the materials relaxed from the strain imposed due to the contraction located at the entrance of the die.

2.1.5 DEPENDENCE ON RESERVOIR DIAMETER

If the exit pressure is assumed to be an elastic phenomena then the magnitude of the exit pressure may be influenced by the strain history of the sample. The reservoir-to-capillary diameter ratio (D_r/D) may be used to vary the total strain on a material as it enters a capillary. Kowalski [121] and Schreiber [122] have reported that the die swell ratio was affected by D_r/D . Han and Kim [8] suggested that the exit pressure depended on D_r/D due to varying the strain history as the melt entered the capillary. This argument assumed that the exit pressure resulted from the residual elastic energy stored in the melt. Han and Kim [8] measured the exit pressure for a high density polyethylene for D_r/D of 3-12. For a D_r/D greater than 12, no change was found for die swell or the exit pressure for a constant L/D capillary. Han and Kim have also published results for the measurement of Separan/H₂O solutions for a capillary rheometer [12]. Reservoir-to-capillary ratios of 4.16 and 2.54 were used to measure geometry effects of elasticity. Die swell increased for the larger D_r/D ratio but a limiting value for the ratio was not calculated for exit pressure measurements.

2.1.6 DEPENDENCE OF ASPECT RATIO FOR A SLIT DIE

In this section the effect on the width-to-height ratio or aspect ratio of a slit die rheometer is reviewed. As discussed previously, the analysis of flow in a slit die assumed a two dimensional flow field. For an ideal two dimensional flow, or flow between infinite parallel plates, the aspect ratio has a limit of infinity. For practical studies, the minimum aspect ratio which produces a nearly two dimensional flow field

must be determined. Eswaran, Janeschitz-Kriegl, and Schijf [37] reported one of the earliest studies on the use of slit die rheometers to measure the steady shear properties of polymer melts. The objective of this work was the comparison of slit and capillary viscometers. The pressure gradients and volumetric flow rates per unit width were compared for aspect ratios of 20, 15, and 10 respectively. Eswaran et al. concluded no effect of slit width, but no comparison was made based on the magnitude of elastic properties.

Han measured the effect of aspect ratio on the exit pressure for a series of polymer melts [9]. The values of the exit pressure were not affected by decreasing the aspect ratio from 20 to 10 for a slit die rheometer with flush mounted pressure transducers. Han commented that at small aspect ratios, less than 10, the flow in a slit must be treated as three dimensional flow problem. A plot of the exit pressure versus shear rate for each polymer melt was linear, but the exit pressure was not determined at the same shear rate for each aspect ratio. This prevents meaningful comparison of the effect of slit width on elastic properties.

A study examining aspect ratios of 20-6.6 using butadiene-styrene block copolymers was published by Leblanc [16]. The exit pressure increased with an increase in aspect ratio. Leblanc suggested that consistent exit pressure measurements were obtained only at high aspect ratios but did not give a minimum limit which should be used as a guide in designing slit die rheometers.

Flow birefringence has been used to study the effect of aspect ratio on whether the influence of the side walls can be disregarded. Wales

[125] used low-density polyethylene with aspect ratios of 10, 12.5, and 30 by measuring the birefringence in the 1-3 plane of a slit die. The results showed no difference between the measurements for the three given aspect ratios, although no measurements of elastic properties were taken in this study.

Han and Kim [12] presented results of exit pressure results for polymer solutions with varying aspect ratios (20,30,50,100). The analysis assumed velocity gradients in one dimension due to the large aspect ratios used. Results for the different slit widths were presented, but the results were reported at constant volumetric flowrate and not at a constant shear rate so the dependence of exit pressure on aspect ratio could not be determined.

The results of Wales [125] and Leblanc [16] contradict whether the aspect ratio affects the measurement of elastic properties. The experimental investigation by Leblanc used a series of thin metal inserts to vary the height (aspect ratio) of the die. The presence of small non-uniformities in the die height may have influenced the exit pressure results. The optical birefringence technique was not subject to these errors. Aspect ratios greater than 10:1 were assumed to be sufficient in obtaining a flow field in the slit die in which velocity components due to the side walls were negligible.

2.1.7 MATHEMATICAL TREATMENT OF THE DIE EXIT

This section outlines the derivation of the use of the exit pressure for measuring normal stresses. The derivation will highlight the most general treatment of the subject in a review article by Boger and Denn

[60] who used a macroscopic momentum balance to analyze exit flows. An alternative general description of exit flows is presented by Choplin and Carreau [63] using a macroscopic mechanical energy balance. Later, a review is presented in which certain simplifying assumptions are imposed on the general equations. Studies which examine these assumptions are also discussed. Finally, a section is presented on the errors associated with exit pressure measurements.

The relationships used to relate the exit pressure and normal stresses were obtained by a macroscopic momentum balance using a control volume which enclosed the exit region of a slit or capillary. The derivation of the equations were similar for both a capillary and slit geometry. Only the capillary geometry will be covered in this section. For a more detailed consideration, the mathematical treatment has been covered in a number of publications [14,58,59,68,123]. The control volume used in the macroscopic momentum balance is represented in Figure 5. The flow into the control volume at $z=0$ was assumed to be fully developed laminar flow. The right hand surface or exit of the control volume was taken at a point within the jet, sufficiently far from the die exit, where the velocity profile was constant across the diameter of the jet. The flow was assumed isothermal, with negligible gravitational, surface tension, or air drag effects. The validity of these assumptions will be reviewed in a later section. The overall momentum balance at steady state is then:

$$0 = \int_0^R 2\pi \rho v_z^2(r, 0) r dr - \pi \rho R_j^2 v_j^2 + \int_0^R 2\pi \Pi_{zz}(r, 0) r dr - \int_0^L 2\pi R \tau_{rz}(R, z) dz \quad (2.2)$$

The first two terms in equation (2.2) represents the contribution of momentum at the entrance and exit planes respectively. The third term re-

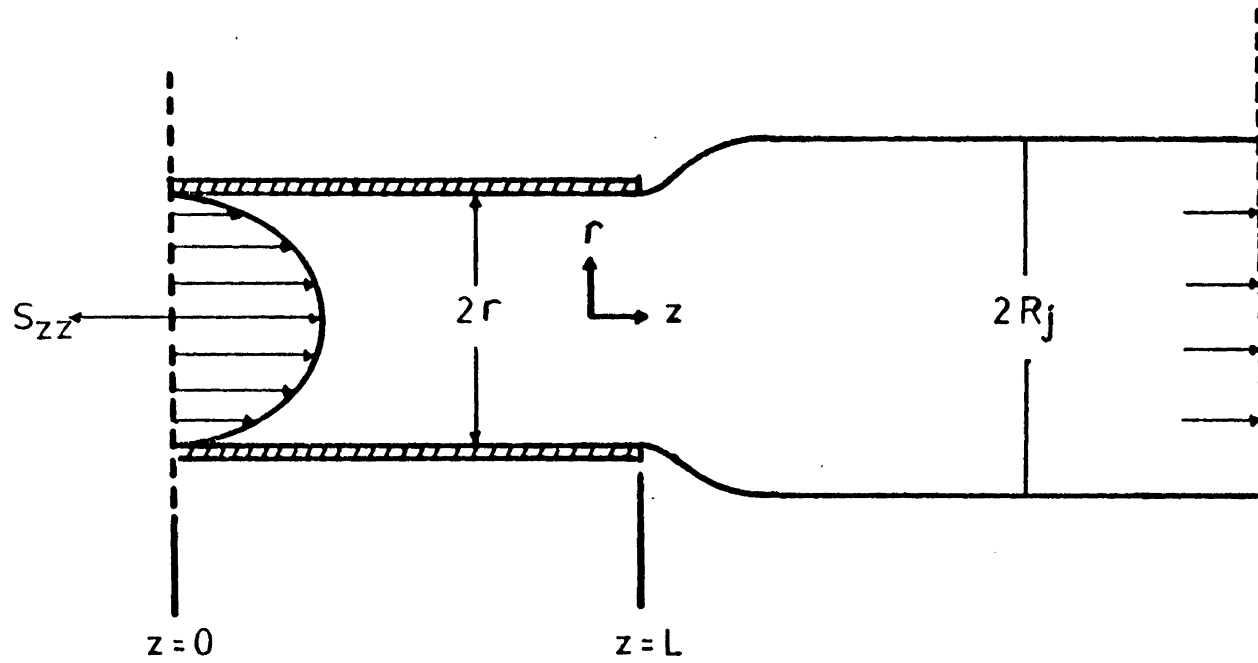


Figure 5. Control Volume for the Macroscopic Momentum Balance

presents elastic forces acting on the entrance plane and the last term accounts for shear forces acting along the tube walls.

The term $\Pi_{zz}(r,0)$, the total stress component acting in the z-direction, can be rewritten using the r component of the equation of motion and an identity used to define the set of normal stresses differences. The $\Pi_{zz}(r,0)$ term may be expressed as

$$\Pi_{zz}(r, 0) = N_1(r) + \Pi_{rr}(R, 0) + \int_r^R N_2(r') \frac{dr'}{r'} \quad (2.3)$$

The term Π_{zz} is now expressed as a combination of normal stresses and the total stress quantity Π_{rr} . The r' in the last term is a dummy integration variable. The integration of equation (2.3) with partial integration of the double integral allows expression of the axial stress term Π_{zz} in equation (2.2) in terms of the viscometric function:

$$\int_0^R 2\pi \Pi_{zz}(r, 0) r dr = \pi R^2 \Pi_{rr}(R, 0) + 2\pi \int_0^R [N_1(r) + \frac{1}{2} N_2(r)] r dr \quad (2.4)$$

The term $\Pi_{rr}(R,0)$ is the pressure measured by a flush mounted pressure transducer, $P_w(0)$. For a constant linear pressure gradient in the capillary, the pressure is extrapolated to the die exit to yield the exit pressure, P_{xc} . The original equation (2.2) can now be rewritten as

$$\begin{aligned} \int_0^R [N_1(r) + \frac{1}{2} N_2(r)] r dr = & - \int_0^R \rho v_z^2(r,0) r dr + \frac{1}{2} \rho v_j^2 R_j^2 - \frac{1}{2} R^2 P_x - RL\tau_w \\ & + R \int_0^L \tau_{rz}(R,z) dz \end{aligned} \quad (2.5)$$

The term $1/2 \rho v^2 R^2$ is often expressed as the magnitude of the reactive thrust, T . This is equal to the momentum flux of an exiting jet:

$$T = \rho \pi R^2 v^2 \quad (2.6)$$

Equation (2.5) may be rewritten in terms of the reactive thrust, T.

$$\int_0^R [N_1(r) + \frac{1}{2}N_2(r)]rdr = \frac{T}{2\pi} - \int_0^R \rho v_z^2(r, 0)rdr - \frac{1}{2}R^2P_x - RL\tau_w + R\int_0^L \tau_{rz}(R, z)dz \quad (2.7)$$

As suggested in chapter one the stress profile inside the exit region may deviate from fully developed flow due to a rearrangement of the velocity profile in the anticipation of the end of the die. A function is defined to express the magnitude of τ_{rz}/τ_w as a function of the dimensionless axial distance along the wall of the die.

$$\tau_{rz} = -\tau_w F(\varepsilon; \tau_w, Re) \quad (2.8)$$

where $\varepsilon = z / L$. The function F is unity in fully developed shear flow and may vary as the fluid approaches the exit of the die. Boger and Denn [60] postulate that the function F is dependent on the stress level in the fluid, τ_w , and there may be Reynolds number dependence. For creeping laminar flow of polymer melts, the inertial contributions will be negligible. The function f is not expected to depend on the Reynolds number for polymer melts at low shear rates. The form of the function is rheologically dependent on the fluid. Equation (2.7) becomes

$$\int_0^R [N_1(r) + \frac{1}{2}N_2(r)]rdr = \frac{T}{2\pi} - \int_0^R \rho v_z^2(r, 0)rdr - \frac{1}{2}R^2P_x + RL\tau_w(\int_0^1 f(\varepsilon)d\varepsilon - 1) \quad (2.9)$$

The normal stresses contained in the above equation are a function of the r-direction. The shear stress in fully developed flow is linear in the r-coordinate as shown below:

$$\tau = (r / R) \tau_w \quad (2.10)$$

where τ is the magnitude of τ_{rz} at any position. The integral expression in equation (2.9) may be written as a function of shear stress, τ . This expression can be solved explicitly for the combination of normal stresses by differentiating the integral in equation (2.9) by τ_w to give

$$N_1(\dot{\gamma}_w) + \frac{1}{2}N_2(\dot{\gamma}_w) = \frac{1}{\pi R^2} \left(T - 2\pi \int_0^R \rho v_z^2(r,0) r dr \right) - P_x - \frac{\tau_w}{2} \frac{\partial P_x}{\partial \tau_w} + \frac{\tau_w}{2\pi R^2} \frac{\partial}{\partial \tau_w} \left(T - 2\pi \int_0^R \rho v_z^2(r,0) r dr \right) \quad (2.11)$$

The analysis for a slit geometry is analogous to that of the capillary for a slit of half height h as shown below in equation (2.12): (Note the secondary normal stress difference does not appear in the expression for slit flow)

$$N_1(\dot{\gamma}_w) = -P_x - \tau_w \frac{\partial P_x}{\partial \tau_w} + \frac{1}{h} \frac{\partial}{\partial \tau_w} \tau_w \left(\rho v_y^2 h_y - \int_0^h \rho v_z^2(y,0) dy \right) + \frac{\partial}{\partial \tau_w} \tau_w^2 \frac{L}{h} \left(\int_0^1 f(\epsilon) d\epsilon - 1 \right) \quad (2.12)$$

The equations relating the normal stresses to the exit pressure derived above do not assume any specific behavior of the fluid at the exit of the die. Han and coworkers [4,5,6,14,28,32,70,123] published a series of papers which used a simplified form of equations (2.11) and (2.12) for the calculation of normal stresses of polymer melts in capillary and slit die rheometers. The sign of the normal stress differences in equations (2.11) and (2.12) is negative for steady shear flow. Using the absolute value of the normal stress differences, equations (2.11) and (2.12) become

$$N_1(\dot{\gamma}_w) + \frac{1}{2}N_2(\dot{\gamma}_w) = P_x + \frac{\tau_w}{2} \frac{\partial P_x}{\partial \tau_w} \quad (2.13)$$

$$N_1(\dot{\gamma}_w) = P_x + \tau_w \frac{\partial P_x}{\partial \tau_w} \quad (2.14)$$

These equations form the basis for the experimental investigation presented in section 5.3. These equations include the assumptions listed in section 2.1.7 in addition to the assumption of steady flow up to the exit of the tube, $F(\epsilon, \tau_w, Re) = 1$ and that for polymer melts and concentrated solutions at low Reynolds numbers that inertial terms are negligible.

The equations (2.13) and (2.14) containing the assumptions of viscometric flow up to the die exit have been used by Han and others [1-40] to measure the value of N_1 in polymer melts and solutions. The major criticism in the use of the exit pressure concerns the validity of the assumption of fully developed flow. Disturbance in the stress field upstream of the die exit contributes to the value of N_1 through the rearrangement function f discussed in the previous section. Experimental investigations have shown the assumption may not be valid for polymer melts and solutions. These results are presented in section 2.2. The quantitative effects of the rearrangement on the measurement of N_1 using the exit pressure and equations (2.13) and (2.14) have not been addressed.

2.1.8 ALTERNATE FORMS OF THE MOMENTUM BALANCES

The equations developed in the proceeding section potentially permit measurement of both the primary and secondary normal stress differences. The magnitude of N_2 for polymer melts is negative and 0.1-0.4 times the

primary normal stress difference[137]. An explicit measurement of N_2 would be useful in characterizing viscoelastic fluids.

An explicit relationship measuring N_2 may be derived by the comparison of the exit pressure measurements in slit and capillary die rheometers. Han [9,66] conducted an experimental investigation using polymer melts which indicated that the exit pressure was equivalent for both slit and capillary dies for the same shear rate range. Using this result, Davies, Hutton, and Walters [57] compared equations (2.13) and (2.14) to obtain a set of equations for N_1 or N_2 from exit pressure data in a capillary

$$N_1 = - P_x - \tau \partial P_x / \partial \tau w \quad (2.15)$$

$$N_2 = + \tau w \partial P_x / \partial \tau w \quad (2.16)$$

Since experimental evidence shows that P_x is a monotonically increasing function of shear stress, equation (2.16) predicts a secondary normal stress difference which is qualitatively correct with experimental data.

The use of equation (2.15) to directly calculate the value of N_1 from a capillary is based on the experimental results by Han that the magnitude of the exit pressure is independent of geometry. Tuna and Finlayson[101] reported numerical exit pressure values for a convected Maxwell fluid. They found that $P_c \neq P_s$ and the difference between the two quantities increased with wall shear stress. These results suggest the capillary die may not be used to measure N_1 through equation (2.15). The magnitude of the exit pressure in different geometries will be examined by deriving a relationship calculating P_x in terms of the stress field present in the exit region of the die for both slit and capillary geometries.

2.2 EXPERIMENTAL ERRORS

In this section are reviewed experimental, theoretical, and numerical studies which critically examine the assumptions used to derive the equations relating the exit pressure to normal stresses. Also, the experimental errors encountered which effect direct measurement of P_x will be discussed.

2.2.1 FLOW AT THE EXIT

The primary criticism of using the exit pressure as a means of measuring normal stresses is the validity of the assumption requiring fully developed flow up to the exit of a capillary or slit. The flow field at the exit is examined using three major techniques. The first examines the velocity profile at the exit by laser anemometry or tracer studies. The stress field is examined by use of flow birefringence studies, and finally, macroscopic momentum and mechanical energy balances are evaluated from detailed pressure gradient measurements.

The use of velocity field measurements in the exit region is currently limited to the study of viscoelastic solutions. Higashitani, Nishio, and Hara [55] measured the velocity distribution around a circular die exit for a viscoelastic fluid (Separan/water). Flow deviation from steady shear flow was reported at $1/3$ diameter upstream from the die exit. They postulated the exit region would exist at higher Reynolds numbers. Wipple and Hill [48] used a similar tracer technique in a solution of polyacrylamide in glycerin and water. Exit disturbances were detected at $2/3$ upstream diameter. Both of these studies concluded a large extensional gradient exists along the wall inside the die.

Schowalter and Allen [45] have also used tracer studies to measure velocity profiles. They concluded that no appreciable change was indicated in the velocity field upstream of the die exit. Minor changes in the velocity field at the exit plane were observed. The velocity field at the exit exceeded theoretical predictions by several percent and this was attributed to acceleration of the fluid near the wall. This conclusion suggests that there may be some disturbance upstream that was not detected by the experimental apparatus.

Laser anemometry has been used to measure the velocity field in viscoelastic fluids by several groups [45-47,49,54]. Goulden and MacSporran [54] investigated accelerating shear flow at the exit of a vertical tube for polyacrylamide solutions. No exit disturbance was apparent upstream into the tube.

In contrast to the findings of Goulden and MacSporran, the group of Clermon, Pierrard, and Scrivener [47] reported a modification of the axial velocity profile up to one diameter upstream. Rama Murthy [46] calculated velocity fields for a tube Reynolds number $0.03 \leq Re \leq 2.94$ largely in the free surface region. Some variation in the velocity profile was apparent at the exit, but the length of the disturbance region was not calculated. Goltlieb and Bird [49] examined the deviation from viscometric flow for a series of five rheologically different liquids at $Re < 1.0$. The existence of an exit region was reported for each of the test liquids. The exit region started at between $1/2$ and $4/3$ radius upstream, with the velocity accelerating along the wall and decelerating near the tube axis. The extent or length of the disturbance seemed to depend on the elasticity of the fluid but the magnitude of the velocity

change was almost independent of elasticity and a function of the flow conditions (Re). Based on this work and previous work by Allen [53], Goltlieb and Bird concluded that exit effects were negligible for flows above $Re = 1$ for polymer solutions.

An alternative method in assessing the existence of fully developed flow at the exit is the use of flow birefringence to examine the stress field. Funatsu and Mori [23] presented an isochromatic pattern of polypropylene melt at the exit. The stress field was disturbed at a distance of approximately $1/3$ radius upstream. The length of the exit disturbance was also found independent of shear rate from 1 to 10 s^{-1} . These flow birefringence photographs also appear in Rheology [52].

Vinogradov et al. [51] presented some birefringence results for flow of narrow MWD polybutadiene samples. The patterns clearly show the stress field disturbance upstream for the exit. A stress concentration of 1 extra fringe order at the exit corner is clearly shown. The actual stresses were not reported.

The most complete stress analysis of the die exit was conducted by Arai and Hatta [50] for exit flow of polyethylene from a slit. They presented a map of the principal stress lines about the exit region. The exit disturbance was seen to extend to a distance of $1/2$ die height upstream. The stresses calculated from the flow birefringence data were qualitatively in agreement with the numerical results of Nickel et al. [74].

Han and Drexler [44] published flow birefringence photographs of exit flow for polystyrene and polyethylene melts. The photographs of the isochromatic patterns demonstrated marked deviation from fully developed

flow upstream of the exit. Han argued, however, that the stress rearrangement was of secondary importance at reasonably high shear rates. An examination of the data presented by Han shows the extrudate drooping as it exits the die. Gravity forces or other body forces can influence the stress fields present. The small contribution of the exit rearrangement term as presented by Han and Drexler has been used extensively by Han to support the use of the exit pressure as a means of obtaining normal stresses.

The assumption of fully developed flow was indirectly studied by evaluating the stresses calculated by a series of pressure transducers using a macroscopic momentum balance analysis. Davies, Hutton, and Walters [57] examined the use of the jet-thrust technique for normal stresses with particular attention to stress rearrangement at the exit plane. The discrepancy between normal stresses measured by jet-thrust and normal stresses measured independently was attributed to stress rearrangement and the disturbance was proportional to the elasticity of the fluid.

Carreau, Choplin and Clermont [127] have used a macroscopic mechanical energy balance over the exit control volume to estimate the contribution of viscous dissipation at the exit. For flow of a polyisobutylene solution in mineral oil through a fine tube, they reported deviation of fully developed flow upstream of the exit. Excess viscous dissipation represented 90 percent of the exit pressure as calculated by viscometric data and the mechanical energy balance. These results were similar to an earlier paper of Choplin and Carreau [63] where the magnitude of the elastic and viscous dissipation correction terms were equivalent. The

assumption of negligible excess dissipation at the exit was judged unacceptable.

In summary, experimental evidence in most cases supports a disturbance upstream of the die exit. The consensus is reflected by Boger and Denn [60] who state that "without a full understanding of the velocity rearrangement term, the exit pressure technique is worthless as a means of measuring normal stresses and can only provide an upper bound of uncertain magnitude."

The previous section dealt with the validity of the basic assumptions used in the derivation of equations (2.13) and (2.14) for the determination of normal stresses from the exit pressure. An error analysis also includes the experimental errors as well as the validity of the basic assumptions. In the next section the numerous practical problems which must be eliminated to obtain consistent, accurate values of the exit pressure are discussed.

2.2.2 EXTRAPOLATION TECHNIQUES

The exit pressure is an extrapolated quantity and therefore dependent on the method used to extrapolate the pressure measurements to the die exit. Han and coworkers [2,4,6-12,14,28,31] published a series of papers in the early 1970's which supported the use of the extrapolated exit pressure as a means of measuring fluid elasticity. By extrapolating the pressure profile in the fully developed flow region to the exit, a positive residual stress was obtained for polymer melts and solutions. The major criteria used in determining a fully developed flow region was the constancy of the pressure gradient. A linear extrapolation technique was

therefore employed by Han to obtain P_x . Only once does Han et al. [3] comment on non-linear pressure profiles. The non-linearity was attributed to the absence of fully developed flow, but no explanation was given for the nonlinear pressure profiles. Han and coworkers did not examine the effects of different extrapolation techniques on the magnitude of P_x . Only P_x values obtained by linear extrapolation were reported.

Linear extrapolation techniques were employed by Blum, Yerushalmi, and Williams [13,33] investigating extrusion rheometers. Linear profiles were observed for the polymer solutions investigated. Okubo and Hori [71] and Springer, Brodkey, and Lynn [15] reported linear results for polymer melts. Neither group discussed the existence of non-linear profiles.

The presence of non-isothermal temperatures and a pressure dependent viscosity function can cause curvature in the pressure profile. Leblanc [16] reported a parabolic pressure profile for butadiene-styrene block copolymers. A reference was made to the earlier work of Han et al. [3] on the conditions for fully developed flow. Leblanc suggested the parabolic shape may be due to elastic effects. A parabolic equation was eventually used for calculation of τ_w and the exit pressure.

A comparison of different extrapolation techniques was discussed by Lodge and deVargas [20]. They compared 2-point and 3-point extrapolation techniques on the data by Leblanc [16] as shown in Figure 6. A 3-point least squares extrapolation gave negative P_x values which were in distinct contrast to the 2-point extrapolation (positive P_x). Both straight line methods gave significantly lower values of P_x than originally reported by Leblanc using a quadratic fit. Previously reported studies of the exit

pressure have not considered the consequences of the extrapolation technique.

Laun [18] has also explored the significance of the pressure profile curvature for LDPE polymer melts. A linear profile yielded negative exit pressure losses for all shear rates examined. A parabolic fit gave values of P_x which were small in magnitude and positive for low and medium shear rate ranges. Laun discussed the pressure curvature based on temperature and pressure dependence. Rauwendaal [21] concluded the presence of non-linear pressure profiles was due to variation in temperature and pressure.

An experimental comparison of various extrapolation techniques was presented by Pike et al. [9] for the flow of polystyrene melts. Large deviations in the value of P_x were observed for various extrapolation techniques. A more recent comparison was presented by Read and Baird [131] for polyethylene melts. The extrapolation technique strongly influenced the magnitude of P_x .

The presence of nonlinear pressure profiles may result from die geometry effects, non-isothermal temperatures, or a pressure dependent viscosity function. The choice of the extrapolation technique used to calculate P_x from non-linear pressure profiles has been shown to strongly influence the final magnitude of the exit pressure. A quadratic extrapolation of the pressure profile $p(z)$ can account for the non-linear pressure profiles reported in the literature, but no experimental evidence has been presented which suggests that a quadratic function yields the "correct" value of P_x . The choice of the extrapolation technique still presents an unanswered question in the measurement of P_x from pressure values obtained along a die. Also, the presence of curvature

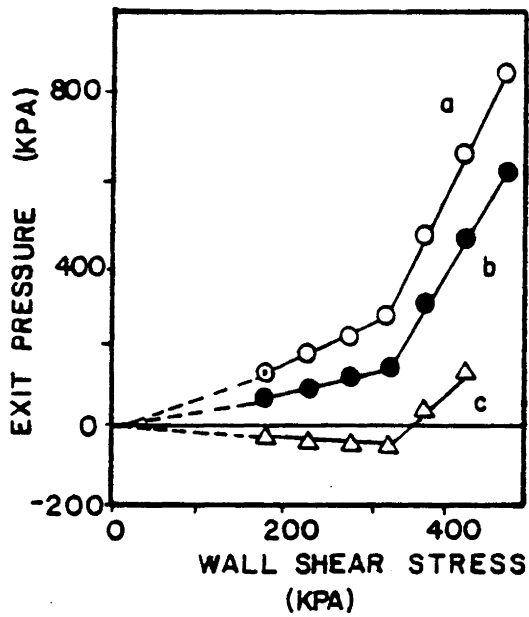


Figure 6. Comparison of Extrapolation Techniques on the Value of P_x
 (a) Quadratic, 3 points. (b) Linear, 2 points. (c)
 Linear, 3 points by least squares. [20]

in the observed pressure profiles suggests that the flow is not fully developed which violates one of the assumptions used in the exit pressure theory.

2.2.3 TEMPERATURE EFFECTS

Viscous heating effects must be considered for polymer melts and concentrated solutions for high shear rate experiments. The high viscosity and low thermal conductivity for most polymer melts can cause significant temperature variation both axially and across the die cross section. Due to the temperature dependent viscosity function, small temperature gradients within the flow geometry may seriously affect the pressure profiles. As the viscosity decreases with increasing temperature, the pressure gradient will decrease along the length of the die.

The magnitude of viscous heating in a slit die rheometer has been estimated by Rauwendaal[21]. He calculated the temperature rise in a polymer melt assuming isothermal conditions at the walls. Viscous dissipation effects were significant ($> 2^{\circ}\text{C}$) for shear rates greater than 1000 s^{-1} for a high density polyethylene melt. Ybarra and Eckert [40] presented a numerical analysis of viscous heat generation in a slit die for power-law fluids. They concluded that viscous heating effects could be minimized by reducing the height of the slit.

Heat transfer problems must be carefully considered in designing equipment used to measure the pressure profile since high temperatures are involved in polymer melt experiments. Thermal insulation and control systems must maintain constant temperature for the entire geometry. Pike [128] reported temperature differences of 2°C between flush mounted

thermocouples in a slit die and a thermocouple immersed in the fluid. Pike suggested the temperatures measured by the thermocouples did not represent the temperature of the fluid, but measured the temperature of the metal in the surrounding walls.

Viscous heating generation was not expected to be significant in the present investigation. The maximum shear rate used in the study was less than 15 s^{-1} . Viscous heating effects were negligible at these shear rates.

2.2.4 HOLE PRESSURE ERROR

In this section the influence of the hole pressure on measurements of P_x are discussed. Han [14,66] reported hole pressure errors for dilute polymer solutions in a slit die rheometer. The hole pressure decreased as the polymer concentration increased. Han also reported negligible hole pressures for polymer melts. These results were criticized by Blum et al. [13] due to the geometry originally used by Han. The transducers used in the experiments by Han were not flush mounted but were recessed from the wall. Blum et al. reported negligible hole pressure error for a concentrated polymer solution. Higashitani and Lodge [129] suggested that the large scatter of the results of Blum may mask the hole pressure error. They reported significant hole pressure errors for an aqueous Separan solution. The hole pressure increased with shear stress. Lodge and deVargas [20] have also reported significant hole pressure in polymer melts at low Re flow. Pike et al. [19,128] have also conducted a series of investigations for the magnitude of the hole pressure in polystyrene and polyethylene melts. Positive hole pressure values were reported for

these systems. The extrapolated exit pressure is reduced by the hole pressure error. Hence, transducers must be flush mounted to obtain accurate pressure measurements.

2.2.5 SURFACE TENSION - INERTIAL EFFECTS

Surface tension can reduce the magnitude of the jet thrust in normal stress measurements. In general for polymer melts the influence is negligible. Joseph [67] has given a full discussion of surface tension effects as related to die swell measurements. The magnitude of the inertial contribution may be measured by the Reynolds number. The high viscosity of polymer melts at low flow rates usually minimizes inertial forces. Inertial effects are therefore usually negligible for polymer melts at low flow rates. High Reynolds number experiments are possible for the flow of viscoelastic solutions. The jet-thrust technique [57,59] employs inertial effects to measure normal stresses for polymer solutions at high shear rates.

2.2.6 PRESSURE DEPENDENT VISCOSITY

The apparent viscosity, η , of a fluid can vary as a function of the hydrostatic pressure imposed on the system. A pressure dependent viscosity function will, to first approximation, yield a parabolic pressure profile. Laun [18] discussed the influence of the pressure dependent viscosity on the curvature of the pressure profile. The pressure profile $p(z)$ can be written as a quadratic function is shown below:

$$p(l) = a + b l + c l^2 \quad (2.17)$$

where l represents the axial distance along the die. The three coefficients are determined from the pressure profiles. For isothermal flow, the pressure coefficient α is obtained from the quadratic function using the following expression.

$$\alpha = 2 b / c^2 \quad (2.18)$$

Laun measured the viscometric properties of LDPE melts in a slit die rheometer. He concluded that in the range $\tau_w > 10^5$ Pa the evaluation using linear pressure profiles yielded significant deviations in the measurement of τ_w and P_x compared to using a quadratic fit for the pressure profiles. The shear stress values varied by +12% and the exit pressure varied by -300% if the pressure dependence of viscosity was neglected. The magnitude of these errors was seen to increase with increasing shear rate.

Lodge and de Vargas [20] used a 2-point method to evaluate the exit pressure. Non-linearities in the analysis were modeled by using a Maclaurin expansion to express the pressures. The coefficient of these higher order terms consisted of deviations due to nonisothermal flow, a pressure dependent viscosity function, and die geometry effects. They concluded for a polyethylene melt that the exit pressure can be influenced by the pressure coefficient of viscosity almost as much as the first normal stress difference.

The pressure dependent viscosity parameter creates a non-linear pressure profile $p(z)$ inside the die. The magnitude of the error increases with increasing wall shear stress as the hydrostatic pressure

inside the die increases. The value of P_x measured by extrapolating the pressure profile must account for the curvature due to the variation of viscosity with pressure.

2.2.7 FINITE TRANSDUCER WIDTH

An error may arise by using finite-width transducers, calibrated using a constant pressure, but used in a non-uniform pressure field. The effective center of the transducer must be known for accurate determination of the pressure gradient and therefore the exit pressure. Original analysis by Higashitani and Lodge [129] dismissed the errors as negligible. Tong [130] later concluded that the effect was positive, proportional to r^2 , and independent of temperature. This error can be minimized by decreasing the transducer width.

The effective center for strain gauge transducer, such as those used in the present investigation, was examined by Pike [128]. By modeling the deflection of the transducer surface under a pressure gradient field, the effective pressure reading was obtained. Pike concluded that the center of the transducer diaphragm was also the effective pressure.

Tong [130] also argued there is an additional effect on the pressure due to the effect of a shear stress on the diaphragm. The shear stress creates additional tensile forces acting on the diaphragm which may alter the pressure measurements. A model representing the tensile forces was constructed based on a two dimensional analysis. Tong concluded that diaphragm deflection was not significantly affected by shear forces and that the effective diaphragm center was also unaffected by shear forces. Pike [128] reached the same conclusion for a strain gauge transducers.

2.2.8 DIE WALL AFFECT

The existence of a converging geometry, resulting from non-parallelism of the die walls, can produce an error in viscosity measurements. Lodge and deVargas [20] discuss the potential effects of changing die height on the pressure gradient. A nonlinear pressure gradient would occur in this case. The effect can be checked by reversing the flow direction as done by Higashitani and Lodge [129] and Tong [130].

In this section the validity of the assumptions used in the theory used to predict N_1 from P_x have been discussed. Flow birefringence results and laser dopler anemometry studies have shown the presence of stress or velocity field rearrangement upstream of the die exit. The assumption of fully developed shear flow until the die exit plane used in the exit theory is violated for polymer melts. Also, a description of the experimental errors associated with direct measurement of the exit pressure were presented. The magnitude of these errors present in the current investigation are discussed in chapter five. In the next section the experimental investigations which use P_x to predict N_1 will be reviewed. The results of these studies should be examined in view of the violation of the assumption used in the simplified equations (2.13) and (2.14) presented by Han.

2.3 PREDICTION OF N_1 FROM THE EXIT PRESSURE.

The measurement of the primary normal stress difference, N_1 , is currently limited to low shear rates ($< 10 \text{ s}^{-1}$) due to the experimental limitations of rotatory instruments. The use of the exit pressure with slit die rheometers offers a technique to extend the range in normal stresses

to shear rates of industrial importance. This section will discuss experiments which directly compare the values of N_1 as obtained using the exit pressure through equation (2.14) and a cone-and-plate rheometer.

Han and Charles [31] were one of the first groups to try to predict N_1 using the exit pressure. The relationship derived, however, was incorrect as the resulting equation produced:

$$N_1 = P_x \quad (2.19)$$

This relationship was then used by Han [9,31], Springer et al. [15], and by White and Kondo [103] to predict elasticity for polymer melts. A direct comparison to rotary rheometers was not made.

The correct derivations of the equations relating the exit pressure to normal stresses were presented by Davies et al. [59], Han [14,123], and Boger and Huilgol [58]. The direct comparison between cone-and-plate and slit/capillary rheometer, using the results of equation (2.14), were reported first by Han et al. [32] for a series of polymer melts. The results are shown in Figure 7 which is taken from Han. It should immediately be noted that the cone-and-plate and the slit and capillary rheometer data were not reported over the same shear rate range. A continuous curve has been drawn through both sets of data arbitrarily without any direct comparison based on equal shear rates. A gap of one decade shear rate is present in the comparison for certain polymer melts.

A comparison of rheogoniometer and slit die normal stresses was presented by Pike et al. [19]. Predicted normal stresses were overestimated by 200-300 percent for the shear rate range $0.1 \leq \dot{\gamma} \leq 15 \text{ s}^{-1}$ for

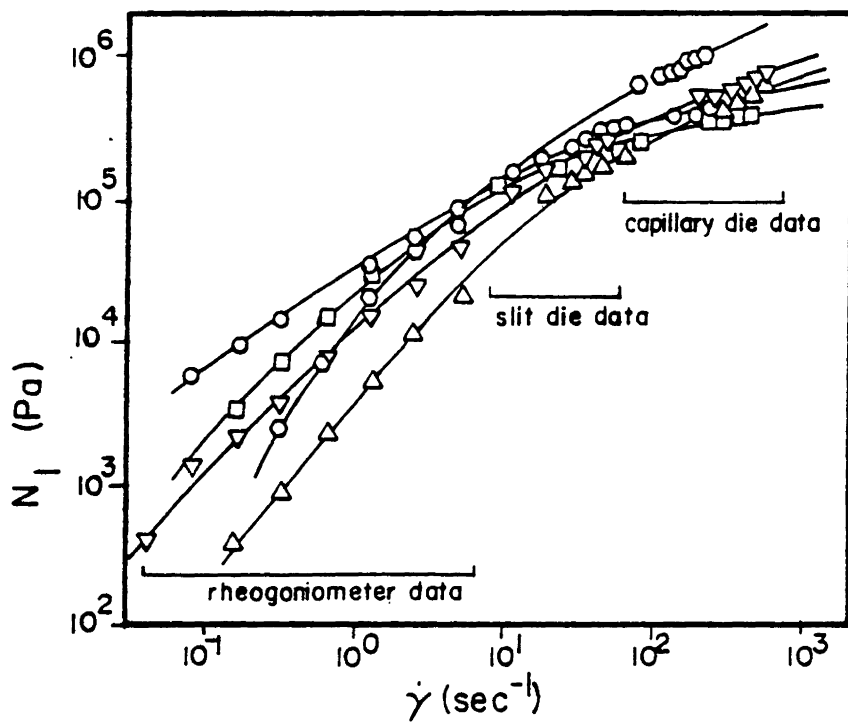


Figure 7. Comparison of N_1 Results From Cone-and-plate and Exit Pressure Technique [123]

polystyrene melts. The lack of agreement was attributed to the difficulty in evaluating the slope $\partial P_x / \partial \tau_w$ and to experimental problems previously discussed in section 2.2.

The use of the exit pressure to measure N_1 has been suggested for shear rates above the shear rate range in which cone-and-plate rheometers can currently measure normal stresses. The only studies, however, which have presented results in the shear rate region where cone-and-plate and slit die results overlap have reported the normal stresses were overestimated by 200-300 percent. The lack of agreement may be traced to both the violation of the assumption of fully developed flow in the exit region implicit in equation (2.14) and the influence of experimental errors on the measurement of P_x . The effect of the rearrangement terms on the prediction of N_1 can be evaluated by examining the stress field at the die exit. The stress optic law can be used to evaluate the results of flow birefringence data to quantitatively determine the stress field in the die exit region. The birefringence studies discussed in the previous section only presented the isochromatic fringe patterns which are proportional to the principal stresses in the fluid. In the next section the use of birefringence and the validity of the stress optic law is reviewed for polymer melts.

2.4 FLOW BIREFRINGENCE AND THE STRESS-OPTIC LAW

A review is presented in this section which describes the use of the stress-optic law for polymer melts. The stress-optic law permits one to obtain the values of the principal stress difference ($\sigma_1 - \sigma_2$) and the principal stress directions, χ , from flow birefringence data. A brief

introduction of the birefringence phenomena will be discussed. A review of the validity of the stress-optic law for polymer melts is then presented.

2.4.1 BIREFRINGENCE

Certain solids and liquids become optically biaxial under the application of a stress. These materials possess three different components of the refractive indices along a set of mutually perpendicular principal optic axes. For polymer melts an optical anisotropy is created due to orientation of the polymer molecules created by an imposed stress field. If polarized light is passed through a transparent material parallel to one of the principal optic axes, the light wave is divided into two components, each with its plane of polarization parallel to one of the other two principal axes. The two component waves travel through the material with different velocities. At the exit of the material the waves recombine with a relative phase difference θ (radians) given by

$$\theta = (2 \pi L \Delta n) / \lambda \quad (2.20)$$

The phase difference θ is also called the relative retardation between the light waves. The Δn term is the difference between the principal refractive indices and is called the birefringence. The constant L represents the optical path length through the medium and λ the wavelength of the polarized light beam.

Early studies by Neumann and Maxwell [132] on birefringence resulted in the formulation of the following stress optic laws:

1. At each point on the material the principal optic directions are parallel to the principal stress directions in the plane of the wave front.
2. The difference in the velocities of the two waves in the medium is proportional to the difference in the principal stresses.

The principal optic and stress directions are defined by the angles, χ_{opt} and χ_{stress} made with a laboratory reference axis. The stress-optic laws are expressed mathematically by:

$$\chi_{opt} = \chi_{stress} = \chi \quad (2.21)$$

$$\Delta n = C (\sigma_I - \sigma_{II}) \quad (2.22)$$

where the constant of proportionality, C , in equation (2.22) is the stress-optic coefficient and σ_I and σ_{II} are the principal stresses.

If the principal stresses are transformed to an arbitrary coordinate frame q_i , the following expressions for the shear stress τ_{12} and the normal stress difference $\tau_{11} - \tau_{22}$ are obtained from equations (2.21) and (2.22)[133].

$$\tau_{12} = \Delta \sigma \sin 2\chi / 2 \quad (2.23)$$

$$\tau_{11} - \tau_{22} = \Delta \sigma \cos 2\chi \quad (2.24)$$

If the linear stress optic rule eq. (2.22) is introduced into these equations, the following expressions are obtained:

$$\tau_{12} = (\Delta n / 2 C) \sin 2\chi \quad (2.25)$$

$$\tau_{11} - \tau_{22} = (\Delta n / C) \cos 2\chi \quad (2.26)$$

where the angle χ is called the extinction angle in flow birefringence measurements. The values of Δn , χ , and C are determined experimentally from optical measurements.

The use of the linear stress optic rule (equation 2.22) for polymeric systems was obtained mathematically by Treloar [134] for an ideal rubber. The birefringence of an ideal rubber system was calculated which related the principal polarizabilities to the stretching ratios. The form of these equations were equivalent to those relating the principal stresses to the stretching ratios. Treloar also arrived at the result in equation (2.22). The stress-optical coefficient obtained by this procedure:

$$C = \frac{2\pi}{45} \frac{(\bar{n}^2 + 2)^2}{\bar{n}} \frac{\alpha_1 - \alpha_2}{kT} \quad (2.27)$$

The magnitude of C is mainly dependent on the back-bone anisotropy, $\alpha_1 - \alpha_2$, of the chain molecules. The temperature dependence of C is determined by the kT term and by the temperature dependence of $\alpha_1 - \alpha_2$. There is no dependence on the molecular weight, the MWD in the sample, or on the segment length in the sample.

It was suggested by Lodge [135] that the linear stress-optic rule could be extended to the flow of uncrosslinked systems. Using his network theory, Lodge showed the stress-optic coefficient C for a polymeric fluid should be equivalent to that predicted by Treloar for a crosslinked rub-

ber. The permanent crosslinks in the rubber were replaced by temporary points of entanglement. For uncrosslinked systems an alternate form of the stress-optic rule was found. The average life time of the entanglement point must be much greater than the time for thermodynamic equilibration for the chain segment system. The validity of the linear relationship in equation (2.22) may deviate from linearity for large stresses or for unsteady flows. The limits of applicability of the stress-optic rule are investigated below for polymer melts.

In this section the limits of the validity of the linear stress-optic rules are discussed for polymer melts. A more complete review of the limits of the stress optic rule can be found in the text by Janeschitz-Kriegl [133]. The linearity of equation (2.22) was investigated using a steady shear flow with equation (2.26). The values of C versus $\dot{\gamma}$ or τ_w were plotted to insure a constant value of the stress optic coefficient. Wales performed a study of this type for a series of polymer melts [125]. Flow birefringence measurements were conducted using cone-and-plate apparatus. For all cases investigated, C was constant over the imposed shear rate range. The upper limit of the shear stress was 8×10^4 Pa due to depolarization effects caused by the "parasitic" velocity gradients produced by the side windows [133,136].

Deviation of the stress-optic rule has been shown by Matsumoto and Bogue [137] in polystyrene melt for an extensional flows at high strain rates. Non-linear response was present for tensile stresses of the order of 10^6 Pa. Since melt fracture generally occurs in shear flow in the range $\tau_w = 0.4-3 \times 10^5$ Pa., the results of Matsumoto and Bogue implied that

deviations from linearity of the stress optic law may not be observable in steady shear flow.

The results of elongational experiments also show the limits of validity of the stress optic law for flow components containing tensile stresses. Extensional gradients in the region along the wall have been reported for flow out of a die. Beginning at tensile stresses greater than 10^6 Pa, the linear stress-optical rule can no longer be valid. The results of the birefringence investigation must be evaluated in terms of these limits.

The validity of the stress optic law in response to a transient deformation was reported by Retting [108]. The birefringence ratio of $\Delta n/\sigma$ was plotted as a function of time for various isothermal tensile experiments at constant crosshead speed. The time for internal equilibrium of the sample was less than the duration of the experiments by Matsumoto and Bogue for temperatures 20°C above T_g . The stress optical law, therefore, was valid for transient experiments for materials in the melt state ($T > T_g + 20^\circ\text{C}$).

Wales [136] investigated the coaxiality of the extinction angles χ_{opt} and χ_{stress} . The values of χ_{stress} are derived from continuum mechanics for simple steady shear flow in a cone-and-plate rheometer. The values of χ_{stress} were evaluated from the values of N_1 and τ obtained from the rheometer. The values of χ_{stress} were in excellent agreement with values of χ_{opt} obtained from flow birefringence measurements. These results indicate the validity of the stress optic rule for polymer melts in steady shear flows.

2.5 NUMERICAL MODELING

In this section the various studies involving the modeling of non-Newtonian fluid mechanics is reviewed. The emphasis is on the use of the Galerkin finite element method to solve the equations of motion, continuity, and constitutive equation for a given domain and boundary conditions. The first section will introduce the general steps used to construct an algorithm for the numerical simulation of the field equations describing fluid flow. The convergence behavior of the numerical techniques is then discussed with emphasis on mesh refinement and the formulation used to model the problem. Finally, the die swell problem will be reviewed with specific reference to the stress and velocity field rearrangement upstream of the die exit.

2.5.1 NUMERICAL SOLUTIONS

The basic equations of motion have been known for a long time, yet fluid flow problems involving complex geometries even for Newtonian fluids have only recently been attempted. The reason for this is that analytical solutions exist only for very simple flow problems. In most cases numerical techniques must be used to approximate the continuous solution over a given domain. Given the difficulties with even simple Newtonian flow problems, the solution of flows of viscoelastic fluids with more complicated geometries such as in plastics manufacture, require numerical techniques using digital computers.

Numerical simulation of fluid problems consists of a series of steps of algorithms to obtain a numerical solution. These steps are outlined schematically in Figure 8.

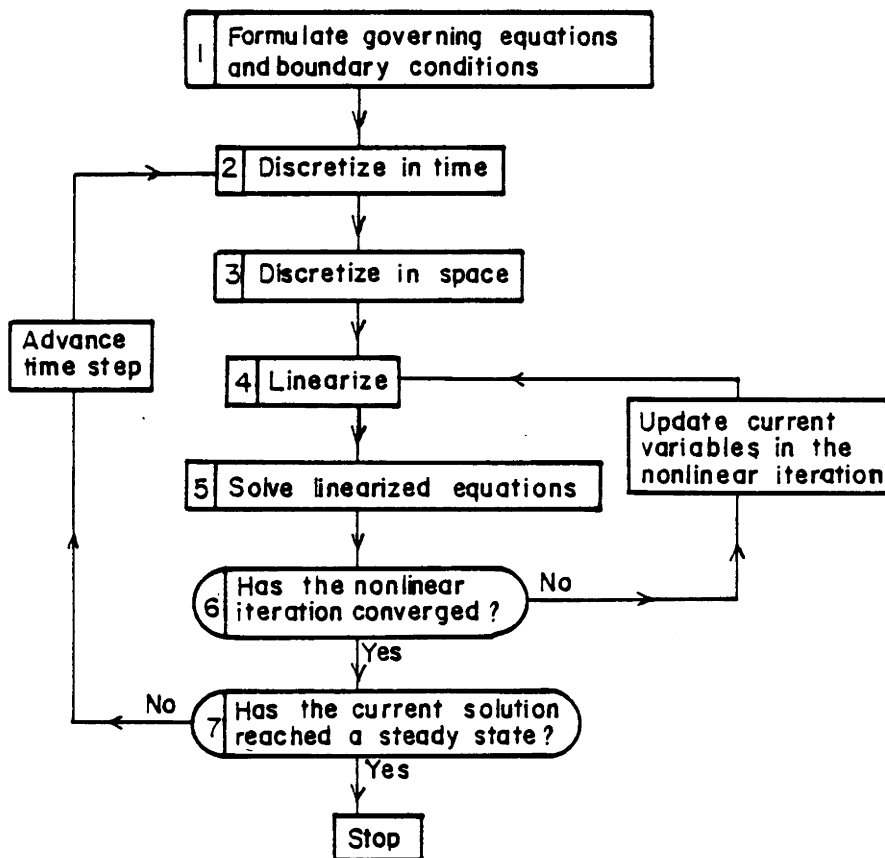


Figure 8. Program Steps Involved in Numerical Simulation of Fluid Flow

2.5.1.1 SYSTEM OF EQUATIONS AND BOUNDARY CONDITIONS

The governing equations for fluid mechanics are the continuity, momentum, and the constitutive equations. The selection of the physical variables required (u, p, T, Ψ) will influence the system of equations. The choice of variables also dictates the type of partial differential equation (elliptic, hyperbolic, parabolic or mixed) which in turn can dictate the choice of boundary conditions.

The boundary conditions are dependent of the nature of the boundary; free surface, inflow, solid(moving or stationary), and slip. For fluids with memory, a history of all past deformations must be specified by specifying the stress components on the inlet boundary.

2.5.1.2 TIME DISCRETIZATION

This step is necessary for transient flows and may be omitted for steady-state flows. The system of equations is approximated over a finite time step, t , after the imposition of initial conditions on the unknown variables. Most methods using time integration use finite difference methods for this step. As shown in Figure 8, the solution of the steady state system occurs within the time discretization loop. These steps are repeated for each time step.

2.5.1.3 SPACE DISCRETIZATION

Space discretization involves the approximation of the primary unknowns on a spacial grid which represents the domain of the problem. The approximation may be generated in several ways, using finite difference methods, finite element methods, boundary integral methods, multigrid

methods or spectral methods. The last three methods have seen little application in fluid mechanics and will not be discussed.

In the finite difference method, the primitive variables are approximated at discrete spatial grid points or nodes. Approximation at an arbitrary point in the domain may be calculated by interpolation. In the finite element method, the variables are approximated by simple functions of the spatial coordinates, defined over finite regions of the domain. These "elements" make up a grid pattern which approximates the shape of the domain. In each case the discretized system yields a non-linear system of algebraic equations for the unknown variables or coefficients.

The choice between the two techniques in most cases is a matter of judgement. Both techniques have distinct advantages over the other. The finite difference technique is the easier to implement, also the theoretical mathematical analysis is well established. Computationally, finite difference techniques usually are faster and require less storage.

The advantage of finite element techniques over other variational techniques is due to three basic features. First, the domain of the problem is represented as a collection of geometrically simple subdomains or elements. This enables modeling of complex non-uniform geometries and free surface complications found in industrial processing equipment. Second, the continuous solution is approximated by a combination of simple approximation functions. This assumes that the continuous solution may be adequately represented by a linear combination of algebraic polynomials. The finite element method implements natural boundary conditions which may also be viewed as an advantage.

2.5.1.4 LINEARIZATION

Nonlinear systems must be solved numerically using an iterative procedure. At each iteration, the system is linearized and the resulting system is solved to provide an updated solution. The linearization is usually accomplished by two methods: a Picard-type iteration, or as a step of a Newton's method. Newton's method and its derivatives allow simultaneous update of all variables, and is becoming more widely used, particularly in finite element calculations.

2.5.1.5 SOLUTION OF SYSTEM OF EQUATIONS

For each iteration of the non-linear loop, a system of linear matrix equations needs to be solved. In general the systems consist of banded, sparse matrices. Several well established methods exist for the solution of sparse systems. The most common technique is based on Gaussian elimination for finite element systems and relaxation methods in the context of finite differences.

2.5.1.6 TERMINATION OF THE NON-LINEAR ITERATION LOOP

The last two steps are repeated until convergence to an approximate solution is attained. For transient problems, the solution procedure is repeated for each time increment until a steady state solution is obtained.

2.5.2 CONVERGENCE LIMITS

The numerical simulation of non-Newtonian flows involves the solution of a system of non-linear equations by some iterative technique. The outstanding problem in the simulation of viscoelastic fluids concerns the

upper limit above which the numerical algorithm fails. In this section a review of the studies examining the convergence behavior of non-Newtonian numerical simulations are presented. The following points present an outline of some relevant conclusions:[138]

1. A limit of the Weissenberg number, We , is found in all published works above which the algorithm fails.
2. Minor changes in the constitutive equation or the algorithm can alter the convergence ranges for which a solution can be obtained.
3. As the elastic nature of the system increases to a critical limit, spurious oscillations often appear in the field variables. The stress components usually are more severely affected causing large and erroneous stress gradients. The spurious oscillations have no physical background, and their wavelength depends upon the mesh.
4. Mesh refinement and corner strategies alter the range of convergence, but there does not seem to be a consistent trend in current published studies.

The cause of the failure in the iterative process has been investigated by Mendelson et al. [141]. The causes were divided into two categories: approximation error and multiplicity or loss of flow field. The approximation error results from the inability of the weighted residuals method to approximate the field equations and the associated boundary

conditions or the inability of the discretization to describe the local behavior of the field variables. The latter cause results in difficulties in approximating steep gradients in the solution by low-order approximation functions and coarse meshes.

The existence of multiple solutions or no unique solution in the numerical calculations can cause convergence failure. A continuation method was used by Mendelson et al. to describe the loss of existence for steady two-dimensional flow. Three possibilities were identified for the solution at a given Deborah number, De ; regular, bifurcation and a limit point. These are represented in Figure 9 with $\chi = \chi(De)$ representing a characteristic variable of the flow field such as the overall pressure drop. A regular point occurs when the solution is a single valued function and locally unique. At bifurcation points the solution becomes multi-valued. Numerical algorithms fail because the methods can not discriminate between the multiple solutions. Limit points occur when the solution behavior turns back on itself at a critical De , and since no solution exists beyond this point, the numerical method fails.

The existence of limit or bifurcation points was examined by Mendelson et al. [141] for a finite element formulation using a convected Maxwell model and a second order fluid. The presence of a bifurcation point was investigated by examination of the determinant of the Jacobian matrix in a Newton's iteration. No bifurcation or limit points were detected. The loss of convergence was attributed to approximation errors. In a more recent report, Yeh et al. [142] found a limit point for an upper-convected Maxwell fluid in axisymmetric contraction. The limit

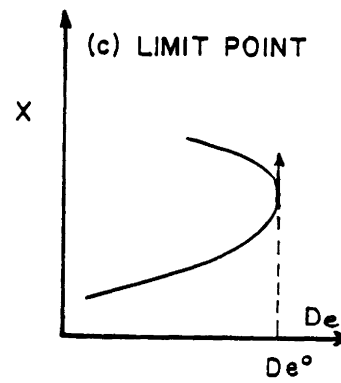
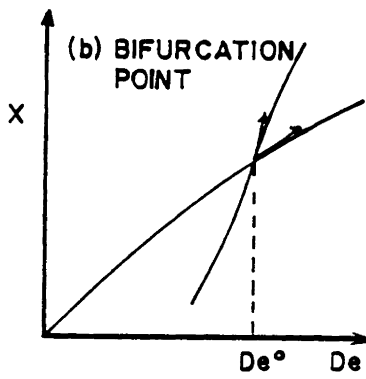
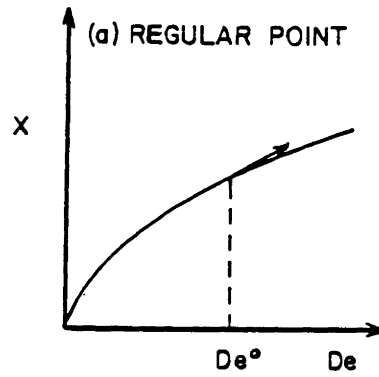


Figure 9. Numerical Solution Behavior for Non-linear Systems
[141]

points were independent of mesh size and the order of the approximation functions.

The stability of the second order fluid and the convected Maxwell model was examined by Tanner [143]. Stability criteria were derived above which no solution was possible for the corresponding numerical solutions. Mesh refinement for the given stability criteria would reduce the range of convergence, and in the limit of $h \rightarrow 0$, no solution was possible for the simple iterative procedure. A Newton-Raphson iterative technique was suggested in improving stability.

Lee and Finlayson [144] examined the stability of a codeformational Maxwell model using both a time integrator solution and the results of an eigenvalue analysis for fully developed flow in a pipe. They concluded that the given formulation was unstable for $We > 4.0$. The results of the eigenvalue analysis suggested that all modes studied were stable.

The effect of mesh size on the convergence behavior as related to the problem of approximation error was discussed by Mendelson et al. [141]. The loss of convergence was preceded by oscillations of the stresses. Stress singularities caused by re-entrant corners or abrupt change in boundary conditions as found in die swell problem can not be adequately approximated by present interpolation polynomials.

Davies, Lee, and Webster [145] have addressed the effect of mesh size directly for the flow of Oldroyd type constitutive equations in a 4:1 contraction. The limiting value of De decreased with increasing mesh refinement. Also, the mesh configuration affects convergence by using an increased number of elements in the area of the corner singularity. The specific cause of breakdown in the solution, the FE formulation itself

or approximation error of the corner singularity, is unknown at this time. Mitsoulis et al. [39] reported mesh refinement increased the limit of convergence for a CEF fluid for a similar flow geometry. Other factors influencing the convergence of non-Newtonian simulations include both the algorithms used to discretize the differential equations and the interaction between discretization error and nonlinear interaction.

The convergence limits of non-Newtonian models all demonstrate a limit of the Weissenberg number above which all algorithms fail. Mesh refinement alters the range of convergence, but a consistent trend in the effect of mesh refinement on convergence has not been established. For models containing sharp changes in boundary conditions, such as re-entrant corners or free surface problems, mesh refinement can actually reduce the limits of convergence [145,94]. The comparison of the results of the numerical simulations to experimental results will therefore be limited to shear rates where the elastic terms in the constitutive equations are not significant. The limit of convergence of numerical models predicting exit pressures will be presented in the next section. Numerical results predicting exit pressure values are found under the general classification of the die swell problem. These studies are presented in the next section.

2.6 THE DIE SWELL PROBLEM

Viscoelastic extrudate swell is of practical interest to the polymer processing industry. Free surfaces are found in extrusion, fiber spinning and blow molding. The main interest in the extrudate swell problem is the presence of an abrupt change in boundary conditions from a no-slip

velocity condition along the die walls to zero shear force imposed on the free surface. In this section a summary of numerical studies investigating die swell behavior of viscoelastic fluids is presented. Particular attention will be directed towards studies which highlight the velocity and stress rearrangement found at the exit region of extrusion dies. Excess pressure loss predictions relating to the exit pressure will also be discussed.

A summary of numerical work on die swell problems is given in Table 2.3. The table includes information of the type of constitutive model used, the finite element formulation, and the maximum value of the stress ratio, $N1 / 2\sigma$, for which convergence was achieved.

The loss of convergence in the numerical solutions as seen in Table 2.3 is limited to Deborah number $\sim 1 - 1.25$. Studies reporting higher limits of the Deborah number have relied on the separation of the extra stress into a viscous and elastic contribution. Crochet and Keunings [95] used an Oldroyd B fluid with a retardation time λ^* to achieve values of the recoverable shear of four. The use of the retardation parameter tends to dampen oscillations in the stresses at the die lip. Mitsoulis et al. [99] used an empirical constitutive equation which employed an empirical power-law function to model normal stress behavior. The models were not viscoelastic, but predicted normal stresses due to the extra empirical terms. The limiting value of the Deborah number reported was 4.5. The success of this model can be attributed to the elimination of the highly non-linear extra stress terms found in differential forms of viscoelastic constitutive equations.

Table 2.3

Summary of Numerical Investigations for the Die Swell
Problem Using non-Newtonian Constitutive Equations

Constitutive	Maximum Value of $N_{1/2\sigma}$ Slit Capillary		Mesh	Reference
2nd-order fluid	0.75		7 x 4	[79]
Maxwell		0.4	3 x 9	[83]
Maxwell	0.75	0.66	2735 DOF	[84]
Maxwell	1.25		5 x 15	[91]
Maxwell	1.25		Mesh	[94]
			Comparison	
Integral Maxwell		0.75	4 x 23	[96]
Oldroyd-B	4	4	3 x 25	[95]
Generalized Dewitt Fluids	4		431 DOF	[86]
Maxwell	1.6	1.6	6 x 18	[101]
CEF	1.0		859 DOF	[98]
Emperical	2.24		858 DOF	[99]
PTT and Leonov				[106]

2.6.1 REARRANGEMENT AT THE DIE EXIT

As discussed in section 2.1, the use of the exit pressure technique as a means of measuring N_1 requires fully developed flow up to the exit of the die. The examinations of streamlines and the contour plots of the resulting stress field obtained from the numerical simulation can be used to evaluate the magnitude of any exit disturbances. The choice of the constitutive equation representing the fluid can also be used to test the influence of shear thinning viscosity, normal stresses, and extensional behavior on the type of rearrangement observed.

Tuna and Finlayson [101] attempted to evaluate the assumptions specific in the theoretical development of the exit pressure for a convected Maxwell fluid and a model with non-zero secondary normal stresses. They reported velocity rearrangement with the velocity profile "flattening out" as the die exit was approached. The magnitude of the rearrangement was reduced as the elasticity of the fluid increased, but remained not fully developed. Tuna and Finlayson concluded that the rearrangement effect did not invalidate the use of the exit pressure as a means of estimating normal stresses. These conclusions were based on the agreement between values of N_1 predicted in steady shear flow and the values of N_1 calculated using the numerically calculated values of P_x and equations (2.13) and (2.14).

Other numerical simulations examine the velocity rearrangement indirectly through the study of die swell. It is useful to present the results concerning some of these studies. Crochet and Keunings have presented a series of two papers which contain velocity rearrangement

information [84,95]. For an upper-convected Maxwell fluid, the velocity profile flattens up to one-half radius from the exit. This behavior was similar to Tuna and Finlayson. In a later paper, however, Crochet and Keunings [95] presented velocity profiles in which the centerline velocity overshoots the fully developed velocity. This effect increased with increasing Deborah number. Based on the large velocity overshoot behavior, numerical calculations were not pursued for higher values of De . This would suggest the overshoot behavior may be an artifact of the numerical simulation. Mitsoulis et al. [98] also reported centerline velocity overshoot behavior for an empirically modified constitutive equation.

Rearrangement in the exit region is also shown by contour plots of the radial velocity for die swell from a circular die. Coleman [86] showed a radial velocity component extending one-half radius upstream from the exit. Caswell and Viriyayuthakorn [96] showed similar behavior for a Maxwell fluid ($De = 0.75$).

The assumption of fully developed flow at the exit of a die was violated according to the results of finite element models examining the die swell problem. The examination of streamline contour plots and the velocity profiles near the die exit showed a marked deviation from the profiles in the viscometric shear flow region. Tuna and Finlayson conducted the only numerical investigation specifically examining the use of P_x in equations (2.13) and (2.14) to measure N_1 . They concluded rearrangement effects were not significant in the use of P_x to predict normal stresses. Their results, however, were limited to low shear rates due to the loss of convergence in the numerical model and they did not

compare their results with experimental investigations. The numerical simulation did not include pressure dependent material parameters, viscous dissipation effects, or other experimental errors which could affect the accuracy of using the exit pressure technique to measure $N1$.

2.6.2 DISCONTINUITY AT THE DIE EXIT

One of the difficulties in modeling die swell concerns modeling the abrupt change in boundary conditions between the imposed velocity boundary conditions inside the die and the stress boundary conditions on the free surface. Mathematically, this results in the presence of a stress discontinuity located at the die lip. The presence of the discontinuity can be shown in Figure 10 by examining the pressure profile of an Oldroyd B fluid presented by Crochet and Keunings [95]. The pressure and stresses all overshoot their fully developed values. The magnitude of this overshoot behavior was altered by the choice of the rheological model or by changing the mesh discretization [94].

The rheological model can influence the magnitude of the singularity by varying the viscosity of the fluid which in turn affects the shear stresses. Boger et al. [78] altered the degree of the shear thinning behavior of the power-law fluid by changing the powerlaw index, n . The larger the powerlaw index, the more pronounced the shear thinning behavior exhibited by the fluid. Reducing the powerlaw index, reduced the magnitude of the overshoot in the wall shear stress. The elongational viscosity may also have an important effect on the singularity and on the overall range of convergence. Crochet and Keunings [84] suggest that the

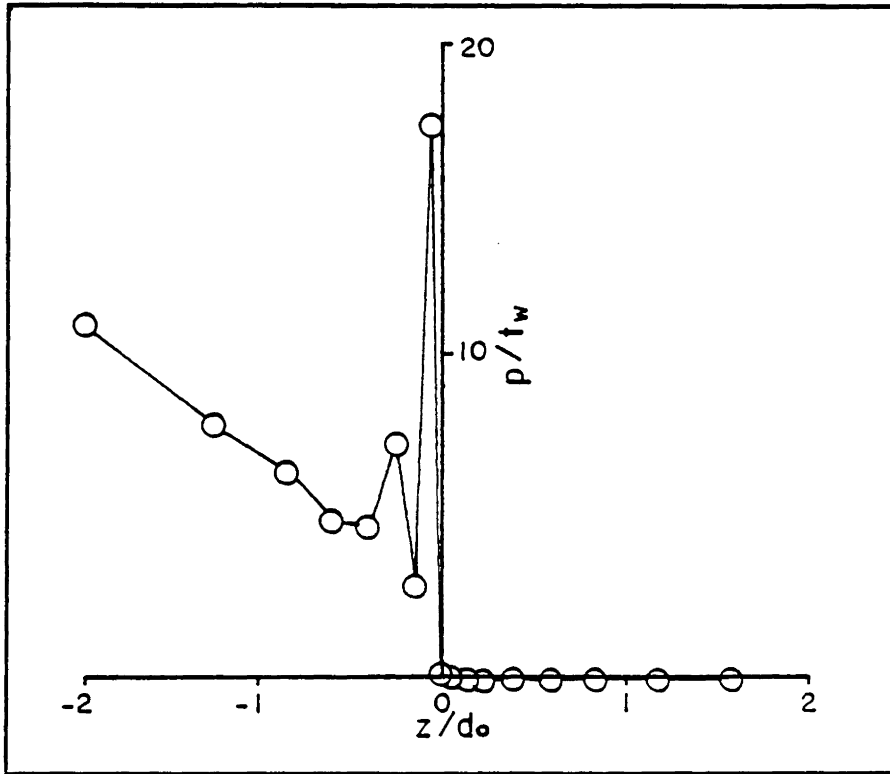


Figure 10. Numerical Pressure Profile Obtained for an Oldroyd B Fluid: The effects of the discontinuity of the pressure profiles are shown. [95]

large extensional stresses encountered for a upper-convected Maxwell fluid eventually caused the lack of convergence.

Bush, Tanner, and Phan-Thien [106] have recently published a study of extrudate swell for Maxwell type models, a Phan-Thien Tanner (PTT), and Leonov models. The elongational viscosity of the Maxwell model is unbounded above a critical strain rate, while the PTT and Leonov model both have limiting values of the extensional viscosity at higher elongational rates. Bush et al. concluded that the flow field near the die lip became more extensional in nature as the elasticity increased. The Leonov model converged for $We = 3$, while the Maxwell model failed, tends to support the conclusion that extensional behavior is important.

An alternative method of reducing the stress singularity is the mesh discretization scheme. Crochet and Keunings [94] compared mesh patterns used by previous investigators examining die swell. They concluded that using a coarse mesh improved the convergence range by smoothing the stress singularity.

The no-slip boundary condition used in modeling die swell has been examined by Silliman and Scriven [80,82]. They used a Galerkin finite element model with and without the presence of slip for indications whether the presence of slip can eliminate the stress singularity at the die exit. The reason for questioning the non-slip hypothesis comes from the need to relieve stress from stress singularities observed at contact lines. Silliman and Scriven reported the alleviation of the stress singularity for a slip boundary condition. The slip condition does not appreciably alter the velocity or pressure profiles, but does reduce die swell for a Newtonian fluid.

The stress singularity exhibited in the numerical models as a result of the change in boundary conditions at the die corner contributes to the loss of convergence in the numerical simulations. The magnitude of the stress discontinuity can be reduced by reducing the stress levels predicted near the die corner by altering the viscosity predictions of the constitutive models. Shear thinning viscosity η and bounded extensional viscosity $\bar{\eta}$ increase the limit of convergence for the associated constitutive equations. The stress discontinuity was eliminated entirely by introducing slip velocity boundary condition along the walls. The effect of a slip boundary condition on the convergence behavior of non-Newtonian constitutive equations, however, has not been examined.

2.6.3 NON-ISOTHERMAL FLOW

Thermal effects have recently been shown to affect the die swell through temperature dependent viscosity function. Experimental measurement of extrusion properties such as the exit pressure and die swell have useful meaning only if heat transfer conditions are taken into account. Thermal effects can be separated from elastic effects by numerical simulations using generalized Newtonian models with temperature dependent viscosity functions.

Heat transfer effects in Newtonian fluids have been investigated by Phouc and Tanner [111] and Ben-Sabar and Caswell [92] using a finite element formulation. Phouc and Tanner introduced the term thermal extrudate swell. They showed large swelling can occur when a large temperature difference exists between the centerline of the die and the wall. Ben-Sabar and Caswell also reported significant die swell for a Newtonian

fluid due to non-isothermal effects. Tanner has recently attempted to explain the non-isothermal swelling using a "Two-layer extrusion theory"[143]. He proposed a relationship between the die swell and the maximum temperature difference between the wall and the fluid centerline. The two layer theory is based on the flow kinematics at the exit in which the outer surface is in tension due to acceleration and the centerline region which is in compression due to deceleration of the fluid. The magnitude of the tensile and compressive forces are important as they may also represent the magnitude of the stress rearrangement at the die exit.

The magnitude of the viscous dissipation occurring in slit flow was investigated by Ybarra and Eckert [40] for a power-law fluid. An analytical series solution treated both isothermal and adiabatic wall cases. Dimensionless temperature rise charts were constructed for powerlaw viscosity model for different wall heat transfer rates. Significant temperature gradients were shown to occur for flow of viscous polymer melts in a slit. The viscous effects could be minimized by using as thin a slit as possible.

2.6.4 EXCESS PRESSURE LOSSES

The exit pressure may be predicted from numerical results by extrapolating the total normal force exerted on the wall to the die exit. This is the same procedure used in experimental investigations. The extrapolation technique was also used in numerical predictions as the exit pressure can not be calculated directly due to the stress singularity at the die lip.

Numerical correlations for the exit pressure have been presented by two groups. Tuna and Finlayson [101] fitted the following function to the numerical results.

$$P_x / \tau_w = 0.28 N_1 / \tau_w + 0.30 \quad (2.28)$$

It should be noted in equation (2.28) that the numerical data does not have the same functional dependence as the exit pressure theory derived in section 2.1. The function in equation (2.28) predicts the magnitude of the exit pressure as a linear combination of normal and shear stress contributions. Reddy and Tanner [110] also presented the same functional dependence for the exit pressure for a second order fluid in a slit die.

An alternate method used in reporting exit losses is the excess pressure loss, Ex defined by

$$Ex = \Delta P / 2\tau_w \quad (2.29)$$

The exit losses were evaluated by the difference ΔP between the upstream pressure in fully developed flow and the pressure loss that would result without the free surface. The wall shear stress, τ_w , was based in fully developed flow at the wall. For Newtonian fluids, $Ex \sim 0.16$ as reported by Crochet and Keunings [84], Reddy and Tanner [113], and Mitsoulis et al. [98]. Increasing elasticity, measured by the Deborah number, resulted in an approximately linear increase in the exit losses. Crochet and Keunings [95] reported the highest elasticity levels for an Oldroyd B fluid. They reported a change in curvature of Ex versus De in the region

of $De = 3$. Beyond this level the stresses began to oscillate near the die lip. For $De \geq 4$ no solutions were attempted. The change in the behavior of Ex may signal the onset of unstable behavior of the finite element formulation. A linear increase in Ex was also observed by Caswell and Viriyayuthakorn [96], Crochet and Keunings [84,94], and Coleman [91] for convected Maxwell models. Mitsoulis et al. [98] reported similar behavior for a second order fluid.

The effect of shear thinning viscosity on the excess pressure losses was investigated for power-law fluids of varying power-law indices. Boger, Gupta, and Tanner [78] reported exit losses increased for decreasing flow behavior index. They concluded the shear thinning viscosity reduced the extent of the exit effects for the power-law fluids observed. Mitsoulis et al. [98] reported, however, decreasing exit correction for decreasing power-law index in slit flow. The disagreement between these results and that of Boger et al. [78] were attributed by Mitsoulis to the deviation between the wall and centerline pressures reported by Boger.

The choice of the constitutive equation on the excess losses was investigated by Bush, Tanner, and Phan-Thien using a boundary element finite element formulation [106]. The results of the Maxwell models described above were compared with the behavior for a Phan-Thien Tanner model and the Leonov model. The slope of Ex versus We was lower for the Leonov and PTT model.

Numerical studies predicted positive values of the excess pressure losses for Newtonian and inelastic shear thinning fluids. These results suggest that the exit pressure contains contributions other than elasticity. The positive exit pressures may be due to the rearrangement

of the velocity field upstream of the die exit. The velocity rearrangement generates additional stresses which may contribute to the value of P_x . Elasticity in the fluid was varied by increasing the Deborah number by changing the material constants in the constitutive equations. The excess pressure losses increased with increasing elasticity. This is in qualitative agreement with experimental results. The Maxwell constitutive equation used by the majority of the researchers in this section, however, do not realistically model the steady shear or elongational behavior of polymers. Also, no comparison to experimental results were made. The numerical simulations in this section serve as a qualitative guide to the expected stress behavior observed in polymer melts.

2.7 RESEARCH OBJECTIVES

The value of the extrapolated exit pressure using the exit pressure theory derived from the macroscopic momentum balance equation has been proposed as a technique to measure the value of N_1 in polymer melts and solutions at high shear rates. The experimental investigations into the validity of the assumptions used in the development of the exit pressure theory have raised serious doubts whether P_x measurements may be used to calculate N_1 . Flow birefringence [23,44,50,51], tracer studies [45,48,55], and laser doppler anemometry [45-47,49,54] studies have been used to examine the validity of the assumption that the flow field remains viscometric up until the die exit. It has been shown that the velocity field rearranges before the die exit. To assess the effect of velocity field rearrangement on the use of the exit pressure technique, quantita-

tive calculations using stress field results for polymer melts must be evaluated. Boger and Denn [60] presented an empirical function f which should account for the rearrangement of the stress field. This correction term can be evaluated once the stress field at the die exit is known. Also, an explicit expression for P_x can be derived in terms of the normal stresses and shear stresses present in the exit region of the die. One objective of this study will be to assess the contributions of the stresses on the magnitude of P_x and the assumptions involved in calculating the value of N_1 by obtaining the stress field at the exit of a die in polymer melts using the flow birefringence technique and the linear stress optic rule. In previous birefringence studies the stress optic rule was not used to calculate the stress field in the exit region of a die and quantitatively evaluate the magnitude of the stresses generated by the velocity field rearrangement upstream of the die exit plane [23,50].

The value of the exit pressure was shown to be influenced by a number of experimental errors. A discussion of the errors associated with P_x measurements was presented by Lodge and de Vargas. No consistent values of P_x have been reported in the literature due to the influence of these errors. The purpose of part of the experimental study will be to experimentally measure the pressure profiles $p(z)$ for a series of polymer melts and discuss the influence of various error contributions on the final reported value of P_x . A slit die has been designed to minimize the effect of temperature on the extrapolated value of P_x . The die design also features an attached oil bath so the extrudate exits the die into a

neutrally buoyant heated environment. This eliminates temperature gradients and gravity effects on the measured value of P_x .

Although the magnitude of the exit pressure has been associated with fluid elasticity, an explicit expression which can be used to calculate P_x directly has not been presented in the literature. One objective will be to derive an expression used to calculate P_x from the stress field at the die exit. The stress field obtained from the experimental flow birefringence investigation will be used to evaluate the contribution of shear stresses and normal stresses on the magnitude of the exit pressure. The stress field rearrangement contribution on the value of P_x can also be calculated.

The numerical simulations investigating the nature of the stress field rearrangement at the die exit and the exit pressure have employed constitutive equations which do not represent the steady shear behavior of real viscoelastic fluids. One objective of the numerical investigation was to develop and test a finite element computer code which would adequately model the flow behavior of polymer melts in steady shear flow. The numerical model will then be used to calculate the velocity and stress field present at the exit of a die by solving the die swell problem. The numerical results will then be directly compared to the stress field obtained by means of the flow birefringence technique.

Finally, the results of the flow birefringence and numerical models will be used to examine the nature of the stress field in a fluid where numerical simulations fail to converge. The stress oscillations exhibited by numerical models at high Deborah numbers can be compared to the stress field obtained using the linear stress optic rule. This comparison

can be used to establish whether the sharp gradients predicted near the die corner are an artifact of the numerical simulation or are actually present in the fluid as measured by the flow birefringence studies.

The purpose of this chapter has been to critically review studies associated with the experimental and numerical calculation of the exit pressure and studies which have examined the nature of the stress or velocity field in the exit region of a die. The objectives of the current investigation were stated in light of the previous work reported in those areas. In the following chapter an outline of the experimental procedures used to obtain the value of P_x and the stress field from flow birefringence is presented. Details of the experimental apparatus and operating procedures are also discussed. In chapter four the numerical techniques used in the finite element simulation of the die swell problem are presented. Finally, in chapter five the results of the experimental and numerical investigations are discussed.

3.0 CHAPTER THREE - EXPERIMENTAL APPARATUS AND PROCEDURE

In this chapter the important aspects of the experimental investigation are discussed in detail. The experimental apparatus, consisting of a modified slit die rheometer, and the associated measurement and control systems are described. The procedure used to obtain the flow birefringence patterns will also be discussed. Finally, a brief outline of the operating procedure used to obtain the experimental results is presented.

3.1 POLYMERS STUDIED

The polymers used in the experimental investigation are described in Table 3.1. The principal material used in the detailed evaluation of the stress field was Styron 678U. The polystyrene melt exhibited excellent thermal, oxidative, and mechanical stability over the shear rate ranges and temperatures of interest. Because of this stability, no special handling or preparation procedures were required. The materials all consisted of bulk pelletized material received in 22 kg. containers.

An accurate assessment of the use of the exit pressure technique as a means for measuring the primary normal stress difference requires that the values of N_1 be available from a standard technique. A cone-and-plate rheometer (Rheometrics RMS 605) was used to measure the rheological properties of the polymer melt systems. The major equations used to calculate the viscometric quantities are described in detail elsewhere [105].

Table 3.1

Polymer Investigated

Polymer	Trade Name	Source	MW or Melt Index
Polystyrene	Styron 678	Dow Chemical	255000
Low-density Polyethylene	NPE 952	Northern Petrochemical	2.0 at 150°C
High-density Polyethylene	Petrothene LY600-00	U.S. Industrial Chemical Co. Inc.	1.5 qt 200°C

A cone-and-plate geometry was used in the present investigation. The fixture was a 2.5 cm. diameter stainless steel (316) cone with a cone angle of 0.1 radian. The practical limit of shear rates for the cone-and-plate instrument was less than 5 s^{-1} for the polymer melts used in this study. Above this shear rate sample loss and edge fracture became significant. Thus, actual comparison of viscosity and normal stress data between the cone-and-plate rheometer and the slit die rheometer was limited to shear rates less than 5 s^{-1} .

3.2 SLIT-DIE APPARATUS

The experimental investigation of the exit pressure consisted of two basic areas. First, direct measurement of the exit pressures was conducted for a series of polymer melts by measurement of the pressure profiles within the slit die geometry. Second, to obtain the stress field in the die exit region, glass windows were installed in the slit die rheometer so polarized light could be passed through the die for flow birefringence measurements. The specifications of the slit die, the pressure measurement, and the temperature control system will be discussed in the next section.

3.2.1 DIE DESIGN AND CONSTRUCTION

The slit die used in the experimental investigation was machined from two rectangular pieces of 316 stainless steel. The dimensions of the die and construction details are shown in Figure 11 and 12. The slit geometry was obtained by machining a rectangular slot which was $2.54 \pm 0.026 \text{ mm}$. deep and $25.4 \pm 0.026 \text{ mm}$ wide into the bottom block. By bolting the two die halves together a slit was formed with an aspect ratio of 10:1.

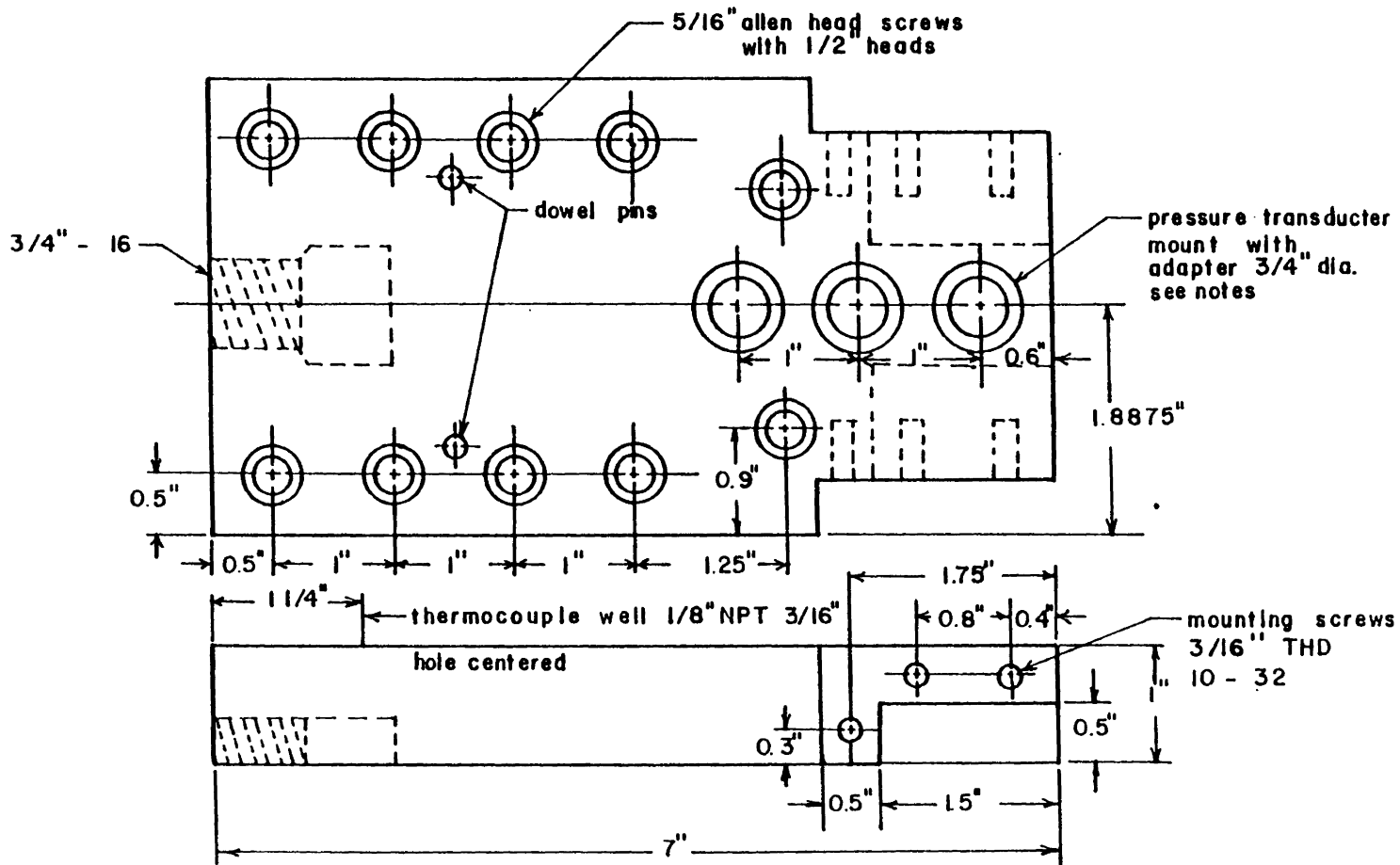


Figure 11. Construction of the Slit Die Rheometer - Top Plate

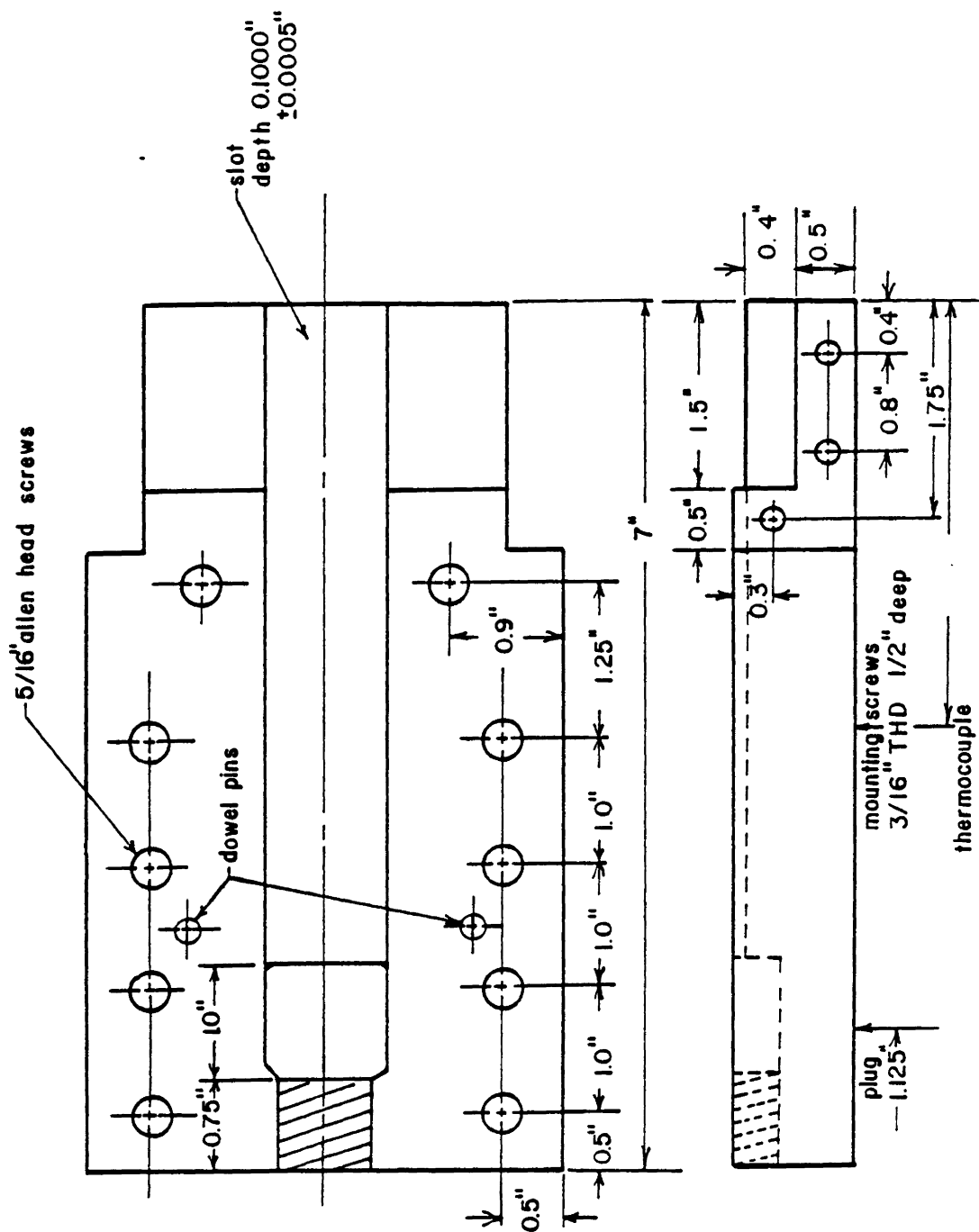


Figure 12. Construction of the Slit Die Rheometer - Bottom Plate

The machine tolerance in the construction of the slit die was 0.026 mm (0.001"). The effect of non-parallelism in the die walls was limited to random variation within the machine tolerance limits or approximately 1 percent of the die height. Machining imperfections were removed by polishing the rectangular slot with abrasive paper in an oil medium.

A reservoir region was included at the entrance of the slit die. The reservoir increased the residence time of the fluid within the die to allow for equilibration of temperature with the set points of the die temperature control system. The reservoir also allowed partial relaxation of the polymer melts, reducing the effect of the previous strain history received in the melt extruder and gear pump assembly.

The pressure gradient in the fluid was measured by a series of three flush mounted transducers located in the upper die block. The transducers were strain gauge construction (Dynisco model PT422A) and their operation is described in the next section. The transducers were flush mounted with the upper die wall to eliminate possible hole pressure error. The transducers were fitted into the die by means of a custom bushing. The transducer diaphragm was flush mounted by machining the adapter bushing until the diaphragm was level with the rest of the die wall.

The measurement of the pressure drop in the steady viscometric flow region required the pressure transducers be located in the fully developed flow region within the die. The location of the pressure transducers was chosen to eliminate errors due to entrance or exit effects. The first pressure transducer, T1, was located 73.7 mm or 30 die heights from the beginning of the slit. For polymer melts systems an entrance region of 1-2 die heights was sufficient for fully developed flow [125]. The last

transducer, T3, was located 15.24 mm or 6 die heights from the die exit. Transducer T3 was located as close to the exit as possible to reduce the extrapolation distance when measuring the exit pressure. The effective center of transducer T3 was far enough upstream to eliminate exit effects for exit lengths reported by Han [44] and Mori and Fonatsu [23] for polymer melts.

The use of flow birefringence to examine the stress field at the die exit required the inclusion of glass windows into the side walls of the die. Commercial quartz windows were mounted on either side of the die in the exit region of the die. This permitted flow birefringence and flow visualization studies in the 1 - 2 plane of the slit. A schematic of the window construction is shown in Figure 13. The windows were mounted in the die by placing the window in a machined section at the die exit and along the bottom support attached to the connecting oil bath. The window was sealed by placing a silicone rubber gasket, a steel spacer plate, and a cover plate through which a series of bolts were attached. By bolting the cover plate over the window assembly, the silicone gasket expanded and prevented any leakage from occurring around the windows.

In order to obtain a clear picture of the stresses at the exit plane of the die, the windows continued past the exit plane and formed a section of the walls of the oil bath. The die swell encountered at the exit was therefore not an unconstrained die swell. The fluid could swell freely in the vertical direction, but was contained between the two windows horizontally after the exit. The windows were extended beyond to the die exit to permit detailed examination of the stress field downstream of the die.

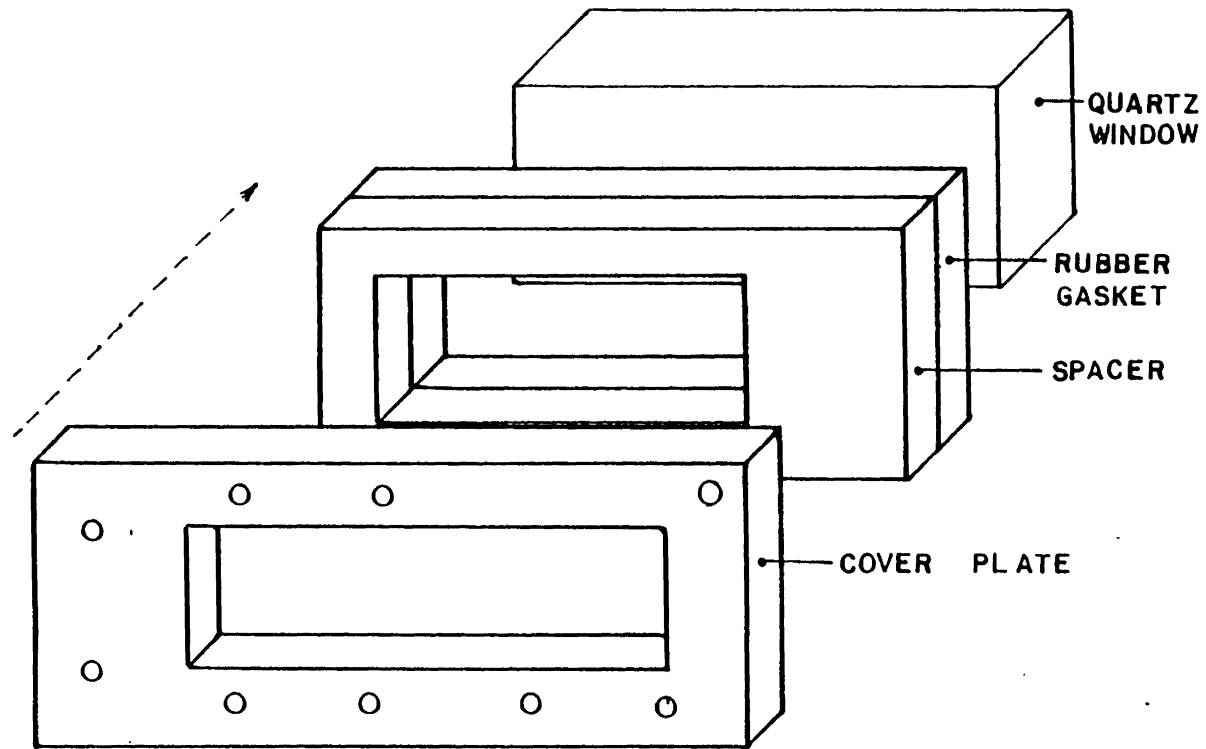


Figure 13. Installation of the Windows into the Die

An oil bath was attached to the slit die to reduce the effect of gravity forces influencing the stress field at the exit and to eliminate sharp temperature gradients at the die exit. Due to the horizontal arrangement of the slit die, the weight of the extrudate could cause an additional set of stresses to be transmitted into the die. The extrudate can sag as it exits the die and the downward force may affect the exit pressure or the stress field rearrangement. For each polymer, a silicone oil was used in the bath which matched the density of the extrudate for the given operating temperature. The neutrally buoyant extrudate should eliminate any additional forces. Dow Corning type 200 silicone oils (20 and 50 centistoke) were used to match the density of the extrudate at the operating temperature of the die. The heated oil also eliminated any sharp temperature gradients between the extrudate temperature and the ambient air temperature.

The heating system for the die was provided by means of four independently controlled sets of electrical resistance heaters. The entry region of the die was heated by two sets of silicone rubber patch heaters (Electrofilm Inc. Valencia California) adhered to the die by a high temperature silicone adhesive (Dow Corning Silastic 736 RTV adhesive). The exit region and the oil bath were heated with 1/4" diameter cartridge heaters purchased from Industrial Heaters, Inc. Each set of heaters was controlled by a single set-point proportional controller (Omega 4001JC) with a iron-constantan thermocouple as the temperature sensor. The thermocouples were mounted in the bottom of the die such that the end of the thermocouple was within 3 mm of the slit wall. A thermal paste (Omega Omegabond 201) was included in the thermocouple well to insure good

thermal contact. The die was insulated by blocks of alumina-silica fiber insulating material.

The accuracy of the rheological measurements from the slit die is dependent on the accuracy of the temperature control system and the pressure measurement system. The calibration procedures and accuracy of these two systems are discussed in the following sections.

3.2.2 PRESSURE MEASUREMENT SYSTEM

In this section the operation of the pressure measurement system is described. The sensor used for this system is a strain gauge type transducer. The basic design of the transducer is first considered and then the calibration procedure is discussed.

3.2.2.1 PRESSURE TRANSDUCER DESIGN AND OPERATION

The strain gauge transducers (Dynisco model PT422A) operate by displacing a volume of mercury between two thin metal diaphragms. The outer diaphragm on the end of the transducer was in contact with the fluid. The diaphragm responded to an applied pressure by deflecting inward and displaced a volume of mercury in the stem reservoir. The displaced mercury transmits the force to the inner diaphragm inducing a deflection on this diaphragm. Strain gauges were mounted on the inner diaphragm and were wired to form a wheatstone bridge circuit. Deflection of the strain gauges produced a millivolt signal proportional to the applied pressure. The signal was transmitted to an amplifier which filtered and amplified the original signal. The output signal 0-1 volts was fed to a strip chart recorder.

The operating characteristics of the specific transducers are given in Table 3.2. Two pressure ranges were chosen to accurately measure the pressures encountered inside the die. As shown by the values in Table 3.2 the transducers exhibit excellent thermal stability characteristics. Pressure variation due to thermal effects was negligible for the small changes in temperature during any one trial, $< 1^{\circ}\text{C}$. The typical performance of the transducers with respect to zero drift is also shown in Table 3.2. It is observed that the transducers exhibited good stability for the given experimental conditions.

The signal amplifier for the pressure transducers contained a zero and span calibration mode. An alternate calibration procedure was necessary in order to improve the accuracy of the measurement system for the determination of the exit pressure. The calibration procedures used in the present study are presented in the next section.

3.2.2.2 PRESSURE CALIBRATION PROCEDURE

The pressure transducers used in the present study were calibrated in-situ under simulated operating conditions. A dead weight tester (Chander Engineering, Model No. 23-1) was employed to impose a known hydrostatic pressure onto the system. In general the procedure consisted of sealing the ends of the die and pressurizing the melt in the die at an elevated temperature. Calibrated weights were placed on a platform of the dead weight tester which transmitted a pressure through an oil reservoir. Oil was pumped into the die until the imposed pressure was equivalent to the force due to the known weights. The calibrated pressures produced by the dead weight tester were accurate to within 0.69 KPa.

Table 3.2

Pressure Transducer Characteristics
Dynisco Model PT422A

Transducer	Range [KPa]	Temperature Stability of Transducer Zero [KPa/°C]	Transducer Zero Drift [KPa/Hr]
1	0 - 3450	1.55	1.5
2	0 - 3450	1.60	1.5
3	0 - 5170	1.70	2.5

A calibration curve relating the imposed pressure from the dead weight tester to the voltage output of the pressure transducer must be constructed for each of the three transducers. The accuracy of the output voltage measurement was improved by using two ranges to measure the 0-1 volt output signal. The 0-0.1 volt range provided by the strip chart recorder was used to record the lower 10 % of the pressure range. The sensitivity of the strip chart recorder was ± 0.001 volt for the range 0-0.1 volt and ± 0.01 volt for the 0-1 volt span. The output for pressure versus output voltage was slightly non-linear. To compensate for slight curvature, the voltage range was broken into two sections. Two least squares lines were constructed to cover each of these regions. This technique yielded the lowest error between the pressure calibration data and the calibration curve for each transducer. A representative set of calibration functions for polystyrene melt at 165°C are given in Table 3.3. An estimate of the error in using the given calibration functions is given by the standard error of estimate (Se)[148]. The value of Se was determined from the original calibration data based on the number of calibration points and the error between the calibration pressure and the predicted pressure from the calibration function. Based on these error estimates a precision estimate of ± 3.0 KPa was made for these transducers.

The pressure transducer calibration procedure was implemented each time the die was dismantled or the transducers were removed from the die. The calibration curves obtained each time were highly reproducible and were independent of the operating temperature for the temperature range $165\text{-}200^{\circ}\text{C}$.

Table 3.3

-Calibration Functions for the Pressure Transducers at
165°C

Transducer	Range [KPa]	Linear Fit Equation		S_e [KPa]
		P - [Pa]	V - [Volts]	
1	0-345	P = 6.5162E3 + 3.6018E6 V		1.0
	345-1100	P = 3.1956E4 + 3.4135E6 V		2.5
2	0-345	P = 5.8531E3 + 3.5311E6 V		0.72
	345-2200	P = 2.3116E4 + 3.4206E6 V		2.1
3	0-510	P = 9.7697E3 + 5.9913E6 V		1.8
	510-2300	P = 3.3640E4 + 5.5933E6 V		5.35

3.3 POLYMER FEED SYSTEM

In this section the apparatus used to feed the polymer to the slit die is discussed. A schematic drawing of the feed system is shown in Figure 14. The major components of the feed equipment consist of a one inch extruder and a gear pump to regulate the volumetric flowrate of the polymer melt.

A Killion 2.54 cm. extruder (serial number K100/184) with a 1 horsepower drive system provided polymer melt to the system. The melt then passed through a static mixer (Kenic ISG 1" dia.) to reduce temperature variations in the melt introduced in the extruder. Constant volumetric flowrates were provided by a Zenith gear pump (HPB 5556, 0.16 cc/rev.). The gear pump was driven by a 3/4 horsepower motor which provided a speed range of 11-113 rpm. An additional speed range was available by installing a gear reducer (Renold Limited 21.4:1 ratio) between the drive motor and the gear pump. The apparent shear rate range available in the slit die was 1.07-11.03 s⁻¹ without the gear reducer and 0.05-0.55 s⁻¹ with the gear reducer.

Flow connections for the feed system consisted of 3/4" steel pipe. Heating for the pipe and the static mixer was provided by glass insulated heating tape. The feed system was then insulated by several layers of glass fiber insulating tape (American Scientific Products). Installation of a bleed valve was necessary because the volumetric output of the extruder was greater than the throughput of the die with the gear reducer in place. The back pressure upstream of the gear pump could be controlled by the valve position of the bleed valve. The back pressure was adjusted

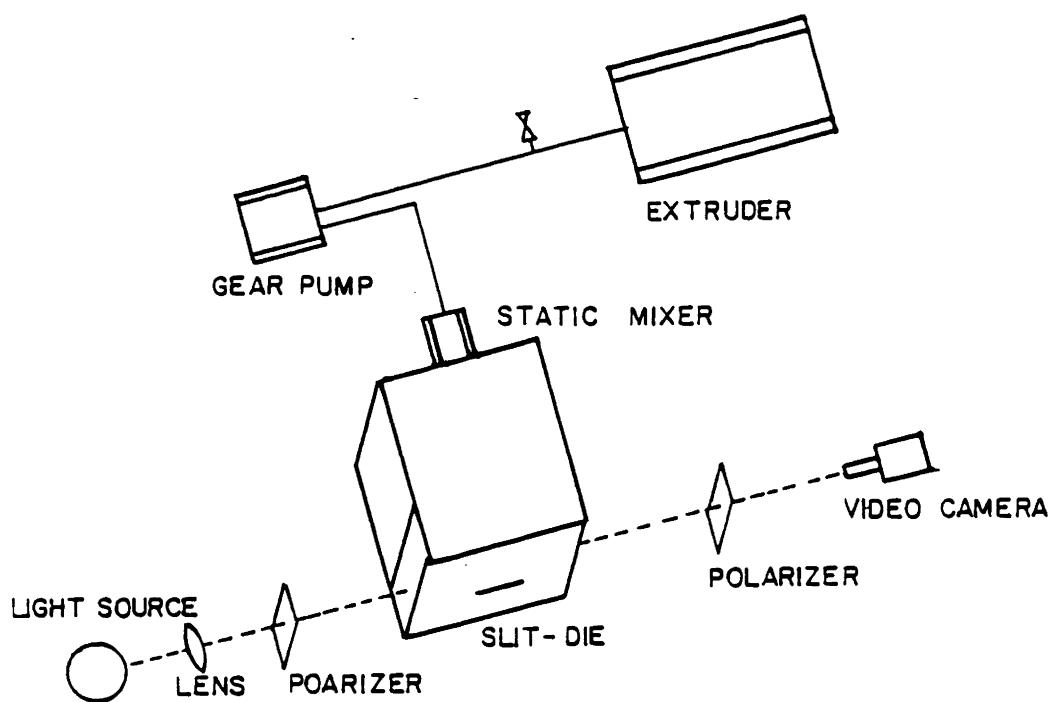


Figure 14. Schematic Diagram of the Polymer Feed System

by slowly closing the valve position until the pressure traces obtained from the slit die were stable. This valve also served as a by-pass for cleaning out the extruder.

In order to calculate the shear rate in the die, it was necessary to accurately measure the volumetric flowrate of polymer delivered to the die. Two techniques were readily available for this purpose. The volumetric flow rate, Q , can be calculated from the mass flow rate of the polymer and the melt density of the material. The accuracy of this technique was limited by the difficulty in obtaining the density of the polymer melts at elevated temperatures. Also, measurement of the mass flowrate was complicated by the presence of an oil bath at the exit of the die. The mass of oil absorbed in or onto the surface of the polymer melt could not be accurately determined. The technique used in the present study for measuring the volumetric flowrate consisted of multiplying the gear pump rpm (obtained with a tachometer) and the volumetric rating of the gear pump in cc/revolution. A comparison between the two techniques was completed for Styron 678 melt at 165°C. Flow rates agreed to within 4% for the two techniques over the apparent shear rate range 1-11 s^{-1} . This technique is also readily adapted for automated measurement.

3.4 TEMPERATURE CONTROL

In this section additional information is presented concerning the control and measurement of the temperature profile of the polymer melt throughout the slit die and the polymer feed system. The temperature control was of importance due to the large variation in fluid viscosity

for small changes in the melt temperature. The temperature of the melt was controlled by heating the metal surfaces to a given set point temperature. The die feed system was divided into three heating zones and the the slit die into four zones for improved temperature control. No interaction between the various control zones was observed. Due to the low volumetric flow rate through the feed system, thermal equilibrium was established in each of the heated regions.

The temperature sensors used in the temperature control system were iron-constantan industrial thermocouple probes (Omega Standard Extruder Probes). Compression fittings were used to attach the thermocouples to the processing equipment. Thermocouples in the polymer feed system were inserted directly into the melt. The thermocouple used to control the gear pump temperature was located in the melt exiting the gear pump. An additional temperature probe was inserted into the gear pump face to insure adequate temperature of the gear pump unit. Starting the gear pump before the unit reached operating temperature could result in damage to the drive pin in the unit.

A stable and uniform melt temperature in the slit die was critical to obtain accurate measurement of the pressure profiles. For this reason, the slit die was divided into four independently controlled temperature zones as described in section 3.2.1. The set points of the controllers were determined by a trial and error procedure. A thermocouple probe was inserted into the die to monitor the actual melt temperature. The set points of the proportional controllers could be set to maintain stable melt temperatures as measured by the thermocouple within the melt. In this manner the temperature settings could be controlled to within $\pm 0.5^\circ$

C throughout the die. This procedure was repeated at the beginning of each experiment. The procedure could also be used while the melt was flowing through the die to check for viscous heating in the melt or variations in the melt temperature caused by control problems in the polymer feed section.

The presence of viscous heating in the polymer melt could severely complicate the temperature control procedure. Viscous heating may be significant in polymer melts due to the materials high viscosity and low thermal conductivity. Tests were conducted to estimate the effects of viscous heating for the polymer melts investigated. Direct experimental measurements were conducted by using a thermocouple probe as described in the previous section. Since the temperature variation along the length of the die was $\pm 0.5^{\circ}\text{C}$, no direct evidence of viscous heating was reported. A check on the experimental measurement was conducted by using a simple analytical expression for the temperature rise of a fluid in an adiabatic channel. Thermal properties of Styron 678 at 165°C were used to estimate the maximum temperature rise in a slit channel. For the shear rate ranges investigated, $0.05 \leq \dot{\gamma} \leq 15 \text{ s}^{-1}$, no significant viscous heating effects were observed.

3.4.1 VISCOSITY MEASUREMENTS

In this section the basic equations used to calculate the viscosity of the material using the slit die viscometer is discussed. The slit die geometry approximates ideal flow between infinite parallel plates provided the aspect ratio is large enough so the effects due to the side walls are negligible. As discussed in section 2.1.6, aspect ratios

greater than 10:1 were sufficient to obtain constant values of η . Under these conditions the derivation of the equations used to calculate η in a slit die can be approximated by flow between two infinitely wide parallel plates [125].

The wall shear stress for pressure driven flow through a slit can be obtained from the equation of motion [137]

$$\sigma_w = \frac{\Delta P}{L} \frac{H}{2} \quad (3.1)$$

The pressure gradient along the flow direction, dP / dx , was determined by measuring the pressure at the wall by means of a flush mounted transducers located at least two locations along the flow direction. The shear rate at the wall was obtained by using the Weissenberg-Rabinowitsch equation which accounts for the non-parabolic velocity profile in the fluid [99,137].

$$\dot{\gamma}_w = \frac{2Q}{wh^2} \left(2 + \frac{d \ln Q}{d \ln \sigma} \right) \quad (3.2)$$

The slope, $d \ln Q / d \ln \sigma$, was obtained from a series of measurements at varying flow rates. The fluid viscosity, η , may now be determined by

$$\eta = \tau_w / \dot{\gamma}_w \quad (3.3)$$

The value of the exit pressure, P_x , was obtained by extrapolating the pressures as a function of axial distance to the exit of the die. The residual stress or pressure above atmospheric pressure is called the exit pressure. A series of three pressure transducers were employed for this

purpose. The choice of the extrapolation technique may influence the magnitude of P_x .

3.5 FLOW BIREFRINGENCE MEASUREMENT

In this section the flow birefringence apparatus and experimental procedures used to obtain the isochromatic and isoclinic fringe patterns are discussed. The objective of the flow birefringence technique was the calculation of the stress components σ_{12} and $\sigma_{11} - \sigma_{22}$ by using the linear stress optic rule. The stress field obtained was based on an arbitrary set of coordinate axes and was used to evaluate the assumptions of the exit pressure theory at the die exit for pressure driven flow in a slit die. The discussion of the experimental procedure will first introduce the experimental quantities of interest and then specific methods used to obtain these quantities are discussed.

As discussed in section 2.4, a light beam passing through a birefringent material will be decomposed into two components. Upon exiting the material the light beam recombines and interference patterns can result due to the phase difference of the two component waves. The relative retardation can be written in terms of the birefringence of the material.

$$\bar{N} = \Delta n L / \lambda \quad (3.4)$$

where $\bar{N}$ is the number of wavelengths of relative retardation of one wave component with respect to the other. If monochromatic light is employed, light and dark bands or fringes which represent different values of $\bar{N}$

throughout the sample volume were present. These patterns are referred to as the isochromatic patterns. The magnitude of the fringe orders could be determined from a point in the sample in which the value of the stresses were known.

A second extinction pattern was identified in the flow field by the use of a white light source. The fringe produced using a white light source is known as the principle optic angle χ which is also called the isoclinic angle. These patterns were produced when the principal optic angle are parallel to the orientation of the polarizer and analyzer. The techniques used to obtain the isochromatic and isoclinic patterns will now be described.

3.5.1 DETERMINATION OF ISOCHROMATIC FRINGE PATTERNS

In this investigation the value of $\bar{N}$ was determined using a full field technique by identifying the location of the dark bands throughout the sample. Light and dark field patterns were used to obtain values of the fringe order $\bar{N} = 0, 1/2, 1, 3/2, \dots$. Optical arrangement for each of these patterns is discussed in the next section. The fringe order for points not lying on a dark fringe were calculated by interpolation.

The experimental apparatus used to measure and record the birefringence patterns is shown in Figure 15. An optical bench was assembled on to which the optic components were attached. The monochromatic light source consisted of a helium-neon laser (Spectra-Physics Model 155) having a wave length of 632.8 nm. The laser beam was passed through a 10x microscope objective lens to expand the diameter of the impinged light beam. The light beam was then collimated perpendicular to the sample

orientation to obtain a parallel light source. Two sets of polarizers were used to obtain the fringe order $\bar{N}$ and the isoclinic angle, χ . Plane polarized light was obtained by passing the light beam through a set of two polarizing filters (Oriel Linear Film Polarizer). A second set of polarizers were used to obtain circularly polarized light. The circular polarizers used consisted of a $1/4$ wave plate laminated, with a 45° optic orientation onto a plane polarizer (Oriel Circular Film Polarizer). The resulting optic information was recorded on a VHS format video recorder for further analysis.

Two types of fringe orders can be obtained by the choice and orientation of the polarizers used in the optical measurement. A light field pattern was obtained by using the orientation of circular polarizers pictured in Figure 15. The light field pattern was characterized by destructive interference which occurs when $\bar{N} = 0, 1/2, 3/2, \dots$ cycles. The relative orientation of the circular polarizers was not important for the measurement of the fringe orders. Circularly polarized light was obtained by orienting the polarizer and analyzer 90° with respect to each other. The quarter wave plates were oriented with the principal optic axis 45° relative to the polarization lanes of the polarizers, and with the fast principal axis of the quarter wave plates parallel [128]. A dark field pattern was obtained by using the same optical components as Figure 15, but with the quarter wave plates removed. The resulting interference patterns represented fringe orders of $\bar{N} = 0, 1, 2, 3, \dots$ cycles.

The complete isochromatic map of the fringe orders was obtained by using both circularly and plane polarized light. The magnitude of the fringe orders was determined by a knowledge of the stress field in fully

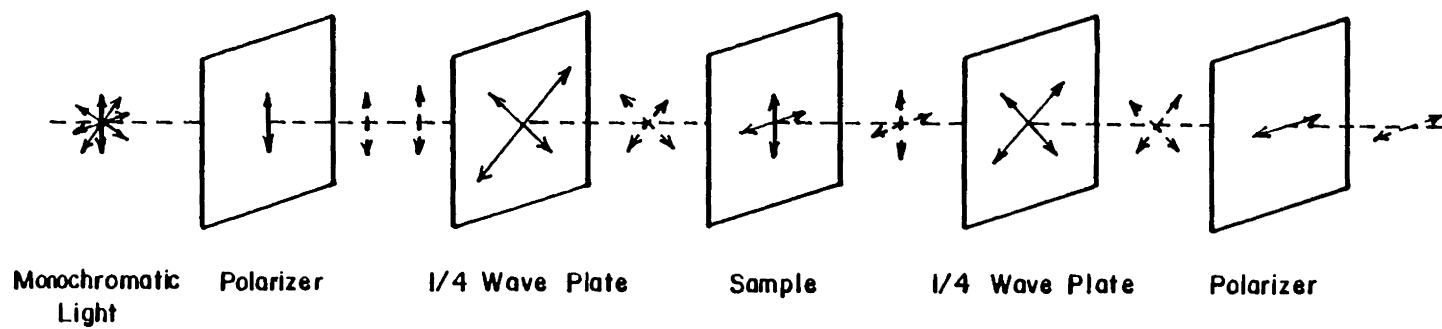


Figure 15. Optical Bench Used in Flow Birefringence Experiments

developed flow and from transient flow experiments. The fringe orders varied from $\bar{N} = 0$ along the centerline where the stresses were zero and increased in value towards the walls where the stresses were highest. The value of the fringes could then be calculated by counting the number of fringes from the centerline to the wall. Areas of complicated flow fields were analyzed by recording birefringence patterns from transient flow experiments. The development of the fringe patterns could be traced from an initial stress free state.

3.5.2 DETERMINATION OF THE ISOCLINIC ANGLES.

The magnitude of the isoclinic angle was determined by the relative orientation between the set of crossed plane polarizers and the laboratory coordinate system used to describe the system. An extinction pattern in the sample resulted when the principal optic direction corresponded with the orientation of the polarizer and analyzer. The principal optic angle along the dark band was then known from the orientation of the polarizers. The isoclinic patterns were distinguished from the isochromatic patterns by using white light source. The isochromatic patterns appeared as a series of fringes of varying color while the isoclinic angle appeared as a dark band. The white light source was an incandescent lamp.

The polarizing optics were mounted in a rotator device so different orientations of the optics were obtained. A scale was provided with a vernier graduated in 1° increments. The 0° reference angle was chosen so that the optic axis of the polarizers was parallel with the flow direction of the slit die rheometer. The extinction angles were obtained throughout the sample by rotating the polarizer and analyzer through 90° . The stress

quantities calculated by equations (2.23 and 2.24) yielded the same sign convention as the numerical results. Calibration procedure for the measurement of the isoclinic angles is described by Pike [128].

3.5.3 STRESS OPTIC COEFFICIENT

The calculation of the stresses from the birefringence requires knowledge of the stress optic coefficient, C , of the material for each operating temperature. The value of C could be determined by solving the equation (2.23) for the stress optic coefficient

$$C = \bar{N} \lambda \sin(2\chi) / 2 W \sigma_{xy} \quad (3.5)$$

The stress optic coefficient could be calculated in undisturbed pressure gradient flow given the value of the shear stress at the wall and N and χ from birefringence measurements. An alternate method was chosen due to the difficulty of measuring the isoclinic angles along the wall. The value of C was calculated near the slit centerline. The value of χ approached 45° near the centerline so the value of $\sin(2\chi)$ approaches one. The shear stress varies linearly from zero along the centerline to the wall value. The value of σ_{xy} near the centerline could now be used to calculate C for a series of shear rates. The error in C by assuming $\chi \rightarrow 45^\circ$ was less than 2 percent when χ differs less than 5° from 45° .

The method above was used to calculate the stress optic coefficient for Styron 678U at 165 and 190°C. The value of the stress optic coefficient $C = 4.54 \times 10^9 \text{ M}^2/\text{N}$ was calculated at 165°C. The results agree to within 6 % of the value $4.8 \times 10^9 \text{ M}^2/\text{N}$ obtained by Wales [125]. The cal-

culations also showed that the value of C was independent of temperature over the range 165-190°C. This has also been observed by Wales [125] and others [133]. The sign of the stress optic coefficient was negative for polystyrene melt, but the absolute value was used to maintain the chosen sign convention.

3.6 OPERATING PROCEDURE

This section will outline general operating procedure used to collect data from the slit die rheometer. The operation of the slit die apparatus is discussed and then measurement of the optical data used in the flow birefringence technique is presented.

3.6.1 SLIT DIE OPERATING PROCEDURE

1. Turn on the main power to the experimental equipment and slowly bring the equipment up to the desired operating temperature. The set point temperatures in the die are increased 40°C/hour to prevent breakage of the glass windows in the die due to unequal thermal expansion. The equipment should remain at the operating temperature for one hour to insure thermal equilibrium. To prevent blockage of solid polymer in the entry of the extruder, the set point of the first zone of the extruder is set 30°C lower than the desired outlet temperature. Also, a water cooling line should be attached to the throat of the extruder.
2. After the equilibration period, the pressure measurement system is initialized. The chart recorder pens are first zeroed. The zero po-

sition and span of the pressure signals are then adjusted using potentiometers found in the pressure signal amplifier.

3. The temperature profile inside the die is checked by inserting a thermocouple probe in the melt. Adjust the temperature set points until a steady temperature profile is obtained.
4. Before starting the extruder, check all temperature sensors for proper operating temperature. Severe damage can result by starting the drive system with solid polymer still in the system.
5. Start the extruder and gear pump drive system. The gear pump speed is set by the variable speed drive. Adjust the back pressure on the gear pump by closing the bleed valve until steady pressure traces are obtained on the strip chart recorder.
6. Polymer should be pumped through the die for 10-20 minutes to remove any degraded material from the system.
7. The data required from the equipment includes volumetric flowrates, chart recorder span, and pressure traces off the recorder. The volumetric flowrate is calculated by measuring the rpm of the gear pump and multiplying by the pump capacity in cc/revolution. The experimental procedure should then be repeated at different motor speeds to obtain results at varying shear rates.

8. After completion of the experimental trials all equipment can be shut off except the controllers to the slit die. Reduce the temperature in the die 20°C / hour to prevent damage to the glass windows.

3.7 FLOW BIREFRINGENCE PROCEDURE

The experimental procedure involved with the measurement of flow birefringence patterns consists of an alignment procedure and collection of the isochromatic and isoclinic patterns. The alignment procedure is necessary to insure the light is well collimated and enters the sample perpendicular to the 1-2 plane of the slit. The light pathway should correspond to the third principal stress direction at each point in the sample volume.

The alignment procedure for the optical apparatus used the property of reflected light in which the angle of the incident beam is equal to the angle of the reflected beam. The laser was oriented so the reflected component of the beam off the glass window of the die was reflected directly back into the laser source. The light rays were collimated using a plano-convex field lens. The lens was adjusted until the laser source was located at the focal point of the field lens. The resulting beam was collimated parallel to the third principal stress direction. The polarizers were positioned perpendicular to the imposed light source. The images of the resulting fringe patterns were recorded on a VHS video camera and video tape recorder. A bi-convex magnification lens was placed between the analyzer and the camera and provided 40x magnification in conjunction with the zoom lens of the video camera.

The following procedure outlines the steps used in the actual collection of the birefringence patterns. It is assumed that the optical alignment procedure has been completed and the slit die feed system has equilibrated at operating temperature.

1. Perform the steps outlined in section 3.6 to check the temperature profiles, initialize the pressure measurement system and start the polymer feed system.
2. The light field pattern is obtained by using the set of circular polarizers with the laser light source. The dark fringes correspond to $\bar{N} = 0, 1/2, 3/2, \dots$ orders. Patterns are recorded with the video system.
3. The dark field pattern is obtained by replacing the circular polarizers in step 2 with a set of plane polarizers. The resulting fringe patterns correspond to $\bar{N} = 0, 1, 2, \dots$ orders.
4. The isoclinic patterns are obtained with a white light source and plane polarizers. The laser light source is replaced by an incandescent light. Recheck the alignment of the light source. Record the isoclinic patterns at 5° angle increments from -45° to 45° orientation.
5. Repeat steps 2 through 4 to obtain birefringence data at other shear rates.

6. The flow birefringence data stored on the video tape system is recorded off the television screen by placing a sheet of mylar film on the screen. The fringe patterns are then traced onto the plastic sheet using color markers. The data is recorded as a function of position by placing the mylar sheet over graph paper. The values of $\bar{N}$ and χ are interpolated at mesh points located on the graph paper.

4.0 CHAPTER FOUR - NUMERICAL METHODS.

One of the objectives of the current investigation was the development of a numerical scheme capable of quantitatively modeling the steady shear behavior of viscoelastic fluids in simple flow situations where comparison to analytical solutions is possible. The numerical model would then be used to simulate more complicated geometries in which analytical solutions become intractable. The majority of numerical studies in the literature examining the exit pressure and die swell rely on constitutive equations with constant viscosity and unrealistic normal stress behavior. In this study emphasis was placed on choosing models which accurately predict the steady shear properties exhibited by polymeric materials such as shear rate dependent viscosity and additional stresses associated with fluid elasticity. The finite element program MAX2D represents an attempt to use simple differential constitutive equations with shear rate dependent material functions to realistically model the viscometric properties of viscoelastic fluids in shear dominated flows. The results obtained from the finite element simulation could then be compared to experimental results obtained using the flow birefringence technique.

In this chapter an overview is presented covering the numerical techniques used in the investigation of the stress field in the exit region of a slit die. In the first section the general finite element formulation used in the solution of non-Newtonian fluid mechanics problems is presented. For the present study a mixed penalty method formulation will be employed. A brief outline in the use of penalty method techniques in fluid mechanics is then presented in section 4.2. The re-

maining part of this chapter will be used to discuss the capabilities and use of the finite element program, entitled MAX2D. The program MAX2D is a mixed penalty finite element formulation which solves the boundary value problem composed of the equations of motion and a differential constitutive equation for a two dimensional Cartesian coordinate system. The general requirements and capabilities of the program are outlined in the section covering data input. Details of the computational algorithms are then discussed. Finally, the presentation of results from the program are outlined in the discussion of the postprocessor.

4.1 GENERAL FINITE ELEMENT FORMULATION FOR FLUID FLOW

A general flow problem for fluid flow consists of solving the field equations [137].

$$\text{Equation of linear momentum:} \quad \frac{\partial(\rho \vec{v})}{\partial t} = - [\rho \vec{v} \vec{v}] - \Pi + \rho \vec{g} \quad (4.1)$$

$$\text{Equation of mass (continuity):} \quad \frac{\partial \rho}{\partial t} = - (\rho \vec{v}) \quad (4.2)$$

$$\text{Constitutive equation:} \quad h(\tau, \dot{\gamma}, \vec{v}, \dots) \quad (4.3)$$

where h is a differential or integral operator acting on the extra stress tensor, τ , the rate of deformation tensor $\dot{\gamma}$, and the velocity vector $\vec{v}$.

The total stress tensor in the equation of motion is defined as the sum of the hydrostatic pressure P and the extra stress terms, τ_{ij} :

$$\underline{\underline{\Pi}} = \underline{\underline{\tau}} + \underline{\underline{\delta}} P \quad (4.4)$$

The above system of equations must be solved simultaneously to determine the primary unknown variables ($\tau, \mathbf{y}, P$). The resulting finite element system is usually called a mixed formulation as the components of the extra stress tensor τ are primary unknown variables. For the case of isothermal creeping flow of an incompressible viscoelastic fluid, the equations reduce to the following using Einstein's tensor notation:

$$-\tau_{ij,j} - P_{,i} = 0 \quad (4.5)$$

$$v_{i,i} = 0 \quad (4.6)$$

$$\tau_{ij} + \lambda \frac{\delta \tau_{ij}}{\delta t} = \eta \dot{\gamma}_{ij} \quad (4.7)$$

The equations are multiplied by a test function w_i and integrated over the element domain to develop the variational form. The weak form of the equations of motion are written:

$$\int_{\Omega} w_j (\tau_{ik,k}^e + P_{,i}^e) d\Omega \quad (4.8)$$

The order of the differential terms in the equation of motion are reduced by using the divergence theorem. Integration by parts of equation (4.8) yields

$$\int_{\Omega} (w_{k,j} \tau_{ij}^e + w_{k,i} P^e) d\Omega^e = \int_{\Gamma} w_k(t_i) d\Gamma^e \quad (4.9)$$

The term on the right side of equation (4.9) are the element traction vectors and are defined in terms of the stresses by

$$t_i = (\tau_{ij} n_j + P n_i) \quad (4.10)$$

The Galerkin finite element formulation is completed by substituting the approximation functions ψ_i for the test functions and for the variables using the form

$$u = \sum u_j \psi_j \quad (4.11)$$

The resulting matrix system has the general form:

$$[K(u)] [u] = [F] \quad (4.12)$$

The left hand side matrix $[K(u)]$, or element stiffness matrix, is usually a non-linear function of the unknown velocities and stresses.

For the resulting mixed formulation requires specification of the order of the interpolation polynomials for each of the unknown variables. It has been shown [138] that the shape functions for the extra stress and the velocity should be of the same order. Also, the shape functions for the pressure should be one degree less than the stress and velocity unknowns in order to have a non-singular stiffness matrix.

4.2 PENALTY METHOD FORMULATION

An alternative formulation to the mixed finite element formulation presented in the previous section seeks to find a solution to the field equations (4.1-4.3) by using a "penalty method". In this method the original system of equations is modified by imposing a constraint on the system. A Lagrange multiplier method is usually used for this purpose. The penalty method usually reduces the problems of conditional extremum

to problems without constraints by using a penalty parameter on the infringement of constraints [42].

The penalty method formulation is useful in the solution of incompressible fluid flow problems by using the continuity equation as a constraint on the system. Examination of the Lagrange multiplier, λ , shows it is the negative of the pressure. Comparison of the terms in the modified functional of the Stokes equation show that the pressure may be given by

$$P_n = - \lambda_n (u_{i,i}) \quad (4.13)$$

The removal of the pressure from the equations of motion is a result of the choice of the Lagrange multiplier. The pressure definition given in equation (4.13) is not the basis of the penalty method, but a consequence of the original Lagrange multiplier [42].

The replacement of the pressure in the equations of motion leads to several computational advantages over the mixed formulation. The penalty method eliminates one of the equations and the pressure as an unknown variable from the system. The reduced system contains fewer degrees of freedom and corresponding reduction in the size of the stiffness matrix. The formulation also eliminates the presence of zero diagonal terms found in the mixed formulation. Another advantage of this method is the elimination of higher order approximation functions for the velocity and stress terms since the pressure has been eliminated.

The existence and uniqueness of the penalty method techniques for the solution of the Navier-Stokes equations has been shown by Reddy [43].

The solutions of the penalty method converge to the solution of the mixed problem as the penalty parameter approaches infinity. The existence of solutions for finite element approximations, however, has not yet been fully established. Oden and coworkers have provided a starting point in proving the existence of solutions [43].

One practical problem associated with the implementation of penalty method is the treatment of the penalty terms associated with the penalty parameter γ . The global stiffness matrix has the general form

$$[K] = [K_1] + \gamma [K_2] \quad (4.14)$$

The penalty formulation becomes exact as the penalty term goes to infinity. During implementation the use of large penalty terms causes the penalty terms to dominate the stiffness matrix. This problem can be avoided by using reduced integration techniques in the integrals encountered in $[K_2]$. Malkus and Hughes [89] have summarized reduced integration techniques for nonlinear incompressible fluid mechanics.

The magnitude of the penalty parameter must be chosen to satisfy the incompressible constraint imposed on the system. Large values of γ do not give accurate numerical results due to round off or machine truncation errors. For slow flow in which the viscous terms dominate, the ratio of λ / η is chosen as a guide [146]. Reddy suggests the value of γ be chosen such that

$$\gamma_e = \eta \times 10^6 \quad (4.15)$$

The upper limit of γ_e will depend on machine accuracy. The finite element code used in the numerical investigation is based on a mixed penalty method formulation of the field equations presented in section 4.1. In the next section the characteristics of the finite element code named MAX2D are presented.

4.3 GENERAL CHARACTERISTICS OF MAX2D

MAX2D is a general purpose in-core finite element program for the solution of two dimensional flow problems for a series of differential constitutive equations. The general application of the program is the solution of boundary value problems for constitutive equations having the general form of the upper convected Maxwell model. The present computer code is based on a model finite element program FEM2D developed by Reddy [146] for the solution of the Stokes equation. The current code contains additional subroutines which enable the inclusion of shear rate dependent viscosity functions, choice of constitutive equations, and the presence of free surface boundary conditions.

The basic structure of MAX2D is shown in Figure 16. The program architecture was designed by using a main driver program with individual subroutines controlling specific calculations in the construction and solution of the final numerical system. The modular construction simplified the incorporation of modifications into the original code. The subroutines and their purpose are now described before a description of the program units is discussed.

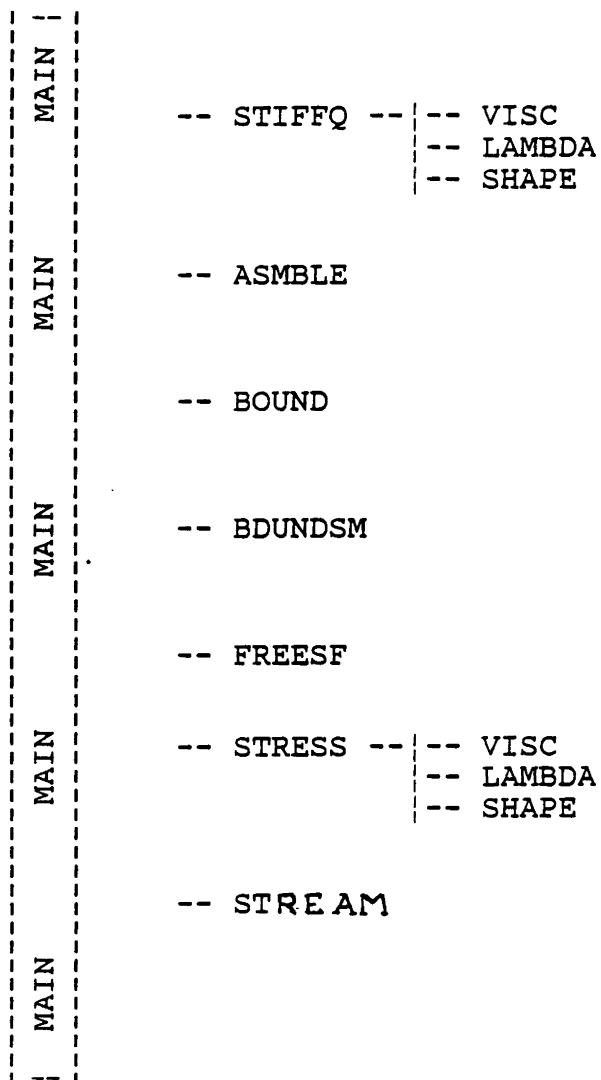


Figure 16. Flow Diagram for the Finite Element Code MAX2D

1. MESH - A mesh generator for rectangular domains. Calculates connectivity matrix, element numbering, and nodal coordinates.
2. STIFFQ - Calculation of the element stiffness matrix. An upper-convected Maxwell model is used as the general constitutive equation. The White-Metzner, generalized Newtonian fluid, and Newtonian models are available by using different options for the viscometric material parameters. Penalty terms are calculated using reduced integration techniques.
3. VISC - Generates the value of the viscosity from a rate dependent viscosity function. Newtonian, power-law, and Carreau models are currently available. Any user defined rate dependent viscosity function may be added.
4. LAMBDA - This returns the value of the fluid time constant λ , found in the differential Maxwell constitutive equation. A shear rate dependent function for λ is used in the White-Metzner constitutive equation. The functional dependence is input by the user. If the value of $\lambda = 0$ is specified, the constitutive equation reduces to the generalized Newtonian fluid.
5. SHAPE - The subroutine evaluates the interpolation functions ψ_i and its derivatives with respect to the global coordinates. Four node rectangular isoparametric elements are currently available.

6. ASMBLE - Places the elements of the element stiffness matrix into their proper location in the global stiffness matrix. The assembly procedure occurs after each element is calculated to reduce storage requirements. A banded storage technique is used due to the sparse system of the global stiffness matrix. The full band width must be used as an asymmetric element stiffness matrix is calculated in STIFFQ.
7. BOUND - Implementation of the specified degrees of freedom into the assembled global stiffness matrix. The specified non-zero values of the secondary degrees of freedom are also entered into the assembled system.
8. SOLVE - Returns the solution of the system of non-symmetric linear banded equations back to the main program. A gaussian elimination technique is used. The presence of a zero on the diagonal of the global stiffness matrix will halt execution.
9. FREESF - This subroutine is available for the calculation of an update in the mesh shape for free surface problems. A fluid streamline representing the boundary is constructed from the current velocity solution vector. The iteration procedure on the free surface is terminated upon completion of a user defined tolerance.
10. STRESS - Solution gradients and secondary quantities are calculated from the primary degrees of freedom at the center of each element.

The pressure is calculated from the solution gradient and the value of the penalty parameter. The pressure, viscosity, shear rate, and extension rate is output for each element.

11. STREAM - This subroutine returns the value of the stream function ψ for each nodal point in the mesh. The fluid stream lines can be constructed using the stream function solutions and a contour plotting routine.

4.4 INPUT DATA USERS GUIDE

This section is intended as a supplemental guide in the use of the finite element code MAX2D. The major groups of data cards are described with a brief explanation of the information required to specify a particular problem. A list of variables and the format required for the data input deck is included in the program listing found in Appendix C. A sample input file is also included in the program documentation.

The information required in the data input deck can be grouped into four major functions. The first group of data cards contains the control card information. These cards are used to specify the major aspects of the desired simulation such as the choice of the constitutive equation, limits on the non-linear iterations, or the presence of free surface boundary conditions. The second group of data cards supply the mesh discretization scheme. This includes the nodal coordinates and the Boolean connectivity matrix. The program contains a simple mesh generating subroutine, but this is limited to rectangular domains. Complex meshes can be created using other mesh generating programs or the mesh

may be entered by hand. The next input section contains the physical constants describing the rheological behavior of the fluid. Constants, such as the zero shear viscosity, fluid density, and the fluid time constants are entered directly. If the fluid contains a shear rate dependent property whose general form is not included in the program, the function must be added by inclusion into the original source code. The last section of the data input phase consists of the implementation of the boundary conditions over the problem domain. Additional comments on the imposition of boundary conditions are presented in the next section.

Two types of boundary conditions must be specified to obtain a non-singular matrix system which can be solved for the unknown variables. For the field equations used in fluid mechanics, the essential boundary conditions consist of the x and y components of the velocity. The natural boundary conditions are specified through a traction vector given by

$$t_x = [\tau_{11} \cdot n_x + \tau_{12} \cdot n_y + P \cdot n_x] \quad (4.16)$$

$$t_y = [\tau_{12} \cdot n_x + \tau_{22} \cdot n_y + P \cdot n_y] \quad (4.17)$$

The values, n_x and n_y , represent the unit normal vector for the given node on the mesh boundary.

The specification of the velocity components along the boundary consists of no-slip velocity condition or a known flow distribution across a domain boundary. Due to the shear rate dependent viscosity behavior of many polymeric fluids, analytical solutions to the input velocities are often not available. The imposition of the velocity field therefore may require an additional numerical procedure in which the input velocity

field is calculated for a simplified model or geometry. This procedure is required for simulations using the Carreau model viscosity function. A second penalty finite element formulation, GNF2D, is used to obtain the numerical solution for the velocity profile using the Stokes equations with a shear rate dependent viscosity function.

For the die swell problem, the velocity profile is calculated at specific values of the wall shear stress, τ_w . A sample mesh was constructed for pressure driven flow in a slit. The boundary conditions for the program GNF2D consist of no-slip velocity conditions along the walls and a known pressure drop, ΔP , calculated from the desired value of τ_w . The calculated pressure drop is then imposed by specifying the traction vector on the upstream surface. The velocity field obtained from the Stokes equation is then used as the input velocity field for the program MAX2D. The major factor in using the program GNF2D rather than MAX2D for the input velocity profiles is the reduced storage requirements and simplicity of GNF2D. The Stokes equation contains two degrees of freedom per node, while the mixed formulation in MAX2D requires simultaneous solution of both the velocity components and the three extra stress components.

The imposition of a known boundary condition is accomplished by specifying the number of the degree of freedom associated with the specific variable and global node. The present finite element formulation contains five degrees of freedom per global node. The order of the variables for each node are the x-velocity, y-velocity, extra stress τ_{11} , τ_{12} , and τ_{22} . The number of the degrees of freedom for the essential

boundary conditions, DOF, can be determined using the following expression.

$$\text{DOF} = 5 N - I \quad (4.18)$$

where N is the global node number in the finite element mesh and I depends on which variable is to be specified. The value I varies from I = 4 for the x-velocity to I = 0 for specification of the extra stress τ_{22} . The degree of freedom for the imposition of a non-zero secondary degree of freedom uses the same expression as equation (4.18) where I = 4 for the traction vector t_x and I = 3 for the traction vector t_y .

The codes GNF2D and MAX2D use available in-core storage for the implementation of the FORTRAN source code. The core storage limits on the computer system available therefore set the upper limit on the size of the matrix system which can be solved. An IBM system 370 computer was used which has a limit of 4.5 Mbytes core storage. The upper limit for the numerical simulation was therefore limited to less than 1600 degrees of freedom.

4.5 PROCESSOR UNIT

Shear rate dependent viscosity functions, inertial terms in the equation of motion, or differential Maxwell type constitutive equations are all non-linear equations. The solution of the finite element formulation must therefore be solved using an iterative procedure. The choice of the initial guess for the values of the non-linear terms and the it-

eration scheme employed will affect both the rate and the limits of convergence.

Non-linear terms in the global stiffness matrix are due to the inertial terms of the equation of motion and the upper convected derivative terms in the Maxwell constitutive equation. Due to the low Reynolds numbers encountered for polymer melt flow, the discussion will concentrate on the treatment of the non-linear stress terms. The upper convected derivative is written as

$$\tau(1) = D\tau - [(\nabla v)^t \tau + \tau (\nabla v)] \quad (4.19)$$

The non-linear terms consist of the dot product of the gradient of the velocity field (∇v) and the stress tensor. Since the velocities and stresses are not known beforehand, the solution of the system requires an iterative procedure. For the first iteration, the velocity field is set equal to zero and the resulting system is solved for the velocity and stresses. For the subsequent iterations, the non-linear terms are evaluated from the velocity solution of the previous iteration. This procedure is continued until a user defined tolerance is met.

The linearization procedure described above is a successive substitution or Picard iterative technique. The initial solution with a zero initial velocity field corresponds to the solution of the Stokes equation for a Newtonian fluid. To improve convergence, a weighted function is used in the update of the velocity used in the non-linear terms. The following function is used in the present numerical investigation

$$v_i = \beta v_i + (1-\beta) v_i \quad (4.20)$$

The velocity for degree of freedom i is calculated from the two previous iterations, n and $n-1$. An acceleration parameter β is chosen to increase the rate of convergence. An optimal value of $\beta = 0.8$ was chosen for the current formulation.

The choice of the functional dependence for the rheological constants η and λ can also introduce non-linear terms into the finite element formulation. The program MAX2D includes option for rate dependent rheological functions by calculating the material functions as a function of the magnitude of the rate of deformation tensor. For the first iteration, the velocity field is set to zero. The program uses the zero shear rate viscosity for η during this iteration. The shear rate $\dot{\gamma}$ is then calculated from the previous velocity solution for subsequent iterations.

The non-linear iteration procedure is continued until the difference between two consecutive solutions is less than some assigned error parameter. The convergence criteria is written as

$$\frac{[\sum (u_i - u_i)^2]^{0.5}}{[\sum (u_i)^2]^{0.5}} \leq \text{Tolerance} \quad (4.21)$$

The error parameter is normalized based on the latest value of the solution vector u_i . A tolerance parameter of 10 percent was chosen for the current investigation.

The presence of a free surface boundary requires an additional iterative procedure to calculate the shape of the free surface. An initial

guess for the free surface is specified which may be written as $F_i(z)$. The problem is then solved by prescribing zero-stress boundary conditions along the free surface. A solution based on the current boundary is then calculated using the non-linear iteration procedure discussed in the previous section. An additional constraint exists on the free surface boundary which requires the boundary to be a stream surface. In general the initial trial surface $F_1(z)$ is not a stream surface, and fluid crosses the boundary. A new surface $F_2(z)$ is computed using the velocity solutions along the boundary $F_1(z)$. The update surface $F_i(z)$ is constructed by using the relation

$$x_{j+1} = x_j + \int u / v \, dy \quad (4.22)$$

The value of the x_j coordinate of the free surface is calculated by using the definition of a fluid stream line to up-date the coordinates of the mesh. The program starts the up-date procedure at an extreme end node (supposed fixed) and computes the successive x coordinates using equation (4.22). The integral in equation is calculated using Simpson's rule. After the new mesh coordinates have been calculated, the solution cycle is repeated. The free surface iteration is halted once the difference in two successive meshes is less than a tolerance parameter. Typically, four free surface iterations are sufficient to calculate the free surface for the die swell calculation.

The subroutine FREESF performs the calculation for the successive surfaces $F_i(y)$ for a two dimensional Cartesian coordinate system. As shown in equation (4.22), the up-date in the mesh surface changes the

x-coordinate of the nodes along the free surface boundary. The orientation of the mesh therefore must be specified so the free surface changes perpendicular to the x-axis.

4.5.1 POST PROCESSOR

Contour plots of the output variables are useful in the graphic presentation of large amounts of data obtained from numerical simulations. The values of the stream functions calculated at the nodal coordinates can be used to construct the stream line contour plot. For incompressible flow, the stream function is the non-zero component of a vector potential which satisfies the equation of mass conservation identically [BSL]. By definition the stream function is written

$$u_1 = - \partial \Psi / \partial x_2 \quad (4.23)$$

$$u_2 = \partial \Psi / \partial x_1 \quad (4.24)$$

The change of the stream function $\delta \Psi$ can be written as an exact differential. The following integral expression results

$$\Delta \Psi = \oint (n_x \cdot v + n_y \cdot u) ds \quad (4.25)$$

The change in the stream function $\Delta \Psi$ can be calculated for each element once an integration path is specified. The change $\Delta \Psi$ is calculated along an element boundary using the element coordinates and the velocities for each element. The integral is evaluated numerically using Simpson's rule. The calculation of the stream function throughout the mesh uses equation

(4.25), starting with an initial value of Ψ specified along a mesh boundary. The value of Ψ is then generated along successive element boundaries. The values of Ψ can then be used to generate the streamline contour plot.

The graphic presentation of data was provided by using the SURFACE II graphics system developed by the Kansas Geological Survey [93]. A contour plot is produced from the coordinates of the nodal mesh points and the "height" of the third variable z . A contour line is created which passes through all points on a surface that have the same value.

The basis of operation in SURFACE II is a rectangular grid of values which is a numerical representation of the surface to be displayed [93]. The grid contains a matrix whose components are the height z and the geographic coordinates x and y . Values of z are calculated for unequally spaced data points by a interpolation procedure. The resulting contour lines are drawn on a Versatec plotter.

The printout for the finite element routine MAX2D consists of three sections. The first section prints a data echo of all the data input file. The data is grouped into control card information, material constants, and specified boundary conditions. The results of the primary degrees of freedom are then printed for each node, including the nodal coordinate and the primary normal stress difference. The final section of the output contains the results from the post processor. The hydrostatic pressure, velocity gradients, and the stream function are reported for each element. The quantities are evaluated at the geometric center of each element.

5.0 CHAPTER FIVE - RESULTS AND DISCUSSION

In this chapter the results of the experimental and numerical investigation exploring the nature of the flow and stress fields at the exit region of a slit die are discussed. The results are used to evaluate the validity of the assumptions in the use of the exit pressure to measure fluid elasticity. Also analytical expressions are evaluated from flow birefringence data from which it is attempted to explain the origin of the exit pressure. In the first section attempts are discussed to predict N_1 from exit pressure measurements for three polymer melt systems. In section 5.4, the results of the flow birefringence studies for flow at the exit of a slit die are examined. The stress field distribution obtained from flow birefringence is quantitatively analyzed using analytical expressions obtained from a macroscopic momentum balance over the system. To supplement the experimental investigation, the stress field distribution was predicted numerically using a finite element technique to model the exit region of a slit die. Numerical results are presented from the finite element code MAX2D. Finally, in section 5.9, a comparison between numerical and experimental stress field distributions is discussed.

5.1 THE USE OF P_x TO PREDICT N_1

In this section the results of the experimental investigation using the exit pressure to predict the primary normal stress difference N_1 are discussed. The extrapolation techniques used to calculate P_x are discussed and their effect on the predicted value of N_1 are presented.

Equation (2.14) developed in section 2.1 was used to obtain N_1 values from the slit die rheometer. The predicted values are then compared with values obtained with a cone-and-plate rheometer. The accuracy of the pressure measurement system of the slit die is verified by first presenting the results using the slit die to measure fluid viscosity.

5.1.1 VISCOMETRIC BEHAVIOR

In this section the viscometric behavior of the polymer melts obtained from the slit die rheometer is compared to results from the cone-and-plate rheometer. A Rheometrics Mechanical Spectrometer (RMS) was used as the basis of comparison for the viscosity and normal stress behavior. The viscosity obtained from the RMS is presented with the viscosity calculated using the pressure gradients and shear rates determined in the slit die rheometer. The results are shown in Figures 17-20 for the polymer melts investigated.

The viscosity behavior for Styron 678 shown in Figure 17 and 18 shows good agreement between the RMS and the slit die rheometer. The consistency of the viscosity values for the two measurement systems provided an indication that the slit die pressure measurement system is functioning accurately. The viscosity data obtained from the cone-and-plate rheometer was limited to shear rates less than $1-3 \text{ s}^{-1}$ due to edge fracture and material loss of the polymer in the test fixture. Comparison of viscosity data at shear rates greater than 10 s^{-1} was obtained from capillary rheometer measurements. Good agreement between slit die and capillary rheometer data was also found for the higher shear rate range.

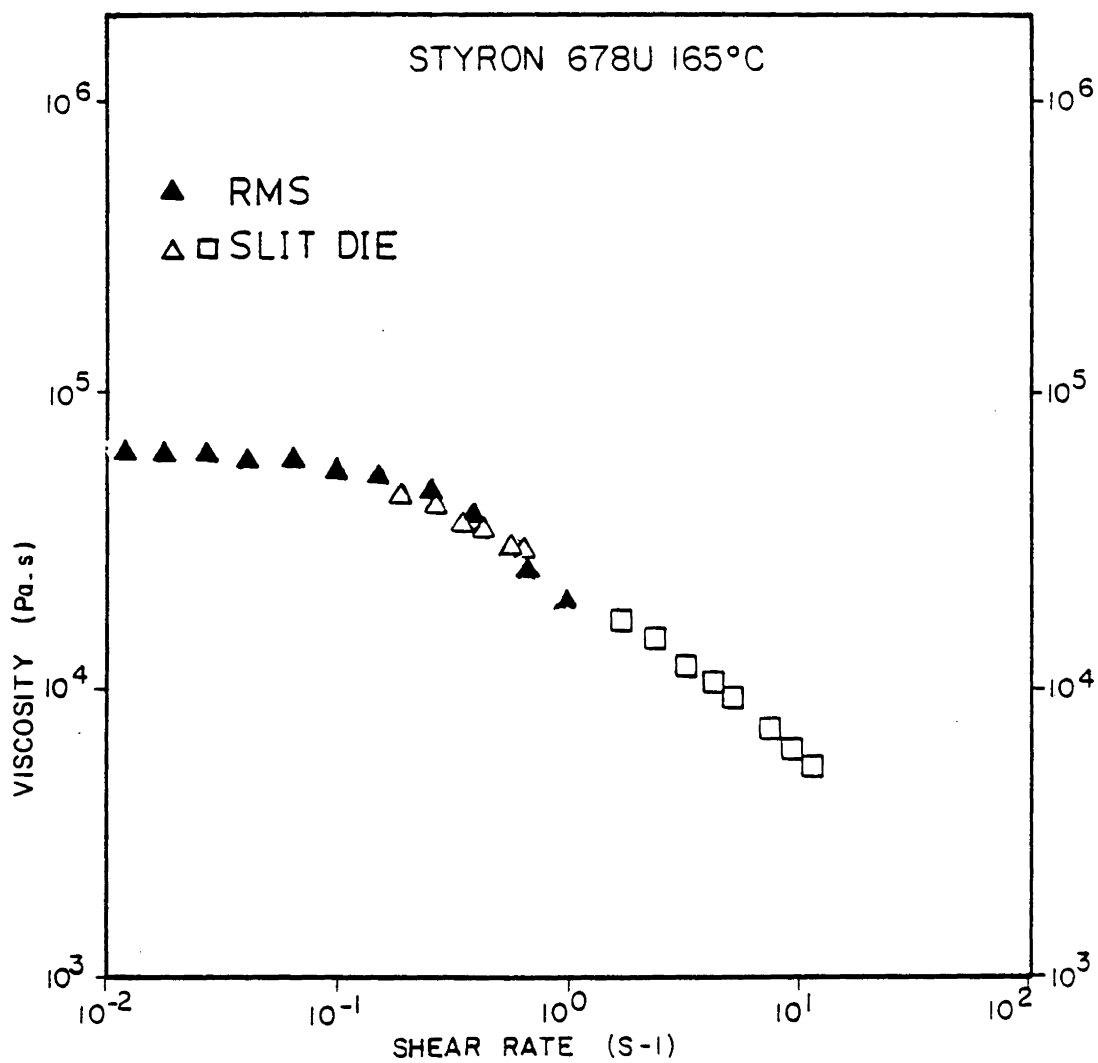


Figure 17. Melt Viscosity of Styron 678 at 165°C

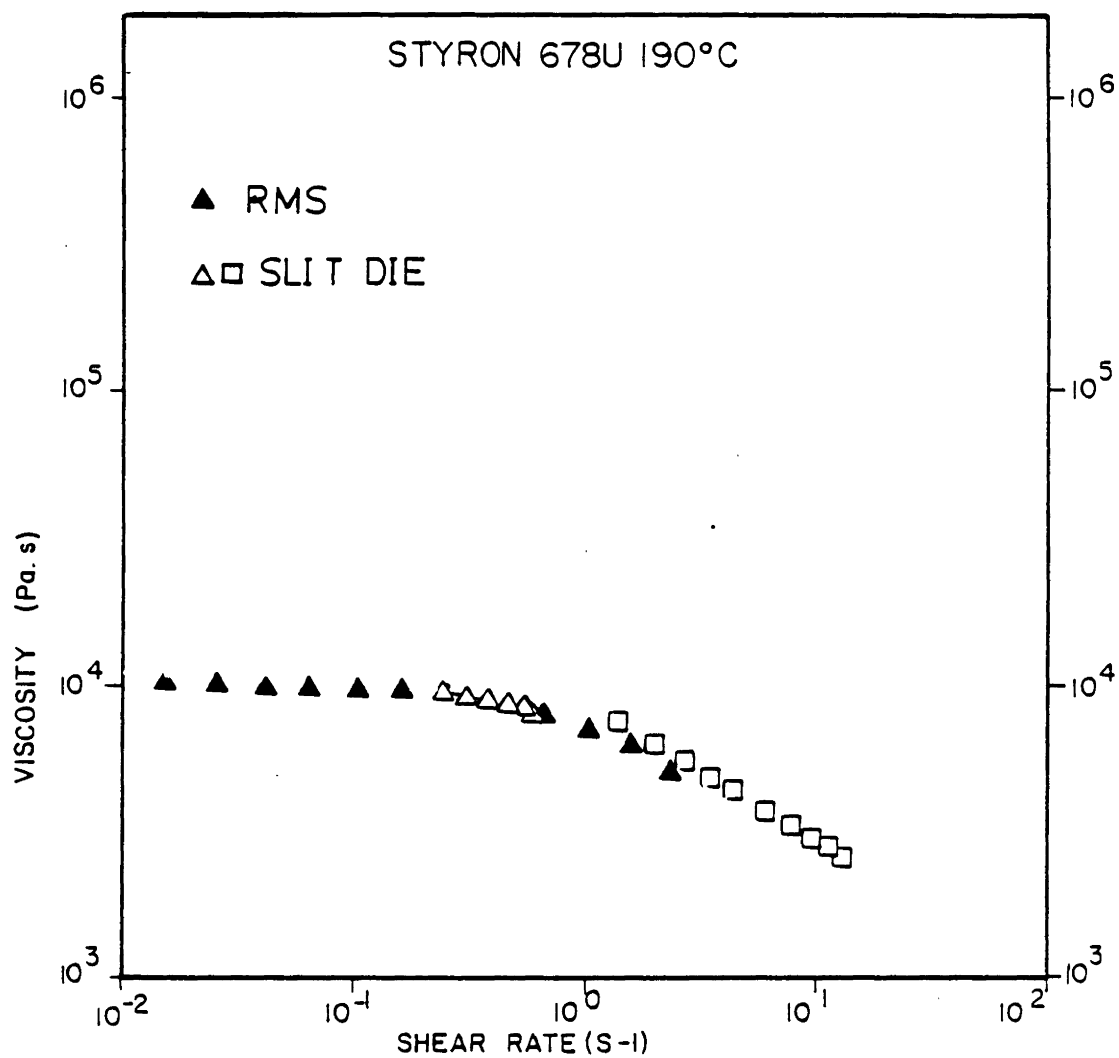
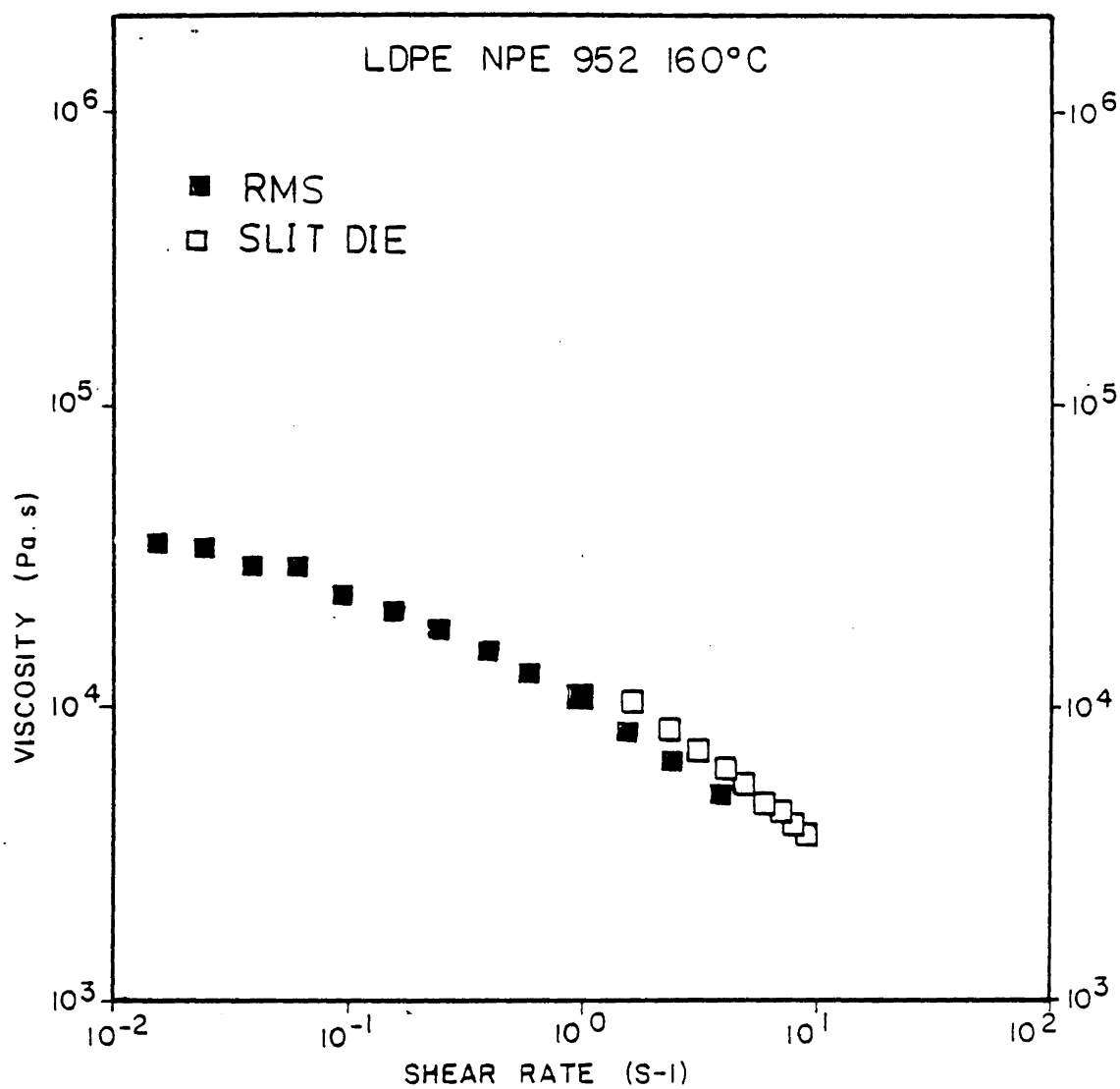


Figure 18. Melt Viscosity of Styron 678 at 190°C



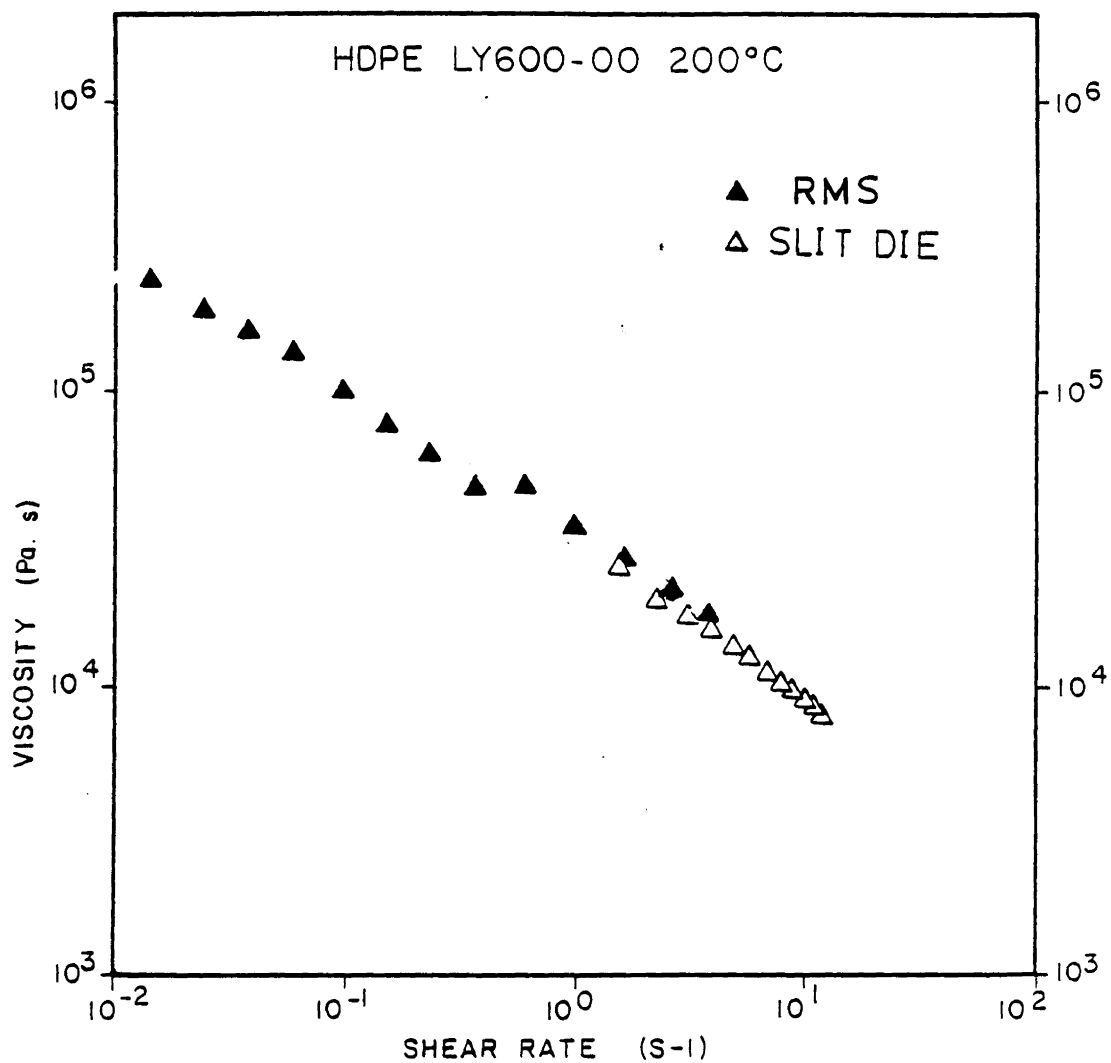


Figure 20. Melt Viscosity of HDPE LY600-00 at 200°C

The precision estimates of the viscosity measurements were obtained by repeated measurement for a given fluid and operating temperature. The repeatability of η was found to be on the order of 10-15 % for the RMS. Multiple measurements using the slit die yielded values of η within $\pm$ 5-10%. The higher precision of η in the slit die may be due to the better temperature control in the slit die rheometer. The slit die temperature variation was $\pm 0.5^{\circ}\text{C}$, while the RMS unit varied in temperature by $\pm 1-2^{\circ}\text{C}$.

The viscosity curve presented in Figure 17 also was used to obtain the material constants for the numerical investigation discussed in a later section. The zero shear rate viscosity, η_0 , was obtained by extrapolating the values of η at the lowest shear rate available.

The good agreement between the viscosity values obtained from the cone-and-plate rheometer and the slit die suggests that the pressure values measured by the flush mounted pressure transducers along the die could be used to obtain accurate values of the wall shear stress. Once the reliability of the pressure measurement system was established, the pressures obtained from the slit die rheometer were used to obtain measurements of the exit pressure for the shear rate range $0.1 \leq \dot{\gamma} \leq 18$. In the next section the pressure profiles and the extrapolation techniques used to evaluate P_x are discussed.

5.1.2 PRESSURE PROFILES - METHOD OF EXTRAPOLATION

As discussed in the introduction, the exit pressure represents the residual stress above atmospheric pressure measured at the exit of a slit or capillary rheometer. The magnitude of the exit pressure, however, can

not be measured directly. P_x must be obtained by extrapolating the pressure profile to the exit of the die. In this section will be discussed the use of various extrapolation techniques and their effect on the magnitude of P_x . The effect and causes of a non-linear pressure gradient will also be discussed.

One of the assumptions used in the derivation in which N_1 is obtained from the exit pressure was a fully developed shear flow at the exit. Han [4] assumed fully developed flow to be as a constant pressure gradient and constancy of an elastic property with increasing die length. In early studies in which the exit pressure was measured for polymer melts, a linear extrapolation technique was used to determine P_x [1-15]. As discussed in the literature review, several authors have reported curvature in the pressure gradient [18,20,21]. Die design, temperature, and pressure dependent viscosity can each introduce non-linearity into the pressure profiles. These effects are discussed elsewhere [18,20]. If, for example, the viscosity is a function of the pressure inside the die, $\eta = \eta(p)$, then the velocity field will vary both in the vertical and axial direction for a slit die, $v_z = v_z(y,z)$. Under conditions in which a non-linear pressure gradient is observed due to the errors detailed by Lodge et al. [20], a fully developed flow field does not exist. This violates one of the basic assumptions used in the exit pressure theory to predict N_1 values evaluated from equation (2.13). In the next section the effect of a non-linear pressure field will be investigated to examine if the exit theory can be used even if one of the primary assumptions concerning fully developed flow has been violated. The question then

exists how best to extrapolate the pressure profile to determine a unique value of the exit pressure.

Two different extrapolation techniques were used in the present study. Linear and quadratic functions having the following form were employed.

$$P = a + b L \quad (5.1)$$

$$P = a + b L + c L^2 \quad (5.2)$$

where the intercept a represents the exit pressure P_x , b is the pressure gradient $\Delta P / \Delta L$, and L is the axial distance along the die. Non-linear pressure profiles were modeled using a quadratic function in equation (5.2). A comparison between a linear and quadratic fit of the experimental pressure measurements are shown in Figures 21-24 for Styron 678 at 190°C and HDPE LY600-00 at 200°C.

The effect of using a linear or a quadratic function to represent the pressure profiles on the extrapolated value of P_x is immediately evident by comparing the intercept for polystyrene in Figures 21 and 22 and for high density polyethylene in Figures 23 and 24. The values of the exit pressure for polystyrene vary from approximately zero for the linear fit to large increasing positive values for the quadratic fit. For high density polyethylene negative values of P_x are calculated for a linear fit versus positive values for the quadratic fit. The choice of the extrapolation technique is therefore critical to P_x especially when $\Delta P / \Delta L$ is not constant.

The level of the hydrostatic pressure inside the die can cause curvature in the fully developed flow region through a pressure dependent

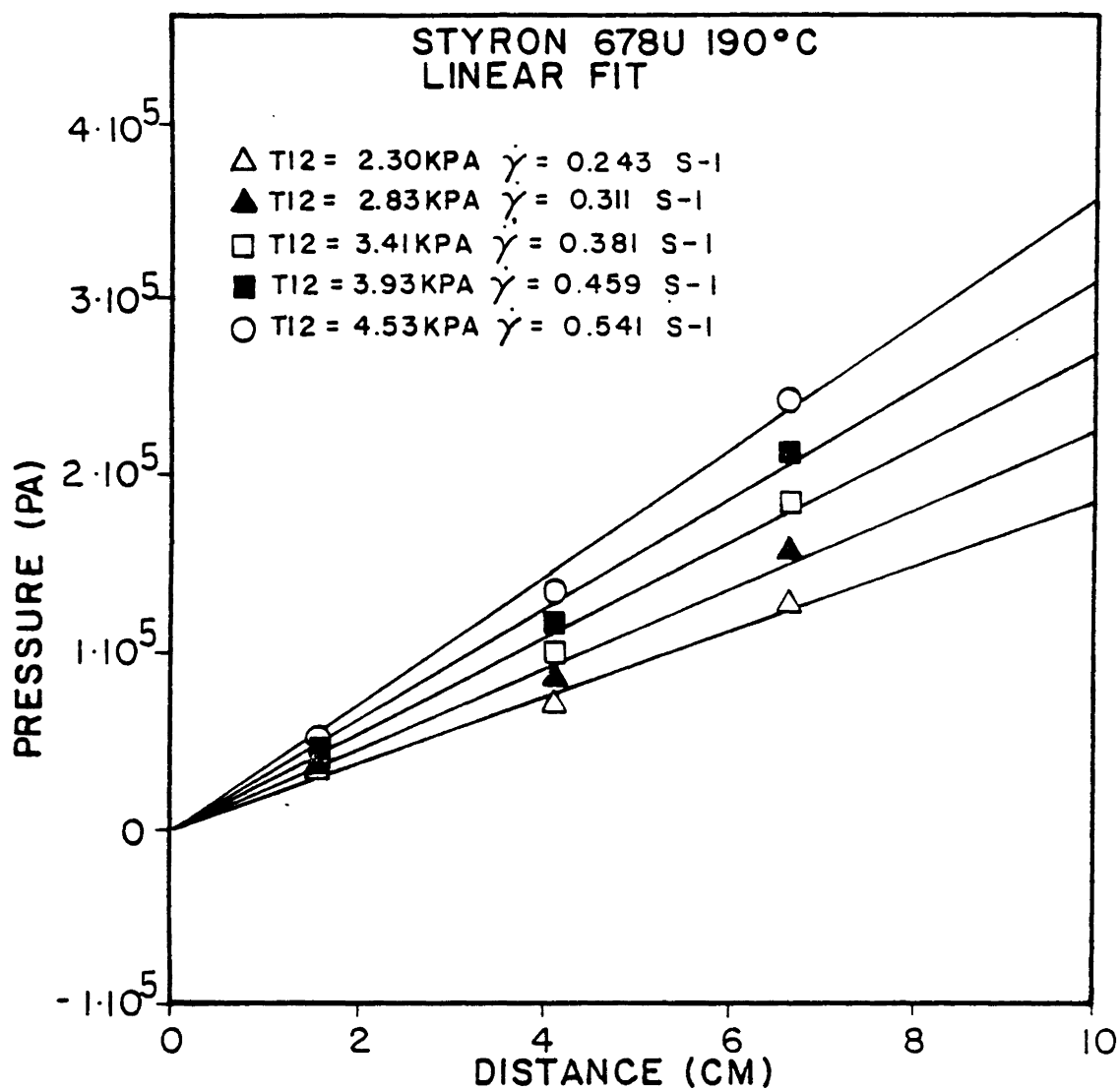


Figure 21. Pressure Profiles of Styron 678 at 190°C - Linear Extrapolation

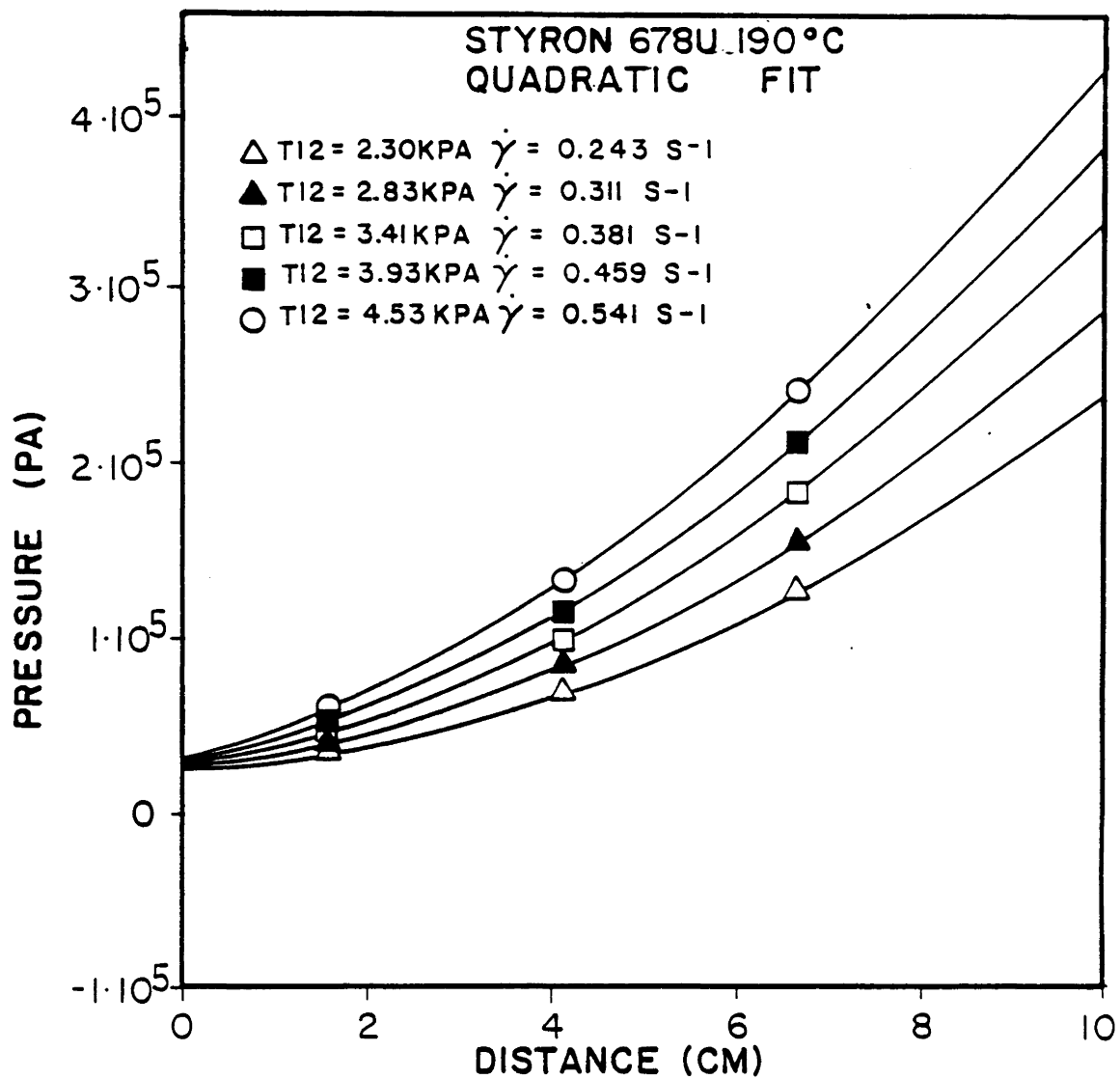


Figure 22. Pressure Profiles of Styron 678 at 190°C: Quadratic function used to model the pressure gradient.

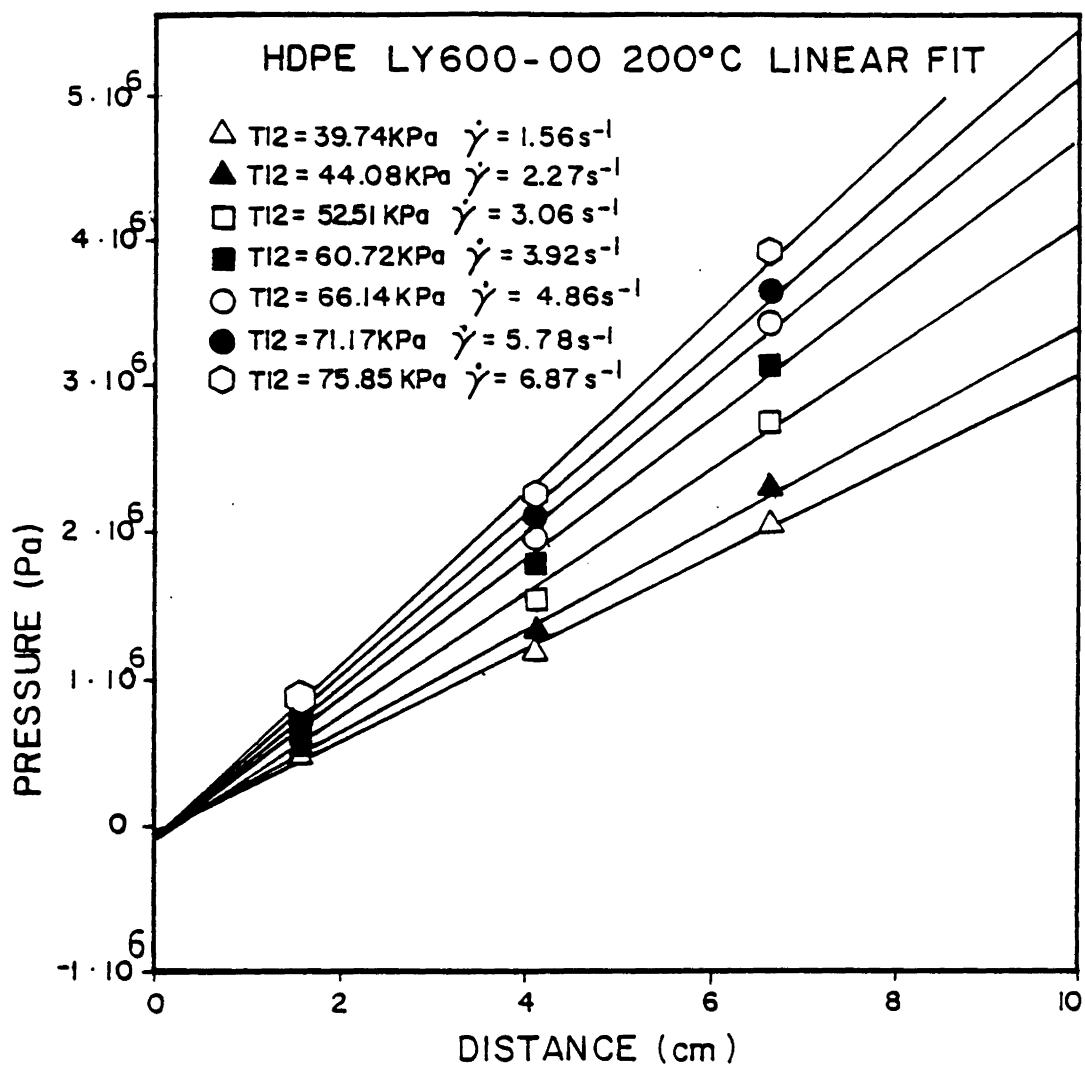


Figure 23. Pressure Profiles for HDPE LY600-00 at 200 °C: Least squares fit of the pressure gradient.

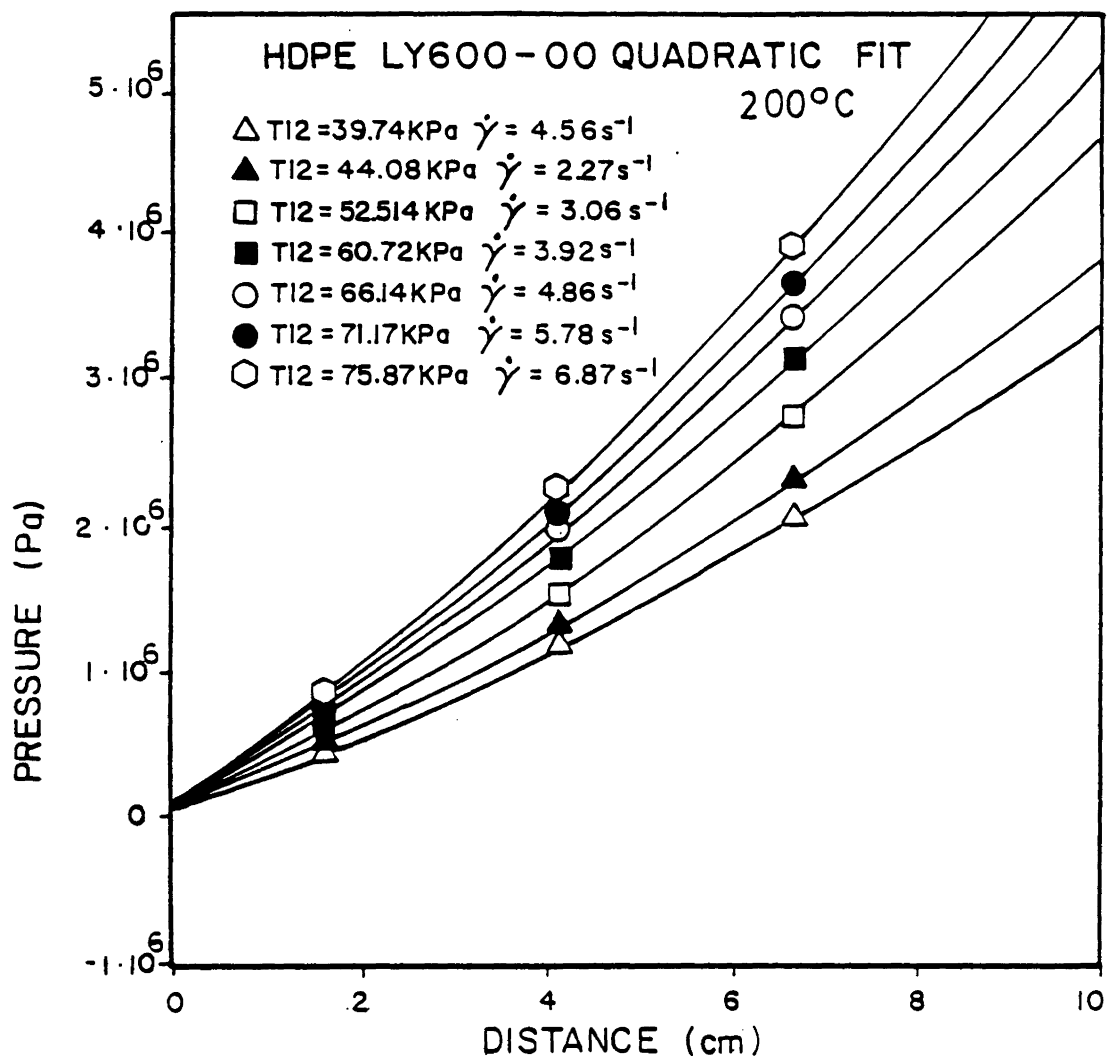


Figure 24. Pressure Profiles for HDPE LY600-00 at 200°C: Quadratic function used to model the pressure gradient.

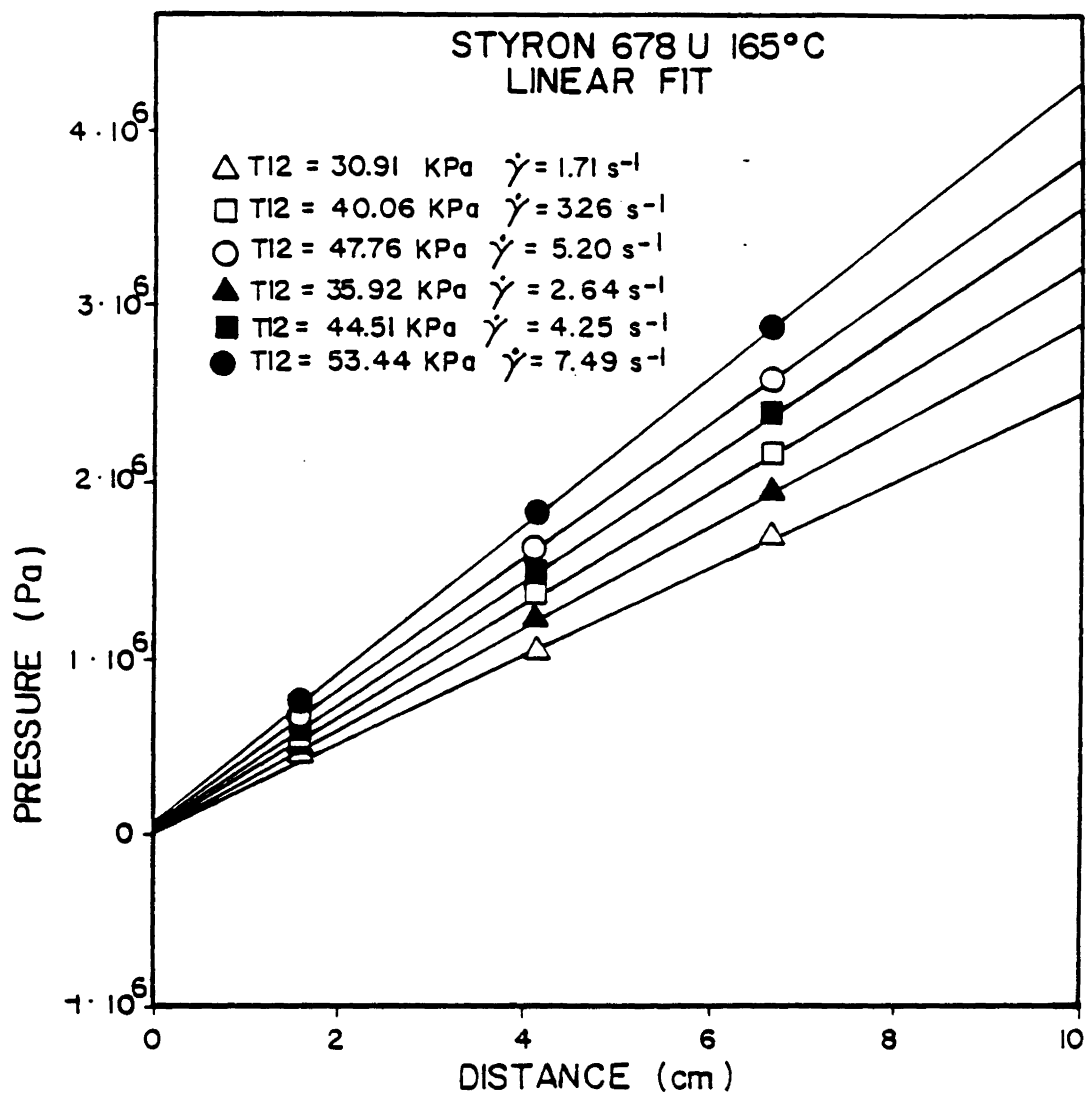


Figure 25. Pressure Profiles for Styron 678 at 165°C: Least squares fit of the pressure profiles.

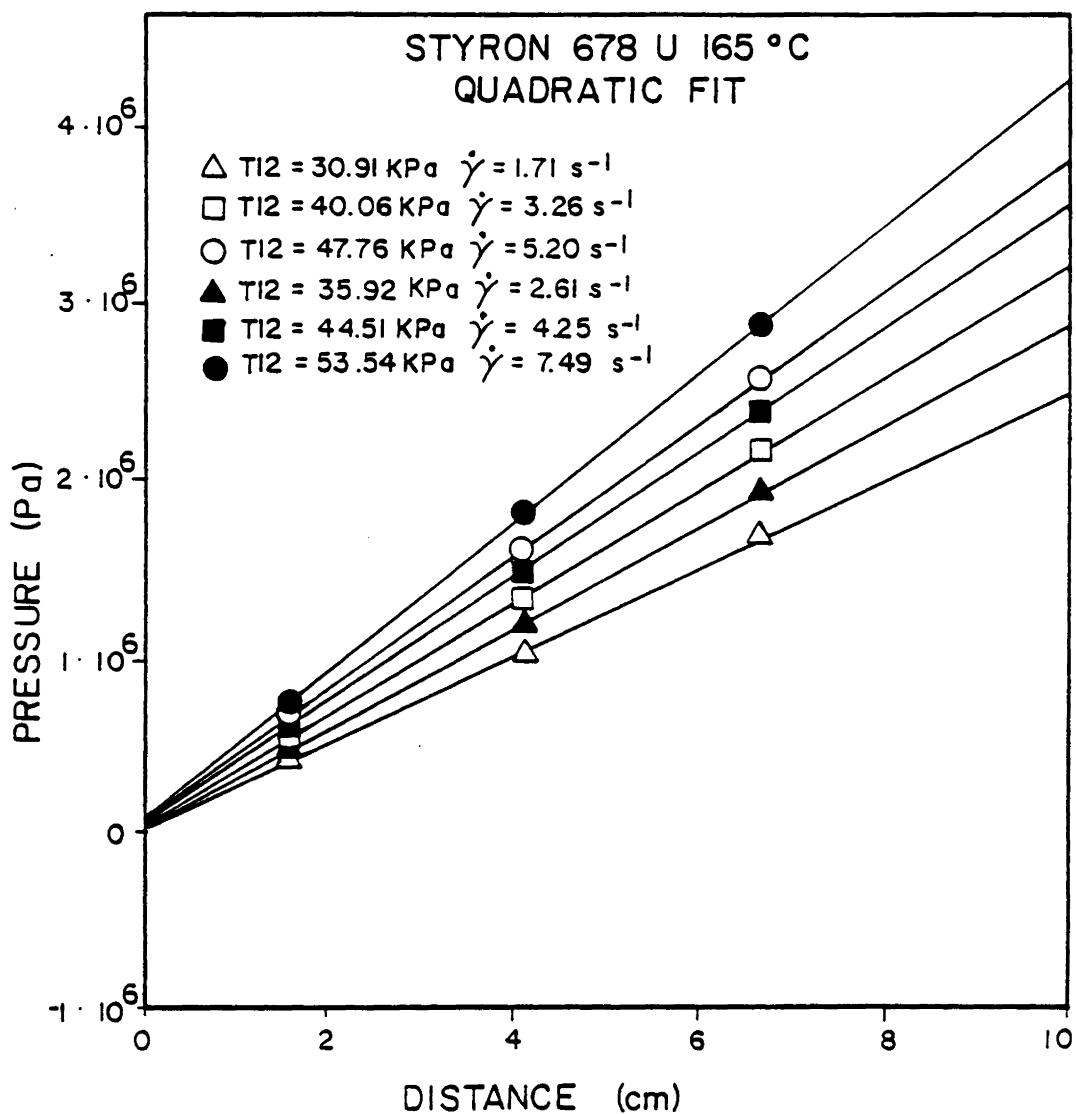


Figure 26. Pressure Profiles for Styron 678 at 165 °C: Quadratic function used to model the pressure profiles.

viscosity or by changing the dimensions of the slit. The value of the pressure coefficient of viscosity, α , can be evaluated approximately using the parameters b and c obtained from the parabolic pressure profiles[18].

$$\alpha = 2 c / b^2 \quad (5.3)$$

The value of α calculated for HDPE LY600-00 at $\dot{\gamma} = 6.9 \text{ s}^{-1}$ was 4.0 E-7 Pa^{-1} . Independent determination of α is possible from the increase of viscosity η with increasing hydrostatic pressure at a constant shear rate. From literature values, the pressure coefficient $\alpha = 1\text{E-9 Pa}^{-1}$ [18]. The values of α calculated in the present investigation were significantly larger than those reported by others [18]. The increase in viscosity was not sufficient to give an explanation for the magnitude of the curvature observed in the pressure profiles.

The significance of the curvature in the pressure profiles was assessed by examining the correlation coefficient for a least squares straight line used to obtain the slope and intercept values for the pressure measurements in the slit die. The correlation coefficients for the pressure profiles shown in Figures 21-26 all were greater than 0.99. Statistically, at first sight, this suggests that the curvature is not significant in the calculation of the pressure gradient $\Delta P/dx$ or the intercept P_x from a least squares fit of the data, but in terms of calculating P_x significant variations are seen.

The effect of hydrostatic pressure on the curvature was investigated by comparing the level of curvature between the pressure profiles of

Styron 678 at 165°C and 190°C. In Figures 25 and 26 are shown the pressure profiles of Styron 678 at 165°C for linear and quadratic profiles. The hydrostatic pressure in the die was a factor of ten greater at 165°C than 190°C. The average correlation coefficient from the least squares fit of the data at 165°C was 1.000. The least squares fit of the data at 165°C is better, as measured by the correlation coefficient, than the fit of the data at 190°C even though the hydrostatic pressure level was an order of magnitude higher. If the pressure dependent viscosity effects had been significant, the linear fit of the data at 165°C in Figure 25 should yield a less accurate fit of the pressure data. The less precise fit of the data at 190°C by the least squares line may be due to error in the pressure transducers relative to the pressure level in the die. For Styron 678 at 190°C, the non-linear behavior may be due to the effect of the accuracy of the pressure measurement system.

5.2 EXIT PRESSURE VALUES FOR POLYMER MELTS

In this section direct experimental values of the exit pressure are presented for the three polymer melt systems investigated. As discussed in the previous section the pressure extrapolation technique can influence the magnitude of the exit pressure. Both linear and quadratic fits of the pressure gradient will therefore be presented.

The dependence of exit pressure on the wall shear stress is shown in Figures 27-32. The various symbols in Figures 27-32 represent data obtained from different experiments. Two important differences are noted by comparing P_x obtained with a linear and parabolic extrapolation scheme. First, the absolute magnitude of the exit pressure differs an order of

magnitude depending on the extrapolation technique. This effect is evident by comparing the exit pressure for the polyethylene samples shown in Figures 29-32. The linear fit yields negative values of P_x while a parabolic fit yields positive values of the exit pressure. The second point which must be examined is the slope of the line passing through the results of P_x versus $\dot{\omega}w$. The prediction of N_1 using equation (2.14) required the calculation of the slope, $d P_x / d \dot{\omega}w$, from experimental data. Once P_x is obtained from a series of shear stress measurements, equation (2.14) was used to calculate N_1 from pressure gradient measurements in a slit die rheometer.

Large variations in the magnitude of P_x in Figures 27-32 were shown to exist depending on whether a linear extrapolation technique or a quadratic fit of the pressure profiles was used. The question arises in measuring P_x , then, which extrapolation technique yields the "correct" value of the extrapolated exit pressure. If significant curvature is present, a statistical argument can be made that a quadratic function should be used to model the pressure profile. The presence of geometric effects, pressure, and temperature dependent properties impose nonlinearities in the function $p(z)$. The quadratic function therefore can accommodate curvature in the pressure $p(z)$ through the quadratic term, cL^2 . This argument can not be supported for the given data as only three pressure transducers were used with a three coefficient model. Four data points must be used to support the statistical argument for the quadratic model. Therefore no experimental evidence was available to conclude which method yields "correct" values of P_x . The choice of the extrapolation technique must be made arbitrarily.

Once exit pressure values are calculated using an extrapolation procedure, the physical significance of the exit pressure values was examined based on the precision estimates calculated from repeated measurement at a constant shear rate. A precision estimate of ± 15 KPa was obtained for exit pressure values. For calculations of N_1 , only shear stress levels greater than 35 KPa were used. The values of P_x shown in Figure 27 for polystyrene are on the same order of magnitude of the error variation. The exit pressure values for $\sigma_w \geq 35$ KPa were generally greater than $1E5$ Pa. The values of P_x were significant based on the precision estimates for the three polymers for $\sigma_w \geq 35$ KPa.

The results of the experimentally calculated values of P_x are used in the exit pressure theory to calculate values of N_1 . The qualitative behavior of the predicted values of N_1 calculated from equation (2.14) was examined by observing the absolute values of P_x obtained using linear and quadratic extrapolation techniques. The exit pressure results for the two polyethylene samples in Figure 29 and 31 showed negative exit pressure values which decreased with increasing shear stress for a linear extrapolation technique. Using the exit pressure technique in equation (2.14) to measure N_1 , the the primary normal stress difference values from Figures 29 and 31 were predicted to be negative in magnitude and decreased with increasing wall shear stress. These predictions are contrary to the observed behavior of N_1 . Numerical simulations using viscoelastic models also show that exit pressure values are positive valued and increased with increasing shear stress [83-86,93,96,101]. The use of the quadratic fit for NPE 952 and LY600-00 yielded positive valued exit pressure measurements and values of P_x versus σ_w which were in qualitative agreement with

the numerical predictions. This argument however does not suggest that the proper value of P_x needed to predict N_1 is calculated by this extrapolation procedure. However, positive values of P_x which increase with $\dot{\sigma}_w$ are required from experimental results if realistic behavior in N_1 is to be obtained.

Once a series of exit pressure measurements at various shear rates are collected, the shear stress dependence of P_x must be calculated from the slope of the plots in Figures 27-32. The slope $dP_x / d\dot{\sigma}_w$ was used in equation (2.14) in the calculation of N_1 from the exit pressure results. The results of the predictions of equation (2.14) are presented in the next section.

One of the goals of the present investigation was to determine under what conditions, if any, could exit pressure data be used to measure the normal stress difference N_1 . The results in this section suggest that exit pressure measurements are difficult to obtain on a consistent basis. The exit pressure technique will be used in the next section to determine the value of N_1 so precision estimates could be calculated using the exit pressure theory to calculate N_1 . The precision estimates reflect errors due to experimental factors, and errors introduced due to violations of the assumptions originally used to derive the exit pressure technique in equations (2.13) and (2.14).

5.3 CALCULATION OF N_1 FROM EXIT PRESSURE RESULTS

In this section the magnitude of the primary normal stress difference N_1 will be calculated from the results of the exit pressure measurement. The results will be compared with a cone-and-plate device which will serve

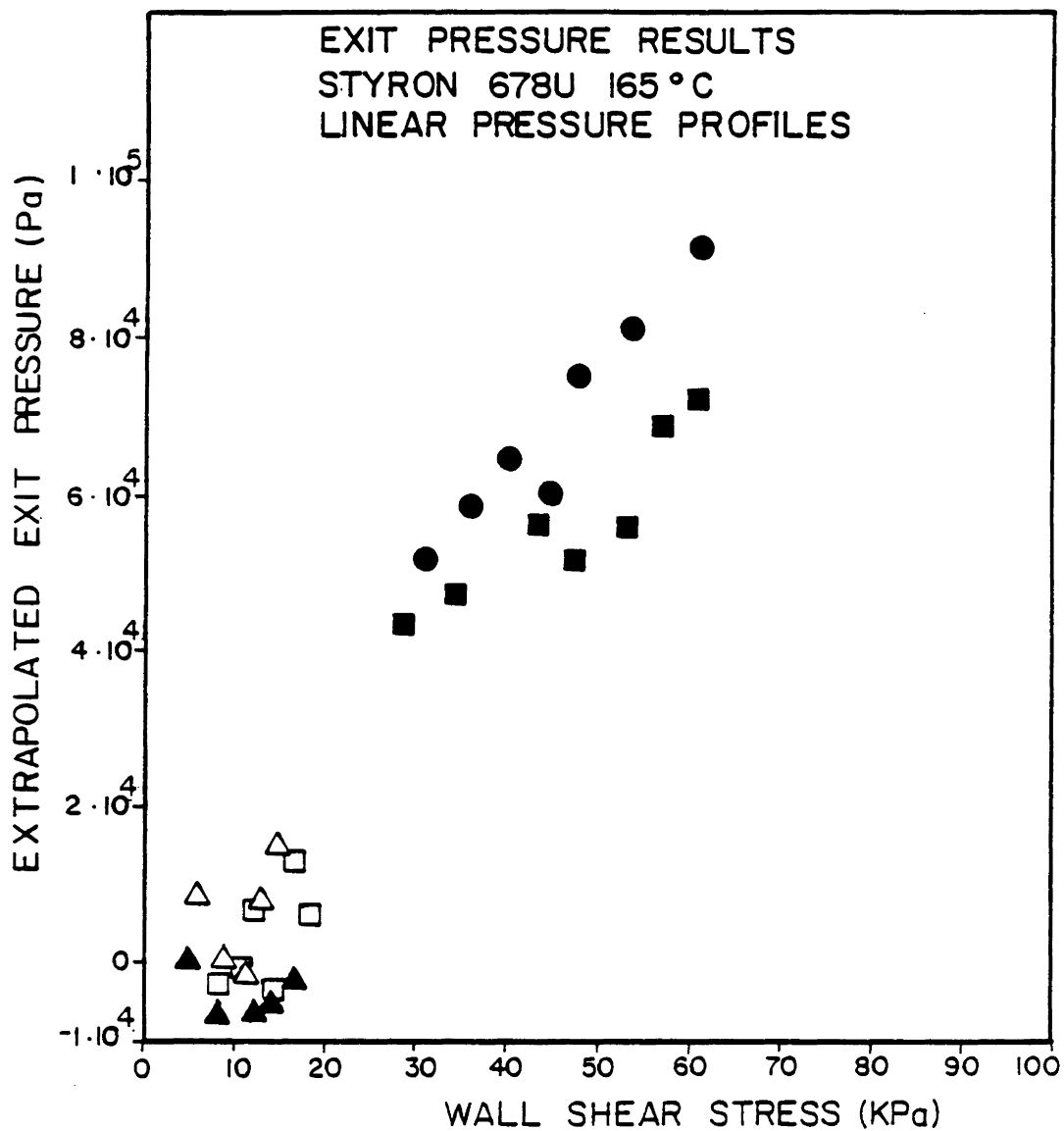


Figure 27. Exit Pressure Results for Styron 678 at 165 °C: Least squares fit of the pressure profiles.

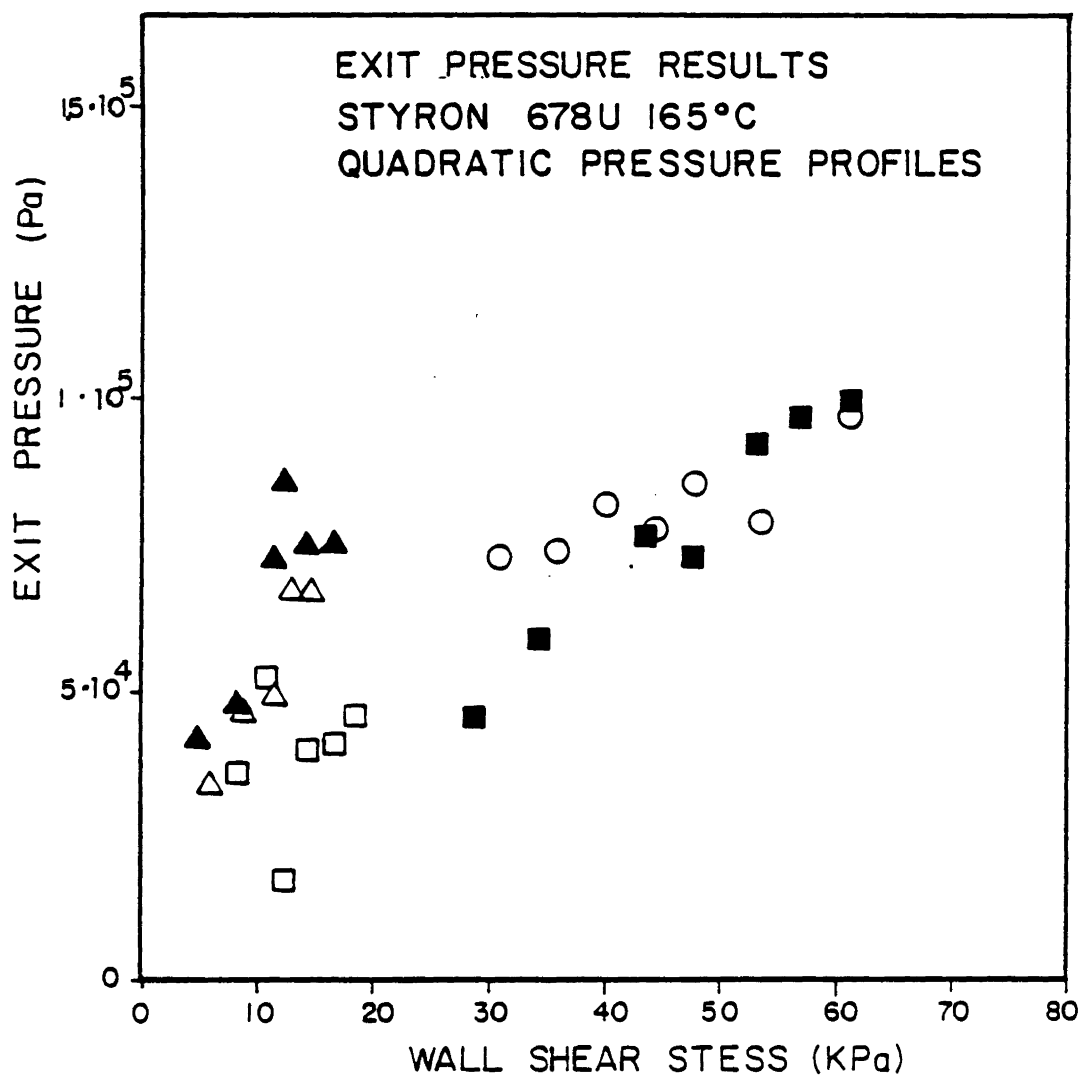


Figure 28. Exit Pressure Results for Styron 678 at 165°C: Quadratic function used to model the pressure profiles.

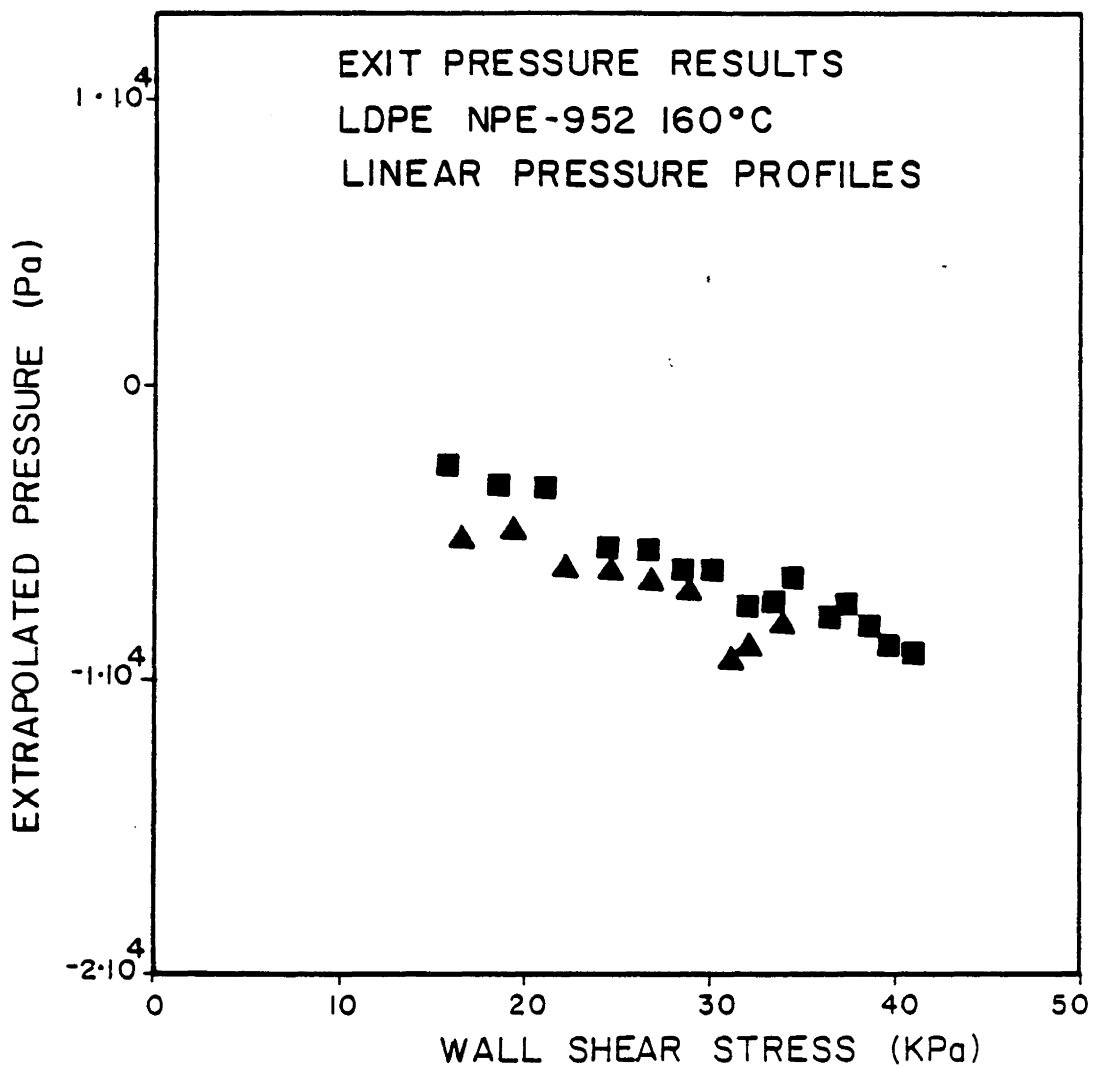


Figure 29. Exit Pressure Results for LDPE NPE 952 at 160°C: Least squares fit of the pressure profiles.

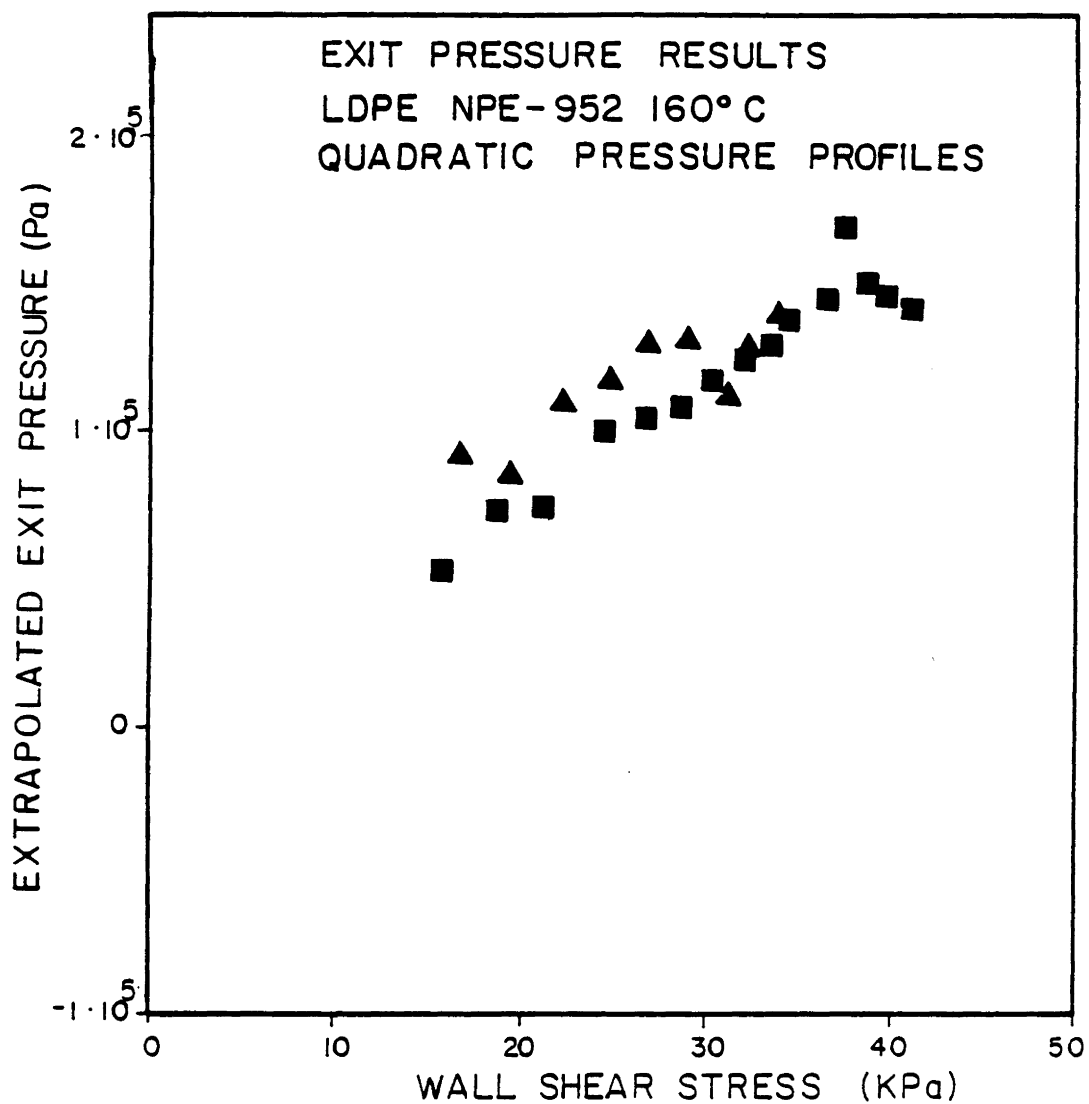


Figure 30. Exit Pressure Results for LDPE NPE 952 at 160°C: Quadratic function used to model the pressure profiles.

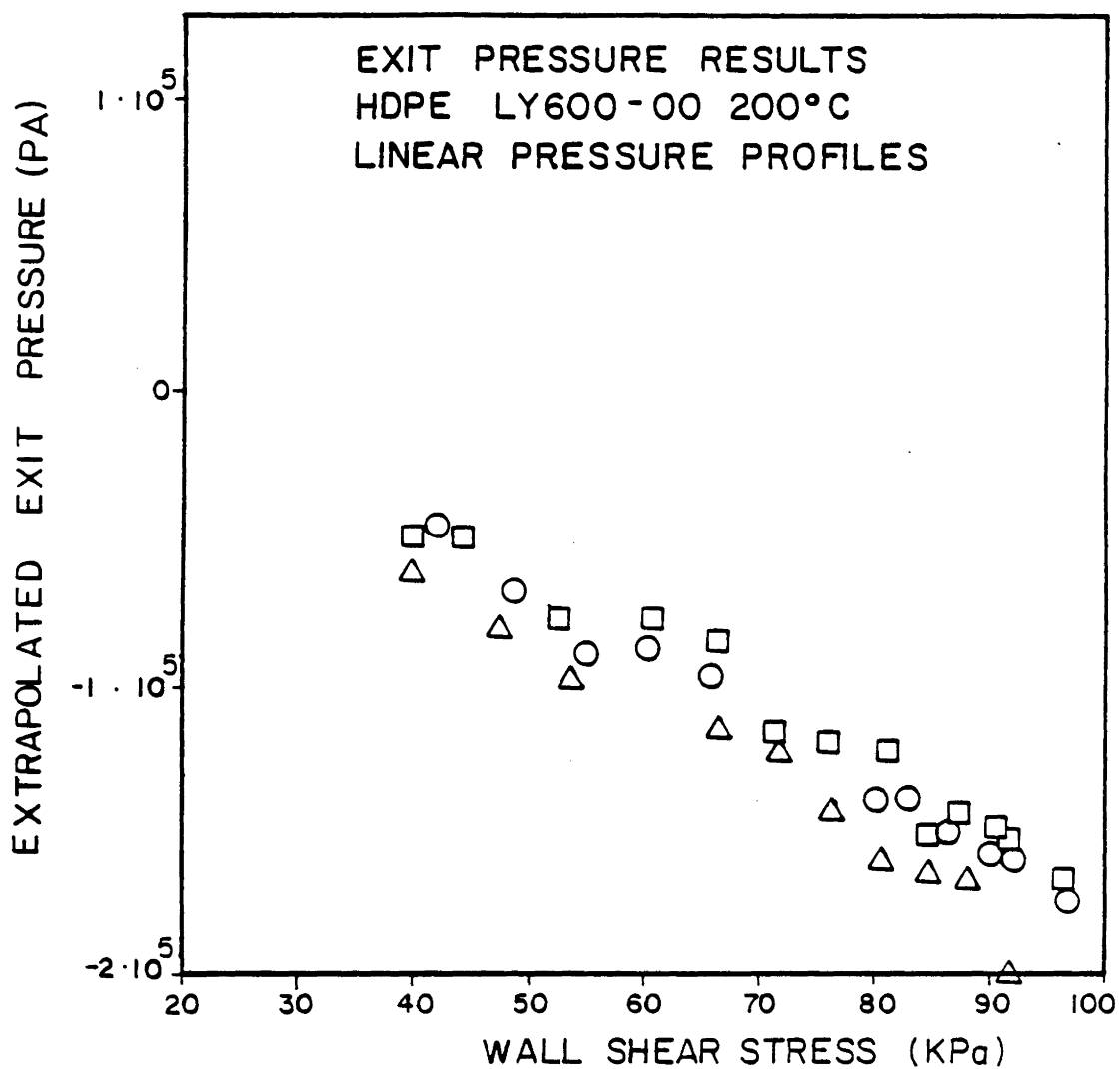


Figure 31. Exit Pressure Results for HDPE LY600-00 at 200°C: Least squares fit of the pressure profiles.

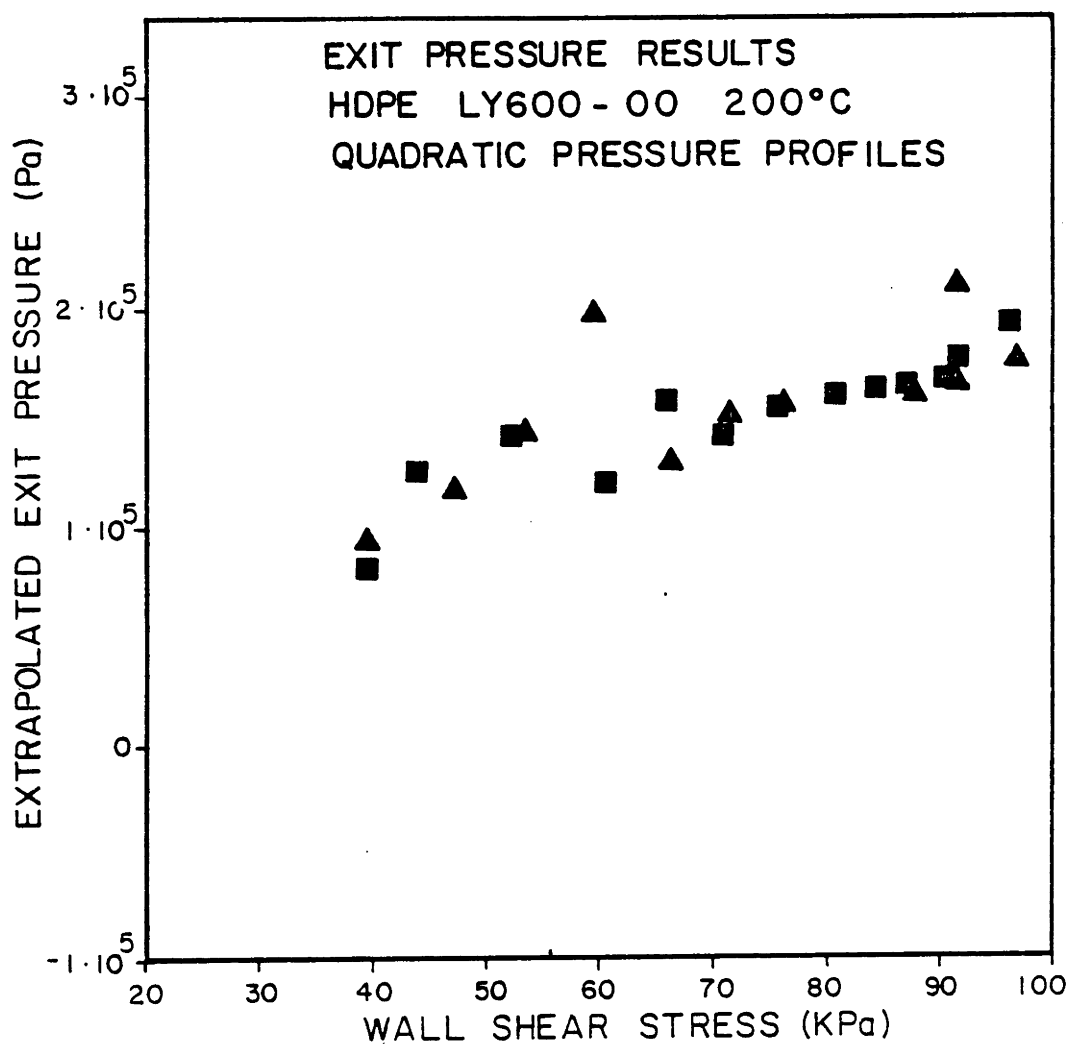


Figure 32. Exit Pressure Results for HDPE LY600-00 at 200°C: Quadratic function used to model the pressure profiles.

as a basis of comparison. The results can also be used to demonstrate the errors subject to using the exit pressure measurements to calculate N_1 by the error estimates in calculated N_1 values. The calculations of N_1 were based on the equations developed in section 2.1 assuming negligible inertial forces and a fully developed velocity field until the die exit.

The normal stress behavior for the three polymer melts is shown as a function of shear rate in Figure 33. The results were obtained using the Rheometrics Mechanical Spectrometer. These values are used as a basis of comparison for the slit die rheometer measurements. The normal stress values were then plotted as a function of shear stress using the results of the viscosity measurements to calculate τ_w . The accuracy of the cone-and-plate apparatus was found to be about $\pm 20\%$ based on repeated measurements of N_1 . The accuracy of the normal stress measurements was less than the viscosity measurements. A complete discussion of the experimental errors associated with obtaining N_1 values from cone-and-plate measurements is discussed elsewhere [68].

Two different equations were used to predict N_1 from the exit pressure data presented in the previous section. In the more common technique equation (2.14) is used as developed in section 2.1.

$$N_1 = P_x + \tau_w \frac{d P_x}{d \tau_w} \quad (5.4)$$

This equation requires the derivative of the exit pressure as a function of the wall shear stress. The following results have used the exit pressure obtained from a parabolic fit of the pressure profiles. A least

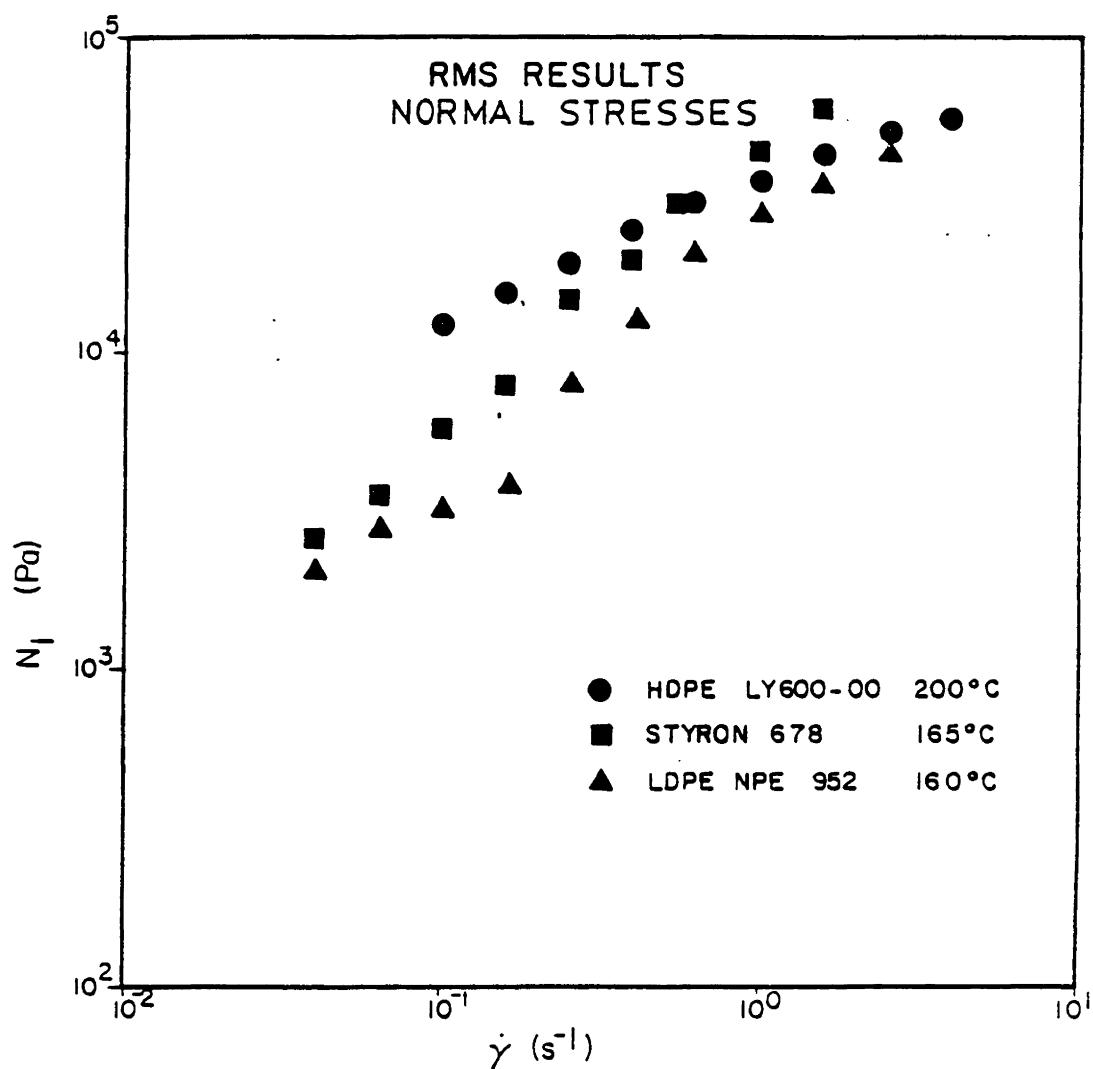


Figure 33. Primary Normal Stress Difference Results from the Cone-and-plate Rheometer.

squares analysis was used on the results given in Figures 29-32 to obtain the derivative $d P_x / d \tau_w$ for each material. An alternate equation was also used to predict N_1 .

$$N_1 = P_x (1 + k) \quad (5.5)$$

This equation was derived by Boger and Denn [60] using a macroscopic momentum balance. This equation assumes that the normal force N_1 can be written as a function of the wall shear stress.

$$N_1(\gamma) = (\text{constant}) \tau_w^k \quad (5.6)$$

The k in equation 5.5 and 5.6 represents the exponential dependence of the shear stress. The value of k was determined from experimental data using the cone-and-plate rheometer. This equation eliminates the differentiation of experimental exit pressures, but still requires a-priori knowledge of the normal stress behavior for the fluid. The constants used in equation (5.4) and (5.5) are listed in Table A.1 for each polymer.

Direct comparison of normal stresses obtained from the Rheometrics Mechanical Spectrometer and the slit die rheometer are shown in Figures 34-36. Figure 35 for NPE 952 contains the most overlap in the two techniques. The results of the normal stresses calculated by the exit pressure technique were clearly larger than the cone-and-plate results. For each polymer, the normal stresses calculated using the exit pressure were 100-200 % greater than the actual normal stress values.

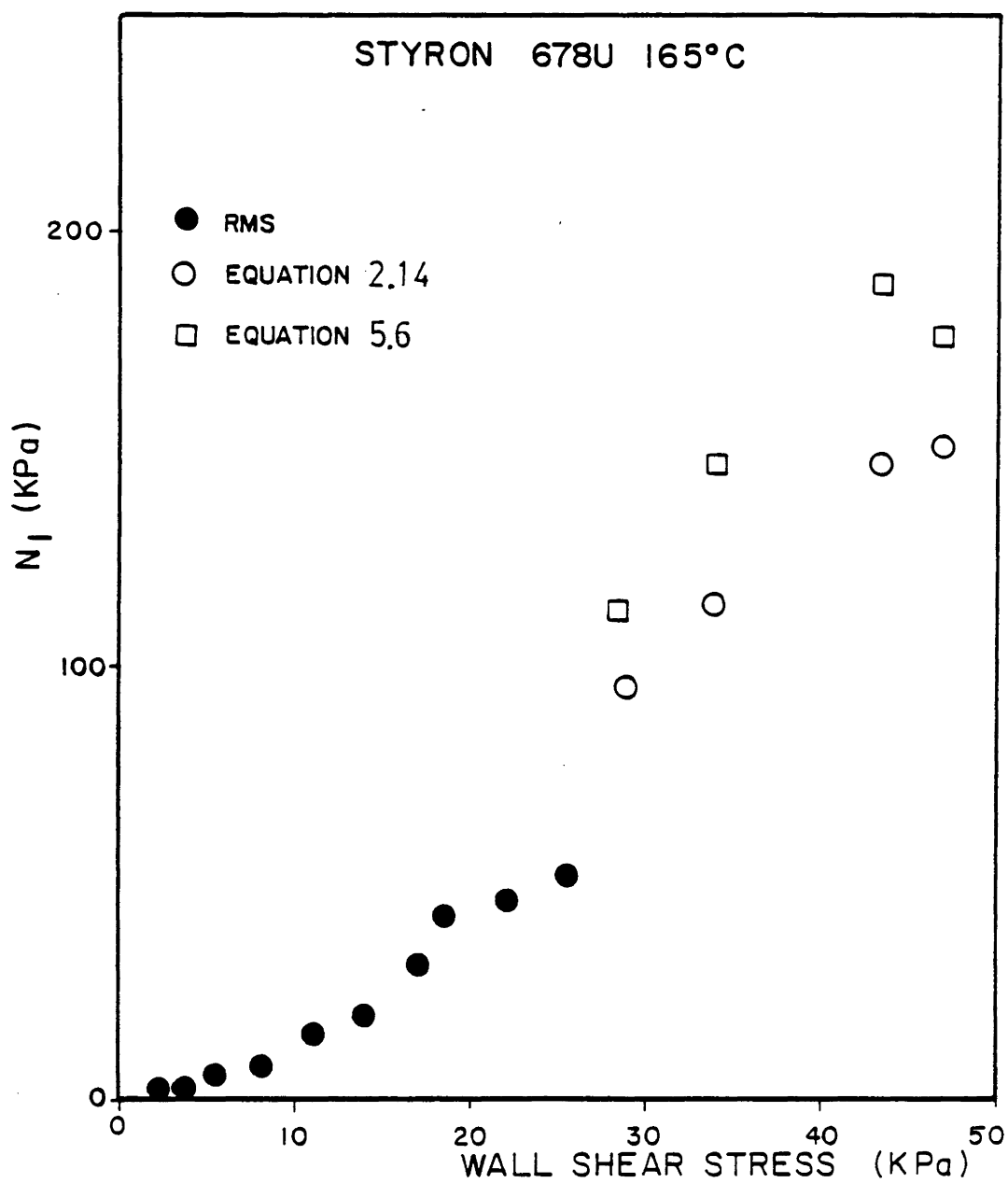


Figure 34. Comparison of values of N_1 for Styron 678 at 165°C

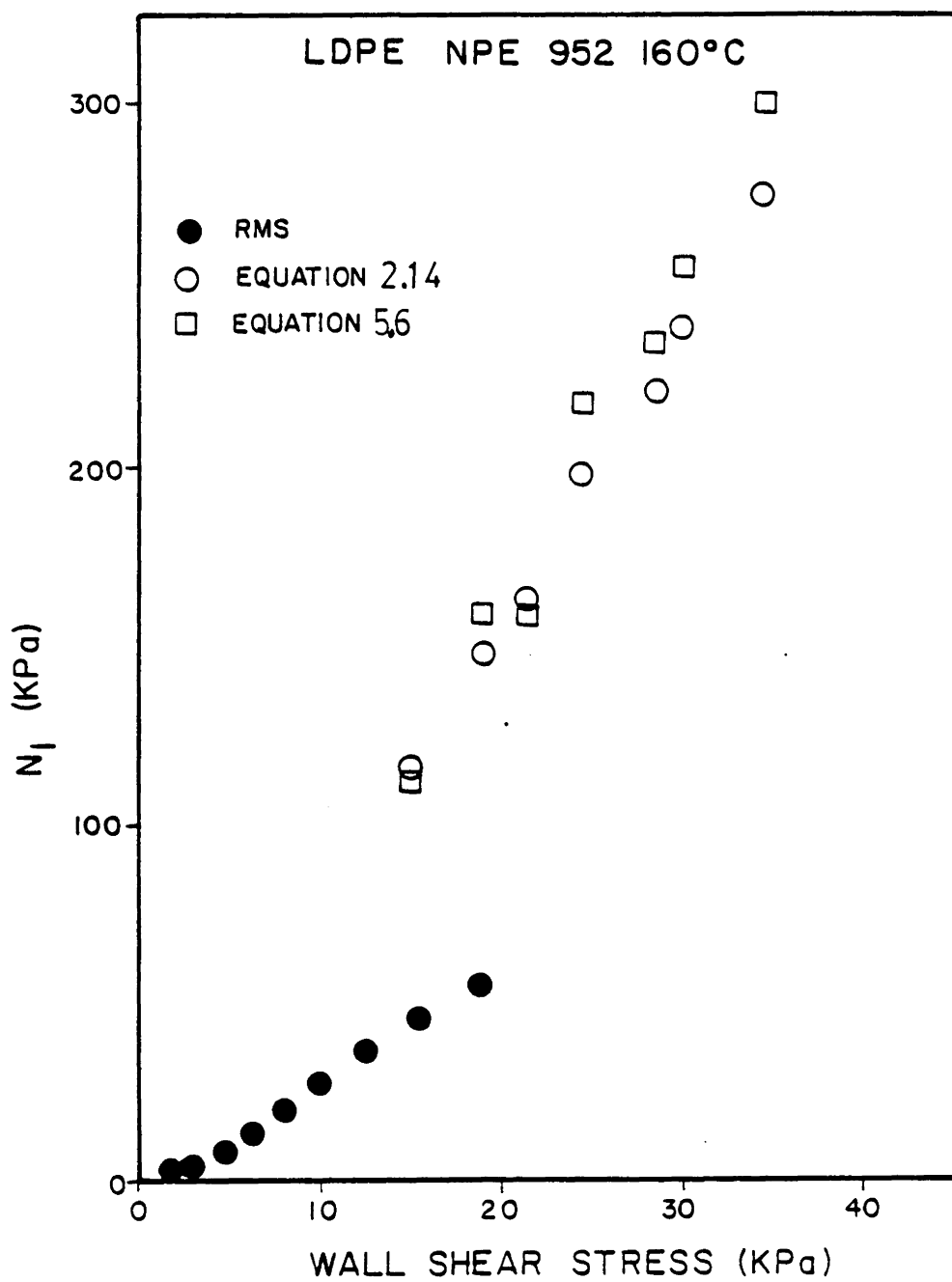


Figure 35. Comparison of values of N_1 for LDPE NPE 952 at 160°C

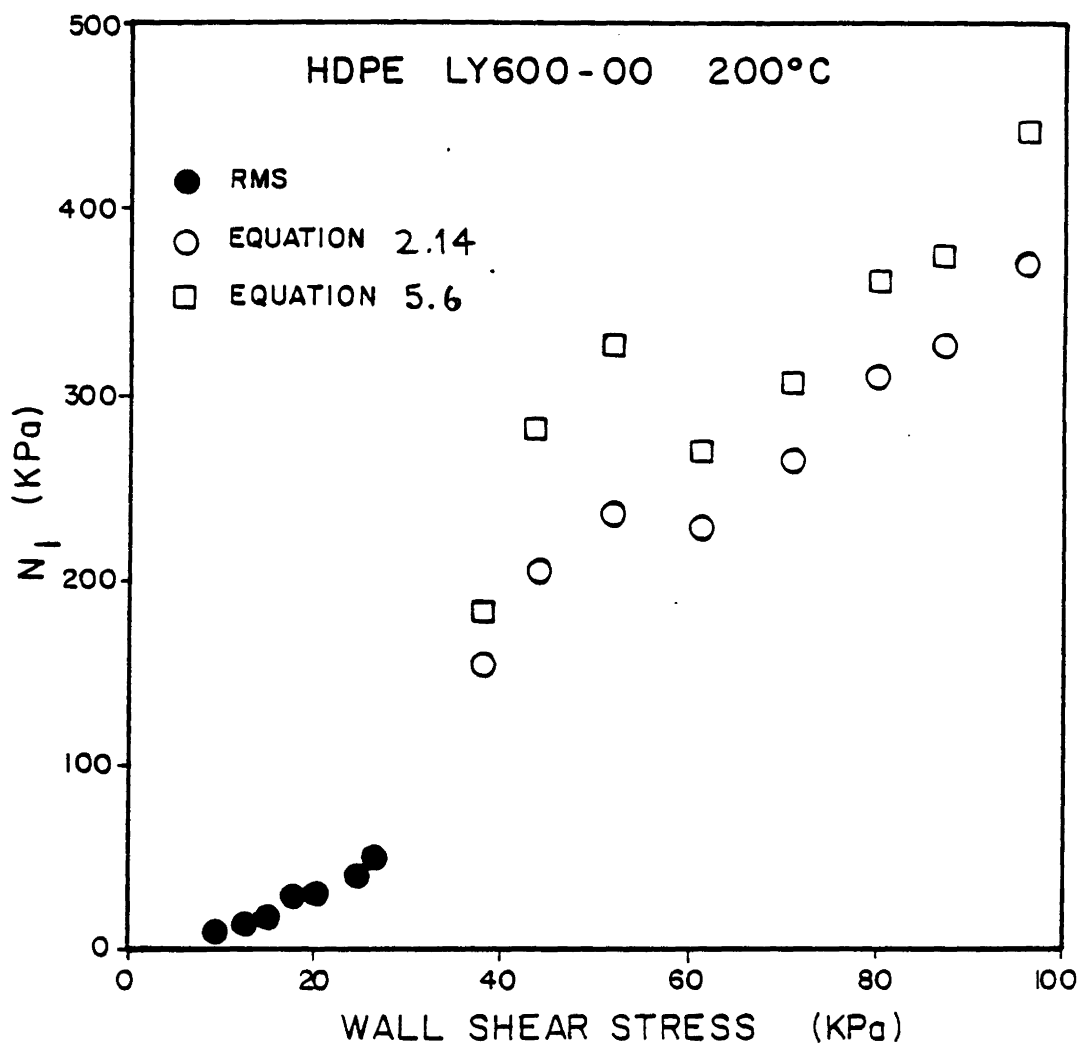


Figure 36. Comparison of values of N_1 for HDPE LY600-00 at 200°C

The large difference between the values in Figures 24-36 may be due to two factors. Various experimental errors discussed in chapter two influence the measurement of the exit pressure which in turn prevents accurate calculation of N_1 from equations (5.4) and (5.5). Another factor may be the validity of the original assumptions used in the derivation of the equations (2.13) and (2.14). A rearrangement of the stress field before the die exit will result in additional stresses which have not been taken into account in the simplified theory.

The normal stress predicted using the existing theory significantly overestimated the value of the primary normal stress difference obtained in steady shear flow. Based on the comparison of the N_1 values calculated using the exit pressure theory and the cone-and-plate rheometer, the exit pressure technique can not be used to measure quantitative values for polymer melts for the shear rate range investigated. As discussed earlier, the validity of the assumptions originally used to derive equations (2.13) and (2.14) may be violated for flow at the exit region of a die. The remainder of this chapter will therefore examine the validity of the assumptions used in the original derivation of equation (2.14). The studies will concentrate on the nature of the stress field in the exit region in a slit die.

5.4 FLOW BIREFRINGENCE STUDIES

One of the objectives of the present investigation was to evaluate the contribution of stresses to the exit pressure by means of a detailed examination of the stress field at the exit of a slit die. The flow birefringence technique was used to qualitatively and quantitatively de-

scribe the stress field for polystyrene and polyethylene melts over the apparent shear rate range $0.1 \leq \dot{\gamma}_{app} \leq 15$. The stress field information was used to evaluate the magnitude of the velocity rearrangement at the exit region of the die by calculating the stress contributions to the exit pressure using a macroscopic momentum balance by comparing the value of P_x with and without flow disturbance at the die exit. The error contributions due to the assumption of fully developed flow up to the exit region may be calculated from these results. This section presents the results of the birefringence studies obtained for flow in the 1-2 plane. Qualitative information is presented for all three polymers by examination of the isoclinic and isochromatic patterns. Detailed stress field information was then calculated for Styron 678 using the results of the birefringence patterns and the linear stress optic rule. Stress contour maps then are presented from which a quantitative assessment of the exit disturbance is conducted. Finally, the shear and normal stress behavior at the die exit is discussed.

5.4.1 ISOCLINIC PATTERNS

In this section a discussion is presented of the isoclinic fringe patterns and extinction angles in the exit region of a slit die. Based on the behavior of the extinction angles, several conclusions can be drawn as to the nature of the stress field and kinematics in the exit region. The isoclinic patterns were collected for Styron 678 at 165°C for a series of shear rates in the range $0.11 \leq \dot{\gamma} \leq 0.4$. The fringe patterns for two values of χ are shown in Figure 37 for Styron 678 at 165°C for a wall shear

stress of 8.10 KPa ($\dot{\gamma} = 0.17 \text{ s}^{-1}$). The flow in the photographs is from right to left.

It is observed that the isoclinic patterns are generally broad diffuse patterns which makes the identification of the extinction patterns difficult. The location of the fringe patterns can be mapped by rotating the polarizing optics and studying the paths of the isoclinic bands through the sample cross section. The accuracy of the location for a specific extinction angle can be improved by changing the orientation of the polarizers $\pm 5^\circ$ about the desired orientation. The isoclinic fringe patterns will translate about the mean location of the extinction angle. The fringe location was taken as the center of the broad band. The estimated accuracy of the values of χ were $\pm 3^\circ$ degrees based on repeated measurements of the isoclinic patterns.

The absence of sharp fringe patterns shown in Figure 37 was believed to be due to parasitic velocity gradients along the side walls of the die. The presence of a velocity gradient tends to rotate the extinction angles out of the 1-2 plane of the slit. The principal directions are no longer uniform throughout the sample volume in the 3 direction of the light beam. This results in a spreading of the extinction band. Measurement of the isoclinic patterns was therefore limited to shear rate ranges below which this effect is negligible. For Styron 678 at 165°C , an upper limit of 0.4 s^{-1} shear rate was observed in the accurate measurement of the isoclinic angles. For the polyethylene samples no isoclinic patterns were obtained. The stress optic coefficient for the polyethylene samples were approximately one half that of polystyrene. The shear rates required to obtain a sufficient number of isochromatic fringe patterns were above the

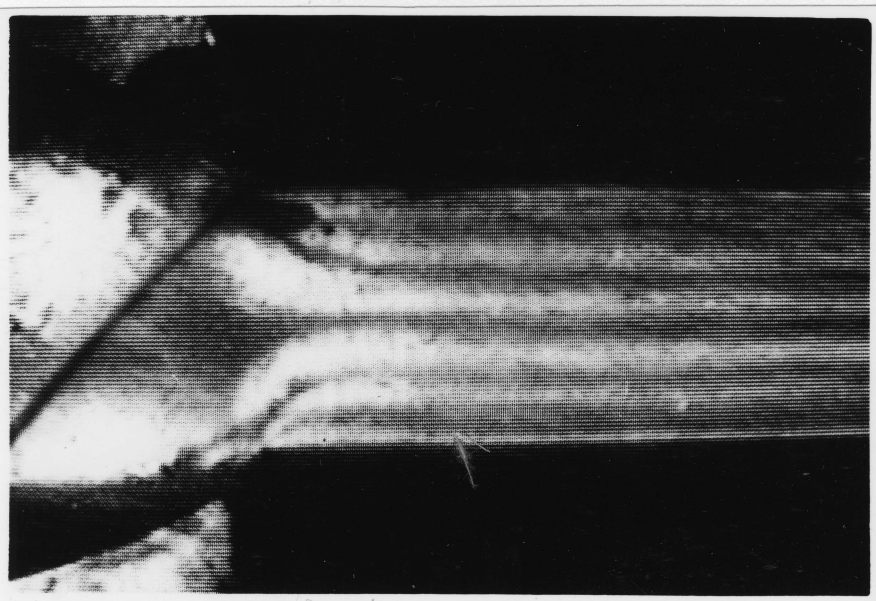
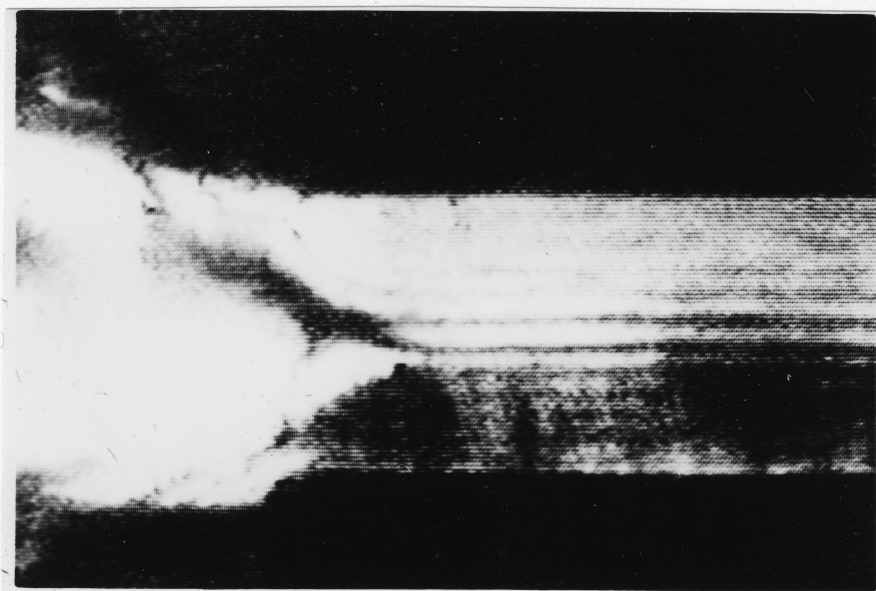


Figure 37. Isoclinic Fringes Obtained for Styron 678 at 165 C: (a) $\dot{\gamma} = 0.17 \text{ s}^{-1}$, $\alpha = 30^\circ$. (b) $\dot{\gamma} = 2.04 \text{ s}^{-1}$, $\alpha = 50^\circ$.

shear rate range in which isoclinic angles could be accurately measured. For the present investigation, complete loss of the isoclinic fringes was observed for shear rates greater than 2 s^{-1} for all polymers and conditions.

The resolution of the isoclinic fringe patterns was also subject to temperature effects. Temperature gradients exist at the glass windows where complete insulation of the die was not possible. The refractive indices of the material can be temperature dependent. The net effect of the temperature gradients is the creation of a lens effect which diverges the light rays passing through the sample [133]. The temperature control throughout the die was controlled to within $\pm 0.5^\circ\text{C}$ of the desired temperature. Since no insulation covered the windows, it is suspected that sharp temperature variations may have existed along the window surface. The temperature gradient at the windows could be reduced by placing an additional glass plate over the windows. This would create an air space which would serve to insulate the die. At elevated temperatures these effects may contribute to the loss of resolution in the isoclinic fringe patterns.

The locations of the isoclinic patterns are combined to form a composite map of the location of the principal stress directions throughout the sample area. An example isoclinic angle map is shown in Figure 38 for Styron 678 at 165°C . An important feature concerning the kinematics of the flow field can be observed by examining the composite map shown in Figure 38. The velocity field rearrangement from a pressure driven shear flow in the die to a shear free flow in the free surface was postulated to consist of regions of fluid acceleration along the slit walls

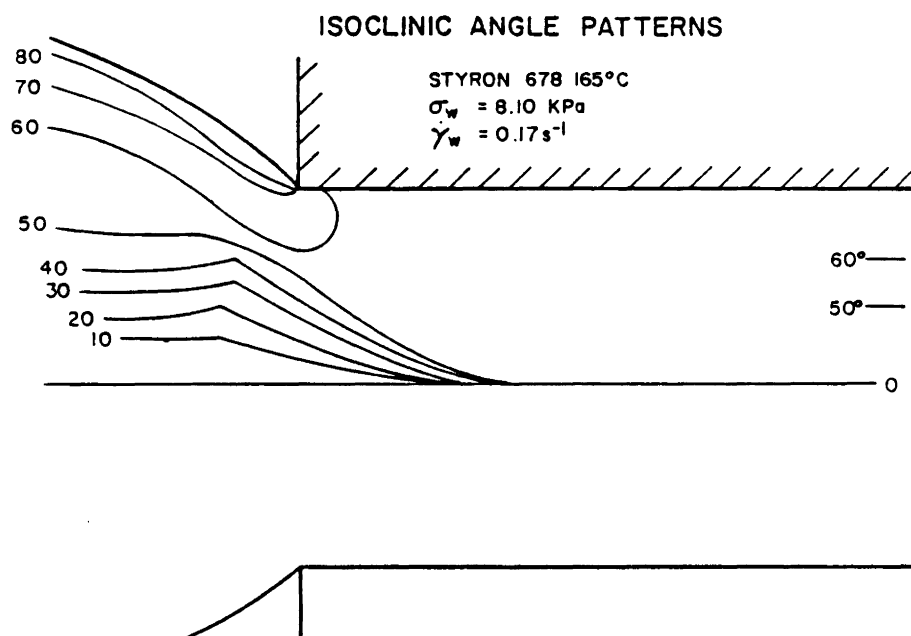


Figure 38. Isoclinic Map Obtained for Styron 678 at 165°C.

and fluid deceleration at the centerline [48,55]. The existence of an extensional flow gradient (deceleration at the centerline) can be assessed by examining the behavior of χ from the centerline to the wall. Acceleration of fluid will create additional normal stress contributions and shear stress gradients as a function inside the die.

The use of the isoclinic angles to detect extensional gradients in slit die geometries has been discussed by Pike [128]. The shear rate for pressure driven flow in a slit should equal zero at the centerline due to symmetry. At a point in the fluid where $\dot{\gamma} = 0$, the stress should become isotropic, so that χ will exhibit all possible values. The fact that χ does not assume all values at the centerline indicates that the flow at the exit may contain extensional flow components upstream of the die exit plane. The isoclinic angle for Styron 678 along the centerline equaled zero within one die height of the exit. This suggests the presence of an additional extensional component in the flow. Knowledge of the kinematics obtained from tracer studies and laser dopler anemometry suggest that the extensional component must consist of a deceleration term.

The compressive or tensile nature of the extensional forces can be obtained directly from the value of the isoclinic angles in the die exit region. As introduced in section 2.4, the stress optic law yields normal stresses given by the expression

$$\sigma_{11} - \sigma_{22} = \Delta n \cos(2\chi) / C \quad (5.7)$$

The values of the extinction angles, χ , vary from 0-90° upstream of the exit as shown in Figure 38. The sign of the stress difference $\sigma_{11} - \sigma_{22}$

will change from positive to negative due to the $\cos(2X)$ term in equation (5.7). Positive values of $\sigma_{11} - \sigma_{22}$ are calculated using equation (5.7) in the region defined by extinction angles less than 45° . In Figure 38, this region encloses a triangular region inside the exit plane and near the slit centerline. The sign convention for the normal stresses follows that of Bird in which a tensile stress is negative and a compressive stress is positive. The isoclinic patterns for Styron 678 show compressive stresses or deceleration of the velocity field near the centerline of the die. A fully developed velocity profile in steady shear flow will exhibit tensile normal stresses which vary from zero along the centerline to a maximum negative value along the walls. The positive normal stress components indicate normal stress differences are generated due to the rearrangement of the stress field at the die exit.

The distribution of isoclinic fringe patterns in the exit region of a slit die was also investigated by Arai and Hatta [50] for a high density polyethylene melt. They presented a composite isoclinic map which corresponds very closely with the results of the present investigation. They commented on the presence of acceleration components along the wall, but did not comment on positive normal stresses or the presence of a velocity deceleration components along the centerline.

The length of the rearrangement region inside the die can also be determined by an examination of the isoclinic map. The length from the exit plane to the location upstream of the die exit where the isoclinic patterns are all parallel represents the region of disturbance in the stress field due to velocity profile rearrangement. An easier technique, however, to assess the length of the exit disturbance involves the exam-

ination of the isochromatic fringe patterns which are discussed in the next section.

The isoclinic patterns obtained for Styron 678 at 165°C for the shear rate range $0.1 \leq \dot{\gamma} \leq 0.4 \text{ s}^{-1}$ have shown a velocity rearrangement at the exit region of a slit die. The positive sign of the isoclinic patterns expressed a deceleration velocity component along the centerline. In the next section the isochromatic patterns will be used to examine the nature of the stress field rearrangement.

5.4.2 ISOCHROMATIC FRINGE PATTERNS

In this section a general description is given of the important features of the isochromatic patterns observed in the exit region of a slit die. Based on these patterns some qualitative comments can be made concerning the nature of the stress field in the exit region. The discussion will concentrate on the length of the exit region and the stress gradients as a function of the shear rate of the fluid.

Two sets of isochromatic patterns for Styron 678 at 165°C are shown in Figures 39 and 40. These patterns represent light and dark field patterns obtained using the optical arrangement discussed in section 3.5. The assignment of values of the fringe order N to the dark bands in Figures 39 and 40 was accomplished through the knowledge of the stress distribution in undisturbed pressure driven flow. For undisturbed flow, the stress varies from a maximum value at the wall to zero at the centerline. It is expected that the value of N will vary similarly. The development of fringe orders can be traced in the fluid by slowly increasing the flow rate. The fringes were seen to evolve from the walls and move towards

the centerline as the shear rate increased. For the dark field pattern, the values of $\bar{N}$ were counted from 0,1,2,3... to the maximum value at the wall.

A composite map of the isochromatic patterns for Styron 678 at 165°C is shown in Figure 41. The values of $\bar{N}$ are seen to increase linearly from the centerline to the wall in the region of undisturbed flow. An exit region was present which was characterized by a disturbance of the fringe patterns from the parallel orientation found in fully developed flow. The exit region will be defined by the length upstream from the die exit in which the isochromatic patterns deviate from their parallel orientation. Since the stresses are proportional to the value of $\bar{N}$, the fringe orders may be qualitatively used to assess the magnitude of the exit disturbance upstream of the die exit.

Isochromatic patterns have been used to qualitatively describe the behavior of fluids in the exit of a die by earlier research groups [22,23,44,50,51]. Flow birefringence patterns were used in assessing the validity of the assumption requiring fully developed flow until the exit. Any deviation of the fringe patterns before the die exit suggests a stress profile rearrangement in anticipation of the free surface. The length of the exit region was measured for the three test polymers in the current investigation by calculating the distance upstream where curvature was evident in the isochromatic patterns. The exit length (L/H) was expressed as a function of the wall shear rate as shown in Figure 42. The experimental points for each polymer in Figure 42 do not show the exit length decreasing as the shear rate increases. The exit length remains approximately constant for the shear rates less than 10 s^{-1} . This behavior was

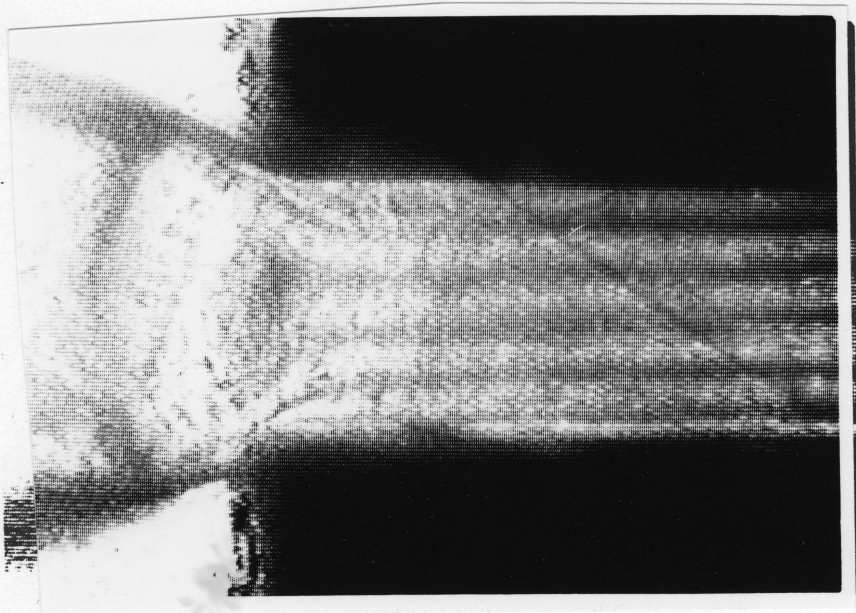


Figure 39. Light-field Isochromatic Fringe Patterns for Styron 678
at 165 C $\sigma_L = 8.23 \text{ KPa}$.

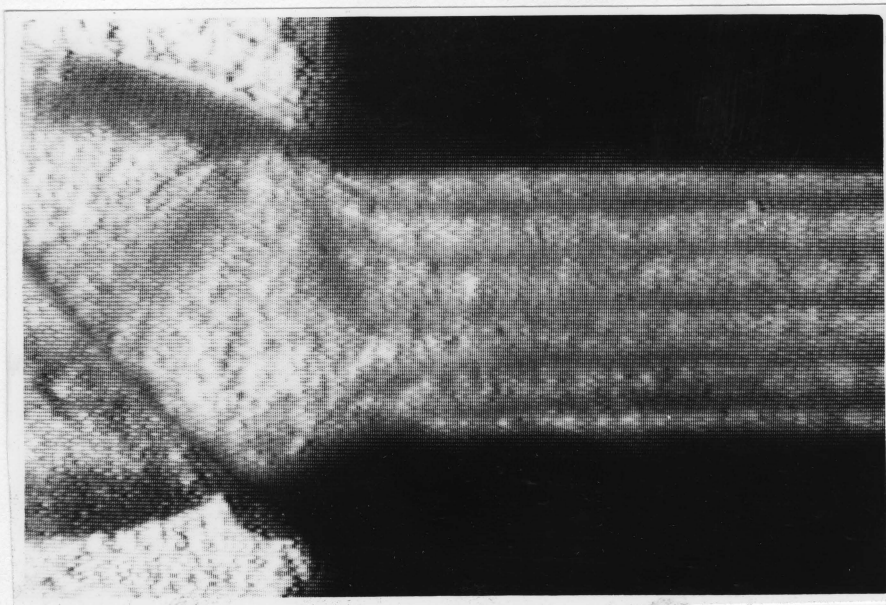


Figure 40. Dark-field Isochromatic Fringe Patterns for Styron 678
at 165 C $\sigma_w = 8.23 \text{ KPa}$.

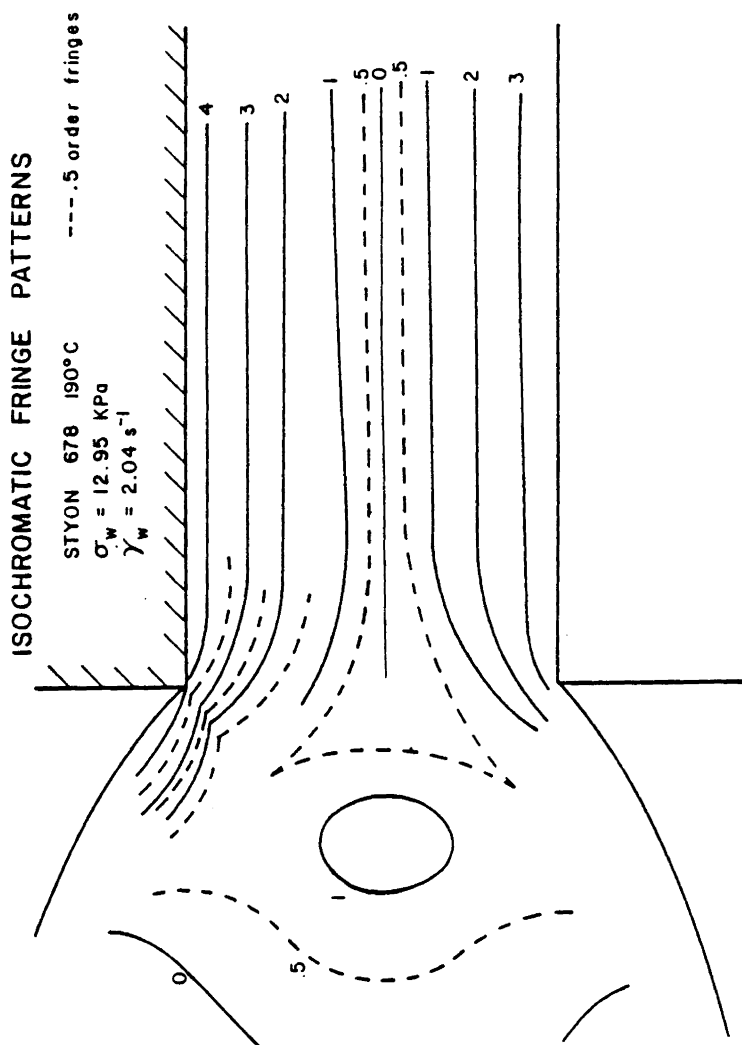


Figure 41. Composite Map of the Isochromatic Fringe Patterns for Styron 678

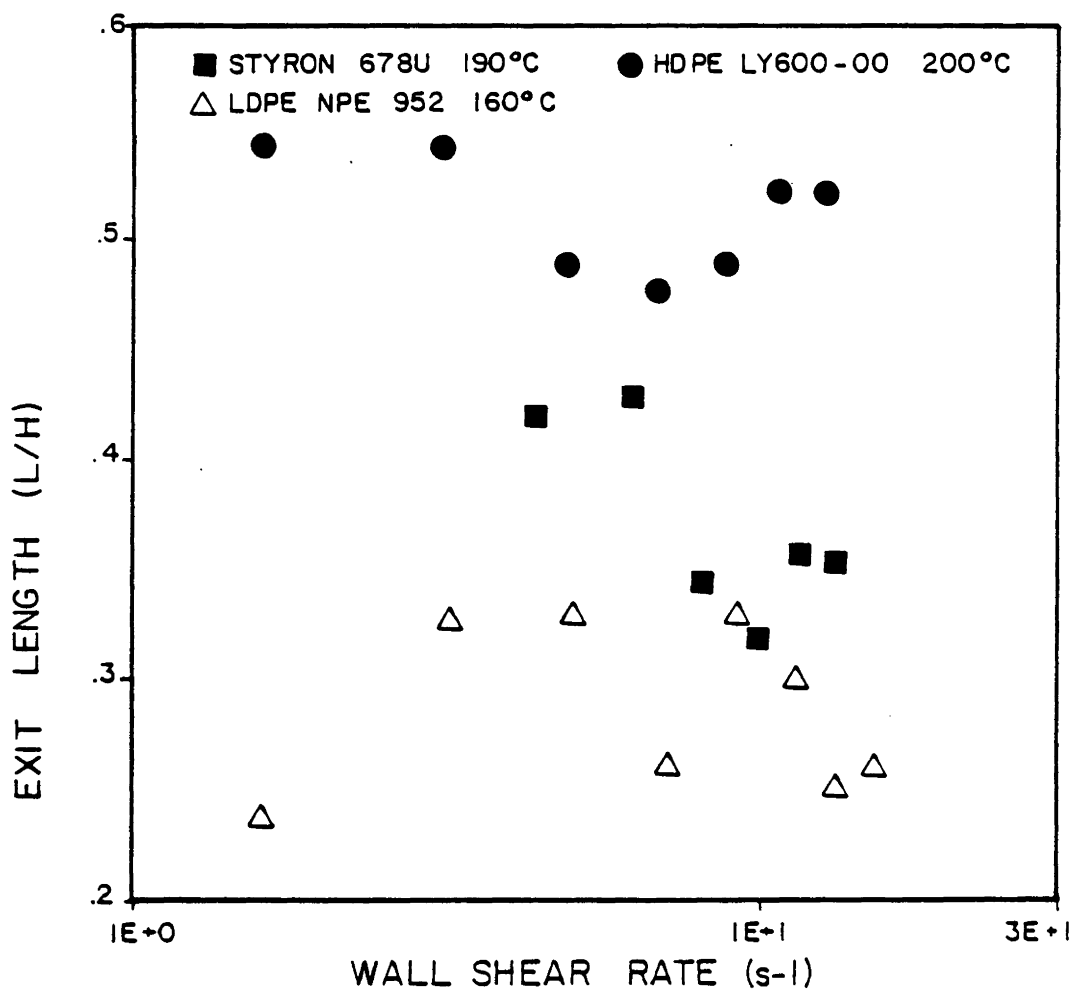


Figure 42. Rearrangement Length Taken From Isochromatic Fringe Patterns

consistent with the flow birefringence results presented by Funatsu and Mori [23] for the flow of polypropylene melts in a rectangular duct.

In contrast to the results above, Han and Drexler [44] concluded that the exit length was negligible above 10 s^{-1} for the polymers investigated. A series of isochromatic patterns for high density polyethylene were presented for increasing shear rates. They concluded that the extent of disturbance of stresses at the exit depended on the shear rate. They postulated that the exit disturbance would become negligible at reasonable high shear rates, $\dot{\gamma} > 10 \text{ s}^{-1}$. The critical shear rate would depend on the specific material. The experimental evidence supporting this assertion was based on the behavior of HDPE for the shear rate range $0.35 \leq \dot{\gamma} \leq 1.59 \text{ s}^{-1}$. An examination of the birefringence patterns by Han and Drexler in [49] shows that the isochromatic patterns may be influenced by the extrudate outside the die. The extrudate is seen to bend downwards as it exits the die. The exit region shown is also obscured by the presence of windows along the side walls. No patterns were visible in the region directly before and after the exit plane. Based on this evidence, the conclusion on the nature of the rearrangement terms by Han must be critically examined. The birefringence patterns clearly show deviation of flow before the exit.

From the stress optic laws in section 2.4, the magnitude of the principal stresses is directly proportional to the fringe order N through

$$N \propto [4\sigma_{xy}^2 + (\sigma_{xx} - \sigma_{yy})^2]^{1/2} \quad (5.8)$$

The behavior of the fringe patterns can then be used to qualitatively assess the behavior of the stress field. Of particular interest in the flow birefringence study was the magnitude of the stress rearrangement in the die. As shown in Figure 41, the fringe patterns are concentrated at the die corner. The stress field near the exit exhibits a higher stress gradient than along the centerline of the die. The stress concentration at the die corner is consistent with numerical predictions. The change in boundary conditions for fluid elements near the die corner may create large stress gradients. This phenomena is observed in the behavior of the fringe patterns in Figure 41.

In addition to large gradients present near the die lip, isochromatic fringe patterns may be used to detect the presence of stress overshoot behavior in the normal stress and shear stresses near the die corner. Overshoot behavior can be examined qualitatively by the presence of extra fringes at the die lip. The presence of an additional fringe was observed for Styron 678 at $\sigma_w = 15.23$ KPa ($\dot{\gamma} = 2.75 \text{ s}^{-1}$). This confirms experimentally some stress overshoot behavior near the die lip. Calculation of stresses at the die lip, σ_w and $\sigma_{zz} - \sigma_{yy}$ (stress discontinuity) was not possible due to the lack of resolution of patterns within 0.05 mm. of the die corner. Interference from the walls, poor equipment alignment, and broad fringe bands prevented an accurate measurement of fringes attached to the die corner.

In the last two sections some conclusions on the nature of the stress field at the die exit can be drawn from the examination of the isochromatic and isoclinic patterns. These conclusions were based on qualitative interpretation of the results of the isoclinic and

isochromatic fringe patterns. The presence of some stress overshoot was observed at the die lip which increased the shear stress gradients near the corners. Also, the nature of the normal stresses were obtained from the birefringence data $\bar{N}$ and χ . From the results of the flow birefringence patterns, the flow field at the die exit was shown to rearrange upstream of the die exit. Fluid deceleration along the centerline and additional stress gradients were created in both the axial and vertical direction. In the next section, the flow birefringence data will be evaluated using the linear stress optic rule. The resulting stress values for σ_{12} and $\sigma_{11} - \sigma_{22}$ can then be used to evaluate analytical expressions which assess the magnitude and significance of stress rearrangement inside the die.

5.4.3 STRESS FIELD DISTRIBUTION

In this section the flow birefringence results in sections 5.4.1 and 5.4.2 are used to calculate the values of σ_{12} and $\sigma_{11} - \sigma_{22}$ for Styron 678 at points in the exit region. The behavior of the stress field can then be examined using contour plots of the stresses or stress profiles at constant z or y coordinates. The objective of this section was the use of the linear stress optic rule to evaluate the shear stress σ_{zy} and normal stress difference $\sigma_{zz} - \sigma_{yy}$ for Styron 678 for a shear rate range of $0.11 \leq \dot{\gamma} \leq 0.4 \text{ s}^{-1}$ ($\sigma_w = 4.8 - 14.2 \text{ KPa}$).

The values of the stresses are calculated using the linear stress optic rule in equations (2.25 and 2.26). A mesh was created in the exit region as shown in Figure 43. The mesh points were equally spaced to facilitate the use of finite difference approximations in the evaluation

of stress gradients. The fringe order $\bar{N}$ and the extinction angle χ were calculated at each mesh point from composite birefringence maps such as presented in the last section. Linear interpolation was used to evaluate $\bar{N}$ and χ at the mesh points in Figure 43. Precision values for the birefringence data were estimated at ± 0.2 fringe orders for $\bar{N}$ and ± 0.052 radians (3°) for χ . These precision estimates were calculated by repeated measurements of $\bar{N}$ and χ from the data recorded on the VHS video system.

The stress distributions in the exit region are shown in Figures 44-47 for Styron 678 at 165°C for wall shear stress values of 8.10 KPa and 14.3 KPa. These contour plots represent the stresses σ_{12} and $\sigma_{11} - \sigma_{22}$. The contour lines in the figures represent 1000 Pa. intervals. Highlighted lines were given for every 5000 Pa. The coordinate system in the figures was given in millimeters. The upstream distance in each figure corresponded to approximately one die height.

It is immediately evident in the figure that both σ_{12} and $\sigma_{11} - \sigma_{22}$ were disturbed before the exit plane. The disturbance was most pronounced near the corner of the die. From these results and the results of the isochromatic and isoclinic patterns in the previous section, the assumption of fully developed flow up to the exit plane has been violated. However, an analysis of the nature of the stress field and the magnitude of the stress near the die corner may yield information whether the assumption is critical in the use of the exit pressure to measure fluid elasticity.

The shear stress τ_{zy} is shown for the shear rate values of 0.17 and 0.39 in Figure 44 and 46. Two important features are present which will

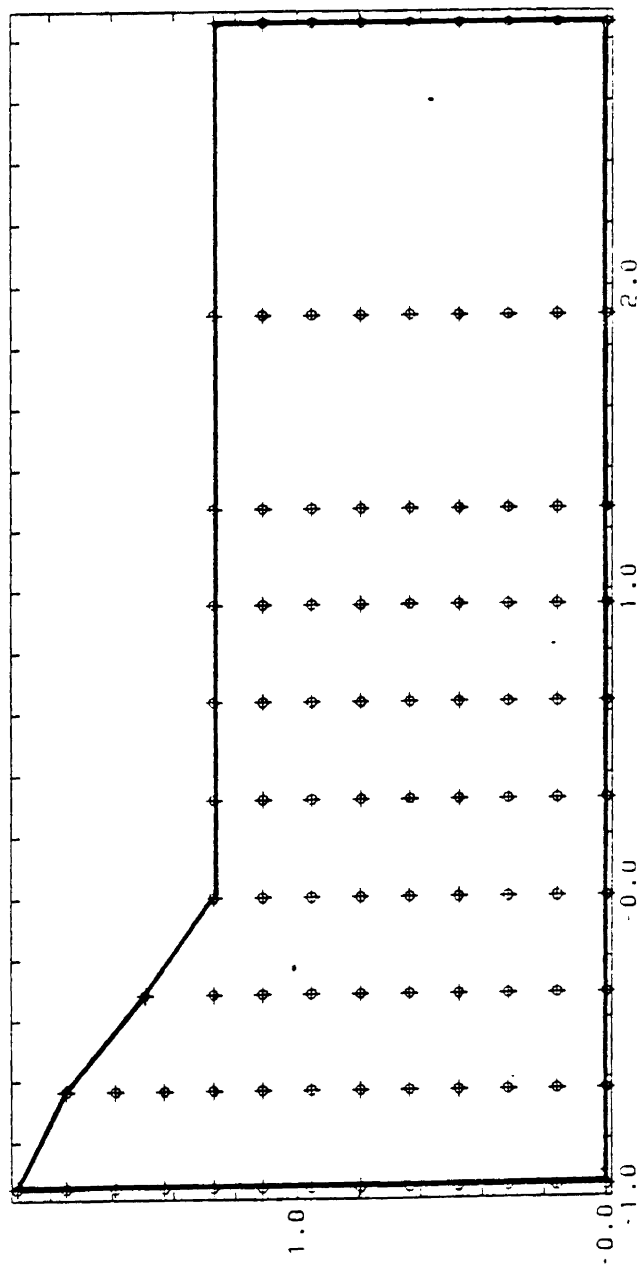


Figure 43. Mesh Points Used to Evaluate Stresses From the Linear StressOptic Rule

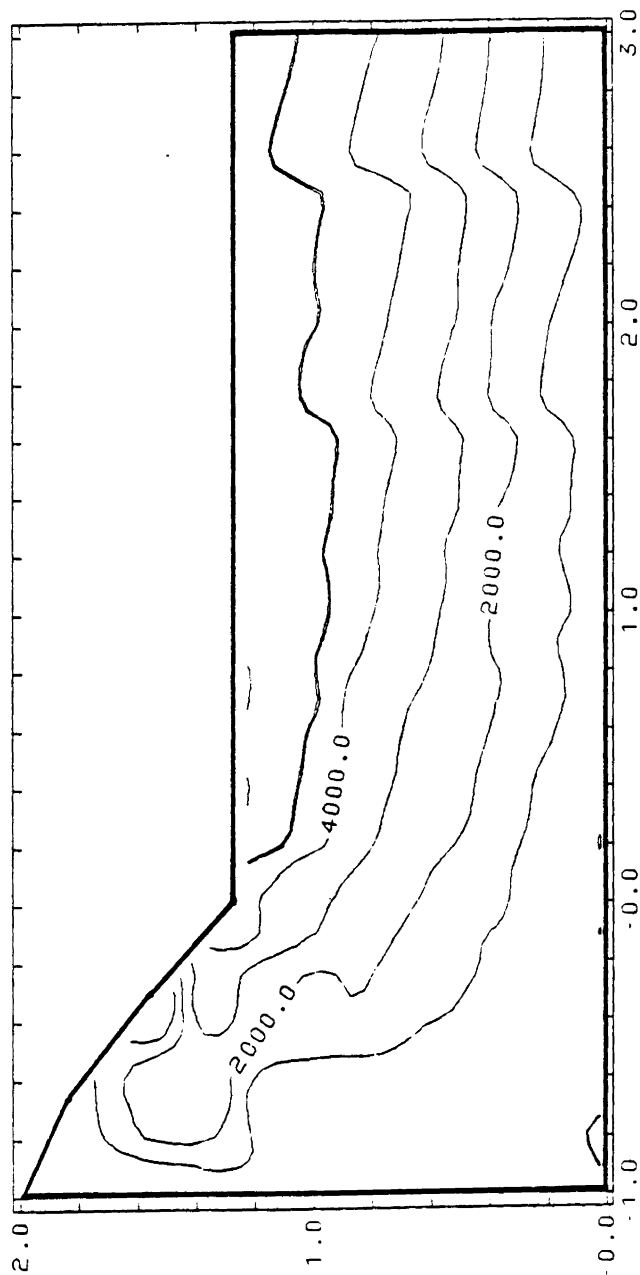


Figure 44. Contour Map of the Shear Stress τ_{12} for Styron 678 at 165°C:
C: Wall Shear Stress = 8.10 KPa.

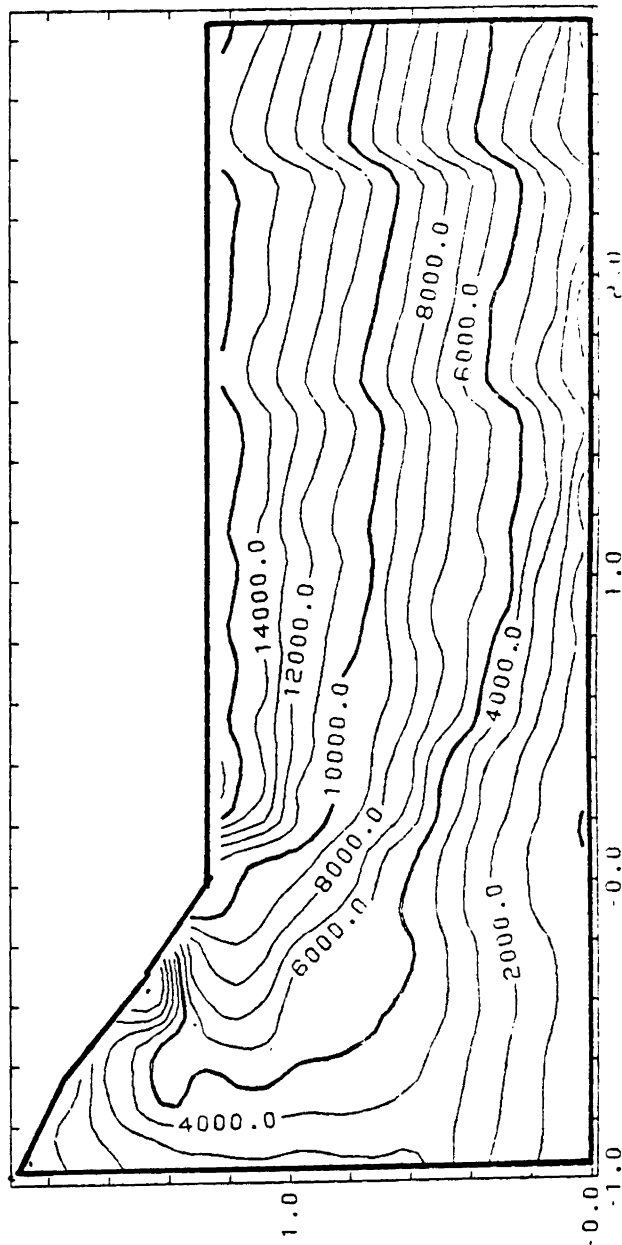


Figure 45. Contour Map of the Shear Stress τ_{12} for Styron 678 at 165 C: Wall Shear Stress = 15.3 KPa.

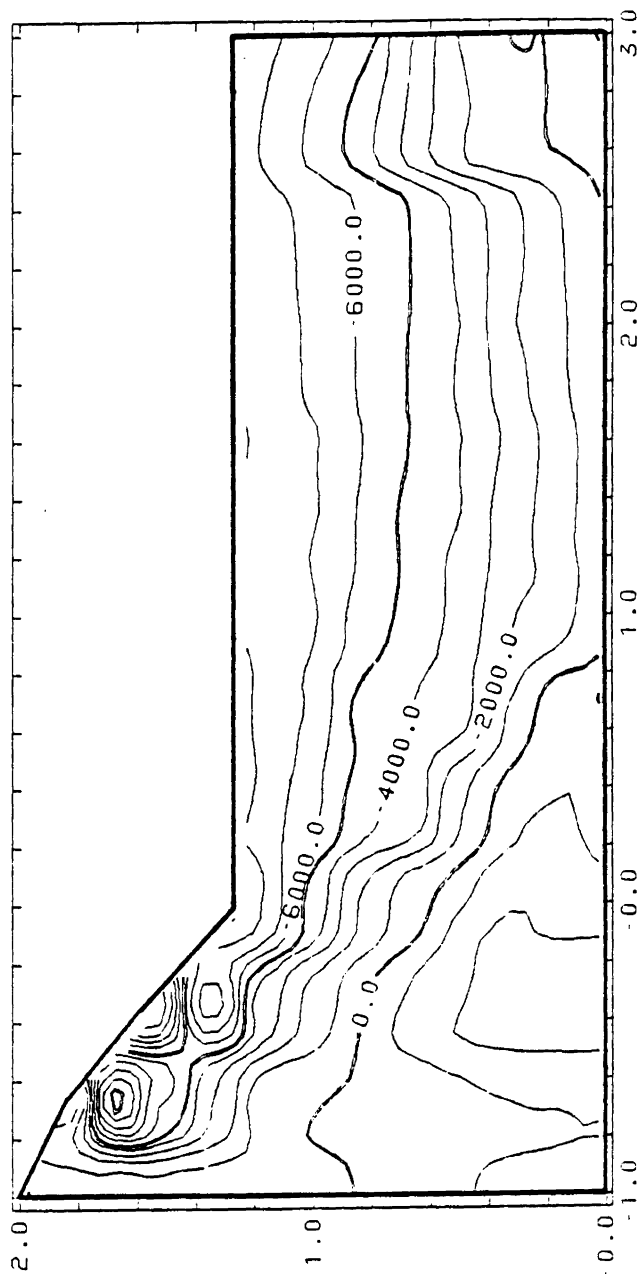


Figure 46. Contour Map of the Normal Stress Difference for Styron 678 (165°C): Wall Shear Stress = 8.10 KPa.

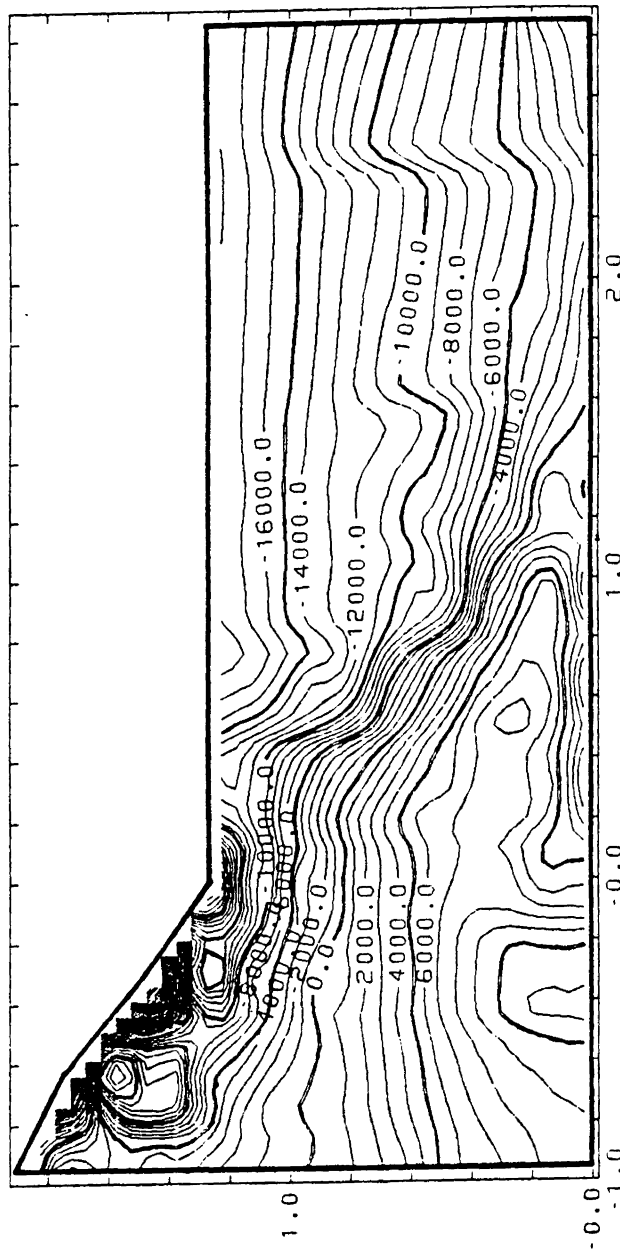


Figure 47. Contour Map of the Normal Stress Difference for Styron 678 (165 C): Wall Shear Stress = 14.3 KPa.

be important in the mathematical analysis presented in the next section. The first feature is the nature of the stress rearrangement near the die exit. As discussed in the previous section, the shear stresses concentrate along the corner. This results in larger stress gradients in the vertical direction near the corner. In fact, this gradient contributes to the magnitude of the exit pressure measured at the die exit. The magnitude of the dependence on the value of P_x is discussed in Section 5.5. The curvature in the stress contours also creates additional shear stress gradients along the axial direction of the die. This stress gradient will result in a pressure difference between the centerline and the stress acting normal to the die wall. Thus, a pressure difference from the centerline to the wall is created due to the rearrangement of the stress field before the exit plane.

The second important point in the shear stress results concerns the stress overshoot at the die lip. As discussed previously the die corner leads to a stress singularity as a result of a discontinuity between the boundary conditions inside and outside of the die. The results of the shear stress measurement of Styron 678 at $\sigma = 14.3$ KPa. showed that the shear stress values along the wall increased as the die exit was approached. The deviation of the shear stress from the value obtained in fully developed flow was measured by the dimensionless stress expressed by $f = \tau_{zy} / \tau_{wall}$ introduced by Boger and Denn [60]. Unfortunately, no measurements were attainable for the stresses at the die lip. A value of f greater than one represents stress overshoot behavior in the wall shear stress, τ_w . The values of f calculated from the shear stress shown in Figure 44 and 46 will be used in section 5.5 to evaluate the magnitude

for stress rearrangement contributions on the measurement of N_1 using equation (2.12) derived by Boger and Denn. Values of the normal stress difference $\sigma_{zz} - \sigma_{yy}$ measured experimentally using the linear stress optic rule are presented in the next section.

The behavior of the normal stresses $\sigma_{11} - \sigma_{22}$ also yields information as to the nature of the stress rearrangement near the die exit. Shown in Figure 45 and 47 are the stress distributions for shear rates of 0.17 and 0.39 s^{-1} . The normal stress distribution can be used to evaluate the magnitude of extensional gradients as the velocity profile rearranges from a fully developed velocity profile inside the die to the free surface jet outside the die. The normal stress quantities are made up of both viscometric normal stresses and extensional components. The steady shear contribution results from the elastic nature of polymer fluids and has a contribution which is negative in magnitude. The normal stresses in steady shear are proportional to $\dot{\gamma}^2$ at low rate of shear. Upstream from the die exit in undisturbed flow, the values of $\sigma_{11} - \sigma_{22}$ in Figures 45 and 47 are seen to increase regularly from zero along the centerline to a maximum at the wall. The regions in Figures 45 and 47 characterized by positive values of $\sigma_{11} - \sigma_{22}$ terms contain normal stresses due to velocity profile deceleration (positive contribution) which are larger in magnitude than the viscometric normal stress contribution. The overshoot behavior of the normal stresses at the die corner contains normal stress contributions from extensional flow gradients (negative contribution) in addition to the viscometric normal stresses.

A schematic of the fluid behavior in the exit region is shown in Figure 48 which would account for the normal stress difference behavior shown

in Figures 45 and 47. Fluid elements along the wall are stretched as the fluid accelerates to the final jet velocity. The conservation of mass requires that fluid elements decelerate along the centerline are subject to compressive forces which contribute to the positive magnitude of the normal stress results in the previous section. The results of the birefringence values of $\sigma_{zz} - \sigma_{yy}$ therefore support the velocity profile schematic shown in Figure 48.

The fact that the flow and the stress field in the exit region were not described by a steady unidirectional shear flow can have a significant effect on the validity of the use of the exit pressure technique to measure the viscometric normal stress N_1 . Since the flow in the exit region was not viscometric up to the die exit, it follows that the exit theory expression given by equation (2.14) may not be valid. The nature of the stress field predicts that additional terms due to stress derivatives in the axial direction will exist and may contribute to the value of N_1 calculated using the macroscopic balances developed in section 2.1.

In this section, the effect of the stress field rearrangement on the predictions of normal stresses using the exit pressure technique was qualitatively examined. The values of the stresses σ_{zy} and $\sigma_{zz} - \sigma_{yy}$ were calculated using the flow birefringence data presented in the previous section and the linear stress optic rule, equations (2.25) and (2.26). The shear stress field was shown to concentrate near the die corner. This created additional shear stress gradients in the axial direction and increased the magnitude of the shear stress gradient in the vertical direction. The nature of the velocity field rearrangement was modeled using a simple schematic presentation of the deformation history of a sample

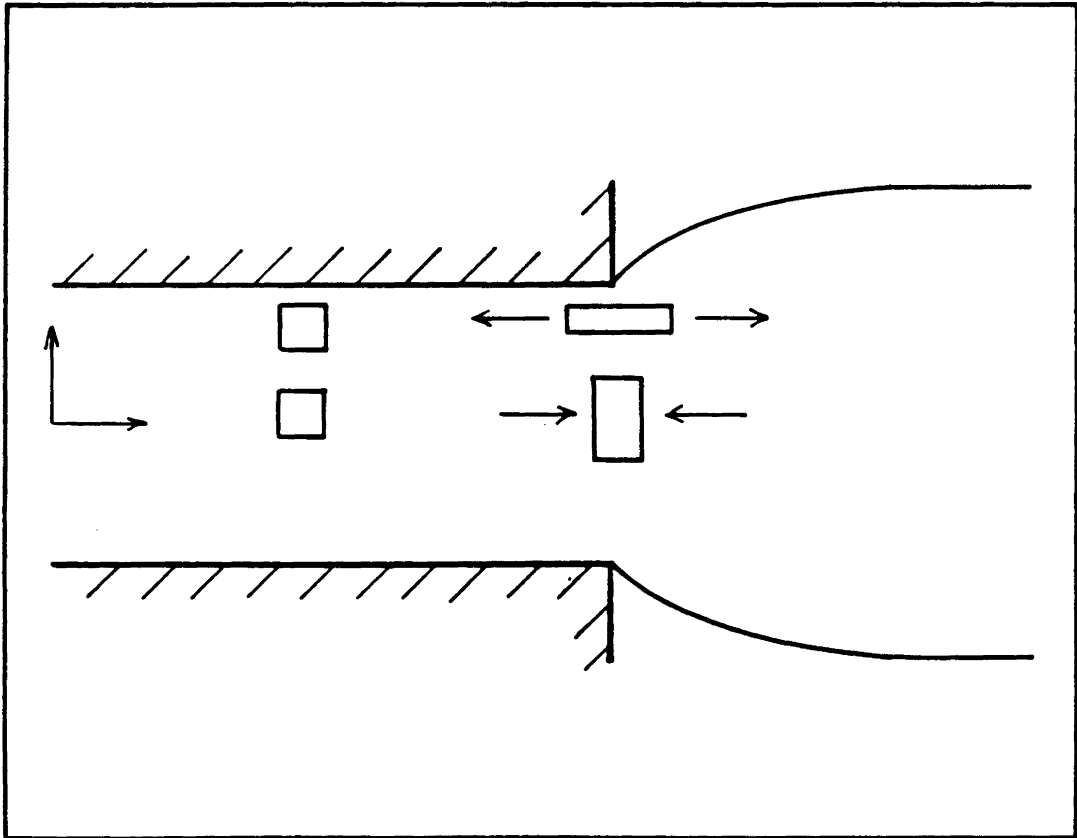


Figure 48. Schematic of the Deformation of Fluid Elements in the Exit Region

fluid element in the die exit region. The normal stress difference values calculated from the birefringence results were used to support the nature of the deformation of fluid elements along the wall and near the centerline of a slit die. The results presented in this section, however, were only qualitative in nature. The values of the stresses obtained using the linear stress optic rule can now be used to evaluate analytical expressions which calculate the contributions of shear and normal stresses to the exit pressure, evaluate the magnitude of stress rearrangement on the use of the exit pressure technique to measure N_1 , and to evaluate errors in the measurement of the pressure drop $\Delta P/\Delta L$ caused by the velocity field rearrangement at the die exit. In the next section the macroscopic momentum balance is used to obtain an analytical expression for calculating P_x from the stress field measurements (σ_{zy} and $\sigma_{zz} - \sigma_{yy}$).

5.5 EVALUATION OF TERMS WITHIN THE MACROSCOPIC MOMENTUM BALANCE

In this section the derivation of equation (2.14) will be examined in light of the birefringence results presented in the previous section. The critical assumption used in the exit pressure analysis for polymer melts is based in viscometric flow until the exit plane. The flow birefringence results have shown a stress field rearrangement from 0.3-1 die heights upstream of the die exit. Boger and Denn [60] proposed the use of a function f to express the deviation of the wall shear stress from that found in fully developed flow. The value of f has been evaluated from the birefringence results. The effect of this correction on the use of equation (2.14) is discussed.

Boger and Denn [60] have adapted an arbitrary function f to describe any deviation in the flow field at the die exit, where $f = \tau_{12} / \tau_w$. The form of the correction term is written as

$$L \tau_w \left(1 - \int_0^1 f(\epsilon; \tau_w, Re) d\epsilon \right) \quad (5.9)$$

The variable $\epsilon = z/L$ represents a dimensionless distance inside the die where the stress field deviates from steady unidirectional shear flow. The limits of integration correspond to the exit plane $z=0$ and the maximum distance upstream of the die $z=L$ where deviation from fully developed flow first occurs. The magnitude of this term should account for rearrangement effects which influence the measurement of N_1 . Once a functional dependence of f is obtained for a given material, the expression given by equation (5.9) is added to the stress contributions due to the exit pressure and the exit pressure derivatives to obtain the value of N_1 . The expression given in equation (5.9) does not however account for the influence on rearrangement effects on the value of P_x . The stress rearrangement effects on extrapolating the pressure profiles to the exit are discussed in section 5.7.

The magnitude of the correction term in equation (5.9) will be influenced by the rearrangement length L and the value of f in the integral term for a given shear stress. The results of the isochromatic patterns showed that the rearrangement length was not a strong function of the shear rate. For constant L , then, the correction term will be dominated by the value of the function f in the exit region. The dependence of the function f may be a function of the stress level, the Reynolds number,

and fluid elasticity. For the present investigation the function f would not be expected to depend on the Reynolds number since the inertial terms are negligible for the creeping flow of polymer melts. The form of the empirical expression for f may also depend on the details of the fluid rheology [60].

The value of f has been calculated in the present investigation using the results of the stress, σ_{12} , obtained from flow birefringence measurements. The shear stress at the wall was calculated at a series of locations upstream from the die corner. The values of f as a function of position are shown in Figure 49 for polystyrene melt. The lines drawn through the data points were used to clarify the behavior of f as a function of distance inside the die. The functional dependence of f as a function of distance inside the die is seen to vary for each of the shear stresses.

One aspect of the rearrangement function f which differed from the behavior shown in the isochromatic studies was the rearrangement length L . In the analysis in equation (5.9), the rearrangement length L represents the distance upstream in which the wall shear stress varies from the magnitude in fully developed flow. The exit region in section 5.4 was defined as the length where curvature in the isochromatic patterns first occurred. The extent of the deviation of the isochromatic patterns for increasing shear rates was approximately constant. The rearrangement length L measured by the function f , however, decreases steadily with shear rate as shown in Figure 49. The length L in Figure 49 was measured as the distance between the die exit $z = 0$ and the upstream distance where $f = 1$. This is due to the fact that L is measured by the behavior of the

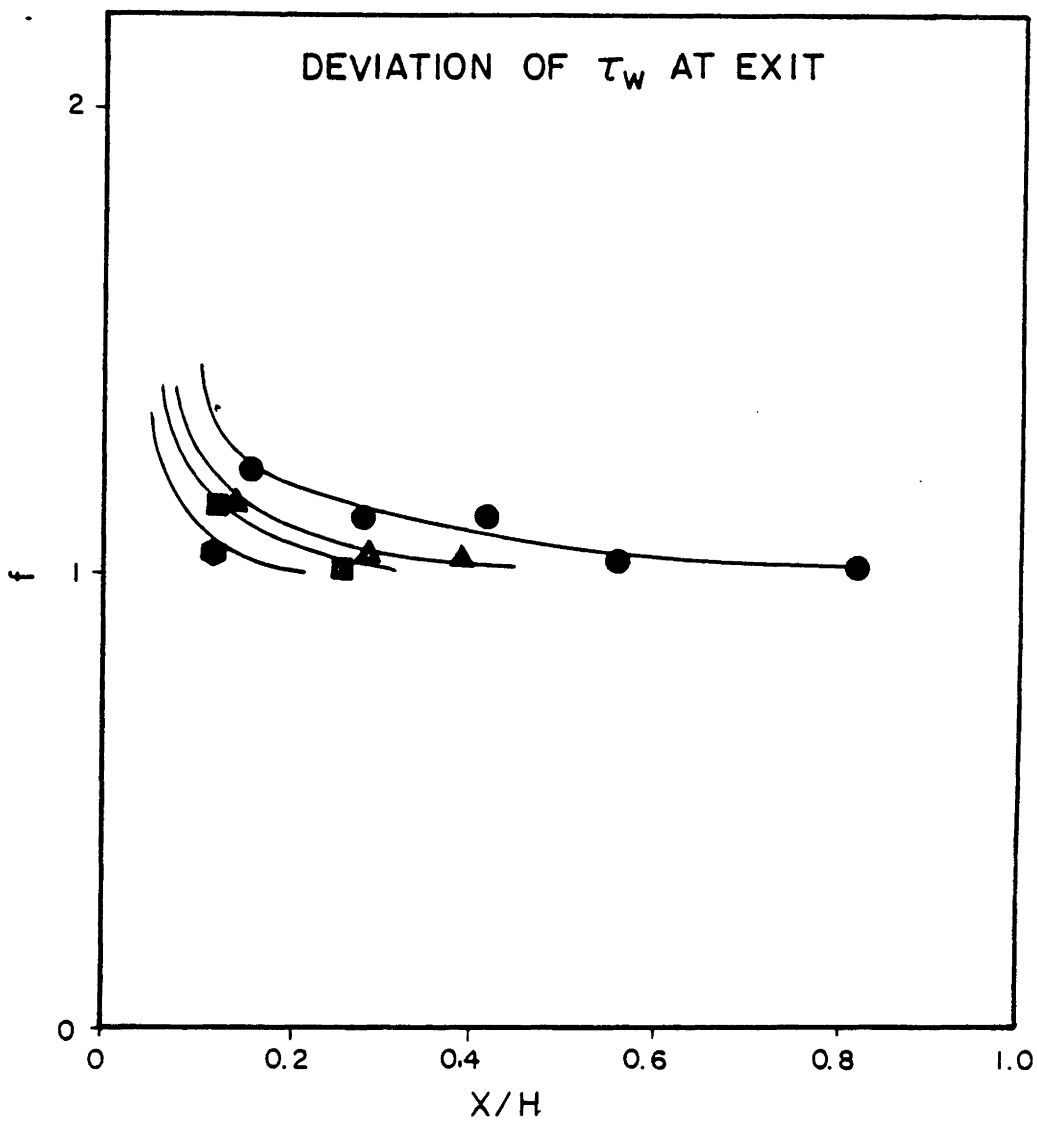


Figure 49. Comparison of the Rearrangement Function f : Styron 678 at 165 C using the results of the flow birefringence investigation. $\bullet$ $\sigma_w = 4.84$ kPa. $\blacksquare$ $\sigma_w = 8.10$ kPa. $\blacktriangle$ $\sigma_w = 10.86$ kPa. $\bullet$ $\sigma_w = 14.3$ kPa.

wall shear stress and the isochromatic patterns which contain contributions due to both shear and extension. The magnitude of the extensional gradients in the flow field increase with increasing shear rates while the length of the shear stress contribution decreased with shear rate. The overall exit region remains approximately constant with shear rate while the length L decreases with shear rate.

The value of the rearrangement correction in equation (5.9) corresponds to the area under the curve in Figure 49. For fully developed flow up until the exit region, the function f equalled one for all locations in the slit. This also corresponds to a zero rearrangement length L . The integral expression in equation (5.9) reduced to integrating a constant ($f=1$) over the dimensionless path length, ϵ . The value of the integral equals negative one, so the value of the entire expression in equation (5.9) yielded zero. The birefringence results showed that the function f was not single valued in the exit region. For each shear rate in Figure 49, the function f increased rapidly as the die corner is approached. This resulted from the stress overshoot behavior described in the previous section. Unfortunately, only the trend in f can be described. The value of f was not available at the die corner due to limitations in resolution of the full field birefringence apparatus. The magnitude of the function f at the corner was predicted to increase with increasing shear rate. The overshoot phenomena should behave similarly to polymer fluids undergoing a stress growth experiment. The overshoot behavior is due to the rapid change in the applied shear rate for a fluid element, which has a similar effect of an imposed time dependent stress field throughout the fluid. This dependence corresponds to the proposed

shear rate dependence proposed by Boger and Denn [60]. An estimate of the magnitude of the correction can be calculated by evaluating the integral expression in equation (5.9) using the values of f shown in Figure 49.

The magnitude of the rearrangement term is proportional to the area under the curves shown in Figure 49. The value of the integral can be calculated numerically given the function f . The value of the rearrangement term will vary with increasing shear rate since both the function f and the integration path L were seen to depend on the shear rate. The exact value of the integral, however, can not be explicitly obtained without the value of f at the die corner. Qualitatively, the area under the curves shown in Figure 49 increased with increasing shear rate. The magnitude of the total contribution in equation (5.9) will therefore reduce the value of the predicted normal stress N_1 due to the stress field rearrangement. In section 5.3, the normal stress values calculated from exit pressure measurements with viscometric flow assumed up to the exit were shown to overestimate the values of N_1 . The addition of equation (5.9) which accounts for stress rearrangement terms to equation (2.14) used to calculate N_1 will decrease the predicted value of N_1 . Also the magnitude of the correction term in equation (5.9) was qualitatively seen to increase in magnitude with increasing shear rate. In order to obtain reasonable agreement between cone-and-plate data and slit die data, the rearrangement terms must be included in the analysis.

The rearrangement term has been suggested to become negligible for shear rates greater than 10 s^{-1} [44]. This assertion was based on the examination of isochromatic patterns at low shear rates. The present

analysis suggests that even if the rearrangement length decreases with increasing shear rate, the stress rearrangement behavior in the shear stresses at the die exit may produce a substantial correction in the predicted value of N_1 . A more complete analysis of the magnitude of the shear stress behavior is required before the rearrangement terms are neglected.

5.6 ORIGIN OF THE EXIT PRESSURE

One of the objectives in the current investigation was the determination of the origin of the exit pressure in terms of the stresses found at the exit of a die. In this section the macroscopic momentum balance was used to express the pressure measured at the wall in terms of the shear stress and normal stress differences at the exit of a die. The expressions obtained were evaluated numerically using stress field data obtained from flow birefringence results and the linear stress optic rule. The magnitudes of the exit pressures were then compared to measured values of P_x obtained by means of extrapolated pressure profiles. Finally, the analytical expressions were used to qualitatively predict the exit pressure behavior for Newtonian and viscoelastic fluids.

An expression was derived to calculate the exit pressure from the macroscopic momentum balance taken over the control volume. The control volume and coordinate system were the same as used in the derivation presented in section 2.1. The flow field in the control volume was assumed to consist of steady state, laminar, incompressible flow. For polymeric fluids at low shear rates, the inertial contributions to the momentum balance were also assumed negligible. The complete derivation

of the exit pressure analysis for slit and capillary die flow is presented in Appendix B of this dissertation. The final expression for the pressure measured at the wall yielded

$$\Pi_{yy}(h,0) = \frac{1}{h} \int_0^L \tau_{zy}(h,z) dz - \frac{1}{h} \int_0^h (\Pi_{zz} - \Pi_{yy}) dy - \frac{1}{h} \int_0^h y \frac{\partial \tau_{zy}}{\partial z} dy \quad (5.10)$$

The stress terms $\Pi_{zz}-\Pi_{yy}$ and $\partial \tau_{zy} / \partial z$ in equation (5.10) were evaluated at the upstream boundary of the macroscopic momentum balance. The atmospheric pressure acting on the free surface jet was used as a reference pressure. A gauge pressure was used to measure the pressure inside the die where, $\Pi_{yy}(hj) = 0$ on the free surface far from the exit.

The pressure acting on the wall at any arbitrary distance upstream from the die exit can be evaluated using the results of equation (5.10). The exit pressure represents the total stress acting normal to the wall at the die exit. The exit pressure can therefore be evaluated from equation (5.10) as the length of the control volume L becomes zero. In the limit as the control volume length inside the die approaches zero, the first term on the right hand side of equation (5.10) becomes zero. The remaining two terms are evaluated at $z=0$ which is now located at the die exit plane. The pressure term $\Pi_{yy}(h,0)$ evaluated at this location is equivalent to the exit pressure, P_x .

The results of the previous analysis yield an expression for the exit pressure in terms of the normal stress field at the exit and rearrangement stresses created by the shear stress gradient along the flow direction:

$$P_x = - \frac{1}{h} \int_0^h (\Pi_{zz} - \Pi_{yy}) dy - \frac{1}{h} \int_0^h y \frac{\partial \tau_{zy}}{\partial z} dy \quad (5.11)$$

The same arguments can be made for the flow in a capillary die using the macroscopic momentum balances. The exit pressure in a capillary may be written as

$$P_x = - \int_0^R \frac{2}{R^2} [(\Pi_{zz} - \Pi_{rr}) + \frac{1}{2} (\Pi_{rr} - \Pi_{\theta\theta})] r dr - \frac{1}{R^2} \int_0^R \frac{\partial \tau_{rz}}{\partial z} r^2 dr \quad (5.12)$$

Equations (5.11) and (5.12) can be used to evaluate the origin and magnitude of the exit pressure for any fluid in a slit or capillary die.

The expressions derived in equations (5.11) and (5.12) can be used to assess the contributions of shear and normal forces in the magnitude of the exit pressure. The first term in equation (5.11) represents the pressure contribution due to normal stresses. For viscoelastic fluids, the normal stress contributions were composed of extensional gradient contributions and viscometric normal stresses. The magnitude of the extensional normal stress contributions can be separated from the viscometric normal stresses by comparing the magnitude of the integral evaluated at the exit region and evaluated in the fully developed flow region of the die. The difference in the normal stress difference contributions must be due either to extensional velocity components or stress overshoot behavior due to the sudden change in boundary conditions at the die exit. Based on the numerical results for inelastic fluids in this study and others [74,78], it is expected that the extra normal components were due to extensional flow gradients.

The second term in equation (5.11) is due to rearrangement in the stress field at or before the die exit plane. A shear stress gradient along the flow direction is created by acceleration or deceleration of fluid for the velocity profile inside the die to the final free jet velocity profile. The stress gradient is weighted by the vertical direction y . Stress rearrangement at the die corner was more heavily weighted than the stress gradient near the centerline.

From the examination of equation (5.11), the exit pressure is composed of two contributions. The first contribution is based on the viscometric normal stresses generated for viscoelastic fluids in steady shear flow. The second contribution is due to rearrangement effects at the exit plane of the die. The velocity field rearrangement causes both normal stress contributions due to velocity acceleration and deceleration and shear stress gradients along the centerline. Han et al. [4] has suggested the exit pressure is an indicator of fluid elasticity. The macroscopic momentum balance results confirm the hypothesis relating P_x quantitatively to N_1 only if the flow remains viscometric up to the exit plane. It has been shown, however, for polymer solutions by laser anemometry and for polymer melts using flow birefringence that the presence of stress field rearrangement upstream of the die exit. The normal stresses predicted using the exit pressure contain additional contributions due to stress gradients created by stress rearrangement inside the die.

Han [14] conducted an experimental investigation in which he compared the magnitude of the exit pressure obtained from a slit die and capillary rheometers. He reported the exit pressure $P_x(\text{slit}) = P_x(\text{capillary})$ for polymer melts. This evidence was then used to obtain an expression which

could be used to measure N_1 as a function of P_x in a capillary die. The theoretical expressions derived in equations (5.11) and (5.12) do not contain the same functional dependence of normal stresses for the two geometries. The value of P_x measured in a capillary die depends on $(\Pi_{zz} - \Pi_{rr}) + 1/2(\Pi_{rr} - \Pi_{\theta\theta})$ which is defined as $N_1 + 1/2 N_2$ in viscometric flow, while the value of P_x measured in a slit die varies as function of $(\Pi_{zz} - \Pi_{yy})$ or N_1 in viscometric flow. For viscoelastic fluids the macroscopic balance equations (5.11 and 5.12) predict the exit pressure to differ between slit and capillary dies. The variation between the two geometries will depend on the fluid rheology of the material. Tuna and Finlayson [101] compared numerically predicted exit pressure values for a convected Maxwell fluid. The values of $P_x(\text{capillary}) \neq P_x(\text{slit})$ for capillary and slit geometries and the difference between the two quantities increased with increasing wall shear stress. Based on the numerical results and the theoretical predictions from equations (5.11) and (5.12), the value of P_x for a given shear stress does depend on the geometry.

In this section an expression was derived which was used to evaluate the value of P_x from the stress field using a macroscopic momentum balance. the magnitude of the exit pressure is composed of contributions due to normal stresses (viscometric and elongational) and axial shear stress gradients. Equation (5.11) can be evaluated numerically from a knowledge of the stress field at the exit region of a die. In the next section the stress field evaluated using the stress optic rule will be used to calculate the contributions of shear and normal stresses to the value of P_x .

5.6.1 EVALUATION OF DERIVATIVES FOR P_x

The expressions derived in the previous section enable the direct calculation of the exit pressure given the stress field at the exit of the die. In this section the stress quantities found in equation (5.11) for a slit die will be evaluated using the results of the flow birefringence investigation. The stress derivatives found in equation (5.11) were calculated by finite difference approximations. The integral expressions were then evaluated using Simpson's rule. The values of the integral terms in equation (5.11) can then be used to evaluate the contributions of the viscometric stresses and exit effects on the exit pressure.

In calculating P_x from the macroscopic balance equation, the integration in equation (5.11) was evaluated using Simpson's rule for the stress field calculated from the flow birefringence results. The integration paths contained equally spaced mesh points from the slit centerline ($y=0$) to the wall ($y=h$). The stress gradient found in the second term of equation (5.11) was evaluated using a first order finite difference approximation described by equation (5.19). The values of the normal stress differences and the stress gradients calculated at the exit plane are summarized for each of the four shear stress levels investigated in Appendix A. Also presented in Appendix A are the magnitudes of the exit pressure P_x and the relative contributions to the exit pressure due to the normal and shear stresses.

The contributions to the final P_x value from each of the two terms of equation (5.11) are shown in Table 5.1 for Styron 678 at 165°C. The

data was obtained for wall shear stress values of 4.84, 8.10, 10.86 and 14.3 KPa ($0.1 \leq \dot{\gamma} \leq 0.45$). For comparison purposes an additional value for P_x (undisturbed) has been included which represents the value of P_x calculated using equation (5.11) assuming viscometric flow continues up to the exit region. The values of $\Pi_{zz} - \Pi_{yy}$ were taken as equal to the normal stress N_1 found in the undisturbed region upstream from the die exit.

A comparison between the P_x values predicted by equation (5.11) and the P_x values obtained from the assumption of viscometric flow showed a lack of agreement caused by assuming a fully developed velocity field up to the die exit. The cause of the disagreement was reflected in the magnitude of the second term in equation (5.11) due to shear stress gradients along the flow direction. The presence of stress field rearrangement upstream of the die exit caused a significant reduction in the predicted value of P_x . The magnitude of the exit pressure was reduced by 75% compared to the value of P_x calculated assuming viscometric flow for $\sigma_w = 10.86$ KPa. The magnitude of exit disturbances can be evaluated by comparing the contributions to the value of P_x with and without an undisturbed stress field at the exit.

The shear stress gradient $\partial\tau_{zy} / \partial z$ was created due to the stress concentration near the die corner. The "bending" of the shear stress contours created a stress gradient in the z direction which was negative in sign. The results of the numerical integration of the shear stress term in equation (5.11) yielded a positive contribution to the exit pressure. The shear stress rearrangement contributed an additional positive contribution which resulted in a calculated exit pressure greater

Table 5.1

Evaluation of the Exit Pressure From Flow Birefringence
Results. Styron 678 at 165°C

Wall Shear Stress [KPa]	Normal Stress Contribution [KPa]	Shear Stress Contribution [KPa]	Px [Pa]	Px Undisturbed [Pa]
4.84	-230	600	370	4040
8.10	1425	2310	3735	7290
10.86	-1425	3472	2045	8790
14.3	-3395	4110	720	16300

than obtained if the shear stress rearrangement term was neglected. The magnitude of the shear stress contribution is shown in Table 5.1. For the shear stress levels investigated, the shear stress term contributed approximately 60% or more to the value of P_x . Based on these results, the shear stress rearrangement can not be neglected from calculations using the exit pressure as a quantitative material parameter indicative of fluid elasticity. The magnitude of the exit pressure calculated using equation (5.11) was dominated by shear stress rearrangement contributions and not viscometric normal stresses as suggested by Han [4].

The magnitude of the normal stress contributions to the exit pressure are calculated from the first term in equation (5.11). As discussed in the previous section, the term $\Pi_{zz} - \Pi_{yy}$ contains contributions due to the viscometric normal stresses and elongational flows. In Table 5.2 is shown the values of $\Pi_{zz} - \Pi_{yy}$ for a wall shear stress value of 8.10 KPa. The magnitude of the normal stresses changes sign from positive values near the centerline to negative contributions near the wall. The presence of positive and negative normal stresses caused cancelation of effects in the integral expression found in equation (5.11). Due to the negative sign on the first term in equation (5.11), the positive normal forces shown in Table 5.2 have a negative contribution to the exit pressure.

The contributions of viscometric normal stresses and elongational components to the normal stress difference $\Pi_{zz} - \Pi_{yy}$ were compared by examining the magnitude of the first term in equation (5.11) evaluated using normal stress values obtained by flow birefringence in the die exit and in the undisturbed flow region. The difference between N_1 values found in undisturbed flow and the observed values of $\Pi_{zz} - \Pi_{yy}$ at the exit

Table 5.2

Normal Stress Contributions at the Exit Plane Styron 678
at 165°C $\sigma_w = 8.10$ KPa

Y-coordinate [mm]	$\pi_{zz}-\pi_{yy}$ Exit Plane [Pa]	N1 Undisturbed Flow [Pa]	Extensional Contributions [Pa]
0	1381	0	1381
0.1671	1298	-1236	2536
0.3342	1919	-2162	4081
0.5013	853	-4016	4869
0.6684	-433	-4942	4509
0.8356	-1889	-5869	3980
1.0027	-4546	-6796	2250
1.1698	-7947	-7414	-533
1.27	-9241	-8031	-1210

may represent normal force contributions due to elongational flow. In Table 5.2 is shown the results of the normal stress contribution for a wall shear stress for Styron 678 at $\sigma_w = 8.10$ KPa. The viscometric normal stresses, N_1 , vary from zero along the centerline ($\dot{\gamma} = 0$) to a maximum value at the wall as the shear rate varies across the slit. The magnitude of the extensional contribution changes sign from positive (compression) values along the centerline to negative values (tension) near the wall. These results agree with the predicted flow field rearrangement from numerical simulations and the birefringence results of Arai and Hatta[50]. The magnitude of the extensional contributions found in Table 5.2 are only qualitative in nature as the velocity gradients at the die exit plane are not known. The magnitude of the contributions due to extensional and shear components can not be separated because the velocity field rearrangement may alter the values of the velocity gradients found in the rate of deformation tensor.

Contrary to the shear stress rearrangement terms, the presence of rearrangement of the stress field upstream of the die exit reduced the contribution of the normal stress difference to the value of P_x . The values of P_x assuming viscometric flow up to the die exit in Table 5.2 were significantly greater than the value of P_x predicted using the normal stress distribution calculated at the die exit from the flow birefringence. Rearrangement effects reduced the normal stress contribution of equation (5.11) by approximately 80 percent compared with the exit pressure predicted neglecting exit effects based on the values of the normal stresses $\Pi_{zz} - \Pi_{yy}$ presented in Table 5.1.

Analysis of the birefringence results using equation (5.11) derived from a macroscopic momentum balance revealed that the origin of the exit pressure contains significant contributions due to stress field rearrangement at the exit plane of a slit die. The argument that the value of the exit pressure is due to viscometric normal stresses generated in shear flow was seen to be incorrect. The stress contributions to the value of P_x due to extensional gradients and shear stress gradients contributed the majority of the residual stresses exhibited at the die exit plane. Based on these results, the exit pressure technique used to measure quantitative values of N_1 based on the value of P_x must be critically examined. The magnitude of the exit pressure was proportional to the value of the normal stress difference $\Pi_{zz} - \Pi_{yy}$ at the die exit plane, but the normal stress contributions which contribute to P_x were made up of contributions from normal stresses generated in shear flow and additional stresses created by the velocity field rearrangement. The use of P_x containing significant contributions due to non-viscometric stresses should not be used to evaluate the primary normal stress difference based on P_x obtained assuming viscometric flow of fluid through a die based on the magnitude of the stress contributions evaluated for polystyrene for the shear rate range $0.1 \leq \dot{\gamma} \leq 0.4 \text{ s}^{-1}$.

Han [44] has argued that above a critical shear rate the exit rearrangement effects are negligible. This argument was based on the decreased rearrangement length observed from flow birefringence isochromatic patterns in polymer melts. Tuna and Finlayson [101] also reported the velocity profiles remain more fully developed as the elasticity of the fluid increased using a finite element simulation.

While the measurement of N_1 using equation (2.14) does depend on a rearrangement length, through the function f , the magnitude of the residual stresses acting on the wall (P_x) is not influenced by the length of the exit region. The integral expressions in equation (5.11) are evaluated at the exit plane and do not contain contributions dependent on the length of the disturbance upstream from the die exit. Any rearrangement in the stress field prior to the die exit may significantly affect the predicted value of P_x . Neglecting rearrangement effects at the die exit yielded significantly different values of P_x evaluated from the flow birefringence results in section 5.4. The use of P_x based on viscometric flow up to the exit to predict viscometric normal stresses will therefore be in error. An additional error due to rearrangement affects the pressure drop near the exit region. This influences the extrapolated value of P_x by introducing an additional pressure drop contribution due to the stress field rearrangement. The extrapolated exit pressure calculated based on the pressures found in the undisturbed flow region does not account for this additional pressure drop. The extrapolated value of P_x will therefore contain an additional error since the ΔP due to stress rearrangement can not be measured with flush mounted pressure transducers. This error is discussed in section 5.7.

5.7 EVALUATION OF TERMS FROM THE EQUATIONS OF MOTION

In this section the equation of motion will be used to derive an expression which may be used to calculate the pressure drop ΔP for an arbitrary flow field in a slit die. The flow birefringence results σ_{zy} and $\sigma_{zz} - \sigma_{yy}$ will be used to evaluate the expression for ΔP derived from the

equation of motion. This expression may be used to evaluate the magnitude of the effects of velocity field rearrangement on the pressure profile used in the calculation of the extrapolated exit pressure. This equation is derived in the first section. The pressure drop equation is then evaluated using a finite difference approximation to calculate stress gradients from stresses obtained from flow birefringence. Possible errors in calculating P_x from extrapolating the pressure profiles are then discussed in light of these results. A second equation is derived from the equation of motion which is used to evaluate the change in total pressure from the centerline to the wall. The magnitude of this term is important as a possible contribution to die swell in viscoelastic fluids.

5.7.1 PRESSURE DROP IN AN ARBITRARY FLOW FIELD

This section will use the equations of linear momentum to express the pressure measured at the wall by a pressure transducer, P_i , in terms of the stress gradients present in the flow field of a slit die. The objective is to obtain an expression relating P_1 and P_2 , the pressure at two arbitrary locations along the wall, and the shear stress τ_{12} and normal stresses $\tau_{11} - \tau_{22}$. The shear and normal component contributions which alter the pressure gradient were identified by evaluating the magnitude of the terms in equation (5.17) using the values of the stresses obtained from the flow birefringence results in section 5.4.

The following definitions were used in the derivation for an arbitrary flow field in a slit die:

$$\Pi = P\delta + \tau \quad (5.13)$$

$$P_{trans.} = (n \cdot \Pi_{yy}) \cdot \delta y \quad (5.14)$$

The coordinate system was the same as presented in Figure 3. The flow direction was identified using subscript (z) and the vertical velocity gradient was identified as subscript (y). The derivation assumed a steady state, laminar, incompressible, pressure driven flow between infinite parallel plates. The second component of the equation of motion is then

$$-\frac{\partial \tau_{zy}}{\partial y} = \frac{\partial \Pi_{zz}}{\partial z} \quad (5.15)$$

The normal stress difference is obtained by adding an identity to both sides of equation (5.15).

$$-\frac{\partial \Pi_{yy}}{\partial z} - \frac{\partial \tau_{zy}}{\partial y} = \frac{\partial \Pi_{zz}}{\partial z} - \frac{\partial \Pi_{yy}}{\partial z} \quad (5.16)$$

The normal stress measured along the wall is obtained by solving for the total stress Π_{yy} term on the left hand side. The equation is then integrated with respect to the z coordinate from 0 to L to obtain the final result. The derivative expressions are evaluated at $y = h$ to obtain the normal stress acting along the wall.

$$\Pi_{yy} - \Pi_{yy} = \int_0^L \frac{\partial(\Pi_{xx} - \partial \Pi_{yy})}{\partial z} dz + \int_0^L \frac{\partial \tau_{zy}}{\partial y} dz \quad (5.17)$$

This expression can be used to evaluate the pressure drop in a slit die containing velocity gradients in the z direction. No assumptions of the velocity field were made in the development of equation (5.17).

The error in a linear extrapolation procedure used to calculate the exit pressure will be obtained by comparing the pressure drop predicted by equation (5.17) with the pressure drop for steady pressure driven flow in a slit. Equation (5.17) was derived for an arbitrary region $z = 0-L$ in a slit die. The results predicted in equation (5.17) simplify to steady pressure driven flow if the region $z=0-L$ is located in the fully developed flow region. For steady shear flow equation (5.17) reduced to the following

$$\Delta P = \tau_w 2 L / H \quad (5.18)$$

The first term in equation (5.17) is not present for steady pressure driven flow as there are no stress gradients in the z direction. If the integration path $z = 0-L$ is now taken to lie in the exit region, the rearrangement of the stress field in anticipation of the die exit will now contribute an additional pressure loss to the total pressure drop, ΔP .

The pressure difference ΔP in the exit region is composed of two contributions. The first term is due to the shear stress gradient $\partial \tau_{zy} / \partial y$. For steady unidirectional shear flow this term is zero. The exit region however contains an overshoot in the shear stress at the corner and a concentration of the shear stresses near the die lip. The value of the shear stress term τ_{zy} will become a function of both the axial and vertical direction, $\tau_{zy} = \tau_{zy}(z,y)$. The second contribution to the exit pressure is due to a normal stress gradient which may be due to extensional flow along the die walls. The magnitude of the stress gradients are qualitatively examined by inspecting the results of the flow

birefringence investigation. These results are presented in the next section.

5.7.2 STRESS PROFILES IN THE EXIT REGION

In this section the stress field found in the exit region is examined with emphasis on the stress gradients found in equation (5.17) developed in the previous section. In Figures 50 and 51 are shown the dimensionless shear and normal stress profiles for polystyrene for different axial distances upstream from the die exit. The slope of each line evaluated at $y/H = 0.5$ is proportional to the slope $\partial\tau_{12} / \partial x_2$ required in equation (5.17). Each curve in Figures 50 and 51 represented the value of the stresses obtained from the flow birefringence results as a function of the dimensionless distance from the exit of the die. The straight line drawn in Figure 50 represents the constant shear stress profile which exists in a fully developed velocity field for pressure driven flow.

The evaluation of the shear stress term in equation (5.17) required the calculation of shear stress gradients at the wall for a series of distances along the flow direction. The deviation from linear behavior of the stress profiles pictured in Figures 50 and 51 represents additional contributions to the pressure drop ΔP due to the concentration of shear stress contours near the die corner. Lines were drawn through the data points to clarify the behavior for the different distances from the exit of the die. The magnitude of the shear stress contribution was dependent on the length of the shear stress rearrangement and the magnitude of the shear gradient evaluated at the wall.

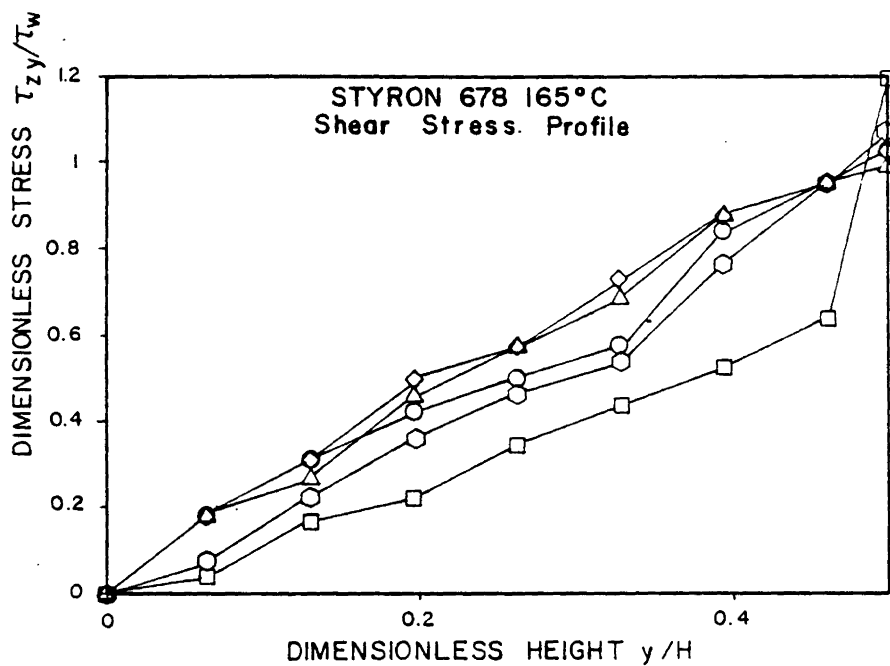


Figure 50. Dimensionless Shear Stress Profiles in the Exit Region: Styron 678 at 165°C for $\sigma_w = 8.10$ KPa. Stress variation from the centerline to the wall.

Dimensionless axial coordinate measured from the die exit. ($\square$) - 0.0 ($\odot$) - 0.278 ($\circ$) - 0.555 ($\triangle$) - 0.8333

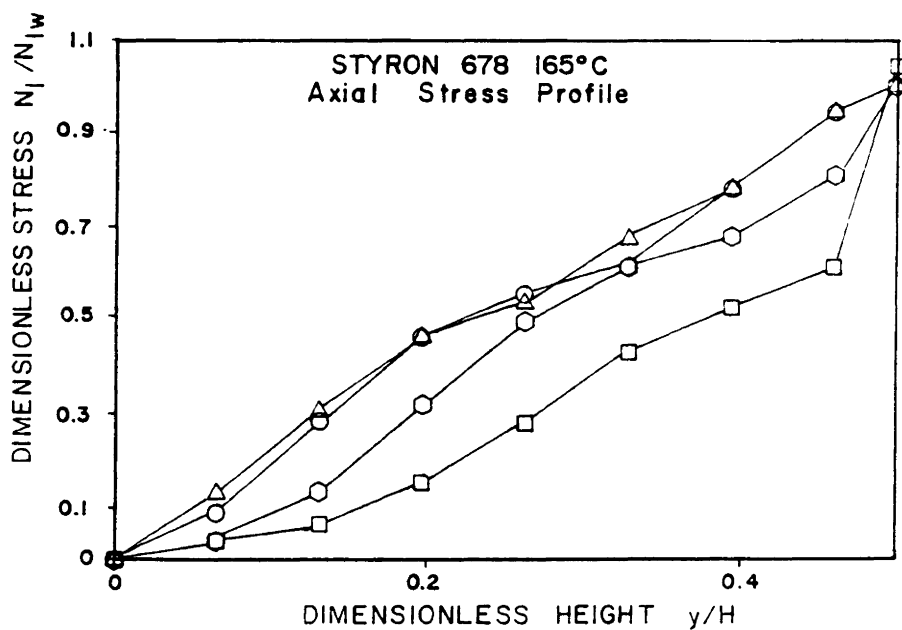


Figure 51. Dimensionless Normal Stress Profiles in the Exit Region: Styron 678 at 165°C for $\sigma_w = 8.10$ KPa. Stress variation from the centerline to the wall.
Dimensionless axial coordinate measured from the die exit. ($\square$) - 0.0 ($\diamond$) - 0.278 ($\circ$) - 0.555 ($\triangle$) - 0.8333

The second contribution to the pressure drop in equation (5.17) is due to the change in the normal stress differences, $\sigma_{zz} - \sigma_{yy}$, along the flow direction. Axial profiles of the normal stresses along the wall are shown in Figure 52 for Styron 678 at 165°C for $\sigma_w = 8.10$ and 10.86 KPa. The gradient $\partial(\sigma_{zz} - \sigma_{yy}) / \partial z$ is proportional to the slope of the curves at each point along the flow direction. The behavior of the normal stresses at the die exit behave similarly to the results of the shear stress gradients. The slope of the curves increases near the die corner. The acceleration of fluid along the wall near the die exit creates an additional contribution to the magnitude of the normal stresses. The magnitude in the normal stress overshoot behavior was seen to increase as the shear rate increases. The comparison of the two curves in Figure 52 shows a larger slope for $\sigma_w = 10.86$ KPa in the region where the data points overlap.

From the above results it is apparent that the rearrangement in the exit region of an extrusion die alters the predicted pressure drop from the pressure drop predicted for steady pressure flow. The origin of these additional stress components due to the stress rearrangement terms found in equation (5.17). The relative magnitude of the rearrangement terms are compared in the next section by evaluating the integral expressions numerically. The significance of these results are then assessed by comparing pressure drop error to exit pressure measurements obtained by extrapolating the pressure profiles.

5.7.3 EVALUATION OF INTEGRALS

The evaluation of the integral expressions in equation (5.17) required

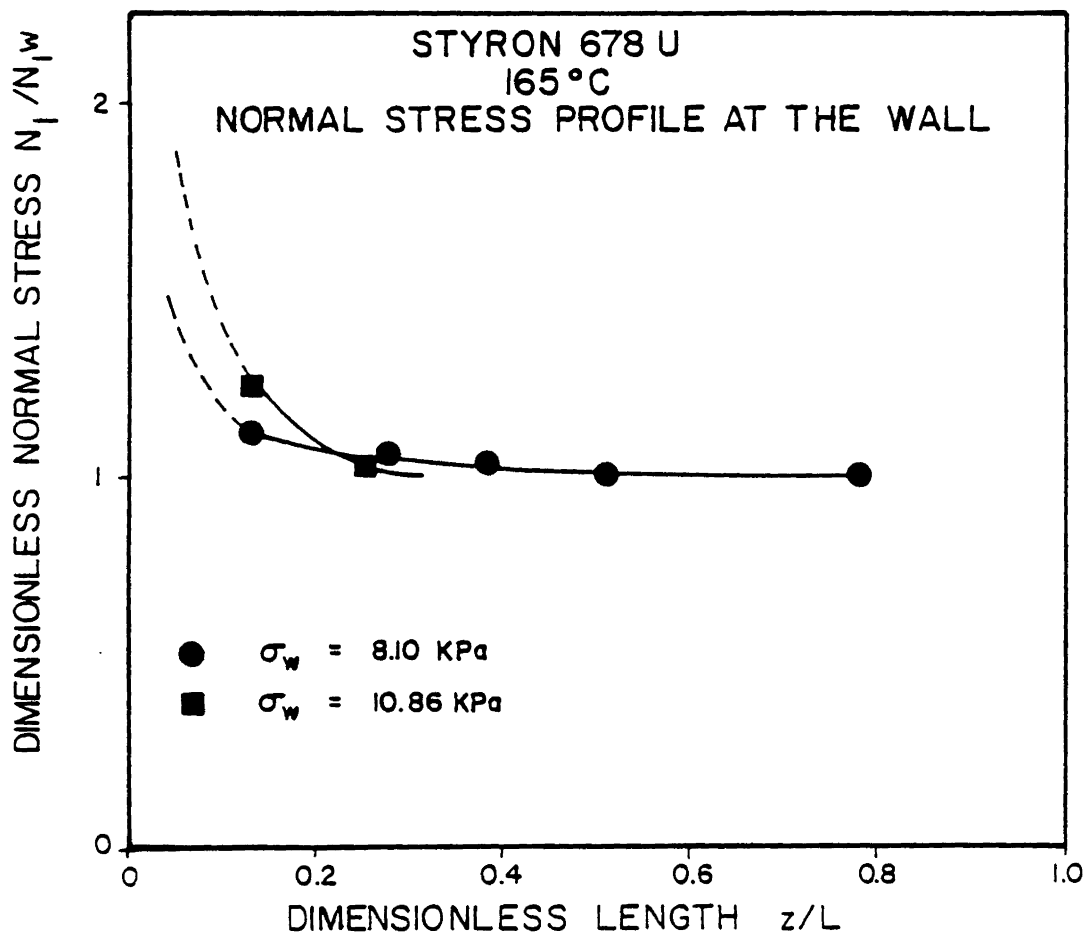


Figure 52. Dimensionless Normal Stress Profiles in the Exit Region: Styron 678 at 165°C. Stress variation along the length of the die measured at the wall.

the evaluation of the stress derivatives from experimental data and then numerical integration of the resulting stress derivatives. The derivatives were calculated using a finite difference approximation based on a mesh of experimental data points. A first order finite difference approximation having the following form was used.

$$\frac{u_n - u_{n-1}}{h} \quad (5.19)$$

where h represents the length between the two data points, $h = x_i - x_{i-1}$. The derivative $\partial \tau_{zy} / \partial y$ was calculated using the shear stress measured at the wall and the data point located nearest the wall. The mesh used for the data points was the same used in the calculation of the stresses presented in section 5.4. The data points were located at equally spaced intervals from the die exit. The integral expressions were evaluated using Simpson's rule.

The calculated value of the terms in equation (5.17) are presented in tabular form for $\sigma_w = 10.86$ KPa. In Table 5.3 are shown the values for the pressure drop ΔP calculated at the exit of the slit die rheometer. The integration path length L was taken as the rearrangement length calculated from the disturbance observed in the stress field upstream of the die exit. The contributions for each term in equation (5.17) are listed separately. The total value of the pressure drop obtained is then compared with the pressure drop for calculated assuming undisturbed flow to the exit.

The results of the integral calculations shown in Table 5.3 can be used to evaluate the relative contribution of shear and normal stresses

Table 5.3

Pressure Drop at the Exit Region of the Slit Die
Calculated Using Flow Birefringence Data Results. Styron
678 at 165°C

Wall Shear Stress [KPa]	Normal Stress Contribution [Pa]	Shear Stress Contribution [Pa]	ΔP [Pa]	ΔP Undisturbed [Pa]
4.84	-730	10600	9870	6780
8.10	-760	12450	11690	9400
10.86	-2900	19945	17045	13975
14.3	-6650	32180	25830	23700

on the magnitude of the pressure drop, ΔP . Comparison of the results in Table 5.3 shows that the normal stress contribution is opposite in sign from the shear stress component. The negative value of the normal stress terms has a negative contribution to the total pressure drop. The magnitude of the normal stress term in each case is - (0.06-0.2) times the pressure drop in the exit region. The shear stress contribution was the dominant factor in the total pressure drop calculated from the flow birefringence results using equation (5.17).

The significance of the stress rearrangement contribution on the calculation of the extrapolated exit pressure was assessed by comparing the pressure losses calculated using equation (5.17) to the extrapolated exit pressure obtained from the slit die rheometer. In Table 5.4 are shown the results of the extrapolated exit pressure obtained by the slit die rheometer compared to the pressure drop error due to stress rearrangement upstream of the die exit. The pressure drop error term ΔP_{error} is the difference between the total pressure drop calculated using equation (5.17) and the pressure drop ΔP obtained by assuming steady viscometric flow in the slit. The pressure drop error in the exit region was approximately constant for the shear stress measured. The magnitude of the error was on the order of ± 6 KPa in polystyrene for $\sigma_w = 14.3$ KPa. This error represents approximately 40 % of the value of P_x for this shear stress. The error due to stress rearrangement in P_x is therefore significant at low shear rates and has not been previously addressed. The significance of this error term compared to the value of P_x decreased with increasing shear rate. The magnitude of this error at higher shear rates will depend on the magnitude of the disturbance in the stress field inside

Table 5.4

Comparison of the Value of P_x With the DP Error Due to
Stress Rearrangement at the Die Exit.
Styron 678 at 165°C

Wall Shear Stress [KPa]	P_x [Pa]	ΔP_{error} [Pa]
4.84	230	3090
8.10	6775	2290
10.86	13000	3070
14.3	15000	2130

the die as the shear rate increases. This error has not been taken into account in previous experimental investigations which reported exit pressure results for viscoelastic fluids. Current extrapolation techniques used to calculate P_x can not account for the larger pressure drop exhibited in the exit region due to velocity profile rearrangement. At low shear rates the stress rearrangement can introduce significant error into the measurement of P_x obtained by extrapolating the pressure profiles to the exit of the die.

In this section the equation of motion was used to derive an expression for the purpose of calculating the pressure drop in the slit die. The equation of motion can also be used to derive an expression which may be used to calculate the pressure difference from the slit centerline to the pressure at the wall. In the next section, the equation of motion will be used to calculate the magnitude of the term $\Pi_{yy} \text{ wall} - \Pi_{yy} \text{ centerline}$ for flow in the exit region of a slit die. This pressure difference may contribute to the die swell observed in the extrusion of viscoelastic materials.

5.8 STRESS DISTRIBUTION FROM THE CENTERLINE TO THE DIE WALL

In this section the magnitude of the normal stress component Π_{yy} will be investigated using an analytical expression derived from the equation of motion. The objective of this section was to evaluate the value of normal stress gradients from the slit centerline to the wall of the die. The magnitude of this pressure drop can be used to assess the deviation in the shear stresses from viscometric flow in the exit region. The presence of a non-zero pressure gradient in the vertical direction may

also be used in the analysis of die swell behavior in viscoelastic fluids. The results of the flow birefringence investigation using the linear stress optic rule can be used to evaluate the magnitude of $\Pi_{yy}(h,L) - \Pi_{yy}(0,L)$ in a slit die.

The expression relating the stress difference $\Pi_{yy}(h,z) - \Pi_{yy}(0,z)$ to the stress distribution in the exit region is obtained from the equation of motion.

$$\Pi_{yy}(h,z) - \Pi_{yy}(0,z) = - \int_0^h \partial \tau_{zy} / \partial z \, dy \quad (5.20)$$

The pressure difference is evaluated by integrating the shear stress gradient $\partial \tau_{zy} / \partial z$ from the centerline to the wall. If the axial coordinate z is chosen in the viscometric flow region, the shear stress gradient along the die is zero. Therefore, for fully developed flow, the total stresses components are constant along the integration path, $\Pi_{yy}(h,z) = \Pi_{yy}(0,z)$. If, however, the shear stress changes in the z direction, such as in the exit region of the die, the normal component Π_{yy} may vary as a function of the y coordinate.

The magnitude of the normal stress difference in equation (5.20) was evaluated using the flow birefringence results for Styron 678 at 165°C. The shear stress gradients were calculated using a finite difference approximation and the integral expression was evaluated using Simpson's rule. In Table 5.5 is shown the shear stress gradients and pressure differences evaluated using equation (5.20) and the stress field obtained from the flow birefringence measurements. The values of the stress difference $\Pi_{yy}(h,z) - \Pi_{yy}(0,z)$ were positive and increased in magnitude with

Table 5.5

$P_{\text{wall}} - P_{\text{centerline}}$ Results
Styron 678 at 165°C

Wall Shear Stress [KPa]	$\pi_{yy}(h,z) - \pi_{yy}(0,z)$ [Pa]
4.84	1350
8.10	2800
10.86	4060
14.3	5790

increasing wall shear stress. The increasing magnitude of the pressure difference suggest the magnitude of the exit disturbance at the exit plane increased with the wall shear stress. These results also suggest that rearrangement effects do not become negligible above a critical shear rate.

The presence of a pressure gradient from the centerline of the slit to the wall can contribute to the magnitude of the die swell phenomena observed in viscoelastic fluids. The positive pressure drop observed for the Styron 678 melt suggests that the stress rearrangement upstream of the die exit created a pressure drop which acts to retard the swelling of the polymer as it exits the die. Similar results using flow birefringence have been reported by Arai and Hatta [50] for the flow of a high density polyethylene melt from a slit die. Arai and Hatta reported a reduction of approximately 15% in the dimensionless normal stresses from the wall to the centerline. They also reported that the same pressure drop changes sign outside of the die. The rearrangement of the velocity field outside of the die created a pressure gradient which increased swelling.

In sections 5.6 and 5.7, the stress field distribution obtained from the flow birefringence investigation and the linear stress optic rule was used to quantitatively evaluate the magnitude of the exit pressure, P_x , the pressure drop in a slit die, ΔP total, and $\Pi_{yy}(h,z) - \Pi_{yy}(h,0)$ for flow in a slit die. The magnitude of these quantities were used to evaluate the magnitude and significance of stress field rearrangement at the exit of a slit die. In the next section the results of the numerical investigation analyzing the stress field behavior at the die exit will

be presented. The mixed penalty method finite element formulation can be used to directly analyze the flow behavior at the die exit using the velocity and stress fields obtained from the numerical simulation. The numerical technique can be used to separate the effect of elasticity on the stress field rearrangement by employing different constitutive equations to model the stress response of a material under deformation.

5.9 NUMERICAL RESULTS

In this section the results of the numerical investigation using the finite element computer code MAX2D are discussed. The objective of the numerical work was the creation of a simple mixed penalty method finite element formulation which could adequately predict viscometric properties in steady shear flow. The model was then used to examine the die swell problem. The White-Metzner constitutive model was chosen in the present investigation because it could be readily adapted to accurately predict the steady shear viscometric behavior of Styron 678 using shear rate dependent material parameters. The previous numerical investigations discussed in section 2.6 employed constitutive models which were not representative of the steady shear behavior of most viscoelastic materials. The viscometric predictions of the White-Metzner model are presented in section 5.9.1. The die swell problem and its relationship to the exit pressure are then discussed. The results of the numerical simulations for the various constitutive models are presented in section 5.9.5.

5.9.1 VISCOMETRIC BEHAVIOR

A series of different constitutive equations were used to represent the viscometric behavior of the polymer melt in steady shear flow. The

numerical investigation attempted to simulate the viscometric shear properties of Styron 678 at 165°C. This material and temperature were chosen so a comparison could be made between the numerical and flow birefringence results. In this section the viscometric behavior of the models is presented based on the viscometric data presented in section 5.1 obtained from a cone-and-plate rheometer.

Four constitutive equations were employed in the numerical investigation. Newtonian, generalized Newtonian fluid (GNF), upper-convected Maxwell (UC Maxwell), and White-Metzner constitutive equations were used to examine the effect of elasticity and shear thinning viscosity behavior on the stress field at the exit of a die. Shear thinning viscosity functions were used in the GNF and White-Metzner model. The Carreau model viscosity function was chosen to model the steady shear viscosity for Styron 678. The material coefficients for the Carreau model viscosity function were obtained using a non-linear least squares data fitting routine obtained from the Statistical Analysis System (SAS) Library on the Virginia Tech computer system.

The steady shear viscosity behavior of the models is shown in Figure 53 for Styron 678. For the Newtonian and UC Maxwell model calculations, a constant viscosity value was used. The value of η for these models was equal to the zero shear rate viscosity. For Styron 678 at 165°C, the value of η_0 was 6.2E4 Pa.s. The Carreau model was used to measure the shear thinning behavior of the polymer melt. The predicted viscosity is shown in Figure 53 for the constants, $\lambda = 15.037$ and $n = 0.48426$. The experimental data points from the RMS are in good agreement with the line predicted for the Carreau model. The Carreau model used in the numerical

model accurately predicts the shear thinning viscosity behavior of Styron 678 for steady shear flow.

The magnitude of the normal stresses, N_1 , in steady shear flow could be varied using the fluid time constant λ found in the UC Maxwell and White-Metzner constitutive equation. The constitutive equations could be solved explicitly for stresses for simple steady shear flow. The normal stresses are predicted by the equation

$$N_1 = 2 \lambda \eta \dot{\gamma}^2 \quad (5.21)$$

For the UC Maxwell model the fluid time constant λ and the viscosity η are constant. Therefore the normal stress behavior for this model is a quadratic function of the shear rate. For the UC Maxwell model the value of $\lambda = 2.5$ was chosen to represent the normal stress behavior for the shear rates of interest. The normal stress behavior for viscoelastic materials, however, may not be adequately modeled by a quadratic function of the shear rate. The normal stress behavior of the fluid in simple steady shear flow was exactly predicted by making the time constant λ a function of the magnitude of the rate of deformation tensor. Equation (5.21) was solved for λ and the values of N_1 and η obtained from cone-and-plate measurements for Styron 678 at 165°C were used to calculate λ as a function of shear rate. In Figure 54 are shown the values of λ obtained from RMS data. The function used to model the shear rate dependence for λ is also shown.

The normal stress predictions for the UC Maxwell and White-Metzner models were calculated using equation (5.21) once the values of λ were

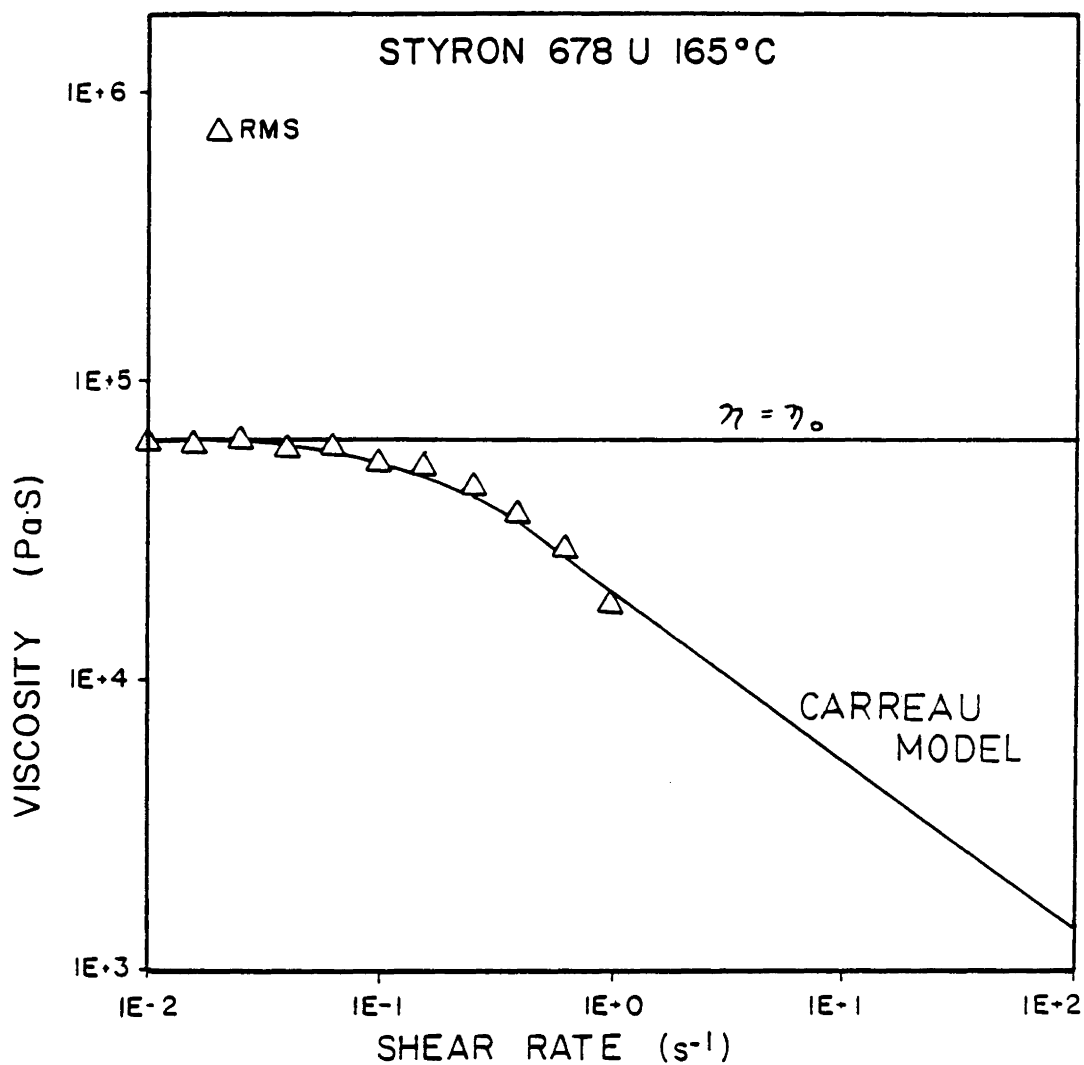


Figure 53. Comparison of Steady Shear Viscometric Properties: RMS and numerical results for Styron 678 at 165°C

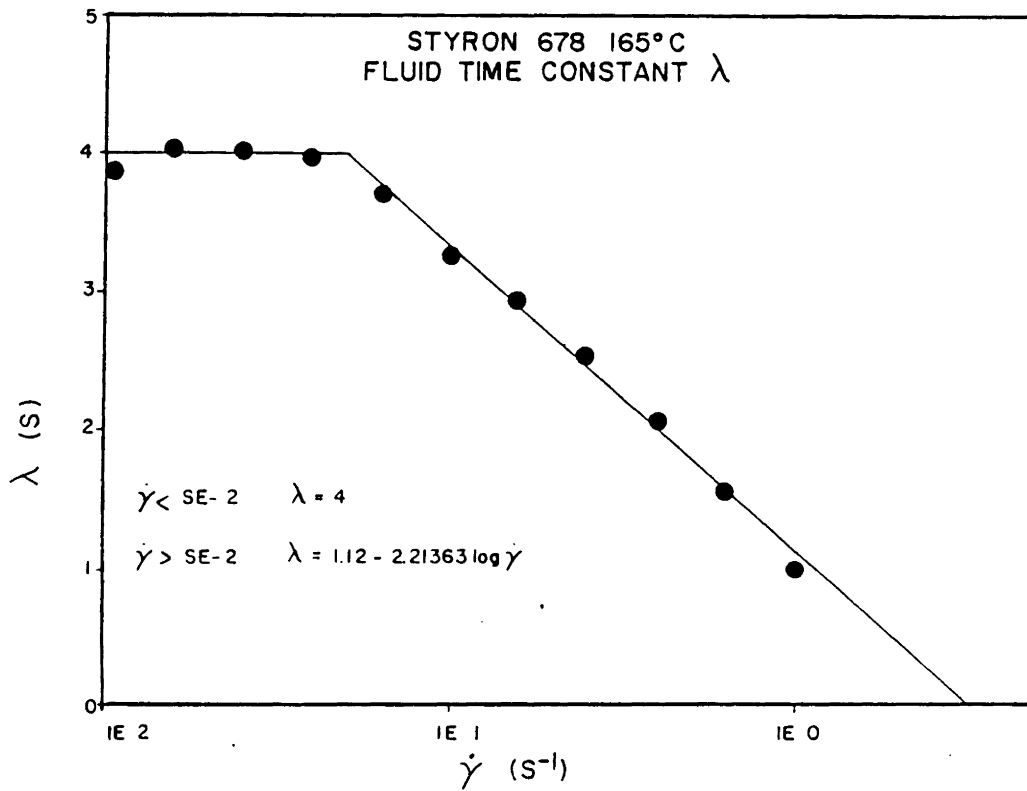


Figure 54. Fluid Time Constant for the White-Metzner Constitutive Equation: Styron 678 at 165°C from steady shear viscometric data.

calculated from experimental data. In Figure 55 is shown the normal stress behavior of the two models compared to the normal stresses obtained by the RMS. The empirical function for λ used in the White-Metzner model predicts N_1 values which are in good agreement with the experimental data while the UC Maxwell predicts N_1 values which do not exhibit the same shear rate dependence as the N_1 values obtained from the RSM for Styron 678.

Since the die exit region contains extensional flow gradients, the response of the constitutive equation in an elongational flow region may be important. The elongational viscosity predicted by the Maxwell type models is limited to a critical extension rate beyond which the extensional viscosity $\bar{\eta}$ becomes unbounded. In Figure 56 is shown the extensional behavior for the Maxwell type models. The extensional viscosity at the zero shear limit was approximately three times the zero shear viscosity. The value of $\bar{\eta}$ is seen to remain approximately constant for low extension rates and then approach an infinite value above a certain extension rate. The White-Metzner with the shear rate dependent function for λ demonstrates a larger range of convergence than the UC Maxwell model. Beyond the critical extension rate, an infinite or negative magnitude of the extensional viscosity may cause the numerical simulation not to converge. The UC Maxwell and the White-Metzner models are therefore not appropriate for flow regions where large extensional gradients are present.

5.9.2 DIE SWELL PROBLEM

The goal of the numerical investigation was the solution of the field

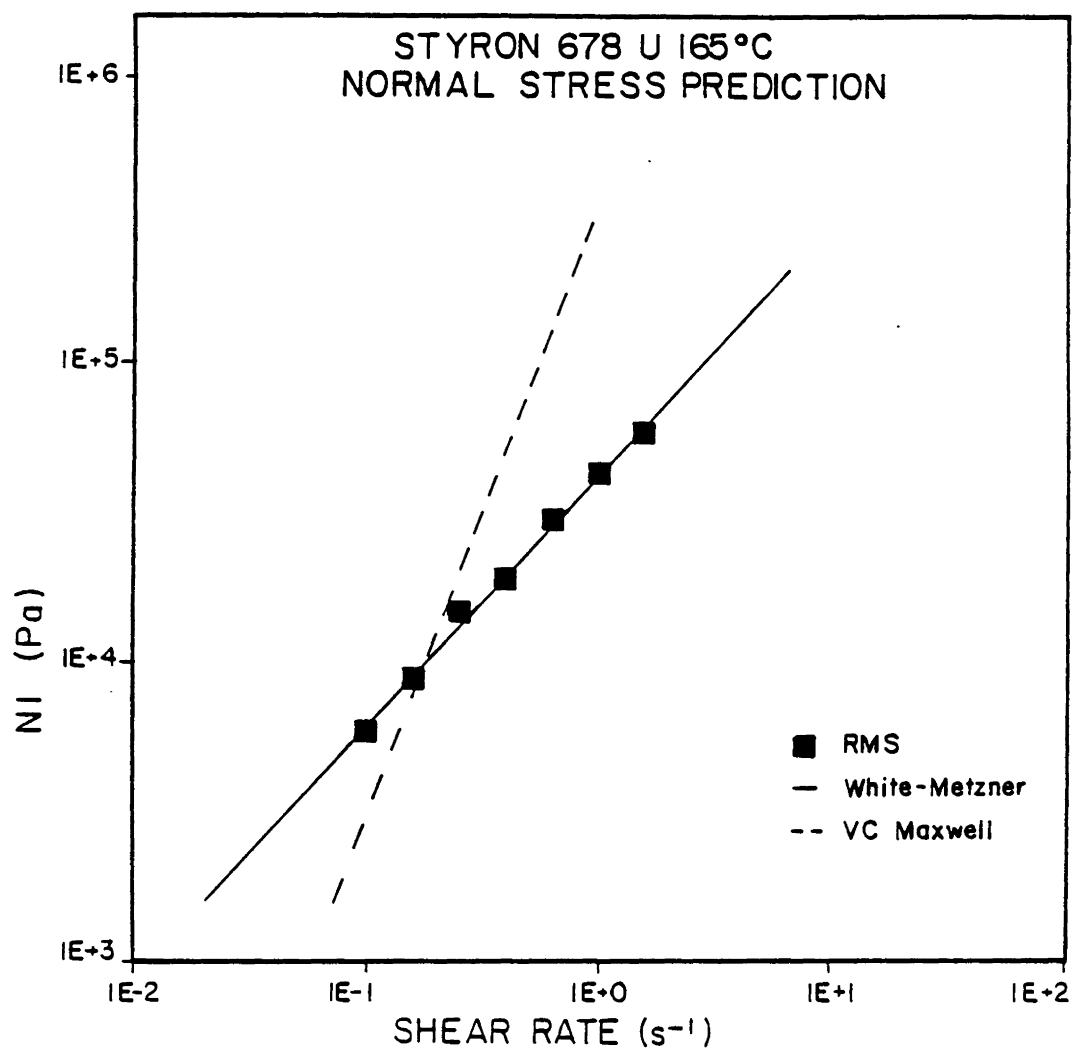


Figure 55. Comparison of Normal Stress Predictions for Numerical Models: Data for Styron 678 at 165°C.

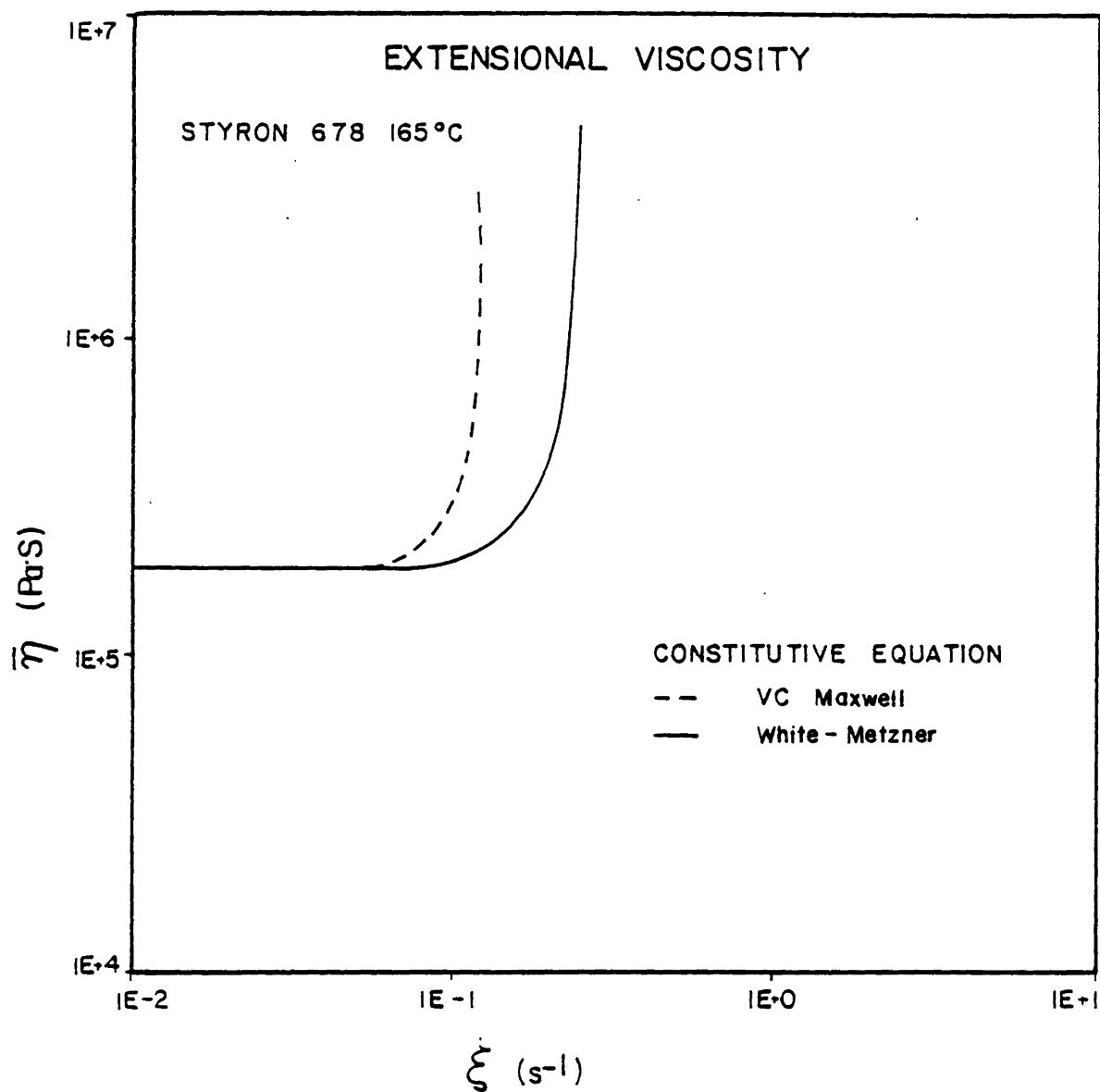


Figure 56. Extensional Viscosity Predictions for the Numerical Models: UC Maxwell and White-Metzner predictions for $\bar{\eta}$ in uniaxial extensional flow for Styron 678 at 165°C.

equations for fluid flow at the exit of a slit die to obtain the velocity field and stress profile at the exit of the die. The stress field obtained from the finite element analysis could be used to assess the validity of the assumptions used in the exit pressure theory. The exit pressure could also be obtained directly from the numerical results. The results of the exit pressure values were then compared with direct experimental measurements. The stress profiles generated by the numerical modeling can also be compared to the flow birefringence results. These results can be used to assess the validity of the nature of the flow field at the die exit numerically and to measure the accuracy of the stress field obtained using the empirically modified White-Metzner constitutive equation by comparing the numerically obtained stresses to the experimentally determined stress field using flow birefringence technique.

The boundary conditions for the die swell problem are shown in Figure 57. Only half the geometry was modeled due to symmetry of the flow field. On solid walls, a non-slip velocity condition were imposed on the fluid. Surface tension and air drag effects were neglected so the traction forces on the free surface were set to zero. For the upstream boundary, a fully developed velocity profile was imposed. For models containing the Carreau model viscosity function, the input velocity field was obtained numerically using a generalized Newtonian model.

The accuracy of the finite element formulation was tested by comparing the results of the shape of the free surface with the results of other numerical studies found in the literature. The die swell ratio was plotted as a function of De for the upper-convected Maxwell fluid flowing through a slit die. In Figure 58 is shown the results of the die swell pred-

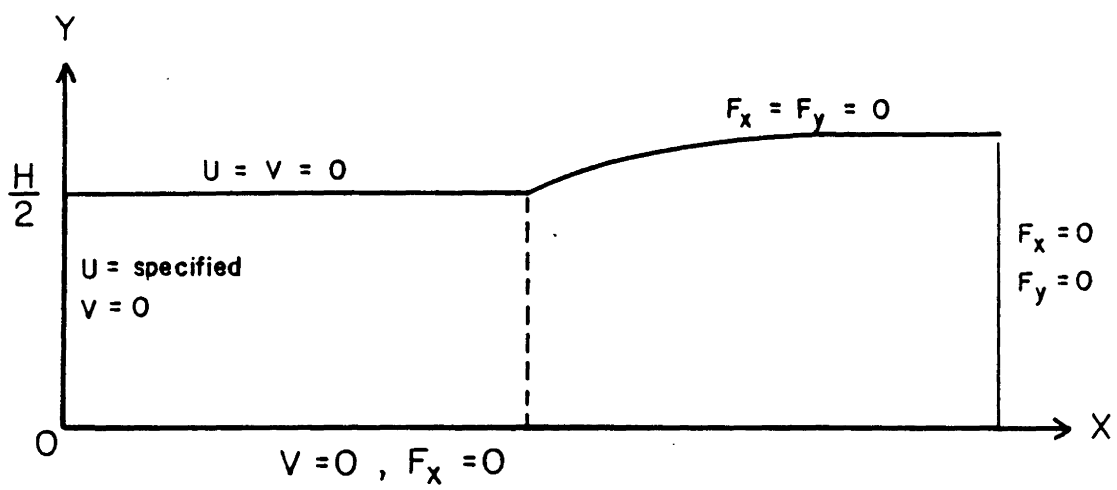


Figure 57. Boundary Conditions for the Die Swell Problem

ictions. The results of the die swell measurements are in good agreement with those by Crochet and Keunings [94,95]. The agreement between the die swell ratios predicted by the present formulation and the mixed finite element formulation by Crochet and Keunings suggests that the present penalty method formulation yields results compared with other non-Newtonian finite element formulations for complicated flow fields.

5.9.3 FINITE ELEMENT MESH

The finite element mesh used in the calculations is shown in Figure 59. The free surface boundary for a deformed mesh is also shown in the figure. The x-coordinates of the boundary nodes on the free surface were displaced by an amount calculated by the subroutine FREESF from the results of the velocity field obtained from the previous iteration. The number of nodes was increased towards the exit region to simulate the large gradients in the primary degrees of freedom, velocities and stresses, as the velocity and stress fields rearrange from pressure driven flow inside the slit to the profile in the free surface jet. The number of nodes required to obtain an accurate representation of the flow field was examined by refining the original mesh.

Two alternative meshes were used to test the effect of mesh refinement on the solution of the problem. In Table 5.6 are listed specifications of the meshes used in the die swell analysis. The behavior of meshes were compared based on the predictions of the flow field. Almost identical flow predictions were obtained using the two alternate mesh configurations. The initial mesh was therefore judged acceptable and was used throughout the numerical investigation.

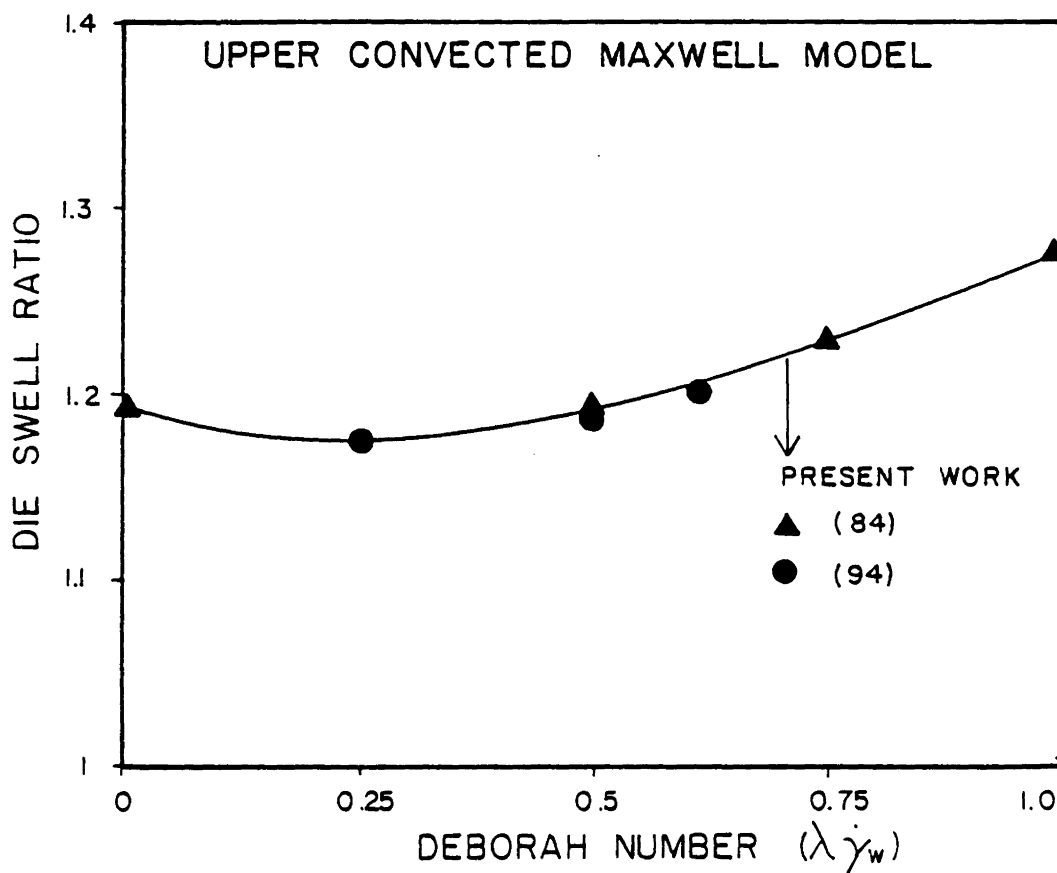
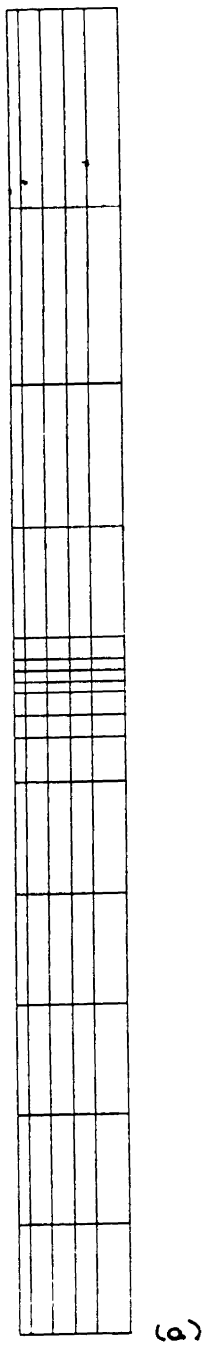


Figure 58. Die Swell Predictions for the Upper-Convected Maxwell Model



WHITE METZNER DIE SWELL T12= 4.84 X-VELOCITY
 PLOT NO. 2 DATE 11/12/85 TIME 12:16:27

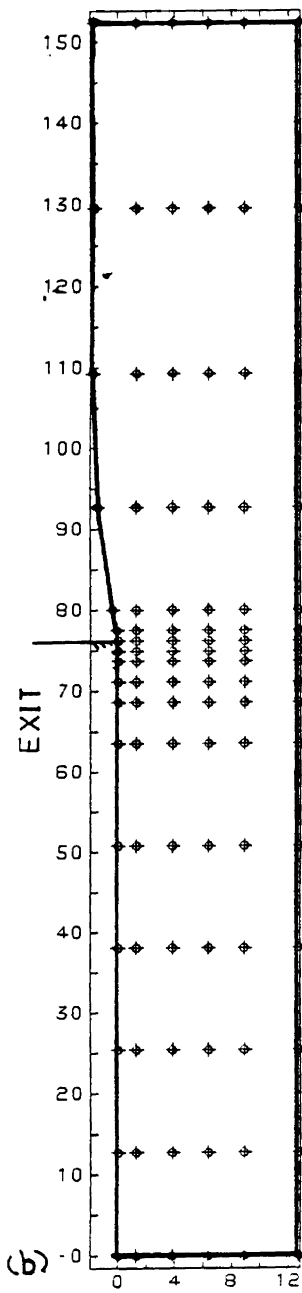


Figure 59. Finite Element Mesh: (a) Original mesh (b) Deformed mesh showing die swell in the free surface.

Table 5.6

Finite Element Meshes Used in the Numerical Die Swell Investigation

Mesh	Size	Number of Elements	Number of Nodes	Total DOF
I	5x16	80	102	510
II	4x16	64	85	425
III	6x16	96	119	595

5.9.4 CONVERGENCE RESULTS

As discussed in section 2/5, the solution of viscoelastic numerical simulations is currently limited to very low elasticity levels measured by the Deborah or Weissenberg numbers. Beyond a critical value of the Deborah number, the iterative solution procedures fail to converge to a steady solution. In this section the convergence limits of the numerical investigation are presented for the UC Maxwell and White-Metzner constitutive equations used in the numerical simulations. Possible contributions to the failure of the procedure are discussed in terms of mesh refinement and the extensional properties of the Maxwell type constitutive models.

The convergence limits for the finite element formulation are shown in Table 5.7. The upper limit of the convergence measured by the Deborah number for the White-Metzner model was $De = 0.61$, while the upper-convected Maxwell model converged to $De = 0.75$. The larger convergence range on the UC Maxwell model may be due to the absence of shear rate dependent material parameters. The viscosity and fluid time constant for the UC Maxwell model were constants. The White-Metzner model, however, used a Carreau model viscosity function and an empirically modified time constant λ . The rate dependent terms reduced the convergence range as the values of η and λ changed after each iteration. This may cause oscillations in the solution vector.

The limitations of the current models to predict realistic stresses in an elongational flow field also created an upper limit for the numerical formulation. The extensional viscosity becomes unbounded beyond a

Table 5.7

· Convergence Behavior for the Finite Element Simulation

Model	Deborah Number	Extension Rate at Die Corner
White-Metzner	0.61	0.250
UC Maxwell	0.75	0.20

critical extension rate for the UC Maxwell and White-Metzner constitutive equations. The value of the extension rates listed in Table 5.7 correspond closely to the critical extension rate discussed in section 5.9.1. The loss of convergence at the given Deborah numbers which also corresponds to the limit of the extensional behavior suggests that the criteria which limits the convergence for these systems may be due to high extensional gradients at the die corner. This behavior is consistent with the convergence studies of Mendelson et al. [141]. The loss of convergence was associated with the failure of the formulation to adequately predict large changes in the solution or stress gradients. The presence of an "infinite" extensional viscosity term in the numerical model would lead to a loss of a steady solution in the iterative procedure.

In this section the convergence limits of the finite element formulation were presented. The White-Metzner constitutive equation failed to converge for $De > 0.61$. This corresponds to a wall shear stress value of 9.0 KPa. for the material constants used to model the steady shear viscometric behavior of Styron 678 at 165°C. In the next section the results of the numerical investigation are presented. Results are presented at $\sigma_w = 4.84$ and 8.10 KPa so the numerical results could be directly compared to the experimental stresses obtained in the flow birefringence investigation.

5.9.5 RESULTS OF THE NUMERICAL VELOCITY AND STRESS FIELDS

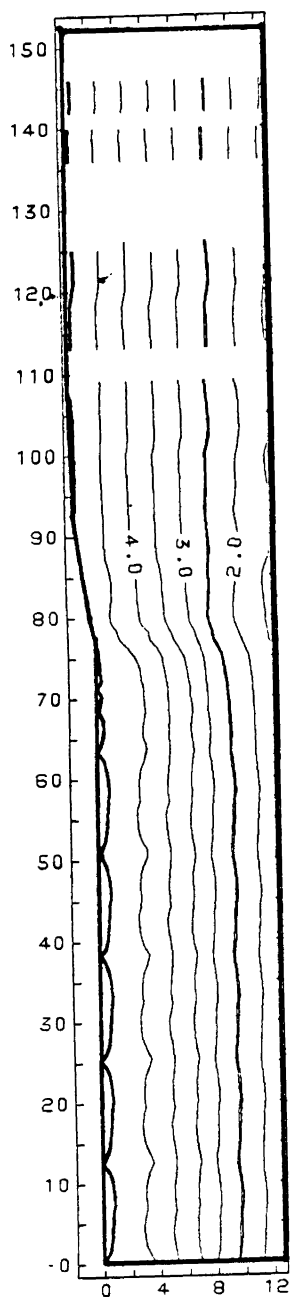
In this section the results of the numerical investigation for the die swell problem are discussed based on the nature of the rearrangement at the exit of the die. Contour plots were used to graphically compare

the gradients of the solution using dimensionless variables. The results of the White-Metzner constitutive equation for Styron 678 are presented for shear stress levels at which flow birefringence results were available.

For the numerical investigation the velocity rearrangement at the exit of the die can be examined using the results of the velocity field and the plot of the streamlines. In Figure 60 is shown the streamlines for the White-Metzner constitutive equation at wall shear stress values of 4.84 and 8.10 KPa. The fully developed flow region, characterized by parallel streamlines, was seen to extend very closely to the die exit plane. Once outside the die, the stream lines deviated in the vertical direction where swelling occurred. The presence of velocity field rearrangement was not observed to change significantly with increasing shear rate.

The rearrangement of the velocity field was also examined by plotting the dimensionless velocity components obtained from the numerical results. The velocity components were written in dimensionless form by dividing the x and y velocity values by the maximum axial velocity, $v_{y \max}$, in the fully developed flow region. The dimensionless axial velocity components (y-velocity) are shown in Figure 61. The velocity rearrangement at the exit of the die was minimal at locations upstream of the die exit. Some rearrangement occurs within $1/2$ die height of the exit plane but very little effect was seen upstream of the die. The x component of the velocity field can be used to show the regions in which the vertical swelling behavior is greatest. In Figure 62 are shown the dimensionless vertical velocity components, v_x , for the White-Metzner model. The ver-

WHITE METZNER DIE SWELL T12=4.84 STREAM FUNCTION PSI
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WHITE-METZNER DIE SWELL T12=8.10 STREAM FUNCTION PSI
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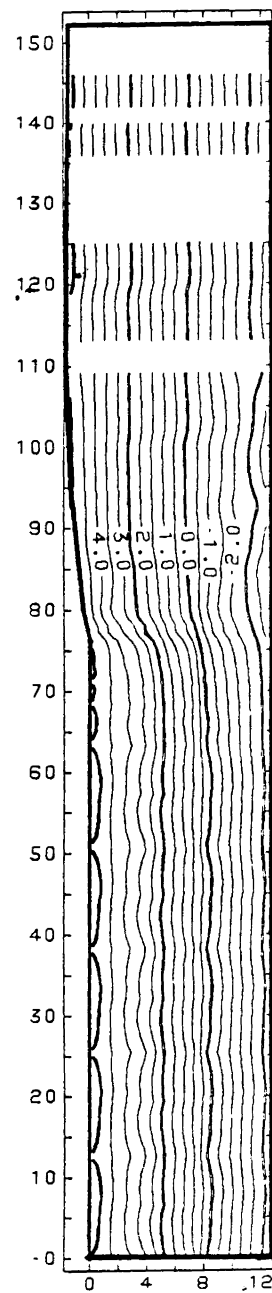


Figure 60. Streamline Contour Plot for Styron 678 at 165°C: White-Metzner constitutive equation (a) $\sigma_w = 4.84$ KPa (b) $\sigma_w = 8.10$ KPa.

tical velocity components were approximately zero in the fully developed flow region and in the free jet. The swelling behavior was observed in the region where the velocity components are concentrated near the die corner. The magnitude of the x-velocity components were greatest near the die corner. The length of the disturbance upstream in the velocity field was negligible based on the error bars of the contour lines.

The numerical velocity profiles did not show significant rearrangement in the velocity profile upstream from the die exit. The velocity field changed into a constant velocity jet within 1 die height, but the velocity disturbance upstream was negligible. The next section will examine the stress field at the die exit to assess whether if the stress field rearrangement effects are negligible in the numerically obtained stress fields.

In the mixed formulation used in the present numerical simulation, the stresses and the velocity components were used as primary variables. The results of the numerical simulation contained the solutions of the extra stress components τ_{11} , τ_{12} , and τ_{22} at each node in the finite element mesh. In Figure 63 are shown the results of the dimensionless shear stress components, τ_{12} / τ_w for the White-Metzner model. The stresses were written in dimensionless form by dividing the shear stresses by the wall value τ_w calculated in the fully developed flow region. Contrary to the numerical velocity field results, the numerical predictions for the shear stress exhibited significant deviation from fully developed flow upstream of the die exit. The steady shear region in Figure 63 was characterized by smooth parallel contour lines near the entrance of the domain. Wiggles which appear in the entrance region were due to the

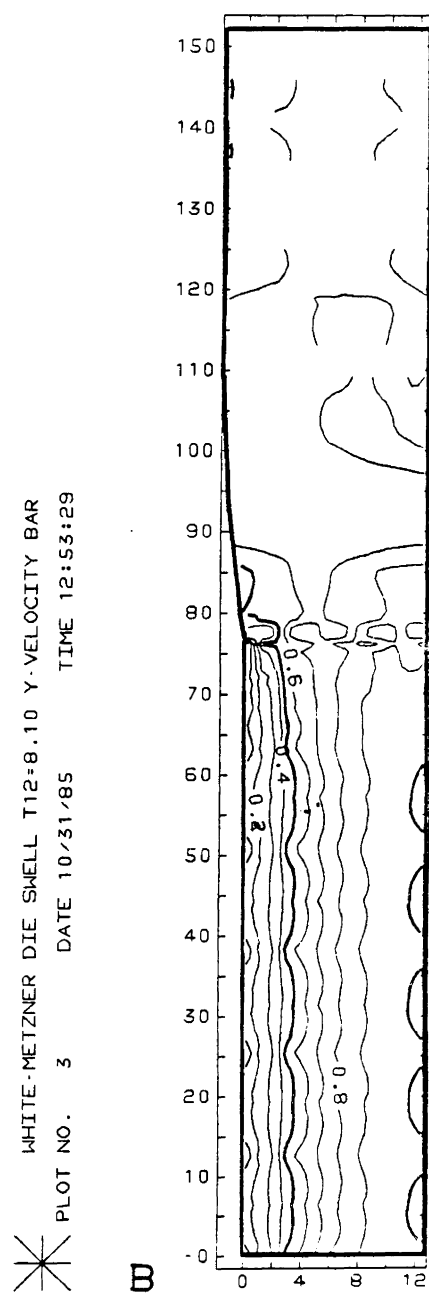
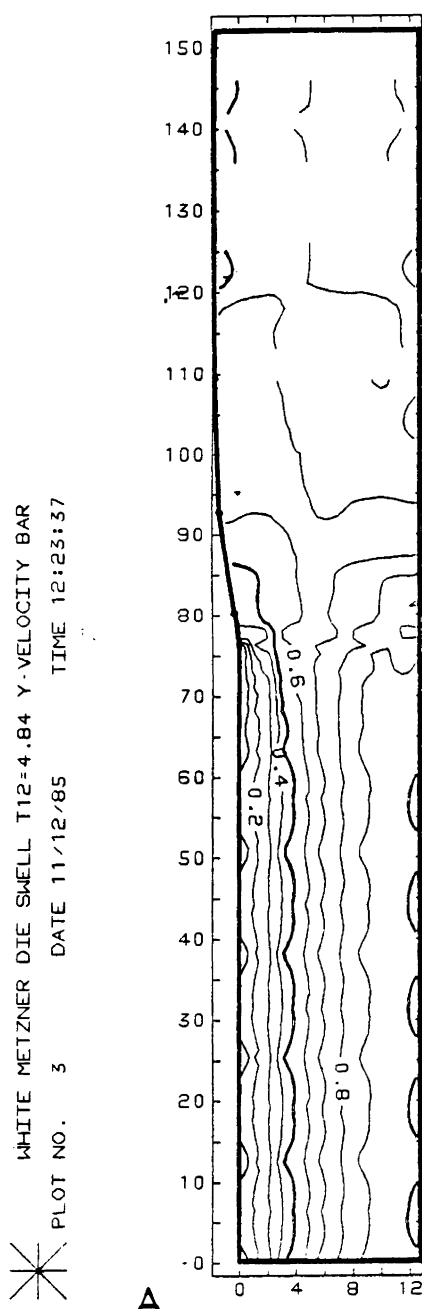


Figure 61. Dimensionless Axial Velocity Contour Plot for Styron 678 at 165°C: White-Metzner constitutive equation (a) $\sigma_w = 4.84$ KPa (b) $\sigma_w = 8.10$ KPa.

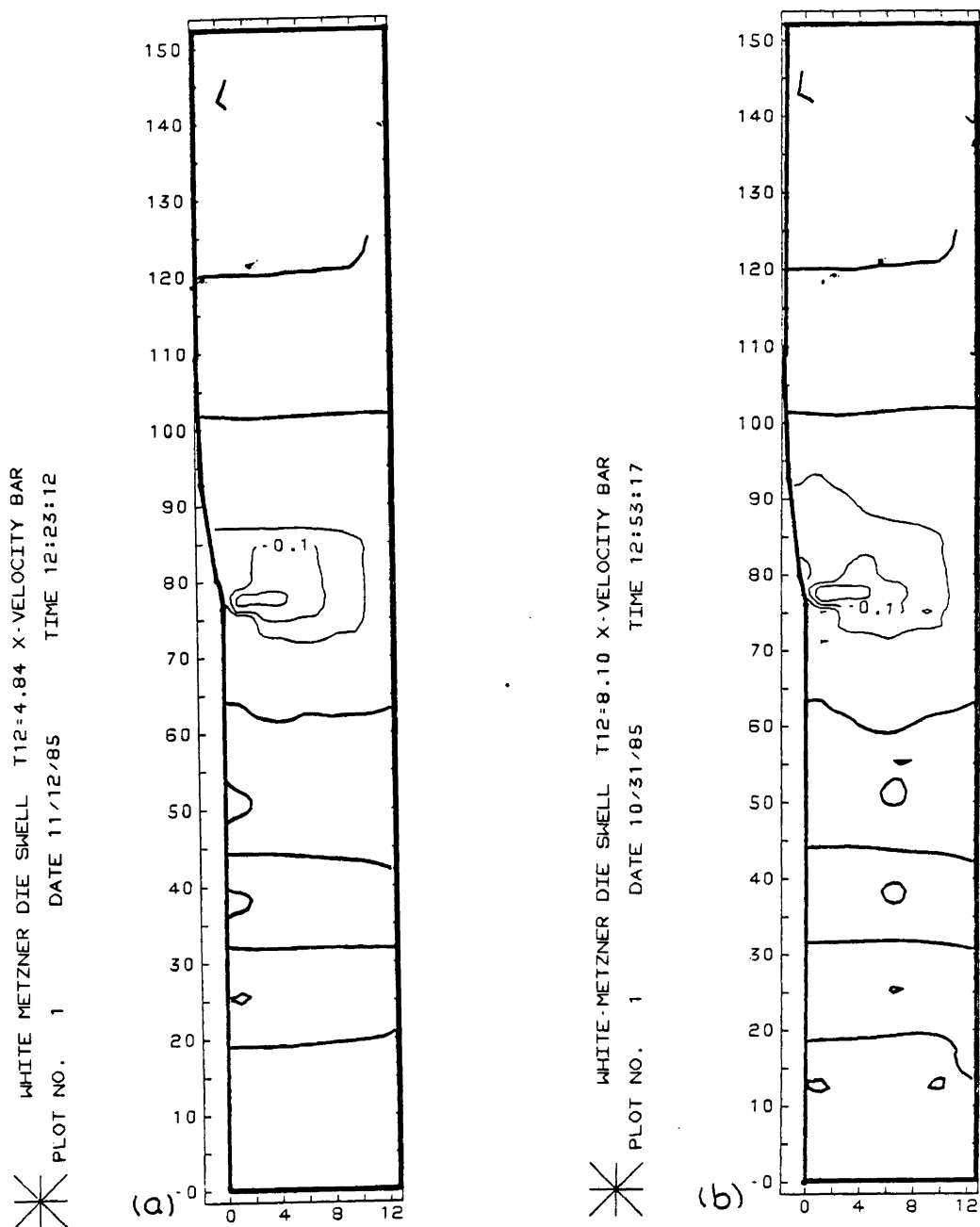


Figure 62. Dimensionless Vertical Velocity Contour Plot: Styron 678 at 165°C - White-Metzner constitutive equation (a) $\sigma_w = 4.84$ KPa (b) $\sigma_w = 8.10$ KPa.

scarcity of data points used in the contour plotting routine. A rearrangement region which was approximately 1/3 die height in length was present for shear stresses investigated. The length of the rearrangement was approximately constant for the wall shear rate range $0.05 \leq \dot{\gamma}_w \leq 0.17$.

The abrupt change in boundary conditions found at the die corner created a stress singularity which must be approximated by the finite element formulation. In the present finite element formulation the change in boundary conditions resulted in the presence of a stress overshoot behavior predicted at the die lip for the UC Maxwell and White-Metzner models. The magnitude of the overshoot increased with increasing wall stress. The contour map for of the results of the White-Metzner model for $\sigma_w = 8.10$ KPa showed a much larger disturbance in the exit plane than for $\sigma_w = 4.84$ KPa. As discussed in section 2.5, the ultimate failure of the numerical simulation may be due to the large gradients predicted at the die corners. The contour maps for the dimensionless shear stresses show the disturbance in the stress profiles increased as the Deborah number of the simulation is increased. The ultimate failure of the iterative procedure has been attributed to the inability of the finite element approximation to model the large stress gradients exhibited by viscoelastic fluids with abrupt change in boundary conditions. The presence of these large stress gradients may be one cause in the loss of convergence in the iterative procedure. This was suggested by several groups.

The normal stress difference results from the numerical models were also used to examine the nature of the stress field at the die exit. The dimensionless normal stress contours can be used to separate the con-

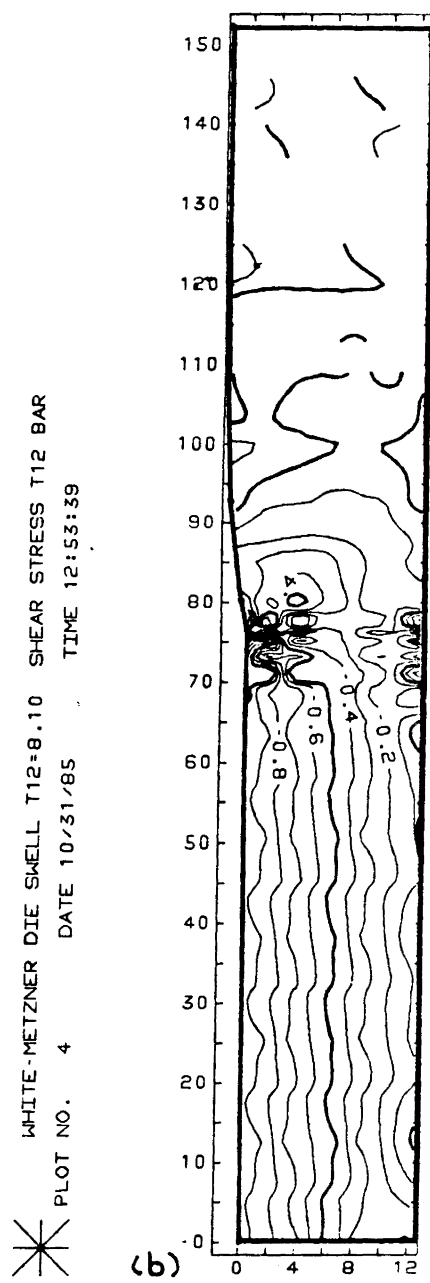
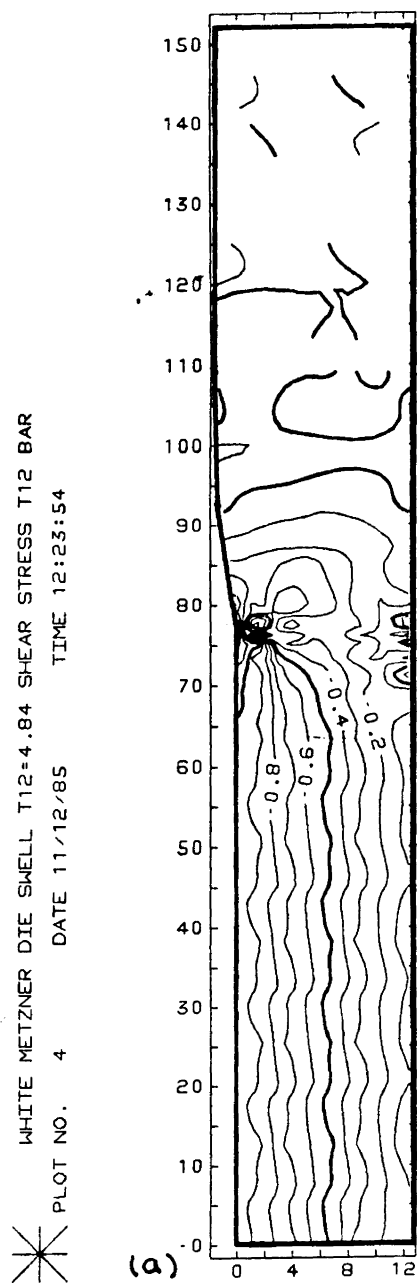


Figure 63. Dimensionless Shear Stress Contour Plot: Styron 678 at 165°C - White-Metzner constitutive equation (a) $\sigma_w = 4.84$ KPa (b) $\sigma_w = 8.10$ KPa.

tributions of elasticity and extension by comparing the results of an inelastic model (GNF constitutive equation) with the White-Metzner predictions. The GNF model contained the the same Carreau model viscosity function as found in the White-Metzner formulation. In Figure 64 is shown the normal stress difference $\tau_{11} - \tau_{22}$ for the GNF model at $\sigma_w = 8.10$ KPa. Dimensionless variables were not used in this plot since $N_1 = 0$ in shear flow for the inelastic model. A large extensional gradient was evident near the corner of the die. The normal stresses were concentrated about the die corner with the highest normal stress difference present on the node at the die lip. A region of fluid deceleration was also evident near the centerline in the die exit region by an examination of the positive values of $\sigma_{zz} - \sigma_{yy}$ exhibited by the inelastic model. For the inelastic GNF model, positive normal stress values are predicted for a decelerating velocity field.

The contributions of both extensional and elastic components were evident in the results for the White-Metzner constitutive equation. In Figure 65 is shown the dimensionless normal stress difference values for wall shear stress values of 4.84 and 8.10 KPa. The dimensionless normal stresses were written as N_1 / N_{1wall} . The viscometric normal stresses vary from approximately zero along the centerline to a dimensionless N_1 value of one at the die wall. This behavior is observed at the entrance of the finite element domain. At the die corner, the normal stresses demonstrate a large overshoot phenomena which are 450% greater than the normal stresses calculated at the wall in steady shear flow. Comparison of the concentration of contour lines at the die lip with the results from the GNF model suggests that the overshoot above viscometric normal

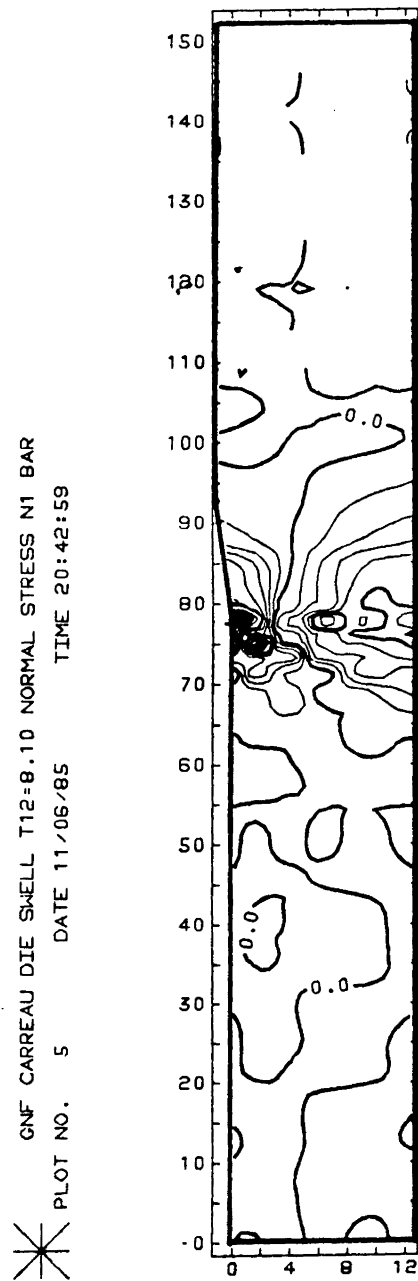


Figure 64. Normal Stress Contour Plot (GNF): Generalized Newtonian Constitutive equation - Carreau model viscosity function - $\sigma_w = 8.10$ KPa.

stresses was due to extensional flow gradients. Positive normal stresses near the centerline were also present for the White-Metzner model. The change in sign of the normal stress results suggest a significant deceleration of fluid along the centerline. The results of the normal stress measurement for the White-Metzner model are in qualitative agreement with the normal stresses observed in the flow birefringence study.

A comparison of the results of the numerical simulation for the velocity field and the stress field have shown different effects on rearrangement terms upstream of the die exit. The velocity field measured by the stream lines and dimensionless velocity components were not significantly affected upstream of the die exit. The stress field, however, began to deviate from fully developed flow up to $1/2$ die height upstream. The rearrangement effects were more readily evident in the stress distribution than in the velocity field.

The shear stress field τ_{12} obtained by flow birefringence was characterized by the concentration of the shear stresses near the die corner and the presence of stress overshoot at the die corner. The rearrangement length was seen to extend approximately $1/3$ die height upstream of the die exit. The numerical results for the White-Metzner model shown in Figure 63 also demonstrated the same characteristics in the shear stress field. The dimensionless stress contours concentrated near the die corner. The numerical results at $\sigma_w = 4.84$ KPa were in good quantitative agreement with the birefringence results. The agreement between the two techniques was less at higher shear rates. The numerical results for $\sigma_w = 8.10$ KPa contained oscillations in the shear stress field. The oscillations may be due to the difficulty in simulating the large stress gra-

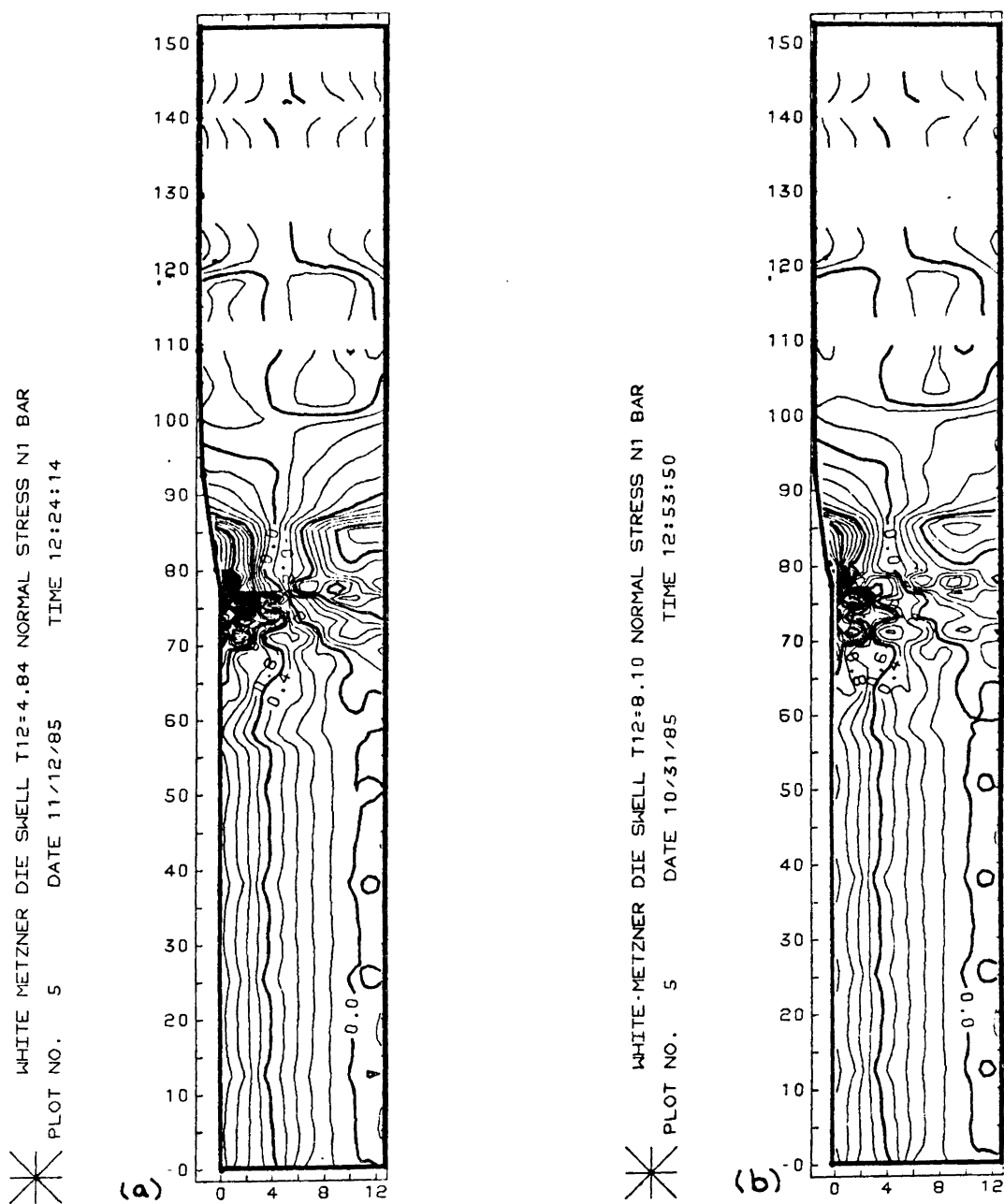


Figure 65. Dimensionless Normal Stress Contour Plot: Styron 678 at 165°C - White-Metzner constitutive equation (a) $\sigma_w = 4.84$ KPa (b) $\sigma_w = 8.10$ KPa.

dients using the finite element approximation functions. The numerical technique failed to converge at higher shear stress levels. The lack of agreement between the numerical and birefringence results at $\sigma_w = 8.10$ KPa was attributed to the oscillations present in the numerical simulation. At low rates of shear, the White-Metzner model accurately predicted the stress rearrangement behavior observed in the experimental investigation. For higher shear rates the failure of the numerical technique caused the lack of agreement and not a the choice of the original constitutive equation.

The presence of the change in boundary conditions at the die exit created a stress singularity which resulted in large overshoot predictions obtained in the stress measurements using the finite element model. The experimental results suggested the presence of a stress overshoot due to the presence of additional fringe patterns near the die lip. The numerical results predicted significant overshoot behavior in both shear and normal forces in the exit region. The numerical predictions, however, overestimated the shear and normal stresses near the die corner. The poor agreement in the results near the die corner was due to the difficulty in the numerical technique to approximate the large gradients at the die corner.

The results of the numerical stress field for the shear stress and normal stress differences were compared with the results of the flow birefringence results presented in section 5.4. The White-Metzner constitutive equation with shear rate dependent material parameters was seen to accurately predict the viscometric behavior of Styron 678 for steady shear flow. The model was then used to predict the stress field

for flow at the exit where an analytical solution was not possible. In general, the numerical model demonstrated good agreement with the results of the flow birefringence analysis for the die swell problem. The penalty method formulation used in the present investigation yields consistent results compared to both experimental results obtained by flow birefringence and other numerical mixed finite element formulations [94,95].

The nature of the velocity field rearrangement was discussed in terms of the extensional velocity gradient in the exit region by measuring the normal stress difference, $\tau_{zz} - \tau_{yy}$. Experimental results for the normal stress difference were seen to change sign from positive values at the centerline (fluid deceleration) to negative values measured at the wall (fluid acceleration). The numerical results for the normal stresses also displayed similar behavior. Contour maps for the White-Metzner model were in agreement with the results of birefringence measurements in predicting the positive normal stresses near the centerline. The numerical normal stresses acting near the wall, however, were overestimated. The normal stresses near the wall were overestimated due to the level of the extensional viscosity predicted using the White-Metzner model and the stress singularity associated with the die corner.

The results of the finite element simulation were in good agreement in the quantitative prediction of the stress behavior observed in the exit region of the slit die dominated by shear gradient flows. The numerical model could not accurately predict the stress field behavior in the region near the die corner. Extensional velocity gradients and stress discontinuity at the die corner limit the range of convergence associated with

the flow region at the die corner. In the next section the values of the numerical stress fields will be used to calculate the value of the exit pressure.

5.9.6 EXCESS PRESSURE LOSSES

The numerical solution of the die swell problem can be used to obtain the total normal force exerted on the wall of the die. In this section the isotropic pressure and extra stress results of the numerical simulation were used to calculate the exit pressure by the a linear extrapolation procedure. Finally, the exit pressure results were compared for the GNF, upper-convected Maxwell, and White-Metzner models as a function of the wall shear stress.

The excess pressure losses were obtained by plotting the total normal force acting on the die wall, Π_y , versus axial distance inside the die. The linear portion of the curve was extrapolated to the die exit which yielded the exit pressure. The extrapolation procedure by which the exit pressures were obtained is illustrated in Figure 66. An extrapolation procedure was required for the numerical results due to the stress singularity at the die corner. The value of P_x measured directly at the die exit overestimated the extrapolated exit pressure by approximately 100 percent.

The calculated values of the exit pressure were plotted as a function of the wall shear stress for the White-Metzner constitutive equation representing the behavior of Styron 678 at 165°C. In Figure 67 are shown the values of the exit pressure as a function of the shear stress, σ_w . The behavior of the exit pressure was qualitatively in agreement with the

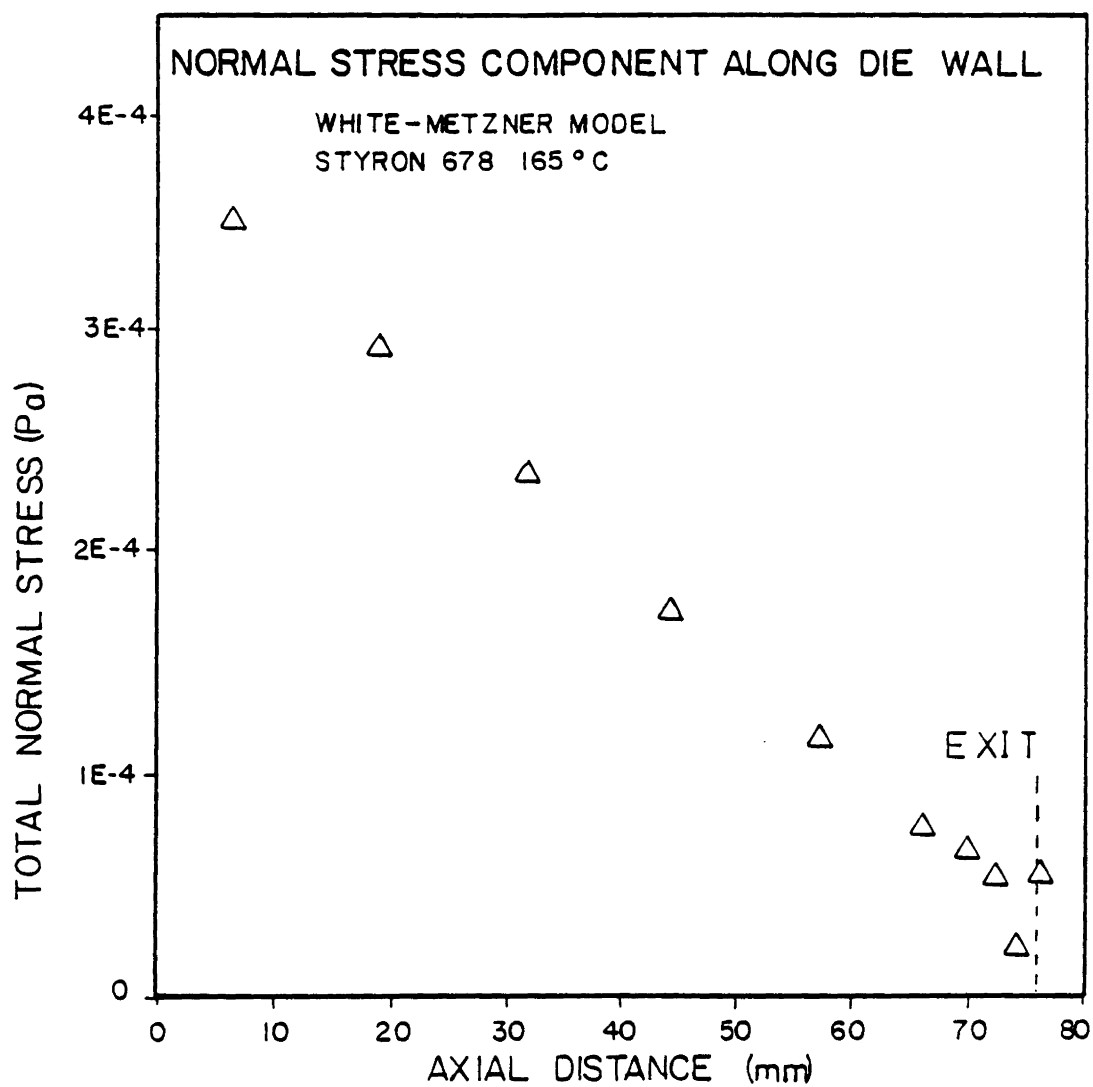


Figure 66. Numerical Pressure Profile Measured at the Wall: Styron 678 at 165 C. White-Metzner constitutive equation - $\sigma_w = 8.10$ KPa.

direct measurements of P_x . The slope of $\partial P_x / \partial \tau_w$ for the numerical simulation was equal to 0.925, while the experimental stress dependence for the exit pressure on σ_w was equal to 1.65. The error estimates on the experimental values of P_x at low shear rates preclude any meaningful comparison of the exit pressures between the numerical and experimental results. The numerical solutions fail to converge below shear stress levels for which experimental errors were not significant in the experimental determination of the exit pressure.

Since direct comparison of numerical and experimental exit pressures were not feasible, an alternative numerical study was conducted to examine the elasticity dependence of numerically calculated exit pressure values. The upper-convected Maxwell model was used to calculate the magnitude of the exit pressure as a function of the Deborah number. In Figure 68 is shown the dependence of the excess pressure loss at the exit of a slit die as a function of the Deborah number. In this figure the exit pressure was written in dimensionless form by dividing the value of P_x at each shear rate by the wall shear stress. The results of this figure may be written as a linear function of the Deborah number. For the upper-convected Maxwell fluid, the results may be expressed as

$$P_x / \tau_w = 0.26 N_1 / \tau_w + 0.30 \quad (5.22)$$

Equation (5.22) was in close agreement with the results of Tuna and Finlayson [101] for a convected Maxwell model and Reddy and Tanner [113] for a Second Order Fluid. Previously published results contained the following dependence for the excess pressure losses.

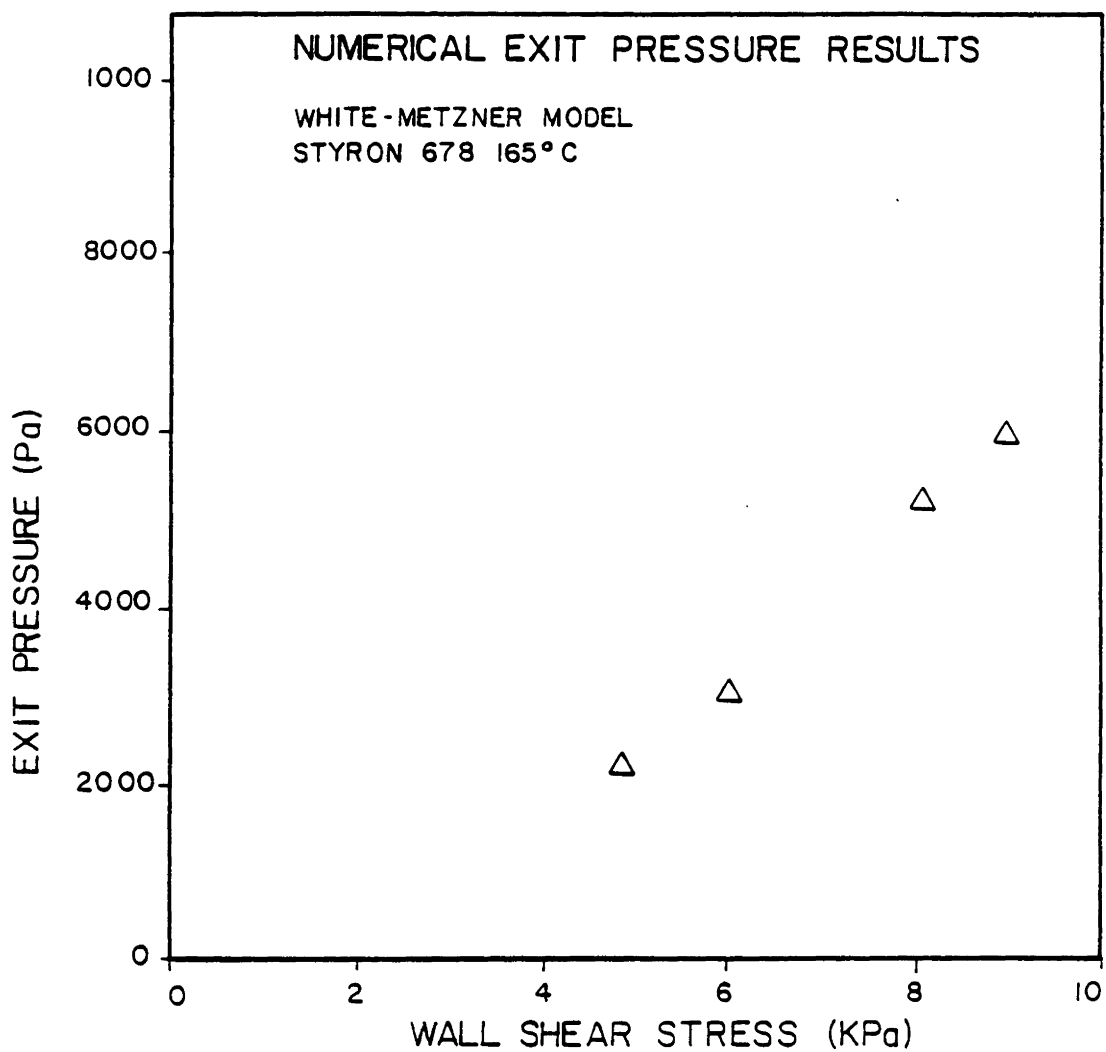


Figure 67. Numerical Exit Pressure Results: Styron 678 at 165°C for the White-Metzner constitutive equation.

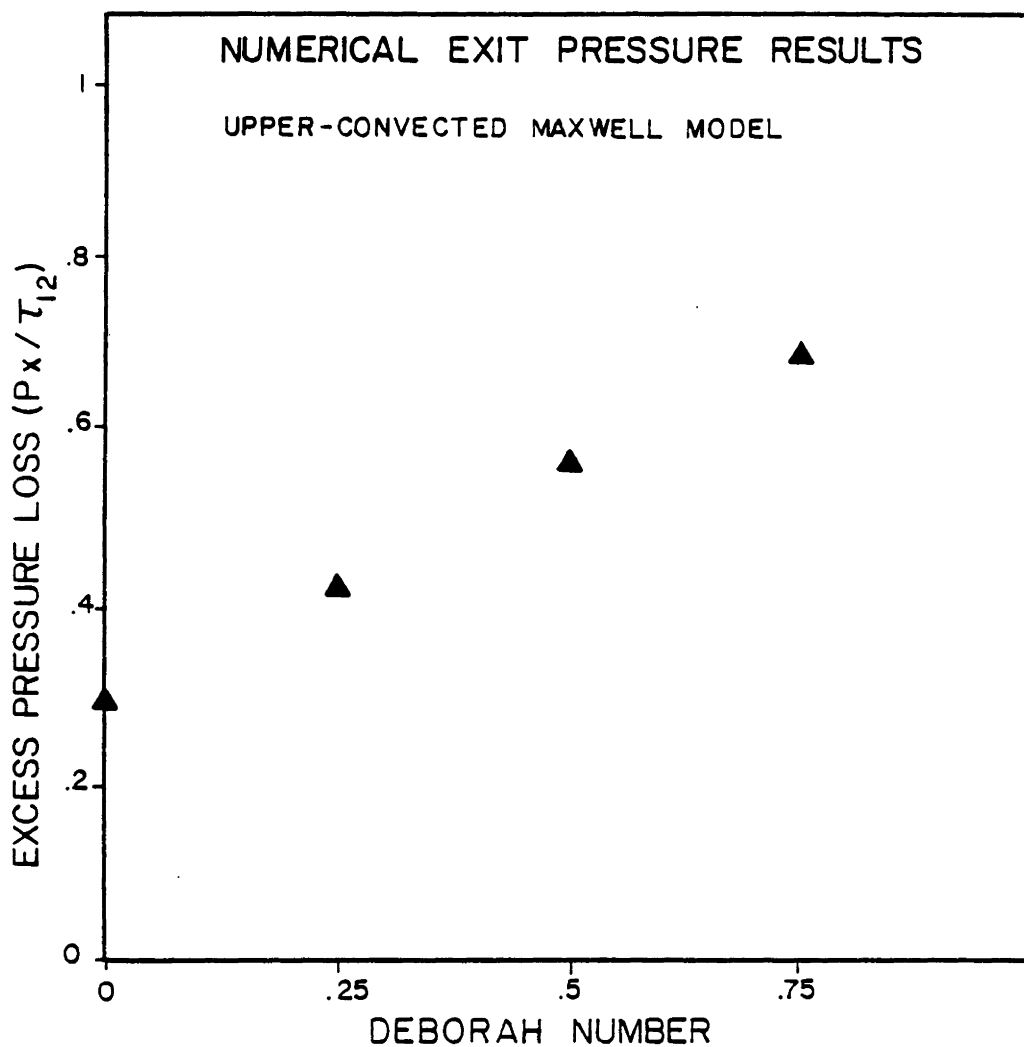


Figure 68. Numerical Excess Pressure Losses: Styron 678 at 165°C for the Upper-Convected Maxwell constitutive equation.

$$P_x/\tau_w = 0.28 N_1/\tau_w + 0.30 \quad [101] \quad (5.23)$$

$$P_x/\tau_w = 0.26 N_1/\tau_w + 0.31 \quad [113] \quad (5.24)$$

The excess pressure in each case increased linearly with the Deborah number. Numerical calculations, however, demonstrate a significant exit pressure for a Newtonian fluid ($De = 0$). The conclusion of Han et al. [4] that a finite exit pressure is proportional to fluid elasticity is not supported by the current numerical results. Similar non-zero exit pressure results were reported by Boger et al. [78] for the flow of a powerlaw fluid in capillary rheometers. The normal stress contribution term in equation (5.17) derived from the macroscopic momentum balance suggests positive exit pressures could be generated for inelastic fluids from the stress terms created by velocity field rearrangement inside the die. Experimental investigations, however, have not reported any significant positive values of P_x .

The exit pressure values presented in this section were shown to be positive in magnitude and to increase with increasing wall shear stress or elasticity level for UC Maxwell or White-Metzner constitutive equations. The numerical results were in qualitative agreement with the direct experimentally obtained values of P_x . The loss of convergence in the numerical simulations prevented meaningful comparison of P_x values at high shear rates. In addition, numerical simulation of the die swell predicted positive P_x values for inelastic fluids, which have not been measured experimentally. The exit pressure values obtained using inelastic constitutive equations was predicted to result from velocity rearrangement and stress overshoot in the stress field upstream of the die

exit. exit effects for inelastic fluids. Based on these results, the positive values of P_x calculated for inelastic fluids may be due to extensional velocity components. Inelastic materials can generate positive values of P_x if tensile stresses in the fluid are generated as the velocity profile rearranges at the exit region of a die.

5.10 ERROR ANALYSIS

In this section the magnitude of the errors existing in the measurement of the primary experimental quantities are presented. These variables are listed in Table 5.8. The error limits of these quantities are summarized, and the propagation of the errors through the calculation of the principal derived quantities is discussed. An estimate of the precision and accuracy of the calculations of P_x from the macroscopic momentum balances and equation of motion is also presented. First, however, a discussion is presented on the magnitude of possible sources of experimental errors which were not dealt with in the previous chapters.

5.10.1 VOLUMETRIC FLOWRATE

The volumetric flowrate delivered to the slit die was measured by using a Zenith metering gear pump. Error in the volumetric flowrate may be introduced due to leakage through the gear pump or due to variation in the volumetric rating of the gear pump (ml/rev). Error estimates were calculated by calibrating the gear pump using the mass flow rate of the polymer extruded from the die. Timed amounts of polymer were collected and weighed using a Metler analytical balance. The melt density of NPE 952 at 150°C was used to calculate the volumetric flowrate. The flow

Table 5.8

Precision Estimates of Principal Quantities

Quantity	Precision Estimates
H	0.025 mm
W	0.025 mm
L1	0.10 mm
P(T ₁)	3 KPa
P(T ₂)	3 KPa
P(T ₃)	5 KPa
Q	5E-5 cc/rev
T	0.5°C
C	0.05E-9 M2/N
N	0.2 Fringes
X	3° = 0.052 radians

rates agreed within 5% with those calculated from the gear pump rpm and rating (0.16 ml/rev).

5.10.2 ERRORS IN THE FLOW BIREFRINGENCE MEASUREMENTS

In this section several sources for generating errors in the flow birefringence experimental variables, $\bar{N}$ and χ are discussed. These include errors due to the broad diffuse nature of the fringes, interpolation of fringe patterns, and errors due to the parasitic velocity gradients along the side walls.

The values of $\bar{N}$ in the slit region used in the flow birefringence were obtained by interpolation of the fringe orders to mesh points located across the flow field. If the value of $\bar{N}$ does not vary linearly, this procedure resulted in erroneous values of $\bar{N}$. An estimate of the interpolation error was estimated by evaluating the deviation between the values of $\bar{N}$ defined by drawing a straight line and a curve through the experimental data. Near the centerline region of the die, the fringe orders do not vary rapidly and the error in calculating $\bar{N}$ was estimated at ± 0.1 fringe order. The error values near the die corner, however, were approximately ± 0.3 fringe orders due to the concentration of isochromatic fringes at the die lip.

Birefringence contributions due to stress generated in the windows created by the window mounting assembly and the force of fluid acting on the window, were measured by pressurizing the die in the absence a pressure gradient. The birefringence was measured during the pressure transducer calibration procedure. The measured birefringence can be attributed to the windows since the polymer melt is in an isotropic state

and the melt birefringence is zero. No birefringence was observed in the windows for an applied hydrostatic pressure of 2000 KPa. The contribution of birefringence due to the windows was therefore neglected.

The values of the isoclinic angle χ were determined by interpolation of the isoclinic maps onto an arbitrary mesh used for calculations. Errors in the value of χ were due to the diffuse nature of the isoclinic bands and the interpolation of the resulting isoclinic maps at discrete locations within the slit. As discussed in section 5.4, the isoclinic patterns consisted of diffuse dark bands in the slit region. The location of the band was based on the average center of the band as the polarizer was rotated $\pm 10^\circ$ about the desired orientation. Error estimates of the values of χ were determined by repeated measurements of χ from the isoclinic fringes recorded on the video tape system. A precision estimate of $\pm 3^\circ$ was assumed from multiple measurements of χ .

5.10.3 PRECISION ESTIMATES OF PRINCIPAL QUANTITIES

In this section the estimated precision of the primary experimental quantities is presented, and the uncertainty in the derived quantities is calculated. Precision estimates for the primary quantities are summarized in Table 5.9.

The error estimates for the derived quantities resulting from the error propagation of the primary experimental quantities were calculated based on the following analysis. The random uncertainty $e(F)$ generated in a derived function $F(x,y,z)$ from propagated uncertainties was estimated by [148].

Table 5.9

Precision Estimates of the Derived Quantities

Quantity	Estimated Precision	Observed Precision
P_x	6 KPa	15 KPa
$\dot{\gamma}_{app}$	4 %	---
σ_w	6 %	10 %
e	8 %	10 %
σ_{zy}	30 %	---
$\sigma_{zz} - \sigma_{yy}$	30 %	---

$$e^2(F) = \left(\frac{\partial F}{\partial x}\right)^2 e^2(x) + \left(\frac{\partial F}{\partial y}\right)^2 e^2(y) + \left(\frac{\partial F}{\partial z}\right)^2 e^2(z) \quad (5.25)$$

where $e(x)$, $e(y)$, and $e(z)$ are the random uncertainty in the primary experimental quantities.

The resulting precision estimates based on this analysis are summarized in Table 5.9. The precision estimates for η and σ_w were compared with precision values obtained from repeatability of the experimental results. The agreement observed between the estimated and experimentally observed precision estimates suggested that the significant sources of error had been adequately identified in the polymer feed system and the pressure measurement system. The estimated precision for the flow birefringence results for σ_{xy} and $\sigma_{zz} - \sigma_{yy}$ increase significantly with decreasing numbers of fringe orders N present. The precision quantities in Table 5.9 were therefore estimated using the lowest values of N and γ and thus these precision estimates represented the maximum expected error in the derived quantities.

The estimated precision for the extrapolated exit pressure was calculated using a graphical procedure based on a linear extrapolation procedure. Exit pressure values from the linear extrapolation technique were based on the construction of a least squares fit of the three pressures obtained from the flush mounted transducers. The error estimates were obtained by calculating the minimum and maximum value of P_x based on the precision estimates for the pressure transducers. The average variation in the extrapolated exit pressure was used as an approximate error for the linear extrapolation technique. The error associated with using a

quadratic fit of the pressure profiles was approximately the same for calculating the value of the exit pressure.

The observed precision of the exit pressure shown in Table 5.9 was approximately 1.5 times larger than the estimated precision based on extrapolation of the pressure profiles. The difference between the precision estimates reflect the number of experimental parameters which can effect the final measurement of P_x for viscoelastic fluids. These include the uncertainty in pressure measurement, extrapolation techniques, temperature effects, geometric effects, and end effects. The precision estimates in P_x were therefore based on the repeatability of direct measurements from the experimental investigation.

5.10.4 PRECISION ESTIMATES OF VALUES CALCULATED FROM FLOW BIREFRINGENCE

The precision with which the derived quantities were obtained from the macroscopic momentum balance and the equation of motion is examined in this section. The precision for these values was estimated by calculating an approximate error in the differentiation and integration of the stress quantities obtained using the results of the flow birefringence analysis. The total uncertainty includes errors due to the uncertainty of the flow birefringence data ($\bar{N}$, χ), temperature inhomogeneity in the window region, errors due to alignment of optical and video system, use of the stress optic rule, interpolation of the data, and errors due to differentiation and integration of the numerical results.

The stress gradients used in the discussion section were evaluated numerically using a finite difference approximation. A backward difference technique was used to evaluate the partial derivatives of the stress

components with respect to the coordinate system. The partial derivative calculated using this technique corresponds to approximating the instantaneous derivative of the stress function by the slope of a line segment representing the curve. The random uncertainty generated for finite difference values was calculated using the function $e(F)$ presented in equation (5.25). The maximum estimated error of the derivative values was approximately 42%, given the error in the stress values σ_{zy} and $\sigma_{zz} - \sigma_{yy}$.

In evaluating the expressions given by the momentum balances and the equation of motion, the integrations were performed using Simpson's rule. These integrations are not exact, and uncertainty limits must be estimated for the numerical integration procedure. The error in the numerical integration procedure was estimated by doubling the number of data points used to evaluate the integrals. The effect of refining the grid on the values of the integrals was used as a measure of the error in the numerical integration technique. This analysis was performed using the birefringence results for Styron 678 at 165°C for $\sigma_w = 8.10$ KPa. The results of the numerical integration were compared using eight and sixteen grid points for the integration of the stress field from the centerline to the wall. The values of the pressure difference $\Pi_{yy}(h,z) - \Pi_{yy}(0,z)$ calculated from equation (5.20) using the two grids agreed within 5%, indicating the level of error in the original grid. The agreement between the two grids indicates that the original grid was acceptable in the evaluation of the integral expressions. The error in the results of the integration procedure, however, does not correspond to the 5% precision estimate given for the numerical integration. This error only represents

the error contribution of the integration procedure. The total error of the results for the derived quantities depends on the sum of the error of the birefringence results σ_{zy} and $\sigma_{zz} - \sigma_{yy}$, the finite difference approximation, and finally on the numerical integration procedure. A conservative estimate of the maximum error expected in the final results from the momentum balances and the equation of motion was expected to be approximately $\pm 50\%$ of the final value of the stress quantities. Even though this error estimate represents a large value of the total for the results of the flow birefringence study, the results presented in this study represent one of the first attempts to obtain quantitative experimental values of the stresses found in the exit region of a die.

6.0 CONCLUSIONS AND RECOMMENDATIONS

6.1 CONCLUSIONS

Based on the results obtained in this investigation it is concluded that:

1. Values of σ_w , η , and $\dot{\gamma}_w$ can be determined, with reasonable accuracy, from direct pressure measurements in the slit die which was constructed for this study. This conclusion is based on results obtained for the experimental conditions $0.05 \leq \dot{\gamma}_w \leq 18 \text{ s}^{-1}$.
2. The values of $\sigma_{zy} = \sigma_w$ and $\sigma_{zz} - \sigma_{yy} = N_1$ evaluated at the wall can be obtained from flow birefringence data with reasonable accuracy. From this conclusion it can also be inferred that the distribution of σ_{zy} and $\sigma_{zz} - \sigma_{yy}$ in the exit region of the slit die can be accurately obtained from flow birefringence and the linear stress optic rule. The range of conditions for which the above conclusions were established is given by : $4.84 \leq \sigma_w \leq 14.3 \text{ KPa}$ and $0.05 \leq \dot{\gamma}_w \leq 2.1 \text{ s}^{-1}$ for Styron 678 at 165°C .
3. The exit pressure technique can not be used to obtain quantitative values of the primary normal stress difference without correcting for the stress rearrangement upstream of the die exit.

4. Consistent values of the exit pressure, P_x , could not be obtained due to the influences of experimental errors on the value of P_x calculated by extrapolating the pressure profiles to the exit of a slit die.
5. The choice of the extrapolation procedure, used to calculate P_x from pressures measured inside the slit die, is arbitrarily made in order to obtain positive values of the exit pressure which increase with increasing shear rate.
6. The magnitude of the primary normal stress difference, N_1 , is overestimated by approximately 200-300% using the calculated values of P_x and the exit pressure technique. This conclusion is based on the results obtained for the experimental conditions $4.84 \leq \sigma_w \leq 28$ KPa and $0.05 \leq \dot{\gamma}_w \leq 5$ s⁻¹ where direct comparison between the N_1 values obtained from a cone-and-plate and the slit die rheometer could be made.
7. The unidirectional shear flow assumption up to the exit plane of the die is violated to some degree.
8. Some overshoot behavior in the shear stress σ_{zy} and normal stress difference $\sigma_{zz} - \sigma_{yy}$ is present at the die exit corner. This conclusion is based on the presence of an additional fringe order at the die corner measured by the flow birefringence technique.

9. The normal stress field, $\sigma_{zz} - \sigma_{yy}$, measured at the exit plane is in compression along the die centerline and is in tension along the die walls. From this conclusion it can be inferred that the velocity field must decelerate along the centerline of the die in anticipation of the die exit.
10. The use of the dimensionless shear stress function f defined in the derivation of the exit pressure technique does qualitatively reduce the value of the primary normal stress difference predicted using the exit pressure theory for the flow conditions in (2) above.
11. The macroscopic momentum balance equation can be used to derive an expression which may be used to calculate the value of P_x directly from the magnitude of the stress field at the exit plane of a slit or capillary die.
12. The shear stress rearrangement upstream of the die exit yields the majority of the stress contributions to the magnitude of the exit pressure for the conditions listed in (2) above based on the expression derived from the macroscopic momentum balance.
13. The rearrangement of the stress field upstream of the die exit increases the pressure drop $\Delta P/\Delta L$ in the exit of the die. The magnitude of the pressure drop is evaluated using an expression derived from the equation of motion and the stress field obtained from flow birefringence for the conditions listed in (2) above. The error in

$\Delta P/\Delta L$ measurements due to rearrangement is approximately constant with increasing shear rate.

14. The total pressure difference $\Pi_{yy}(h,z) - \Pi_{yy}(0,z)$ at the die exit is positive for the flow conditions investigated in (2) above. The magnitude of the pressure difference increased with increasing shear rate. The sign of the pressure drop would tend to reduce the magnitude of swelling behavior exhibited in the extrusion of viscoelastic fluids from a slit die.

6.2 NUMERICAL INVESTIGATION

1. The mixed penalty method finite element formulation, MAX2D, yields numerical solutions consistent with conventional mixed finite element formulations for the die swell problem.
2. The White-Metzner constitutive equation used in MAX2D may be used to accurately predict the steady shear rheological properties for Styron 678 at 165°C. These results are based on the conditions $0.01 \leq \dot{\gamma}_w \leq 4 \text{ s}^{-1}$ where a comparison to experimental results from the cone-and-plate rheometer could be obtained.
3. The numerical stress field obtained from MAX2D using the White-Metzner constitutive equation were in good qualitative agreement with the stress field obtained using the flow birefringence experimental technique for the range $4.84 \leq \sigma_w \leq 9.00 \text{ KPa}$.

4. The numerically obtained values of the exit pressure increased with increasing shear stress. The predicted value of P_x/τ_w could be expressed as a linear function of the Deborah number.
5. The numerical simulation predicted a positive value of the exit pressure using an in-elastic generalized Newtonian fluid constitutive equation.
6. The range of convergence for the finite element models using the White-Metzner constitutive equation was limited to Deborah number less than 0.61. The addition of a shear rate dependent viscosity and fluid time constant to the upper-convected Maxwell model reduced the range of convergence of the finite element simulation.

6.3 RECOMMENDATIONS

The following recommendations are made for improving the existing apparatus and for further experimentation.

1. Replace the windows in the die with metal inserts so that the value of P_x can be obtained for polymer melts at higher shear rates. Exit pressure values could then be obtained where the pressure dependence of viscosity is significant.
2. Automate the pressure measurement system so the pressures and the pressure gradients are calculated directly from the signal of the

pressure transducers. The slit die could then be used as an on-line viscometer.

3. Since the value of the exit pressure is influenced by the magnitude of the stress overshoot at the die corner, future studies should be directed at obtaining birefringence data at the die lip. An optical bench could be used to improve the alignment of the optical apparatus. Also, a high powered laser using a photosensitive light detector could be used to measure birefringence on a point-by-point basis rather than the full field technique employed in the present study. This may improve the resolution of the optical birefringence technique in the region immediately surrounding the die corner.
4. The analysis of the birefringence results using the linear stress optic rule was limited to polystyrene melt. To examine the influence of polymer structure or fluid elasticity, alternative polymers should be investigated to examine if the nature of the disturbance at the die exit is significantly affected by polymer rheology.
5. Numerical studies on the die swell problem should employ constitutive equations such as the Leonov or Phan-Thien Tanner models which have an upper limit on the extensional viscosity. This would eliminate the limitation of the upper convected Maxwell and White-Metzner models to low extensional rates beyond which the extensional viscosity becomes unbounded.

6. The effect of the stress singularity at the die corner encountered in the numerical investigation can be reduced by employing slip boundary conditions along the wall.

REFERENCES

1. B. C. Sakiadis, AICHE J. , 8:3, 317 (1962).
2. C. D. Han and M. Charles, AICHE J. , 16:3, 499 (1970).
3. C. D. Han, M. Charles, and W. Philippoff, Trans. Soc. Rheol. , 13:4, 455 (1969).
4. C. D. Han, M. Charles, and W. Philippoff, Trans. Soc. Rheol. , 14:3, 393 (1970).
5. C. D. Han and M. Charles, Trans. Soc. Rheol. , 14:3, 409 (1970).
6. C. D. Han, T. C. Yu, and K. U. Kim, J. Appl. Polym. Sci. , 15, 1149 (1971).
7. C. D. Han and T. C. Yu, J. Appl. Polym. Sci. , 15, 1163 (1971).
8. C. D. Han and K. U. Kim, Polym. Eng. Sci. , 11:5, 395 (1971).
9. C. D. Han, J. Appl. Polym. Sci. , 15, 2567 (1971).
10. C. D. Han, J. Appl. Polym. Sci. , 15, 2579 (1971).
11. C. D. Han, J. Appl. Polym. Sci. , 15, 2591 (1971).
12. C. D. Han and K. U. Kim, Rheol. Acta, 11, 323 (1972).
13. D. B. Blum, J. Yerushalmi, and D. J. Williams, Canadian J. of ChE. , 50, 581 (1972).
14. C. D. Han, Trans. Soc. Rheol. , 18:1, 163 (1974).
15. P. W. Springer, R. S. Brodkey, and R. E. Lynn, Polym. Eng. Sci. , 15:8, 583 (1975).
16. J. L. Leblanc, Polymer, 17, 235 (1976).
17. R. E. Eckert and E. J. Novotny Jr. , Rheol. Acta, 17, 552 (1978).
18. H. M. Laun, Rheol. Acta, 22, 171 (1983).
19. R. D. Pike, D. G. Baird, and M. D. Read, SPE Technical Papers, 29, 312 (1983).
20. A. S. Lodge and L. de Vargas, Rheol. Acta, 22, 151 (1983).

21. C. Rauwendaal, SPE Technical Papers, 30, 282 (1984).
22. T. Arai, Fifth International Congress on Rheology, Kyoto, Japan (Oct., 1968).
23. Y. Mori and K. Funatsu, Proc. Fifth Int. Cong. Rheol., 4, 537 (1970).
24. Y. Tomita and T. Kobayashi, Fifth Int. Cong. on Rheol., Kyoto, Japan (Oct., 1968).
25. C. D. Han and M. Charles. Trans. Soc. Rheol., 15, 147 (1971).
26. C. D. Han. AIChE J., 16, 1087 (1970).
27. C. D. Han and R. R. Lamonte, Polym. Eng. Sci., 11, 385 (1971).
28. C. D. Han and J. U. Kim, Rheol. Acta, 11, 313 (1972).
29. N. D. Sylvester, PhD. Diss. (ChE) Carnegie-Mellon. Univ., Pittsburgh, Pa. (1968).
30. C. R. Shertzer, PhD. Diss. (ChE) U. Del., Newark, Del. (1965).
31. C. D. Han and M. Charles, Polym. Eng. Sci., 10, 148 (1970).
32. C. D. Han, K. U. Kim, N. Siskovie, and C. R. Huang, J. Appl. Polym. Sci., 17, 95 (1973).
33. D. B. Blum, J. Yerushalmi, and D. J. Williams, Can. J. of ChE., 50, 587 (1972).
34. E. J. Novotny and R. E. Eckert, Trans. Soc. Rheol., 18, 1 (1974).
35. R. E. Eckert and E. J. Novotny, Nature-Physical Sci., 241 (1973).
36. E. J. Novotny and R. E. Eckert, Trans. Soc. Rheol., 17, 227 (1973).
37. H. Eswaren, H. Janeschitz-Kriegel, and J. Schiff, Rheol. Acta, 3, 83 (1963).
38. M. G. Hansen and J. B. Jansma, Proc. VIII Int. Cong. Rheol., 2, 193 (1980).
39. R. M. Ybarra, PhD. Diss. Purdue U., (1980).
40. R. M. Ybarra and R. E. Eckert, AIChE J., 26, 751, (1980).
41. J. Gravis and S. Middleman, J. Appl. Polym. Sci., 7, 493 (1963).
42. J. N. Reddy, Int J. for Num. Meth. in Fluids, 2, 151 (1982).

43. J. T. Oden, Computers and Structures, 8, 445 (1978).
44. C. D. Han and L. H. Drexler, Trans. Soc. Rheol., 17:4, 659 (1973).
45. W. R. Schowalter and R. C. Allen, Trans. Soc. Rheol., 19:1, 129 (1975).
46. A. V. Rama Murthy, Trans. Soc. Rheol., 20, 503 (1976).
47. J. R. Clermont, J. M. Pierrard, and O. Scrivener, J. Non-Newt. Fluid Mech., 1, 175 (1976).
48. B. A. Whipple and C. T. Hill, AIChE J., 24:4, 664 (1978).
49. M. Gottlieb and R. B. Bird, I and E. C. Fund., 18, 357, (1979).
50. T. Arai and H. Hatta, J. Soc. Rheol. (Japan), 2, 173 (1979).
51. G. V. Vinogradov, N. I. Insarova, B. B. Boiko, and E. K. Borisenkova, Polym. Eng. Sci., 12, 323 (1972).
52. H. P. Tordella, Rheology, F. R. Eirich, ed., Vol. 5, Academic Press, N.Y. (1969).
53. R. C. Allen, PhD. Diss. Princeton U., (1970).
54. D. D. Goulden and W. C. Mac Sporrán, J. Non-Newt. Fluid Mech., 1, 183 (1976).
55. K. Higashitani, H. Nishino, and I. Hara, Proc. 7th Int. Cong. Rheology, 478 (1976).
56. C. D. Han, Trans. Soc. Rheol., 15, 371 (1971).
57. J. M. Davies, J. F. Hutton, and K. Walters, J. Phys. D: Appl. Phys., 6, 2259 (1973).
58. D. V. Boger and R. R. Huilgol, Trans. Soc. Rheol., 21:3, 447 (1977).
59. J. M. Davies, J. F. Hutton, K. Walters, J. Non-Newt. Fluid Mech., 3, 141 (1977).
60. D. V. Boger and M. M. Denn, J. Non-Newt. Fluid Mech., 6, 163 (1980).
61. S. Okubo and Y. Hori, J. of Rheol., 25:1, 147 (1981).
62. C. D. Han, J. of Rheol., 25, 1, 139 (1981).

63. L. Choplin and P. J. Carreau, J. Non-Newt. Fluid Mech., 2, 119 (1981).
64. A. S. Lodge, Elastic Liquids, Academic Press, N.Y. (1964).
65. C. D. Han, J. Appl. Polym. Sci., 14, 1775 (1970).
66. C. D. Han, AIChE J., 18, 116 (1972).
67. D. D. Joseph, Arch. Rat. Mech. Anal., 56, 99 (1974).
68. K. Walters, Rheometry, Chapman and Hill, London (1974).
69. A. B. Metzner, W. T. Houghton, R. A. Sailor, and J. L. White, Trans. Soc. Rheol., 5, 133 (1961).
70. C. D. Han and T. C. Yu, Rheol. Acta, 10, 398 (1971).
71. S. Okubo and Y. Hori, J. Rheol., 23, 625 (1979).
72. S. Richardson, Rheol. Acta, 9, 193 (1970).
73. S. Richardson, Proc. Camb. Phil. Soc., 67, 477 (1970).
74. R. E. Nickell, R. I. Tanner, and B. Caswell, J. Fluid Mech., 65, 189 (1974).
75. R. I. Tanner, R. E. Nickell, and R. W. Bilger, Computer Methods in Appl. Mechanics and Eng., 6, 155 (1975).
76. C. J. Coleman, JNNFM., 3, 288 (1977/78).
77. J. R. A. Pearson and R. Trottnow, J. Non-Newt. Fluid Mech., 4, 195 (1978).
78. D. V. Boger, R. Gupta, and R. I. Tanner, J. Non-Newt. Fluid Mech., 4, 239 (1978).
79. K. R. Reddy and R. I. Tanner, J. Rheology, 22:6, 661 (1978).
80. W. J. Silliman and L. E. Scriven, Phys. Fluids, 21:11, 2115 (1978).
81. L. D. Sturges, JNNFM., 6, 155 (1979).
82. W. J. Silliman and L. E. Scriven, J. Comp. Phys., 34, 287 (1980).
83. P. W. Chang, T. W. Patten, and B. A. Finlayson, Computers Fluids, 7, 285 (1979).
84. M. J. Crochet and R. Keunings, J. Non-Newt. Fluid Mech., 7, 199 (1980).

85. M. Viriyayuthakorn and B. Caswell, J. Non-Newt. Fluid Mech., 6, 245 (1980).
86. C. J. Coleman, J. Non-Newt. Fluid Mech., 7, 289 (1980).
87. B. J. Omodei, Comp. and Fluids, 8, 275 (1980).
88. C. S. Frederiksen and A. M. Watts, J. Computational Physics, 39, 282 (1981).
89. D. S. Malkus and T. R. Hughes, Comp. Meth. in Appl. Mech. and Eng., 15, 1557 (1980).
90. L. D. Sturges, J. Non-Newt. Fluid Mech., 2, 357 (1981).
91. C. J. Coleman, J. Non-Newt. Fluid Mech., 8, 261 (1981).
92. E. Ben-Sabar and B. Caswell, J. Rheol., 25:5, 537 (1981).
93. M.J. Crochet and R. Keunings, J. Non-Newt. Fluid Mech., 10, 85 (1982).
94. R. J. Sampson, Surface II Graphics System, Series on Spatial Analysis, Kansas Geological Survey, Lawrence, Kansas (1978).
95. M. J. Crochet and R. Keunings, J. Non-Newt. Fluid Mech., 10, 339 (1982).
96. B. Caswell and M. Viriyayuthakorn, J. Non-Newt. Fluid Mech., 12, 13 (1983).
97. A. I. Leonov and A. N. Prokunin, Rheol. Acta, 23, 62 (1984).
98. E. Mitsoulis, J. Vlachopoulos, and F. A. Mirza, Polym. Eng. Sci., 24:9, 707 (1984).
99. E. B. Bagley, J. Appl. Phys., 28, 624 (1957).
100. E. Mitsoulis and J. Vlachopoulos, Advances in Polymer Technology, 107 (1979).
101. N. Y. Tuna and B. A. Finlayson, J. Rheol., 28:2, 79 (1984).
102. R. I. Tanner, Appl. Polym. Symp., No. 20, 201 (1973).
103. J. L. White and A. Kondo, J. Appl. Polym. Sci., 21, 2289 (1977).
104. D. H. Michael, Mathematika, 5, 1, 82 (1958).
105. Rheometrics Inc., Rheometrics Mechanical Spectrometer Operations Manual, Union, New Jersey (1978).

106. M. B. Bush, R. I. Tanner, and N. Phan-Thien, *J. Non-Newt. Fluid Mech.*, 18, 143 (1985).
107. R. R. Huilgol and R. I. Tanner, *J. Non-Newt. Fluid Mech.*, 2, 89 (1977).
108. W. Retting, *Colloid and Polym. Sci.*, 257, 689 (1979).
109. B. J. Omodei, *Comp. and Fluids*, 7, 79 (1979).
110. K. R. Reddy and R. I. Tanner, *Comp. and Fluids*, 6, 83 (1978).
111. H. B. Phuoc and R. I. Tanner, *Int. Conf. on Finite Element Methods*, 1979.
112. R. Racin and D. C. Bogue, *J. Rheol.*, 23, 263 (1979).
113. K. R. Reddy and R. I. Tanner, *Trans. Soc. Rheol.*, 22, 661 (1978).
114. R. I. Tanner, *J. Non-Newt. Fluid Mech.*, 7, 265 (1980).
115. E. Mitsoulis, J. Vlachopoulos, and F. A. Mirza, *Polym. Proc. Eng.*, 1, 281 (1983).
116. R. Keunings and M. J. Crochet, *J. Non-Newt. Fluid Mech.*, 14, 279 (1984).
117. D. V. Boger and Binnington, *Trans. Soc. Rheol.*, 21:4, 515 (1977).
118. A. B. Metzner, E. L. Carley, and I. K. Park, *Mod. Plast.*, 37:11, 133 (1960).
119. E. B. Bagley, S. H. Storey, and D. C. West, *J. Appl. Polym. Sci.*, 7, 661 (1963).
120. C. D. Han and L. H. Drexler, *J. Appl. Polym. Sci.*, 17, 2329 (1973).
121. E. C. Kowalski, PhD. Diss. (ChE), Polytechnic Inst., Bklyn., N.Y. (1963).
122. H. P. Schreiber, *Polym. Eng. Sci.*, 6, 317 (1966).
123. C. D. Han, Rheology in Polymer Processing, Academic Press, N.Y. (1976).
124. R. R. Huilgol, *Polym. Engr. Sci.*, 18, 643 (1978).
125. J. L. S. Wales, The Application of Flow Birefringence to Rheological Studies of Polymer Melts, Delft University Press (1976).

126. C. D. Han, Y. J. Kim, and H. Chuang, *Polym. Eng. Rev.*, 3, 1 (1983).
127. P. J. Carreau, L. Choplin, and J. Clermont, *Polym. Eng. Sci.*, 25:11, 669 (1985).
128. R. D. Pike, PhD Diss., Virginia Tech, Blacksburg, Virginia 1984.
129. K. Higashitani and A. S. Lodge, *Trans. Soc. Rheol.*, 19, 307 (1975).
130. P. P. Tong, PhD. Diss., Univ. of Wisconsin, Madison, 1980.
131. M. D. Read and D. G. Baird, *SPE Technical Papers*, 31, 121 (1985).
132. H. T. Jessop and F. C. Harris, Photoelasticity, Cleaver-Humes Press, London 1949.
133. H. Janeschitz-Kriegl, Polymer Melt Rheology and Flow Birefringence, Springer-Verlag, New York (1983).
134. L. R. G. Treloar, The Physics of Rubber Elasticity, 3rd Ed., Clarendon Press, Oxford (1975).
135. A. S. Lodge, *Nature*, 176, 838 (1955).
136. T. Matsumoto and D. C. Bogue, *J. Polym. Sci., Phys. Ed.*, 15, 1663 (1977).
137. R. B. Bird, R. C. Armstrong, and O. Hassager, Dynamics of Polymeric Liquids, Vol. 1, John Wiley & Sons, New York (1977).
138. M. J. Crochet, A. R. Davies, and K. Walters, Numerical Simulation of Non-Newtonian Flow, Elsevier, New York (1984).
139. G. Astarita, *J. Non-Newt. Fluid Mech.*, 1, 203 (1976).
140. J. L. White and A. B. Metzner, *J. Appl. Polym. Sci.*, 7, 1867 (1963).
141. M. A. Mendelson, P. Yeh, R. A. Brown, and R. C. Armstrong, *J. Non-Newt. Fluid Mech.*, 10, 169 (1982).
142. P. W. Yeh, M. E. Kim, R. C. Armstrong, and R. A. Brown, *J. Non-Newt. Fluid Mech.*, 16, 167 (1984).
143. R. I. Tanner, *J. Non-Newt. Fluid Mech.*, 10, 169 (1982).
144. M. W. Johnson and D. Segalman, *J. Non-Newt. Fluid Mech.*, 2, 255 (1977).
145. A. R. Davies, S. J. Lee, and M. F. Webster, *J. Non-Newt. Fluid Mech.*, 16, 117 (1984).

146. J. N. Reddy, An Introduction to the Finite Element Method, McGraw Hill, New York, 1984.
147. D. P. Showmaker, C. W. Garland, and J. I. Steinfeld, Experiments in Physical Chemistry, McGraw Hill, New York, 1974. I. Miller and J. E. Freund, Probability and Statistics for Engineers, Prentice-Hall, Englewood Cliffs, N. J. (1977).
148. J. Meissner, Pure Appl. Chem., 42:4, 551 (1975).

APPENDIX A.

Presented in this Appendix are the values of P_x calculated from the stress field obtained in the flow birefringence investigation using the expression derived from the macroscopic momentum balance equation. Also listed in this Appendix are the stress gradients calculated which are used to evaluate the magnitude of the pressure drop $\Delta P/\Delta L$ in the exit region of the slit die.

Table A.1

Shear Stress Dependence of the Exit Pressure Used to
Calculate N_1 From P_x

Polymer	$\partial P_x / \partial \sigma_w$	k (Equation 5.6)
Styron 678 165 °C	1.65	1.48
LDPE NPE 952 160 °C	4.021	1.19
HDPE LY600-00 200 °C	1.835	1.28

Table A.2

Evaluation of P_x From Flow Birefringence Results. Stress Gradients at the Die Exit Plane. Styron 678 at 165°C.

$$\sigma_w = 4.84 \text{ KPa}$$

y-coordinate [mm]	$(\pi_{zz} - \pi_{yy})$ [Pa]	$y \partial \sigma_{zy} / \partial z$ [Pa]
0	0	0
0.1764	992	-130
0.3528	1693	-463
0.5292	1134	-703
0.7056	346	-511
0.8819	-404	-273
1.0583	-1937	-1231
1.27	-5326	+2500
	-----	-----
Integral Contribution	-230 Pa	+598 Pa
Calculated Exit Pressure = 370 Pa		

Table A.3

Evaluation of P_x From Flow Birefringence Results. Stress Gradients at the Die Exit Plane. Styron 678 at 165°C.

$$\sigma_w = 8.10 \text{ KPa}$$

y-coordinate [mm]	$(\pi_{zz} - \pi_{yy})$ [Pa]	$y \frac{\partial \sigma_{zy}}{\partial z}$ [Pa]
0	1381	0
0.1671	1298	-27
0.3342	1919	-330
0.5013	853	-863
0.6684	-433	-1506
0.8356	-1889	-1590
1.0027	-4546	-4263
1.1698	-7947	-6210
1.27	-9241	+4780
	-----	-----
Integral Contribution	1425 Pa	2311 Pa
Calculated Exit Pressure = 3736 Pa		

Table A.4

Evaluation of P_x From Flow Birefringence Results. Stress Gradients at the Die Exit Plane. Styron 678 at 165°C.

$$\sigma_w = 10.86 \text{ KPa}$$

y-coordinate [mm]	$(\pi_{zz} - \pi_{yy})$ [Pa]	$y \frac{\partial \sigma_{zy}}{\partial z}$ [Pa]
0	2210	0
0.1671	2680	-64
0.3342	2439	-503
0.5013	3385	-1866
0.6684	2247	-3422
0.8356	808	-3480
1.0027	-3400	-3587
1.1698	-8500	-5815
1.27	-14810	+6430
	-----	-----
Integral Contribution	-1425 Pa	3472 Pa

Calculated Exit Pressure = 2045 Pa

Table A.5

Evaluation of P_x From Flow Birefringence Results. Stress Gradients at the Die Exit Plane. Styron 678 at 165°C.

$$\sigma_w = 14.30 \text{ KPa}$$

y-coordinate [mm]	$(\pi_{zz} - \pi_{yy})$ [Pa]	$y \delta \sigma_{zy} / \delta z$ [Pa]
0	5524	0
0.1587	5360	100
0.3175	7447	-25
0.4762	6907	-530
0.6349	4139	-2380
0.7936	1000	-5215
0.9524	-3070	-7945
1.1111	-11050	-11350
1.27	-25390	+12000
	-----	-----
Integral Contribution	-3395 Pa	4110 Pa
Calculated Exit Pressure = 720 Pa		

Table A.6

Evaluation of the Pressure Drop in an Arbitrary Flow Field. Styron 678 at 165°C. $\sigma_w = 4.84$ KPa

z-coordinate [mm]	$\delta \sigma_{zy} / \delta y$ [Pa/mm]	$\delta (\pi_{zz} - \pi_{yy}) / \delta z$ [Pa/mm]
0	11875	-1005
0.353	6779	0
0.706	4520	0
1.058	4520	-780
1.411	4520	-780
1.764	4520	0
2.117	4520	0
	-----	-----
Integral Contribution	10600 Pa	-730 Pa

Calculated Pressure Drop = 9870 Pa

Table A.7

Evaluation of the Pressure Drop in an Arbitrary Flow Field. Styron 678 at 165°C. $\sigma_w = 8.10$ KPa

z-coordinate [mm]	$\delta \sigma_{zy} / \delta y$ [Pa/mm]	$\delta (\pi_{zz} - \pi_{yy}) / \delta z$ [Pa/mm]
0	23405	-2695
0.334	4571	0
0.668	4571	-925
1.003	4687	0
1.337	4687	0
1.671	4687	0
2.005	4520	0
	-----	-----
Integral Contribution	12450 Pa	-759 Pa

Calculated Pressure Drop = 11690 Pa

Table A.8

Evaluation of the Pressure Drop in an Arbitrary Flow Field. Styron 678 at 165°C. $\sigma_w = 10.86$ KPa

z-coordinate [mm]	$\delta \sigma_{zy} / \delta y$ [Pa/mm]	$\delta(\pi_{zz} - \pi_{yy}) / \delta z$ [Pa/mm]
0	30250	-10120
0.334	13190	-3620
0.668	6970	0
1.003	6970	0
1.337	6970	0
1.671	6970	0
2.005	6970	0
	-----	-----
Integral Contribution	19945 Pa	-2900 Pa
Calculated Pressure Drop = 17045 Pa		

Table A.9

Evaluation of the Pressure Drop in an Arbitrary Flow Field. Styron 678 at 165°C. $\sigma_w = 14.3$ KPa

z-coordinate [mm]	$\delta \sigma_{zy} / \delta y$ [Pa/mm]	$\delta (\pi_{zz} - \pi_{yy}) / \delta z$ [Pa/mm]
0	44325	-41890
0.317	14700	0
0.635	12440	0
0.952	12440	0
1.270	12440	0
1.587	12440	0
1.905	12440	0
	-----	-----
Integral Contribution	32480 Pa	-6650 Pa

Calculated Pressure Drop = 32830 Pa

Appendix B. Exit Pressure for a Slit Geometry

In this appendix the expression for P_x given by equation (5.10) is derived. This expression includes the stress gradient $\frac{\partial \tau_{zy}}{\partial z}$ which exists due to the rearrangement of the stress field upstream of the die exit. The first section will derive an expression for P_x in a slit die geometry assuming that the flow field in the slit can be approximated by flow between infinitely wide parallel plates.

The derivation will employ a macroscopic momentum balance over a control volume which encloses the exit region of a slit die. The notation used in the derivation is shown in Figure 2. The derivation assumes that the flow in the control volume is isothermal steady state flow and that gravity, surface tension, and air drag effects are negligible. The components of the macroscopic momentum balance equation under these conditions are given by

$$0 = W \int_0^h \rho v_z^2(y,0) dy - 2W h v_j^2 + \int_0^h 2W \Pi_{zz}(y,0) dy - 2W \int_0^L \tau_{zy}(h,z) dz \quad (B.1)$$

For polymer melts the Reynolds number at low shear rates is much less than one. The inertial terms from the macroscopic balance will therefore be neglected for the flow of polymer melts at low shear rates. Equation B.1 reduces to

$$\int_0^h \Pi_{zz}(y,0) dy = \int_0^L \tau_{zy}(h,z) dz \quad (B.2)$$

The Π_{zz} term can be rewritten in a more useful form by expressing it in terms of the stress measured along the wall. The y-component of the equation of motion yields the following expression:

$$\frac{\partial \Pi_{yy}}{\partial y} = - \frac{\partial \tau_{zy}}{\partial z}$$

NOTE: This exercise is to substitute an expression for Π_{zz} into the fully developed flow equation. Hence, the y-comp. of momentum equation (B.3) not contain any term because $\tau_{zy}(y)$ (no y derivative)

Integrate the expression from $y = y'$ to $y = h$.

$$\Pi_{yy}(y,0) = \Pi_{yy}(h,0) + \int_y^h \frac{\partial \tau_{zy}}{\partial z}(y') dy' \quad (B.4)$$

The viscometric normal stress is defined by

$$N_1(y) = \Pi_{zz}(y,0) - \Pi_{yy}(y,0) \quad (B.5)$$

Equation B.4 can now be written in terms of the normal stress difference N_1 .

$$\Pi_{zz}(y,0) = N_1(y) + \Pi_{yy}(h,0) + \int_y^h \frac{\partial \tau_{zy}}{\partial z}(y') dy' \quad (B.6)$$

The expression for Π_{zz} in equation B.6 can be substituted into the integral in equation B.2.

$$\int_0^h \Pi_{zz}(y,0) dy = \int_0^h N_1(y) dy + h \Pi_{yy}(h,0) + \int_0^h \int_y^h \frac{\partial \tau_{zy}}{\partial z}(y') dy' dy \quad (B.7)$$

Perform partial integration of the double integral.

$$\int \Pi_{zz}(y,0) dy = \int_0^h N_1(y) dy + h \Pi_{yy}(h,0) + \int_0^h y \frac{\partial \tau_{zy}}{\partial z}(y) dy \quad (B.8)$$

The integral expression in equation B.8 can be used to eliminate the Π_{zz} term in equation B.2.

Substitution of the results into equation B.2 yields

$$h \Pi_{yy}(h,0) + \int_0^h N_1(y) dy + \int_0^h y \frac{\partial \tau_{zy}}{\partial z}(y) dy = \int_0^L \tau_{zy}(h,z) dz \quad (B.9)$$

Since the flow in the exit region of the die may contain additional stresses due to extensional velocity gradients, the normal stress difference is not equivalent to N_1 . The primary normal stress difference is written in terms of its stress components. The pressure at the upstream boundary of the control volume is obtained by solving equation B.9 for Π_{yy}

$$\Pi_{yy}(h,0) = \frac{1}{h} \int_0^L \tau_{zy}(h,z) dz - \frac{1}{h} \int_0^h \Pi_{zz} - \Pi_{yy} dy - \frac{1}{h} \int_0^h y \frac{\partial \tau_{zy}}{\partial z}(y) dy \quad (B.10)$$

1.1 Exit Pressure for a Capillary Geometry

In the preceding section of this appendix, an expression was derived from the equation of motion which can be used to evaluate the magnitude of the exit pressure in a slit die. In this section the macroscopic momentum balance will be used to obtain a similar expression which may be used to obtain the value of the exit pressure in a capillary. The notation for the derivation is shown in Figure 5. The analysis for flow in a capillary will be analogous to that in a plane slit, but the secondary normal stress difference will enter into the derivation. The components of the macroscopic momentum balance for the capillary are

$$0 = \int_0^R 2\pi \rho v_z^2(r,0) r dr - \pi \rho R_j^2 v_j^2 + \int_0^R 2\pi \Pi_{zz}(r,0) r dr - \int_0^L 2\pi R \tau_{rz}(R,z) dz \quad (B.11)$$

The inertial terms from equation (B.11) are neglected for the flow of polymer melts at low Reynolds numbers. Also, the Π_{zz} term can be rewritten in a more useful form by expressing it in terms of the stresses measured at the wall. The r component of the equation of motion yields the following expression.

$$\frac{\partial \Pi_{rr}}{\partial r} + \frac{1}{r} (\Pi_{rr} - \Pi_{\theta\theta}) + \frac{\partial \tau_{rz}}{\partial z} = 0 \quad (B.12)$$

Integrate the resulting expression from $r = r'$ to $r = R$.

$$\Pi_{rr}(r,0) = \Pi_{rr}(R,0) + \int_r^R [\Pi_{rr}(r', 0) - \Pi_{\theta\theta}(r', 0)] \frac{dr'}{r'} + \int_r^R \frac{\partial \tau_{zr}}{\partial z}(r') dr' \quad (B.13)$$

The viscometric normal stresses are defined by

$$N_1 = \Pi_{zz}(r,0) - \Pi_{rr}(r,0) \quad (B.14)$$

$$N_2(r) = \Pi_{rr}(r,0) - \Pi_{\theta\theta}(r,0) \quad (B.15)$$

Equation (B.11) can now be written in terms of the normal stress differences N_1 and N_2 .

$$\Pi_{zz}(r,0) = N_1(r) + \Pi_{rr}(R,0) + \int_r^R N_2(r') \frac{dr'}{r'} + \int_r^R \frac{\partial \tau_{zr}}{\partial z}(r') dr' \quad (B.16)$$

The expression for Π_{zz} above is substituted into the integral given in equation (B.12).

$$\begin{aligned} \int_0^R 2\pi \Pi_{zz}(r,0) r dr &= \int_0^R 2\pi [N_1(r) + \Pi_{rr}(R,0)] r dr + \int_0^R \int_r^R 2\pi N_2(r') \frac{dr'}{r'} r dr \\ &\quad + \int_0^R \int_r^R 2\pi \frac{\partial \tau_{zr}}{\partial z}(r') dr' r dr \end{aligned} \quad (B.17)$$

Perform partial integration of the double integral.

$$\int_0^R 2\pi \Pi_{zz}(r,0) r dr = 2\pi \int_0^R 2\pi [N_1(r) + \frac{1}{2}N_2(r)] r dr + \pi R^2 \Pi_{rr}(R,0) + \int_0^R \pi \frac{\partial \tau_{zr}}{\partial z}(r) r^2 dr \quad (B.18)$$

Equation (B.11) without the inertial terms can now be written in terms of the normal stress differences and the total stress component measured at the wall.

$$2\pi \int_0^R [N_1(r) + \frac{1}{2}N_2(r)] r dr + \pi R^2 \Pi_{rr}(R,0) + \int_0^R \pi \frac{\partial \tau_{zr}}{\partial z} r^2 dr - \int_0^L 2\pi R \tau_{rz}(R,z) dz = 0 \quad (B.19)$$

The pressure at the upstream boundary of the control volume is obtained by solving equation (B.20) for Π_{rr}

$$\Pi_{rr}(R,0) = \int_0^L \frac{2}{R} \tau_{rz}(R,z) dz - \int_0^R \frac{2}{R^2} [\Pi_{zz} - \Pi_{rr} + \frac{1}{2}(\Pi_{rr} - \Pi_{\theta\theta})] r dr \quad (B.20)$$

$$- \int_0^R \frac{1}{R^2} \frac{\partial \tau_{rz}}{\partial z}(r) r^2 dr$$

APPENDIX C.

Presented in this Appendix is the program listing of the mixed penalty method finite code MAX2D. Documentation for the program is included in the listing. A sample data file modeling the steady shear flow between two infinite parallel plates is also included in the documentation.


```

C          SOLUTION
C  VISC      -  VISCOSITY FUNCTION AS A FUNCTION OF THE MAGNITUDE OF
C              THE RATE OF DEFORMATION TENSOR
C.....
C
C  COMMON BLOCKS :  DEFINE THE STORAGE REQUIREMENTS FOR THE FINITE
C                   ELEMENT PROBLEM. DIMENSIONS MUST BE CHANGED FOR
C                   COMMON STATEMENTS THROUGHOUT THE PROGRAM TO
C                   CHANGE CURRENT MEMORY CONFIGURATION.
C
C  COMMON/MSH/  X(NNM),Y(NNM),DX(21),DY(21),NOD(NNM,9)
C              WHERE NNM - NUMBER OF NODES IN THE MESH
C
C  COMMON/STR/  GSTIF(NRMAX,NBW)
C              NRMAX - TOTAL NUMBER OF DEGREES OF FREEDOM IN THE
C              MESH.  NRMAX = NEM * NDF
C              NBW = VALUE OF THE FULL BAND WIDTH FOR THE
C              ASSEMBLED GLOBAL STIFFNESS MATRIX
C
C.....
C
C  D E S C R I P T I O N   O F   T H E   V A R I A B L E S
C
C  AMU.....ZERO SHEAR RATE VISCOSITY
C  AMBDA....VALUE OF THE FLUID TIME CONSTANT IN SUBROUTINE STIFFQ
C           USER MAY SUPPLY A FUNCTION TO EVALUATE LAMBDA AS A FUNCTION
C           OF THE RATE OF DEFORMATION TENSOR
C  BETA.....ACCELERATION PARAMETER FOR THE PICARD ITERATION TECHNIQUE
C  C1,C2....MATERIAL CONSTANTS FOR FLUID FLOW PROBLEM
C           C1= ZERO SHEAR VISCOSITY ON INPUT
C           C2= VALUE OF PENALTY PARAMETER ON INPUT
C  C4,C5....MATERIAL CONSTANTS FOR NON-NEWTONIAN VISCOSITY FUNCTIONS
C           C4= M-CONSTANT FOR POWERLAW MODEL OR LAMBDA FOR THE CARREAU
C           MODEL
C           C5= EXPONENT N USED IN BOTH THE POWERLAW AND CARREAU MODEL
C  ELSTIF...ELEMENT COEFFICIENT (OR 'STIFFNESS') MATRIX
C  ELXY.....GLOBAL COORDINATES OF ELEMENT NODES:
C           ELXY(I,1)=XE(I);  ELXY(I,2)=YE(I), I=1,NPE.
C  EPS.....TOLERANCE PARAMETER FOR NONLINEAR ITERATIONS
C  ERR.....GLOBAL ERROR FOR THE CURRENT SOLUTION
C  F(I).....ELEMENT FORCE VECTOR
C  GF(I)....ARRAY OF PREVIOUS SOLUTION FOR PICARD ITERATION
C  GP(I)....ARRAY OF I-2 SOLUTION FOR PICARD ITERATION
C  GSTIF....GLOBAL COEFFICIENT MATRIX.  ASSEMBLED AND STORED IN
C           BANDED FORM.
C  IBDF(I)...ARRAY OF SPECIFIED BOUNDARY DEGREES OF FREEDOM
C  IBN(I)....ARRAY OF BOUNDARY ELEMENTS FOR CONVECTIVE B. C.
C  IBSF(I)...ARRAY OF SPECIFIED NONZERO FORCES.
C  ICONV....INDICATOR FOR APPLIED FORCES ON THE BOUNDARIES
C           ICONV=1, BOUNDARY FORCE IS PRESENT

```

```

C          ICONV=0, NO FORCES
C  IEL.....INDICATOR FOR TYPE OF ELEMENT
C          IEL=0, FOUR-NODE QUADRILATERAL ELEMENT
C          IEL=1, QUADRATIC QUADRILATERAL
C  IFREE.....INDICATOR FOR FREE SURFACE PROBLEM
C          IFREE=0, NO FREE SURFACE PRESENT
C          IFREE=1, FREE SURFACE CALCULATION
C  IMESH.....INDICATOR FOR MESH GENERATION
C          IMESH=0, MESH INFORMATION IS TO READ INTO PROGRAM
C          IMESH=1, MESH IS GENERATED IN PROGRAM
C  IMODEL....CONSTITUTIVE EQUATION FOR THE CURRENT PROBLEM
C          IMODEL=0, GENERALIZED NEWTONIAN FLUID
C          IMODEL=1, UPPER-CONVECTED MAXWELL
C          IMODEL=2, WHITE-METZNER MODEL
C  INOD(I,J).THE J-TH NODE OF THE I-TH ELEMENT FOR THE ELEMENTS
C          (ON THE APPLIED BOUNDARY FORCES)
C  IPRNT.....FLAG FOR SUCCESSFUL COMPLETION OF THE FREE SURFACE
C          CALCULATION IPRNT = 1 - CONVERGENCE OF FREE SURFACE -
C  ISTRM.....STREAM FUNCTION CALCULATION FLAG
C          ISTRM=0, NO STREAM FUNCTIONS
C          ISTRM=1, CALCULATE STREAM FUNCTIONS FOR STREAM LINE PLOT
C  ITER.....VALUE OF THE ITERATION NUMBER FOR NON-LINEAR ITERATION
C  ITMAX.....MAXIMUM NUMBER OF ITERATIONS FOR THE NONLINEAR ANALYSIS
C  ITFMAX....MAXIMUM NUMBER OF ITERATIONS FOR THE FREE SURFACE
C          CALCULATIONS
C  ITYPE.....VISCOSITY MODEL TO BE USED:
C          ITYPE=0, NEWTONIAN VISCOSITY
C          ITYPE=1, POWER-LAW FLUID VISCOSITY FUNCTION
C          ITYPE=2, CARREAU MODEL VISCOSITY FUNCTION
C  IVFS()....ARRAY OF NODES WHICH ARE ON THE FREE SURFACE
C  NBE.....NUMBER OF BOUNDARY ELEMENTS FOR APPLIED BOUNDARY FORCES
C  NBW.....BAND WIDTH OF THE COEFFICIENT MATRIX, GSTIF
C  NCMAX....COLUMN DIMENSION OF GSTIF IN THE DIMENSION STATEMENT
C  NDF.....NUMBER OF DEGREES OF FREEDOM PER NODE
C  NEQ.....TOTAL NUMBER OF EQUATIONS IN THE PROBLEM (=NNM*NDF)
C  NEM.....NUMBER OF ELEMENTS IN THE MESH
C  NFS.....NUMBER OF FREE SURFACE NODES (MUST INCLUDE THE NODE WHICH
C          ATTACHES TO THE SOLID SURFACE)
C  NHBW.....HALF BAND WIDTH OF THE COEFFICIENT MATRIX, GSTIF
C  NN.....TOTAL NUMBER OF DEGREES OF FREEDOM PER ELEMENT (=NPE*NDF)
C  NNM.....NUMBER OF NODES IN THE FINITE ELEMENT MESH
C  NOD(I,J)..GLOBAL NODE NUMBER CORRESPONDING TO THE J-TH NODE OF
C          ELEMENT I (CONNECTIVITY MATRIX)
C  NPE.....NUMBER OF NODES PER ELEMENT
C  NPRNT....INDICATOR FOR PRINTING ELEMENT MATRICES AND VECTORS
C          NPRNT=1, PRINT ELEMENT MATRICES
C          NPRNT=0, NO PRINT
C  NRMAX....ROW DIMENSION OF GSTIF IN THE DIMENSION STATEMENT
C  NSBF.....NUMBER OF SPECIFIED NONZERO BOUNDARY 'FORCES'
C  NSDF.....NUMBER OF SPECIFIED PRIMARY DEGREES OF FREEDOM
C  NX,NY....NUMBER OF ELEMENTS IN THE X AND Y DIRECTION, RESPECTIVELY

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C                                     STREAM LINE CONTOUR PLOTS
C 31-35      IFREE      FREE SURFACE INDICATOR FLAG
C                                     IFREE=0, NO FREE SURFACE
C                                     IFREE=1, FREE SURFACE BOUNDARY PRESENT
C 36-40      ITMAX      MAXIMUM NUMBER OF ITERATIONS FOR NONLINEAR
C                                     ANALYSIS.
C 41-45      ITFMAX     MAXIMUM NUMBER OF FREE SURFACE ITERATIONS
C
C 46-50      NPRNT      PRINT INDICATOR FOR ELEMENT MATRICES AND
C                                     VECTORS  NPRNT=1 PRINT; NPRNT=0 NO PRINT
C
C
C *DATA CARD 3  (16I5)      SKIP CARDS 3,4, AND 5 IF IMESH=1
C
C 1-5        NEM         NUMBER OF ELEMENTS IN THE MESH
C 6-10       NNM         NUMBER OF NODES IN THE MESH
C
C
C *DATA CARD 4  (16I5)      NEM CARDS AND NPE ENTRIES/CARD
C
C 1-45       NOD(I,J)     I-TH ROW OF THE CONNECTIVITY MATRIX.
C
C
C *DATA CARD 5  (8F10.4)    8 ENTRIES PER CARD
C
C 1-80       X(I), Y(I)    X AND Y CORINATES OF NODE I.
C
C
C *DATA CARD 6  (16I5)      SKIP CARDS 6,7,AND8 IF IMESH=0
C
C 1-5        NX          NUMBER OF SUBDIVISIONS IN THE X-DIRECTION
C 6-10       NY          NUMBER OF SUBDIVISIONS IN THE Y-DIRECTION
C
C
C *DATA CARD 7 AND 8  (8F10.4)  IEL*NX+1 ENTRIES FOR NX AND IEL*NY+1
C                                     ENTRIES FOR NY
C
C 1-80       DX(I)        DISTANCE BETWEEN NODES ALONG X-DIRECTION
C 1-80       DY(I)        DISTANCE BETWEEN NODES ALONG Y-DIRECTION
C
C
C *DATA CARD 9  (8F10.4)    CONSTANTS DEPENDING ON PROBLEM TYPE
C
C 1-10       C1           ZERO SHEAR VISCOSITY
C 11-20      C2           PENALTY PARAMETER
C 21-30      EPS          TOLERANCE PARAMETER FOR ITERATIONS
C 31-40      C4           M-CONSTANT FOR POWERLAW OR LAMBDA FOR
C                                     THE CARREAU MODEL.
C 41-50      C5           EXPONENT N USED IN BOTH THE POWERLAW AND
C                                     THE CARREAU MODEL.
C
C

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C
C *DATA CARD 10 (8F10.4)      PROBLEM CONSTANTS
C
C 1-10      BETA      ACCELERATION PARAMETER FOR PICARD ITERATION
C 11-20     TOL       TOLERANCE FOR THE FREE SURFACE ITERATION
C 21-30     RHO       FLUID DENSITY USED IN INERTIAL TERMS
C 31-40     PSINIT    VALUE OF THE STREAM FUNCTION AT ELEMENT
C                      NUMBER 1 AND LOCAL NODE 1. USED AS INITIAL
C                      VALUE FOR STREAM FUNCTION CALCULATION
C 41-50     TMCNST    VALUE OF THE FLUID TIME CONSTANT FOR THE
C                      UPPER CONVECTED MAXWELL MODEL
C
C
C *DATA CARD 11 (16I5)      IF NDSF=0, ENTER ZERO IN COLUMN 5 AND
C                          SKIP CARDS 11 AND 12
C
C 1-5       NSDF       NUMBER OF SPECIFIED PRIMARY DEGREES OF
C                      FREEDOM.
C
C
C *DATA CARD 12 (16I5)      READ NSDF ENTRIES
C
C 1-80      IBDF(I)    SPECIFIES DEGREES OF FREEDOM
C
C
C *DATA CARD 13 (8F10.4)    READ NSDF ENTRIES
C
C 1-80      VBDF(I)    VALUES OF THE SPECIFIED DEGREES OF FREEDOM
C                      IN ARRAY IBDF(I).
C
C
C *DATA CARD 14 (16I5)      IF NSBF=0, ENTER ZERO IN COLUMN 5 AND
C                          SKIP CARDS 14 AND 15.
C
C 1-5       NSBF       NUMBER OF SPECIFIES NONZERO SECONDARY
C                      DEGREES OF FREEDOM.
C
C
C *DATA CARD 15 (16I5)      READ NSBF ENTRIES
C
C 1-80      IBSF(I)    SPECIFIED NONZERO SECONDARY DEGREES OF
C                      FREEDOM.
C
C
C *DATA CARD 16 (8F10.4)    READ NSBF ENTRIES
C
C 1-80      VBSF(I)    VALUES OF SECONDARY DEGREES OF FREEDOM
C
C
C *DATA CARD 17 (16I5)      IF IFREE = 0, ENTER 0 IN COLUMN 5 AND

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C                                     SKIP DATA CARD 18
C
C 1-5      NFS      NUMBER OF NODES ON THE FREE SURFACE BOUNDARY
C              (MUST INCLUDE THE NODE WHERE THE FREE
C              SURFACE ATTACHES TO THE SOLID WALL.
C
C
C *DATA CARD 18      (16I5)  READ NFS ENTRIES
C
C 1-80      IVFS(I)  NODE NUMBERS OF THE LOCATION OF THE NODES ON
C              THE FREE SURFACE BOUNDARY. START NUMBERS
C              FROM THE POINT OF ATTACHMENT AND CONTINUE
C              OUT ALONG THE FREE SURFACE.
C
C.....
C
C   S A M P L E   D A T A   F I L E
C   -----
C
C   STEADY SIMPLE SHEAR FLOW  SIGN OF PRIMARY NORMAL STRESS DIFFERENCE
C   1   4   1   0   1   0   0   5   1   0
C   4   5
C 12.7  12.7  12.7  12.7  0.0
C 3.81  2.54  2.54  2.54  1.27  0.0
C 11100.0 1110.0  0.01  4.0  0.67
C 0.8  0.01  0.0  5.0  0.1
C 28
C   1   2   6   7   11  12  16  17  21  22  27  47  52  72  77  97
C 102 122 126 127 131 132 136 137 141 142 146 147
C 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
C 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
C 0.0  0.0  1.0  0.0  1.0  0.0  1.0  0.0
C 1.0  0.0  1.0  0.0
C 0
C 0
C.....
C
C   PROGRAM UNIT *** MAIN ***
C
C.....
C   FUNCTION :
C   DRIVER PROGRAM FOR MOD1 FINITE ELEMENT PROGRAM.  MAIN CONTAINS
C   DATA INPUT, NON-LINEAR ITERATIVE LOOPS, FREE SURFACE ITERATION
C   LOOPS, DATA ECHO SECTION, SOLUTION OUTPUT AND FORMAT STATEMENTS
C
C.....
C   DEFINITION OF VARIABLES :
C   1 - INPUT :
C       SEE DATA CARD LISTING IN DOCUMENTATION
C
C   2 - OUTPUT :

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C      NHBW - NUMBER OF THE HALF BAND WIDTH FOR THE MESH
C      ITERFS - CURRENT NUMBER OF THE FREE SURFACE ITERATION
C      ELSTIF(20,20) - ELEMENT STIFFNESS MATRIX
C      X(NEM), Y(NEM) - COORDINATES OF THE NODES IN THE FINITE ELEMENT
C      MESH
C      NOD(NEM,NPE) - CONNECTIVITY MATRIX FOR THE MESH
C      ITER - ITERATION NUMBER FOR THE NON-LINEAR SOLUTION
C      ERR - VALUE OF THE TOTAL GLOBAL ERROR BETWEEN SOLUTION I AND
C      I - 1.
C      GSTIF(5*I-4,NBW) - X VELOCITY OF SOLUTION VECTOR
C      GSTIF(5*I-3,NBW) - Y VELOCITY
C      GSTIF(5*I-2,NBW) - STRESS T11
C      GSTIF(5*I-1,NBW) - STRESS T12
C      GSTIF(5*I, NBW) - STRESS T22
C
C.....
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION GF(595),GP(595),W(2,9),VEL(20),IBDF(100),VBDF(100),
1      IBSF(25),VBSF(25),TITLE(20),IVFS(20)
      COMMON/MSH/X(120),Y(120),DX(21),DY(21),NOD(120,9)
      COMMON/STF/ELSTIF(20,20),ELXY(4,2),A0,A1
      COMMON/VIS/C4,C5,AMBDA,RHO,ITER
      COMMON/STR/GSTIF(595,90)
      DATA NRMAX,NCMAX/595,90/
C
C      .....
C      .
C      .           P R E P R O C E S S O R   U N I T           .
C      .
C      .....
C
C      R E A D I N   T H E   I N P U T   D A T A   H E R E
C
      READ 400,TITLE
      READ 520, IEL,NPE,IMODEL,ITYPE,IMESH,ISTRM,IFREE,ITMAX,ITFMAX,
*      NPRNT
      IF(ITYPE.EQ.2 .AND. IEL.EQ.0)STOP
C      READ IN MESH DATA FOR USER SUPPLIED MESH - MUST INCLUDE NUMBER OF
C      ELEMENTS AND NODES PLUS CONNECTIVITY MATRIX AND NODAL COORDINATES
      IF(IMESH.EQ.1)GOTO 30
      READ 520, NEM,NNM
      DO 20 N=1,NEM
20  READ 520, (NOD(N,I),I=1,NPE)
      READ 580, (X(I),Y(I),I=1,NNM)
      GOTO 40
C      READ IN NUMBER OF SUBDIVISIONS AND DIMENSIONS USED TO GENERATE
C      THE MESH WITHIN THE PROGRAM FOR RECTANGULAR DOMAINS.
30  READ 520, NX,NY
      NXX1=IEL*NX+1
      NYY1=IEL*NY+1
      READ 580, (DX(I),I=1,NXX1)

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      READ 580, (DY(I),I=1,NYY1)
      CALL MESH( IEL,NX,NY,NPE,NNM,NEM)
C
C
40 READ 585, C1,C2,EPS,C4,C5
   READ 585, BETA,TOL,RHO,PSINIT,TMCNST
50 READ 520, NSDF
C   SKIP INPUT IF NSDF = 0
   IF(NSDF.EQ.0)GOTO 60
   READ 520, (IBDF(I),I=1,NSDF)
   READ 580, (VBDF(I),I=1,NSDF)
C
60 READ 520, NSBF
C   SKIP INPUT OF SPECIFIED FORCES IF NSBF = 0
   IF(NSBF.EQ.0)GOTO 70
   READ 520, (IBSF(I),I=1,NSBF)
   READ 580, (VBSF(I),I=1,NSBF)
C
C   INPUT OF NUMBER AND LOCATION OF NODES ON THE FREE SURFACE
70 READ 520, NFS
   IF(NFS.EQ.0) GOTO 72
   READ 520, (IVFS(I),I=1,NFS)
C
C   E N D   O F   T H E   D A T A   I N P U T
C.....
C
C   SET INTERNAL VARIABLES NEEDED FOR COMPUTATION
C
C   C2 IS THE PENALTY PARAMETER WHICH IS MULTIPLIED BY FACTOR OF 1E6
C   TO CREATE LARGE VALUE REQUIRED FOR CALCULATIONS
72  C2=C2*1.0D6
   ITER = 0
   ITERFS = 0
   NDF = 5
   NEQ=NNM*NDF
   NN=NPE*NDF
C
C   D A T A   E C H O   S E C T I O N
C
   WRITE(6,550)
   WRITE(6,400) TITLE
   WRITE(6,790)
   WRITE(6,910)
   WRITE(6,660) IEL,IMODEL,ITYPE
   WRITE(6,650) IMESH,IFREE,ISTRM
   WRITE(6,655) NPRNT,ITMAX,ITFMAX
   WRITE(6,665) BETA,EPS,TOL,PSINIT
   WRITE(6,675) RHO,C1,C2,TMCNST
   IF(ITYPE.EQ.1) WRITE(6,770)
   IF(ITYPE.EQ.1) WRITE(6, 720) C4,C5
   IF(ITYPE.EQ.2) WRITE(6,780)

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        IF(ITYPE.EQ.2) WRITE(6, 725) C4,C5
        WRITE(6, 450) NDF,NEM,NNM,NEQ
        WRITE(6, 500)
C      BOOLEAN CONNECTIVITY MATRIX
        DO 75 I=1,NEM
75    WRITE(6, 440) I,(NOD(I,J),J=1,NPE)
        IF(NSDF.EQ.0) GOTO 77
        WRITE(6, 460) NSDF
        WRITE(6, 520)(IBDF(I),I=1,NSDF)
        WRITE(6,595)
        WRITE(6,480) (VBDF(I),I=1,NSDF)
77    IF(NSBF.EQ.0) GOTO 100
        WRITE(6, 640) NSBF,(IBSF(I),I=1,NSBF)
        WRITE(6, 600)
        WRITE(6, 480) (VBSF(I),I=1,NSBF)
100   IF(NFS.EQ.0) GOTO 105
        WRITE(6,920) NFS
        WRITE(6,520) (IVFS(I),I=1,NFS)
C
C      .....
C      .
C      .                P R O C E S S O R   U N I T
C      .
C      .....
C
C
C      COMPUTE THE HALF BAND WIDTH
C
105   NHBW=0
        DO 110 N=1,NEM
        DO 110 I=1,NPE
        DO 110 J=1,NPE
            NW=(IABS(NOD(N,I)-NOD(N,J))+1)*NDF
110   IF (NHBW.LT.NW) NHBW=NW
C
        NBW = 2*NHBW
        WRITE(6, 590) NHBW
C
C      INITIALIZE THE GLOBAL STIFFNESS MATRIX AND FORCE VECTOR
C
125   DO 130 I=1,NEQ
        GF(I)=0.0
        GP(I) = 0.0
130   GSTIF(I,NBW) = 0.0
        IF (IFREE.EQ.0) GOTO 800
C
C      FREE SURFACE CALCULATION LOOP BEGINS HERE
C      SECTION HAS STOP SEQUENCE TO END FREE SURFACE ITERATIONS
C      WRITE STATEMENT PRINTS HEADING FOR EACH FS ITERATION
C
1010  ITERFS = ITERFS + 1

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      ITER = 0
C     TRAP TO CHECK FOR NUMBER OF FREE SURFACE ITERATIONS
      IF(ITERFS.GT.ITFMAX) WRITE(6,925) ITFMAX
C     STOP PROGRAM IF NUMBER OF ITERATIONS HAS BEEN EXCEEDED
      IF(ITERFS.GT.ITFMAX) GOTO 840
      WRITE(6,930) ITERFS
C
C
C     BEGIN ITERATION ON NON-LINEAR VISCOSITY FUNCTION
C
      800 ITER = ITER + 1
      IF(ITER.GT.ITMAX) WRITE(6, 396) ITMAX,ERR
      IF(ITER.GT.ITMAX) GOTO 815
C     DEFINE PREVIOUS SOLUTIONS VECTORS IN DO LOOP FOR USE IN
C     PICARD ITERATION.  USES TWO PREVIOUS SOLUTIONS FOR NEXT GUESS
      DO 810 I = 1,NEQ
      GP(I) = GF(I)
      GF(I) = GSTIF(I,NBW)
      DO 810 J = 1,NBW
      810 GSTIF(I,J) = 0.0
C
C     DO-LOOP ON THE NUMBER OF ELEMENTS TO CALCULATE THE ELEMENT
C     MATRICES, AND ASSEMBLY OF THE ELEMENT MATRICES BEGINS HERE
C
      140 DO 300 N=1,NEM
C
C     ASSIGN ELEMENT DATA FROM GLOBAL SOLUTION AND COORDINATES
      DO 150 I=1,NPE
      NI=NOD(N,I)
      L = 5*I - 4
      LI = NI*NDF - 4
C
C     ASSIGN NEW VALUE TO THE NONLINEAR VELOCITY TERMS
C
      VEL(L) = BETA*GF(LI) + (1.0-BETA)*GP(LI)
      VEL(L+1) = BETA*GF(LI+1) + (1.0-BETA)*GP(LI+1)
C     ELEMENT - GLOBAL COORDINATE CORRESPONDENCE
      ELXY(I,1)= X(NI)
      ELXY(I,2)= Y(NI)
      150 CONTINUE
C
C     CALCULATE ELEMENT STIFFNESS MATRIX IN SUBROUTINE STIFFQ
      CALL STIFFQ(NPE,NN,IEL,ITYPE,C1,C2,C5,VEL,IMODEL,TMCNST)
C     OUTPUT OF ELEMENT STIFFNESS MATRIX
      IF(N.NE.NPRNT.OR.ITER.GT.1)GOTO 200
      WRITE(6,680) N
      DO 160 I=1,NN
      160 WRITE(6, 670) (ELSTIF(I,J),J=1,NN)
C
C     ASSEMBLE ELEMENT MATRICES TO OBTAIN GLOBAL MATRIX
C

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200 CALL ASMBLE(NPE,NDF,NHBW,NEM,N)
C      END OF DO LOOP OVER THE NUMBER OF ELEMENTS FOR ELEMENT
C      STIFFNESS MATRIX
300 CONTINUE
C
C      ASSEMBLED MATRIX EQUATIONS ARE NOW READY FOR IMPLEMENTATION OF
C      THE BOUNDARY CONDITIONS ON PRIMARY AND SECONDARY VARIABLES
C
      CALL BOUND(VBSF,VBDF,IBSF,IBDF,NSBF,NBW,NSDF)
C
C      CALL SUBROUTINE 'BDUNSM' TO SOLVE THE SYSTEM OF EQUATIONS FOR THE
C      PRIMARY DEGREES OF FREEDOM (THE SOLUTION IS RETURNED IN
C      GSTIF(I,NBW)
C
      CALL BDUNSM (NEQ,NHBW)
C
C      .....
C      .
C      .           P O S T P R O C E S S O R   U N I T           .
C      .
C      .....
C
C      GO TO LINE 800 FOR FIRST ITERATION - MUST HAVE TWO SOLUTIONS FOR
C      ERROR COMPARISON
370 IF(ITER.EQ.1) GOTO 800
      ERR = 0.0
C      DO LOOP CALCULATES THE GLOBAL ERROR OVER ALL DEGREES OF FREEDOM
      DO 375 I = 1,NEQ
375 ERR = ERR + (GF(I)-GSTIF(I,NBW))**2
      WRITE(6, 730) ITER,ERR
C
C      REPEAT ITERATIONS IF ERROR IS GREATER THAN USER DEFINED TOLERANCE
C
      IF(ERR.GT.EPS) GOTO 800
C
815 IF(IFREE.EQ.0) GO TO 840
      CALL FREESF(IVFS,NFS,TOL,NBW,NMAX,IPRNT,ITERFS)
C
C      IPRNT FLAG RETURNS = 1 IF FREE SURFACE ITERATIONS HAVE CONVERGED
C      IF = 0 BRANCH TO ANOTHER ITERATION
      IF(IPRNT.EQ.0) GOTO 1010
      WRITE(6,935) ITERFS
C
C      O U T P U T   O F   S O L U T I O N   V E C T O R
C
840 WRITE(6, 540)
      WRITE(6, 750)
      WRITE(6, 485)(I,X(I),Y(I),GSTIF(5*I-4,NBW),GSTIF(5*I-3,NBW),GSTIF(
*      5*I-2,NBW),GSTIF(5*I-1,NBW),GSTIF(5*I,NBW),
*      GSTIF(5*I-2,NBW)-GSTIF(5*I,NBW),I=1,NNM)
C

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C   P O S T   P R O C E S S I N G   S E C T I O N
C
      WRITE(6, 760)
      WRITE(6, 620)
      DO 390 N=1,NEM
      DO 380 I=1,NPE
      NI=NOD(N,I)
      L=NI*NDF-4
C
C   ASSIGN VALUES OF SOLUTION VECTOR FOR CALCULATION OF POST PROCESSOR
C   VARIABLES
      W(1,I)=GSTIF(L,NBW)
      W(2,I)=GSTIF(L+1,NBW)
      ELXY(I,1)=X(NI)
380  ELXY(I,2)=Y(NI)
390  CALL STRESS(N,NPE,ELXY,W,C1,C2,ITYPE,IEL,IMODEL,TMCNST)
C       CALCULATION OF THE STREAM FUNCTION IF REQUESTED
      IF(ISTRM.EQ.0) GOTO 820
      CALL STREAM(NNM,PSINIT,NEM,NPE,NDF,NBW)
820  STOP
C
C.....
C
C       F O R M A T S
C
C.....
396  FORMAT(/,2X,120(1H*),/,2X,120(1H*),//,40X,
      *'NON - LINEAR CONVERGENCE NOT MET',//,
      *45X,'MAXIMUM ITERATION =',I3,//,
      *55X,'GLOBAL ERROR =',E12.5,//,
      *2X,120(1H*),/,2X,120(1H*),/)
400  FORMAT(20A4)
440  FORMAT (10X,20I5)
450  FORMAT (10X,'NUMBER OF DEGREES OF FREEDOM PER NODE..=',I4,/,
      *10X,'ACTUAL NUMBER OF ELEMENTS IN THE MESH....=',I4,/,
      *10X,'NUMBER OF NODES IN THE MESH.....=',I4,/,10X, 'TOTAL
      2NUMBER OF EQUATIONS IN THE MODEL...=',I4,/)
460  FORMAT (/,5X,'NO. OF SPECIFIED DEGREES OF FREEDOM.....=',I3,/,
      *5X,'ARRAY OF THE SPECIFIED DEGREES OF FREEDOM=',/)
480  FORMAT (6(2X,E12.5))
485  FORMAT (5X,I4,2X,8E15.5)
500  FORMAT (/,5X,'BOOLEAN (CONNECTIVITY) MATRIX NOD(I,J) ',/)
520  FORMAT (16I5)
540  FORMAT (/,3X,'SOLUTION VECTOR:',/)
550  FORMAT(/,2X,120(1H*),/,2X,120(1H*),//,40X,
      *'MOD1 FINITE ELEMENT SIMULATION',//,
      *50X,'MICHAEL READ AUG, 1985',//,
      *2X,120(1H*),/,2X,120(1H*),/)
580  FORMAT (8F10.4)
585  FORMAT (5F10.4)
590  FORMAT (//,5X,'HALF BAND WIDTH OF GLOBAL STIFFNESS MATRIX =',I3)

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595 FORMAT (/ ,5X,'VALUES OF THE PRIMARY DEGREES OF FREEDOM',/)
600 FORMAT(/ ,5X,'VALUES OF THE SPECIFIED FORCES:',/)
620 FORMAT (/ ,6X,'ELE.NO.',3X,'PRESSURE ',6X,'SHEAR RATE ',7X,
*'VISCOSITY',8X,'LAMBDA',11X,'EXTENSION RATE',/)
640 FORMAT(/ ,5X,'NO. OF SPECIFIED FORCES =' ,I5,/,5X,'SPECIFIED FORCE
1DEGREES OF FREEDOM :',15I5,/)
650 FORMAT(10X,'MESH GENERATION FLAG.....=' ,I2,/,
*15X,'= 0 , USER DEFINED MESH',/,
*15X,'= 1 , PROGRAM WILL GENERATE RECTANGULAR MESH',//,
*10X,'FREE SURFACE PROBLEM FLAG.....=' ,I2,/,
*15X,'= 0 , NO FREE SURFACE',/,
*15X,'= 1 , FREE SURFACE PRESENT',//,
*10X,'STREAM FUNCTION CALCULATION FLAG.....=' ,I2,/,
*15X,'= 0 , NO STREAM LINES',/,
*15X,'= 1 , CALCULATE STREAM FUNCTION FOR STREAM LINE PLOT',/)
655 FORMAT(10X,'ELEMENT MATRICES PRINT FLAG.....=' ,I2,/,
*15X,'= 0 , NO PRINTING',/,
*15X,'= 1 , PRINT ELEMENT AND GLOBAL STIFFNESS MATRICES',//,
*10X,'MAXIMUM NUMBER OF NON-LINEAR ITERATIONS..=' ,I2,//,
*10X,'MAXIMUM NUMBER OF FREE SURFACE ITERATIONS =' ,I2,/)
660 FORMAT(10X,'ELEMENT TYPE.....=' ,I2,/,
*15X,'= 1 , BILINEAR QUADRILATERALS',//,
*10X,'CONSTITUTIVE EQUATION.....=' ,I2,/,
*15X,'= 0 , GENERALIZED NEWTONIAN FLUID',/,
*15X,'= 1 , UPPER-CONVECTED MAXWELL MODEL',/,
*15X,'= 2 , WHITE-METZNER MODEL',//,
*10X,'VISCOSITY MODEL.....=' ,I2,/,
*15X,'= 0 , NEWTONIAN VISCOSITY',/,
*15X,'= 1 , POWERLAW MODEL',/,
*15X,'= 2 , CARREAU MODEL',/)
665 FORMAT(10X,'ACCELERATION PARAMETER BETA.....=' ,E10.3,//,
*10X,'ERROR TOLERANCE ON NON-LINEAR ITERATIONS=' ,E10.3,//,
*10X,'ERROR TOLERANCE ON FREE SURFACE .....=' ,E10.3,//,
*10X,'INITIAL VALUE FOR STREAM FUNCTION AT ',/,
*10X,'ELEMENT 1, LOCAL NODE 1.....=' ,E10.3,/)
675 FORMAT(/ ,20X,'F L U I D P A R A M E T E R S',//,
*10X,'FLUID DENSITY.....=' ,E10.3,/,
*10X,'ZERO SHEAR RATE VISCOSITY.....=' ,E10.3,/,
*10X,'PENALTY PARAMETER.....=' ,E10.3,/,
*10X,'TIME CONSTANT (MAXWELL MODEL).....=' ,E10.3,/)
670 FORMAT(5E15.5)
680 FORMAT(3X,'ELEMENT MATRICES:',I4,/)
720 FORMAT(/ ,10X,'ETA M .....=' ,E12.5,/,
*10X,'ETA N .....=' ,E12.5,/)
725 FORMAT(/ ,10X,'LAMBDA.....=' ,E12.5,/,
*10X,'EXPONENT N.....=' ,E12.5,/)
730 FORMAT(2X,'ITERATION NUMBER = ',I4,5X,'ERROR = ',E12.5)
750 FORMAT(5X,'NODE',6X,'X COORDINATE',3X,'Y COORDINATE',3X,
*'X VELOCITY',5X,'Y VELOCITY',5X,'STRESS T11',5X,'STRESS T12',
* 5X,'STRESS T22',7X,'N1',//)
760 FORMAT(/ ,5X,'P O S T P R O C E S S O R U N I T',///)

```

```

770 FORMAT(//,15X,'POWER LAW MODEL VISCOSITY FUNCTION COEFFICIENTS')
780 FORMAT(//,15X,'CARREAU MODEL VISCOSITY FUNCTION COEFFICIENTS')
790 FORMAT(//,5X,'D A T A           E C H O           S E C T I O N',/)
910 FORMAT(//,3X,'C O N T R O L   C A R D   I N F O R M A T I O N',//)
920 FORMAT(//,10X,'NUMBER OF NODES ON THE FREE SURFACE.....=',I2,/,
  *10X,'ARRAY OF FREE SURFACE NODES.....',/)
925 FORMAT(/,2X,120(1H*),/,2X,120(1H*),//,40X,
  *'N O   F R E E   S U R F A C E   C O N V E R G E N C E ',//,45X,
  *'M A X I M U M   I T E R A T I O N =' ,I3,//,
  *2X,120(1H*),/,2X,120(1H*),/)
930 FORMAT(/,2X,120(1H*),/,2X,120(1H*),//,40X,
  *'F R E E   S U R F A C E   I T E R A T I O N',//,47X,
  *'I T E R A T I O N ',I3,//,
  *2X,120(1H*),/,2X,120(1H*),/)
935 FORMAT(/,2X,120(1H*),/,2X,120(1H*),//,37X,
  *'F R E E   S U R F A C E   C O N V E R G E N C E   M E T ',//,50X,
  *'I T E R A T I O N ',I3,//,
  *2X,120(1H*),/,2X,120(1H*),/)
1000 STOP
      END
      SUBROUTINE ASMBLE(NPE,NDF,NHBM,NEM,N)
C      .....
C      FUNCTION :
C      -----
C      THE SUBROUTINE ASSEMBLES THE ELEMENT STIFFNESS MATRIX INTO ITS
C      POSITION IN THE GLOBAL STIFFNESS MATRIX (GSTIF).  THE ASSEMBLY
C      IS DONE IN BANDED FORM.  NON-SYMMETRIC MATRICES REQUIRE STORAGE
C      OF THE FULL BAND WIDTH.
C      .....
C      DEFINITION OF VARIABLES :
C      1 - INPUT ARGUEMENTS :
C      -----
C      NPE - NUMBER OF NODES PER ELEMENT
C      NDF - NUMBER OF DEGREES OF FREEDOM PER NODE
C      NHBM - HALF BAND WIDTH
C      NEM - NUMBER OF ELEMENTS IN THE MESH
C      N - CURRENT ELEMENT BEING PROCESSED IN CALCULATION OF ELEMENT
C      STIFFNESS MATRICES
C      ELSTIF(20,20) - ELEMENT STIFFNESS MATRIX
C      GSTIF(NEQ,NBW) - GLOBAL STIFFNESS MATRIX
C      NOD(NNM,9) - CONNECTIVITY MATRIX FOR MESH
C
C      2 - OUTPUT ARGUMENTS :
C      -----
C      GSTIF(NEQ,NBW) - GLOBAL STIFFNESS MATRIX WHICH NOW INCLUDES THE
C      CONTRIBUTIONS FROM ELEMENT N.
C
C      3 - SUBROUTINES CALLED
C      -----
C
C      NONE

```

```

C
C.....
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/MSH/X(120),Y(120),DX(21),DY(21),NOD(120,9)
      COMMON/STF/ELSTIF(20,20),ELXY(4,2),A0,A1
      COMMON/STR/GSTIF(595,90)
C      LOOP OVER NUMBER OF NODES PER ELEMENT
      DO 280 I=1,NPE
      NR=(NOD(N,I)-1)*NDF
      DO 280 II=1,NDF
      NR=NR+1
      L=(I-1)*NDF+II
      DO 260 J=1,NPE
      NCL=(NOD(N,J)-1)*NDF
      DO 260 JJ=1,NDF
      M=(J-1)*NDF+JJ
      NC=NCL+JJ-NR+NHBW
      IF (NC) 260,260,250
C      ADD CONTRIBUTION OF ELEMENT STIFFNESS MATRIX INTO GLOBAL
C      STIFFNESS MATRIX
      250 GSTIF(NR,NC)=GSTIF(NR,NC)+ELSTIF(L,M)
      260 CONTINUE
      280 CONTINUE
      RETURN
      END
      SUBROUTINE BDUNSM (N,ITERM)
C.....
C  PURPOSE :
C  -----
C      SOLVER FOR NON-SYMMETRIC SYSTEM OF LINEAR BANDED EQUATIONS.
C      SOLUTION IS STORED IN GSTIF(N,2*ITERM).
C
C.....
C  DEFINITION OF VARIABLES :
C  1 - INPUT ARGUMENTS :
C      -----
C
C      N - TOTAL NUMBER OF EQUATIONS TO BE SOLVED
C      ITERM - NUMBER OF THE HALF BAND WIDTH (NHBW)
C      GSTIF(NEW,NBW) - GLOBAL STIFFNESS MATRIX
C
C  2 - OUTPUT ARGUMENTS :
C      -----
C
C      GSTIF(I,NBW) - THE SOLUTION OF THE SYSTEM OF EQUATIONS IS
C                    RETURNED IN THE LAST COLUMN (NBW)
C
C  3 - SUBROUTINES CALLED :
C      -----
C
C      NONE

```

```

C
C.....
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/STR/GSTIF(595,90)
      CERO=1.D-6
      PARE=CERO**2
      NBND=2*ITERM
      NBM=NBND-1
C      ..... BEGIN ELIMINATION OF THE LOWER LEFT
      DO 80 I=1,N
      IF (DABS(GSTIF(I,ITERM)).LT.CERO) GO TO 10
      GO TO 20
10  IF (DABS(GSTIF(I,ITERM)).LT.PARE) GO TO 110
C      WRITE(6, 160)
C      WRITE(6, 130) GSTIF(I,ITERM),I
20  JLAST=MIN0(I+ITERM-1,N)
      L=ITERM+1
      DO 40 J=I,JLAST
      L=L-1
      IF (DABS(GSTIF(J,L)).LT.PARE) GO TO 40
      B=GSTIF(J,L)
      DO 30 K=L,NBND
30  GSTIF(J,K)=GSTIF(J,K)/B
      IF (I.EQ.N) GO TO 90
40  CONTINUE
      L=0
      JFIRST=I+1
      IF (JLAST.LE.I) GO TO 80
      DO 70 J=JFIRST,JLAST
      L=L+1
      IF (DABS(GSTIF(J,ITERM-L)).LT.PARE) GO TO 70
      DO 50 K=ITERM,NBM
50  GSTIF(J,K-L)=GSTIF(J-L,K)-GSTIF(J,K-L)
      GSTIF(J,NBND)=GSTIF(J-L,NBND)-GSTIF(J,NBND)
      IF (I.GE.N-ITERM+1) GO TO 70
      DO 60 K=1,L
60  GSTIF(J,NBND-K)=-GSTIF(J,NBND-K)
70  CONTINUE
80  CONTINUE
90  L=ITERM-1
      DO 100 I=2,N
      DO 100 J=1,L
      IF (N+1-I+J.GT.N) GO TO 100
      GSTIF(N+1-I,NBND)=GSTIF(N+1-I,NBND)-GSTIF(N+1-I+J,NBND)*GSTIF(N+1-
*      I,ITERM+J)
100 CONTINUE
      WRITE(6, 160)
      RETURN
110 WRITE(6, 140)
      STOP

```

C

```

140 FORMAT ( ' COMPUTATION STOPPED IN BNDEQ BECAUSE ZERO APPEARED ON
      1MAIN DIAGONAL *** ERROR IN BOUNSM ***' )
160 FORMAT ( /// )
      END
      SUBROUTINE BOUND(VBSF,VBDF,IBSF,IBDF,NSBF,NBW,NSDF)
C      .....
C      PURPOSE :
C      -----
C      THIS SUBROUTINE IMPLEMENTS THE KNOWN BOUNDARY CONDITIONS INTO
C      THE ASSEMBLED GLOBAL STIFFNESS MATRIX (GSTIF).
C      .....
C      DEFINITION OF VARIABLES :
C      1 - INPUT ARGUMENTS :
C      -----
C
C      VBSF - VALUES OF THE NON-ZERO SECONDARY DEGREES OF FREEDOM
C      VBDF - VALUES OF THE SPECIFIED DEGREES OF FREEDOM
C      IBDF - SPECIFIED DEGREES OF FREEDOM
C      IBSF - SPECIFIED NON-ZERO SECONDARY DEGREES OF FREEDOM
C      NSBF - NUMBER OF SPECIFIED NON-ZERO SECONDARY DOF
C      NBW  - NUMBER OF THE FULL BAND WIDTH
C      NSDF - NUMBER OF SPECIFIED PRIMARY DEGREES OF FREEDOM
C      GSTIF(NEW,NBW) - GLOBAL STIFFNESS MATRIX
C
C      2 - OUTPUT ARGUMENTS :
C      -----
C
C      GSTIF(NEQ,NBW) - GLOBAL STIFFNESS MATRIX RETURNS TO DRIVER
C                      READY FOR SOLUTION TO SYSTEM
C
C.....
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/STR/GSTIF(595,90)
      DIMENSION VBSF(25),VBDF(100),IBSF(25),IBDF(100)
      NHBW = NBW/2
C
C      IMPOSE SPECIFIED BOUNDARY FORCES
C
C      IF (NSBF.EQ.0) GO TO 340
C      DO 310 I=1,NSBF
C      II=IBSF(I)
C      310 GSTIF(II,NBW) = GSTIF(II,NBW) + VBSF(I)
C
C      IMPOSE SPECIFIED PRIMARY DEGREES OF FREEDOM
C
C      340 DO 342 I = 1,NSDF
C      IB = IBDF(I)
C      VB = VBDF(I)
C      DO 344 J = 1,NBW
C      344 GSTIF(IB,J) = 0.0

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```

        GSTIF(IB,NHBW) = 1.0
342 GSTIF(IB,NBW) = VB
        RETURN
        END
        SUBROUTINE FREESF(IVFS,NFS,TOL,NBW,NMAX,IPRNT,ITERFS)
C.....
C   PURPOSE :
C   -----
C   SUBROUTINE FREESURFACE UPDATES THE COORDINATES OF THE GLOBAL NODES
C   TO ALLOW FOR A FREE SURFACE IN A FINITE ELEMENT BOUNDARY VALUE
C   PROBLEM. THE CALCULATION USES A FORM OF THE CONSERVATION OF MASS
C   TO FIND THE POSITION OF THE NODAL COORDINATES IN WHICH THE NORMAL
C   VELOCITY IS ZERO. FREE SURFACE ITERATION STOPS WHEN THE DIFFER-
C   ENCE IN COORDINATE POSITION CHANGE IS LESS THAN A KNOWN TOLERANCE
C   VALUE.
C.....
C   DEFINITION OF VARIABLES :
C   1 - INPUT ARGUMENTS :
C   -----
C   GSTIF( )- GLOBAL STIFFNESS MATRIX USED TO OBTAIN VELOCITY SOLUTION
C   FOR FS CALCULATION.
C   IVFS( )- ARRAY OF GLOBAL NODE NUMBERS OF FREE SURFACE NODES.
C   ITFMAX - MAXIMUM NUMBER OF ITERATIONS FOR FS UPDATE
C   NFS    - NUMBER OF FREE SURFACE NODES (MUST INCLUDE THE NODE ON THE
C   DIE LIP FOR DIE SWELL EXAMPLE)
C   NBW    - NUMBER OF BAND WIDTH IN GLOBAL STIFFNESS MATRIX
C   NMAX    - GLOBAL NODE NUMBER OF NODE WITH LARGEST ERROR IN FS UPDATE
C   TOL    - TOLERANCE OF FREE SURFACE (SF) ITERATION SCHEME
C   X(),Y()- ARRAY OF GLOBAL NODE COORDINATES
C   NOD(NEM,9) - CONNECTIVITY MATRIX
C
C   2 - OUTPUT ARGUMENTS :
C   -----
C
C   IPRNT - FLAG FOR SUCCESSFUL COMPLETION OF FS ITERATION
C
C   3 - INTERNAL :
C   -----
C   ERRMAX - MAXIMUM ERROR IN FS CALCULATION
C   DELTH  - SUMMATION OF INTEGRAL REPRESENTING CHANGE IN Y-COORDINATE
C   WT( )  - WEIGHTS OF THE NEWTON-COTES QUADRATURE
C   H      - STEP SIZE IN NEWTON-COTES QUADRATURE
C   YBAR( ) - ARRAY OF Y-COORDINATES FOR QUADRATURE EVALUATION
C   XOLD( ) - ARRAY OF NODAL COORDINATES FROM PREVIOUS ITERATION
C   XORGIN( ) ARRAY OF NODAL COORDINATES OF INITIAL VALUES FOR THE
C   FREE SURFACE.
C.....
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/STR/ GSTIF(595,90)
        COMMON/MSH/X(120),Y(120),DX(21),DY(21),NOD(120,9)

```



```

        DIMENSION IVFS(20),XOLD(20),WT(3),YBAR(3),F(3),XORGIN(20)
        DATA WT/0.16667,0.66667,0.16667/
C
C      DEFINE FUNCTION USED TO CALCULATE INTEGRATION PATH FOR THE FREE
C      SURFACE
        FREE(U1,U2,V1,V2,A,B,Z)=(U1*(B-Z)+U2*(Z-A))/(V1*(B-Z) + V2*(Z-A))
        DELTH = 0.0
        IPRNT = 0
C      STORE THE ORIGINAL COORDINATES OF THE FREE SURFACE IN ARRAY XORGIN
        IF(ITERFS.GT.1) GOTO 5
        DO 60 K = 1,NFS
60      XORGIN(K) = X(IVFS(K))
C
C      STORE VALUES OF NODAL COORDINATES FOR COMPARISON WITH PREVIOUS TRIAL
        DO 10 J = 1,NFS
            XOLD(J) = X(IVFS(J))
10      CONTINUE
C
C      FIRST FREE SURFACE NODE CALCULATION
        DELTH = (Y(IVFS(2)) - Y(IVFS(1)))*(GSTIF(IVFS(2)*5-4,NBW)
        * /GSTIF(IVFS(2)*5-3,NBW))/2.0
        X(IVFS(2)) = XORGIN(2) + DELTH
C
C      LOOP ON THE NUMBER OF NODES FOR THE FS CALCULATION
C
        DO 20 J= 3,NFS
            H = (Y(IVFS(J)) - Y(IVFS(J-1)))/2.0
            VINT = 0.0
            DO 30 I = 1,3
                YBAR(I) = Y(IVFS(J-1)) + H*(DFLOAT(I)-1.0)
                F(I) = FREE(GSTIF(IVFS(J-1)*5-4,NBW),GSTIF(IVFS(J)*5-4,NBW),
                * GSTIF(IVFS(J-1)*5-3,NBW),GSTIF(IVFS(J)*5-3,NBW),Y(IVFS(J-1)),
                * Y(IVFS(J)),YBAR(I))
30      VINT = VINT + WT(I)*F(I)
C      VSIMP IS VALUE OF INTEGRAL FOR DELTA H FOR THIS NODE
        VSIMP = 2.0*H*VINT
        DELTH = DELTH + VSIMP
        X(IVFS(J)) = XORGIN(J) + DELTH
20      CONTINUE
C
C      FIND THE MAXIMUM ERROR BETWEEN THE VALUES OF THE NODAL COORDINATES
C      FOR TWO SUCCESSIVE FS ITERATIONS
        ERRMAX = 0.0
        DO 40 J = 1,NFS
            DIFF = DABS(XOLD(J) - X(IVFS(J)))
            IF(DIFF.GT.ERRMAX) NMAX = J
            IF(DIFF.GT.ERRMAX) ERRMAX = DIFF
40      CONTINUE
C
        WRITE(6,100)
        WRITE(6,110) NMAX,ERRMAX

```

```

        WRITE(6,120)
        WRITE(6,130) (X(IVFS(I)),I=1,NFS)
100  FORMAT(/,5X,'FREE SURFACE SUBROUTINE ERROR ANALYSIS',/)
110  FORMAT(5X,'MAXIMUM ERROR FOUND AT NODE NUMBER (NFS) .....=',I3,/,
      *5X,'ERROR .....=',E12.5,/)
120  FORMAT(5X,'UP-DATED VALUES OF THE FREE SURFACE COORDINATES ( X(N)
      *)',/)
130  FORMAT(5(2X,E12.5))
      IF(ERRMAX.GE.TOL) GO TO 50
C    FREE SURFACE CONVERGES IF ERROR IS LESS THAN TOLERANCE (TOL)
C    SET FLAG = 1 AND RETURN TO MAIN PROGRAM
      IPRNT = 1
50   RETURN
      END
      SUBROUTINE LAMBDA(GAMADT,AMBDA,IMODEL,TMCNST)
C    .....
C    PURPOSE :
C    -----
C    USER SUPPLIED FUNCTION FOR THE TIME CONSTANT OF THE CONSTITUTIVE
C    EQUATION. LAMBDA SHOULD BE A FUNCTION OF THE MAGNITUDE OF THE
C    RATE OF DEFORMATION TENSOR
C    .....
C    DEFINITION OF VARIABLES
C    1 - INPUT ARGUMENTS :
C    -----
C
C    GAMADT - MAGNITUDE OF THE RATE OF DEFORMATION TENSOR
C    IMODEL - FLAG FOR WHICH CONSTITUTIVE EQUATION IS USED
C    TMCNST - VALUE OF THE TIME CONSTANT FOR THE UPPER CONVECTED
C             MAXWELL MODEL. USER INPUT
C
C    2 - OUTPUT ARGUMENTS :
C    -----
C
C    AMBDA - TIME CONSTANT FOR WHITE-METZNER MODEL (FUNCTION OF THE
C            MAGNITUDE OF THE RATE OF DEFORMATION TENSOR)
C    .....
      IMPLICIT REAL*8(A-H,O-Z)
      GO TO(10,20,30),IMODEL+1
C    GNF FLUID DESCRIBED BY LAMBDA = 0
10   AMBDA = 0.0
      GOTO 40
C    FLUID TIME CONSTANT EQUAL TO CONSTANT FOR UPPER-CONVECTED MAXWELL
C    MODEL.
20   AMBDA = TMCNST
      GOTO 40
C    WHITE-METZNER MODEL MAY HAVE USER DEFINED FUNCTION FOR THE TIME
C    CONSTANT LAMBDA. FUNCTION SHOULD BE A FUNCTION OF
C    THE MAGNITUDE OF THE RATE OF DEFORMATION TENSOR.

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C          STYRON 678U 190 C
C30 IF (GAMADT.LT.1D-2) AMBDA = 2.0
C    IF (GAMADT.GE.1D-2) AMBDA = 0.43504 - 0.45297*DLOG10(GAMADT)
C    *          + 0.1388*(DLOG10(GAMADT))*2
C          STYRON 678U 165 C
30  IF (GAMADT.LT.5D-2) AMBDA = 4.0
    IF (GAMADT.GE.5D-2) AMBDA = 1.120 - 2.21363*DLOG10(GAMADT)
40  RETURN
    END
    SUBROUTINE MESH(IEL,NX,NY,NPE,NNM,NEM)
C.....
C    PURPOSE :
C    -----
C
C    THE SUBROUTINE GENERATES ARRAY NOD(I,J), COORDINATES X(I),Y(I),
C    AND MESH INFORMATION (NNM,NEM,NPE) FOR RECTANGULAR DOMAINS. THE
C    DOMAIN IS DIVIDED INTO LINEAR TRIANGULAR ELEMENTS OR QUADRILA-
C    TERAL ELEMENTS (NX BY NY NONUNIFORM MESH IN GENERAL).
C
C    .....
C    DEFINITION OF VARIABLES :
C    1 - INPUT ARGUMENTS :
C    -----
C    IEL - FLAG FOR TYPE OF ELEMENT USED IN MESH CALCULATION
C    NX,NY - NUMBER OF ELEMENTS IN THE X AND Y DIRECTIONS, RESPECT-
C            IVELY
C    DX(I) - DISTANCE BETWEEN NODES ALONG THE X-AXIS
C    DY(I) - DISTANCE BETWEEN NODES ALONG THE Y-AXIS
C    NPE - NODES PER ELEMENT
C
C    2 - OUTPUT ARGUMENTS :
C    -----
C    NNM - NUMBER OF NODES IN THE FINITE ELEMENT MESH
C    NEM - NUMBER OF ELEMENTS IN THE MESH
C    NOD() - BOOLEAN CONNECTIVITY MATRIX
C    X(I) - X COORDINATE OF NODE I
C    Y(I) - Y COORDINATE OF NODE I
C
C.....
    IMPLICIT REAL*8 (A-H,O-Z)
    COMMON/MSH/X(120),Y(120),DX(21),DY(21),NOD(120,9)
    IF(IEL.GT.0)GOTO 100
C
C    MESH OF QUADRILATERAL ELEMENTS WITH FOUR,EIGHT, OR NINE NODES
C
100 NEX1=NX+1
    NEY1=NY+1
    NXX = IEL*NX
    NYY = IEL*NY
    NXX1 = NXX + 1
    NYY1 = NYY + 1

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```

      NEM=NX*NY
      NNM = NXX1*NY1 - (IEL-1)*NX*NY
      IF (NPE .EQ. 9)NNM=NXX1*NY1
      K0 = 0
      IF (NPE .EQ. 9) K0=1
C
C   GENERATE THE ARRAY NOD(I,J)
C
      NOD(1,1) = 1
      NOD(1,2) = IEL+1
      NOD(1,3) = NXX1+(IEL-1)*NEX1+IEL+1
      IF (NPE .EQ. 9)NOD(1,3)=4*NX+5
      NOD(1,4) = NOD(1,3) - IEL
      IF(NPE .EQ. 4)GO TO 200
      NOD(1,5) = 2
      NOD(1,6) = NXX1 + (NPE-6)
      NOD(1,7) = NOD(1,3) - 1
      NOD(1,8) = NXX1+1
      IF (NPE .EQ. 9)NOD(1,9)=NXX1+2
200 IF(NY .EQ. 1)GOTO 230
      M = 1
      DO 220 N = 2,NY
      L = (N-1)*NX + 1
      DO 210 I = 1,NPE
210 NOD(L,I) = NOD(M,I)+NXX1+(IEL-1)*NEX1+K0*NX
220 M=L
230 IF(NX .EQ. 1)GO TO 270
      DO 260 NI = 2,NX
      DO 240 I = 1,NPE
      K1 = IEL
      IF(I .EQ. 6 .OR. I .EQ. 8)K1=1+K0
240 NOD(NI,I) = NOD(NI-1,I)+K1
      M = NI
      DO 260 NJ = 2,NY
      L = (NJ-1)*NX+NI
      DO 250 J = 1,NPE
250 NOD(L,J) = NOD(M,J)+NXX1+(IEL-1)*NEX1+K0*NX
260 M = L
C
C   GENERATE THE COORDINATES X(I) AND Y(I)
C
270 YC=0.0
      IF (NPE .EQ. 9) GOTO 310
      DO 300 NI = 1, NEY1
      I = (NXX1+(IEL-1)*NEX1)*(NI-1)+1
      J = (NI-1)*IEL+1
      X(I) = 0.0
      Y(I) = YC
      DO 280 NJ = 1,NXX
      I=I+1
      X(I) = X(I-1)+DX(NJ)

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280 Y(I) = YC
    IF(NI.GT.NY .OR. IEL.EQ.1)GO TO 300
    J = J+1
    YC = YC+DY(J-1)
    I = I+1
    X(I) = 0.0
    Y(I) = YC
    DO 290 II = 1, NX
    K = 2*II-1
    I = I+1
    X(I) = X(I-1)+DX(K)+DX(K+1)
290 Y(I) = YC
300 YC = YC+DY(J)
    RETURN
C
310 DO 330 NI=1,NYY1
    I=NXX1*(NI-1)
    XC=0.0
    DO 320 NJ=1,NXX1
    I = I+1
    X(I) = XC
    Y(I) = YC
320 XC = XC + DX(NJ)
330 YC = YC + DY(NI)
    RETURN
END
SUBROUTINE SHAPE(NPE,XI,ETA,SF,GDSF,DET,ELXY)
C .....
C PURPOSE :
C -----
C THE SUBROUTINE EVALUATES THE INTERPOLATION FUNCTIONS (SF(I)) AND
C ITS DERIVATIVES WITH RESPECT TO NATURAL COORDINATES (DSF(I,J)),
C AND THE DERIVATIVES OF SF(I) WITH RESPECT TO GLOBAL COORDINATES
C FOR FOUR, EIGHT, AND NINE NODE RECTANGULAR ISOPARAMETRIC ELEMENTS.
C .....
C DEFINITION OF VARIABLES :
C 1 - INPUT ARGUMENTS :
C -----
C NPE - NUMBER OF NODES PER ELEMENT
C XI, ETA - COORDINATES OF THE ELEMENT NODES
C ELXY - GLOBAL COORDINATES OF THE LOCAL NODES WITHIN AN ELEMENT
C
C 2 - OUTPUT ARGUMENTS :
C -----
C SF(I).....INTERPOLATION FUNCTION FOR NODE I OF THE ELEMENT
C DSF(I,J)....DERIVATIVE OF SF(J) WITH RESPECT TO XI IF I=1 AND
C WITH RESPECT TO ETA IF I=2.
C GDSF(I,J)....DERIVATIVE OF SF(J) WITH RESPECT TO X IF I=1 AND
C WITH RESPECT TO Y IF I=2.
C XNODE(I,J)...J-TH (J=1,2) COORDINATE OF NODE I OF THE ELEMENT
C NP(I).....ARRAY OF ELEMENT NODES (USED FOR DEFINING SF AND DSF)

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C      GJ(I,J).....JACOBIAN MATRIX
C      GIINV(I,J)...INVERSE OF THE JACOBIAN MATRIX
C      .....
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      DIMENSION ELXY(4,2),XNODE(9,2),NP(9),DSF(2,9),GJ(2,2),GJINV(2,2),
1      SF(9),GDSF(2,9)
C      DATA XNODE/-1.0D0,2*1.0D0,-1.0D0,0.0D0,1.0D0,0.0D0,-1.0D0,0.0D0,
2      2*-1.0D0,2*1.0D0,-1.0D0,0.0D0,1.0D0,2*0.0D0/
C      DATA NP/1,2,3,4,5,7,6,8,9/
C
C      FNC(A,B) = A*B
C
C      BRANCH TO SPECIFIC SHAPE FUNCTIONS REQUIRED IN SUBROUTINE BASED ON
C      THE NODES PER ELEMENT
C      IF (NPE-8) 60,10,80
C
C      QUADRATIC INTERPOLATION FUNCTIONS (FOR THE EIGHT-NODE ELEMENT)
C
10 DO 40 I = 1, NPE
    NI = NP(I)
    XP = XNODE(NI,1)
    YP = XNODE(NI,2)
    XI0 = 1.0+XI*XP
    ETA0 = 1.0+ETA*YP
    XI1 = 1.0-XI*XI
    ETA1 = 1.0-ETA*ETA
    IF(I.GT.4) GO TO 20
    SF(NI) = 0.25*FNC(XI0,ETA0)*(XI*XP+ETA*YP-1.0)
    DSF(1,NI) = 0.25*FNC(ETA0,XP)*(2.0*XI*XP+ETA*YP)
    DSF(2,NI) = 0.25*FNC(XI0,YP)*(2.0*ETA*YP+XI*XP)
    GO TO 40
20 IF(I.GT.6) GO TO 30
    SF(NI) = 0.5*FNC(XI1,ETA0)
    DSF(1,NI) = -FNC(XI,ETA0)
    DSF(2,NI) = 0.5*FNC(YP,XI1)
    GO TO 40
30 SF(NI) = 0.5*FNC(ETA1,XI0)
    DSF(1,NI) = 0.5*FNC(XP,ETA1)
    DSF(2,NI) = -FNC(ETA,XI0)
40 CONTINUE
    GO TO 130
C
C      LINEAR INTERPOLATION FUNCTIONS (FOR FOUR-NODE ELEMENT)
C
60 DO 70 I = 1, NPE
    XP=XNODE(I,1)
    YP=XNODE(I,2)
    XI0=1.0+XI*XP
    ETA0=1.0+ETA*YP
    SF(I)=0.25*FNC(XI0,ETA0)

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        DSF(1,I)=0.25*FNC(XP,ETA0)
70 DSF(2,I)=0.25*FNC(YP,XI0)
        GO TO 130
C
C    QUADRATIC INTERPOLATION FUNCTIONS (FOR THE NINE-NODE ELEMENT)
C
80 DO 120 I=1,NPE
    NI = NP(I)
    XP = XNODE(NI,1)
    YP = XNODE(NI,2)
    XI0 = 1.0+XI*XP
    ETA0 = 1.0+ETA*YP
    XI1 = 1.0-XI*XI
    ETA1 = 1.0-ETA*ETA
    XI2 = XP*XI
    ETA2 = YP*ETA
    IF(I .GT. 4)GOTO 90
    SF(NI) = 0.25*FNC(XI0,ETA0)*XI2*ETA2
    DSF(1,NI)=0.25*XP*FNC(ETA2,ETA0)*(1.0+2.0*XI2)
    DSF(2,NI)=0.25*YP*FNC(XI2,XI0)*(1.0+2.0*ETA2)
    GO TO 120
90 IF(I .GT. 6)GO TO 100
    SF(NI) = 0.5*FNC(XI1,ETA0)*ETA2
    DSF(1,NI) = -XI*FNC(ETA2,ETA0)
    DSF(2,NI) = 0.5*FNC(XI1,YP)*(1.0+2.0*ETA2)
    GO TO 120
100 IF(I .GT. 8)GO TO 110
    SF(NI) = 0.5*FNC(ETA1,XI0)*XI2
    DSF(2,NI) = -ETA*FNC(XI2,XI0)
    DSF(1,NI) = 0.5*FNC(ETA1,XP)*(1.0+2.0*XI2)
    GO TO 120
110 SF(NI) = FNC(XI1,ETA1)
    DSF(1,NI) = -2.0*XI*ETA1
    DSF(2,NI) = -2.0*ETA*XI1
120 CONTINUE
130 DO 140 I = 1,2
    DO 140 J = 1,2
        GJ(I,J) = 0.0
        DO 140 K = 1,NPE
140 GJ(I,J) = GJ(I,J) + DSF(I,K)*ELXY(K,J)
        DET = GJ(1,1)*GJ(2,2)-GJ(1,2)*GJ(2,1)
        GJINV(1,1) = GJ(2,2)/DET
        GJINV(2,2) = GJ(1,1)/DET
        GJINV(1,2) = -GJ(1,2)/DET
        GJINV(2,1) = -GJ(2,1)/DET
        DO 150 I = 1,2
            DO 150 J = 1,NPE
                GDSF(I,J) = 0.0
            DO 150 K = 1, 2
150 GDSF(I,J) = GDSF(I,J) + GJINV(I,K)*DSF(K,J)
        RETURN

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END
SUBROUTINE STIFFQ(NPE,NN,IEL,ITYPE,AK1,AK2,Q,VEL,IMODEL,TMCNST)
C .....
C PURPOSE :
C -----
C STIFFNESS MATRIX FOR ISOPARAMETRIC QUADRILATERAL ELEMENTS
C CALCULATION OF THE ELEMENT STIFFNESS MATRIX FOR THE 3 TYPES OFF
C CONSTITUTIVE EQUATIONS AVAILABLE.  GNF, MAXWELL, AND WHITE-METZNER
C .....
C DEFINITION OF VARIABLES :
C 1 - INPUT ARGUMENTS :
C -----
C NPE - NODES PER ELEMENT
C NN - NN = NDF*NPE  SIZE OF ELEMENT STIFFNESS MATRIX
C IEL - ELEMENT TYPE IEL = 1 BILINEAR QUADRATIC SHAPE FUNCTIONS
C ITYPE - VISCOSITY MODEL FLAG
C AK1 - ZERO SHEAR RATE VISCOSITY
C AK2 - PENALTY PARAMETER
C Q - DUMMY ARGUMENT (NO LONGER ACTIVE)
C VEL() - VELOCITY VALUES AT THE ELEMENT NODES (FOR NONLINEAR
C ANALYSIS.
C IMODEL - FLAG FOR TYPE OF THE CONSTITUTIVE EQUATION
C TMCNST - VALUE OF THE TIME CONSTANT FOR THE UPPER CONVECTED
C MAXWELL MODEL.
C THE FOLLOWING VARIABLES ARE PASSED INTO THE PROGRAM THROUGH
C COMMON BLOCKS.
C
C ELXY() - COORDINATES OF THE ELEMENT NODES
C AO,A1 - DUMMY VARIABLES
C C4 - VISCOSITY CONSTANT M FOR POWERLAW MODEL
C LAMBDA FOR CARREAU MODEL
C C5 - EXPONENT N FOR BOTH POWERLAW AND CARREAU MODEL VISCOSITY
C AMBDA - VALUE OF THE FLUID TIME CONSTANT FOR MAXWELL TYPE
C CONSTITUTIVE EQUATIONS
C RHO - FLUID DENSITY
C ITER - ITERATION NUMBER FOR THE NON-LINEAR ITERATIONS
C
C 2 - OUTPUT ARGUMENTS :
C -----
C ELSTIF(20,20) - ELEMENT STIFFNESS MATRIX
C
C 3 - INTERNAL :
C -----
C GAUSS - COORDINATES OF THE GAUSSIAN INTEGRATION POINTS WITHIN
C THE ISOPARAMETRIC ELEMENTS
C WT - WEIGHT USED FOR THE NUMERICAL INTEGRATION
C NGP - NUMBER OF GAUSS POINTS ACROSS AN ELEMENT
C DUDX,DUDY,DVDX,DVDY - THESE ARE THE DERIVATIVES OF THE
C VELOCITIES EVALUATED AT THE GAUSS POINTS
C GAMADT - MAGNITUDE OF THE RATE OF DEFORMATION TENSOR -

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C          EVALUATED AT THE CENTER OF EACH ELEMENT
C          S(I,J) - PSI1*PSI2 THE FOLLOWING VARIABLES ARE THE TERMS IN
C          THE ELEMENT STIFFNESS MATRIX INTEGRATED OVER THE
C          ELEMENT DOMAIN. THEY CONTAIN CONTRIBUTIONS FROM
C          THE TWO SHAPE FUNCTIONS IN THE TERMS FOR THE ELEMENT
C          STIFFNESS MATRIX
C          S01(I,J) - PSI1 * D PSI2 / D X - DERIVATIVE OF THE BASIS
C          WITH RESPECT TO THE X-COORDINATE DIRECTION
C          S02(I,J) - PSI1 * D PSI2 / D Y - DERIVATIVE OF THE BASIS
C          WITH RESPECT TO THE Y-COORDINATE DIRECTION
C          S01V1(I,J) - X-VELOCITY * PSI1 * D PSI2 / D X
C          X-VELOCITY TERM IS KNOWN FROM PREVIOUS ITERATION
C          S02V2(I,J) - Y-VELOCITY * PSI1 * D PSI2 / D Y
C          SV11(I,J) - D X-VEL / D X * PSI1 * PSI2
C          SV12(I,J) - D X-VEL / D Y * PSI1 * PSI2
C          SV21(I,J) - D Y-VEL / D X * PSI1 * PSI2
C          SV22(I,J) - D Y-VEL / D Y * PSI1 * PSI2
C          XI,ETA - LOCATION OF THE GAUSS POINTS (X AND Y COORDINATES
C          FOR NUMERICAL INTEGRATION IN SUBROUTINE SHAPE
C          CONST - INTEGRATION CONSTANT FOR THE NUMERICAL INTEGRATION
C          CONTAINING DET OF TRANSFORMATION AND GAUSS WEIGHTS
C          UX,UY - DERIVATIVES OF THE X-VELOCITY USED TO EVALUATE THE
C          RATE OF DEFORMATION TENSOR
C          VX,VY - DERIVATIVES OF THE Y-VELOCITY USED TO EVALUATE THE
C          RATE OF DEFORMATION TENSOR
C
C          4 - SUBROUTINES CALLED :
C          -----
C          SHAPE - EVALUATION OF THE SHAPE FUNCTIONS
C          VISC - EVALUATE THE MAGNITUDE OF THE VISCOSITY FUNCTION
C          LAMBDA - CALCULATE THE VALUE OF THE FLUID TIME CONSTANT FOR
C          THE MAXWELL TYPE CONSTITUTIVE EQUATIONS
C.....
C          IMPLICIT REAL*8(A-H,O-Z)
C          COMMON/STF/ELSTIF(20,20),ELXY(4,2),A0,A1
C          COMMON/VIS/C4,C5,AMBDA,RHO,ITER
C          DIMENSION SF(9),GDSF(2,9),GAUSS(4,4),WT(4,4),S(4,4),S01(4,4)
C          *          ,S02(4,4),SV11(4,4),SV12(4,4),SV21(4,4),SV22(4,4),
C          *          S01V1(4,4),S02V2(4,4),VEL(20)
C
C          DATA GAUSS/4*0.000,-.5773502700,.5773502700,2*0.000,-.7745966700,
C          20.000,.7745966700,0.000,-.8611363100,
C          3-.3399810400,.3399810400,.8611363100/
C
C          DATA WT/2.000,3*0.000,2*1.000,2*0.000,.5555555500,.8888888800,
C          2.5555555500,0.000,.3478548500,2*.6521451500,.3478548500/
C
C          NDF = NN/NPE
C          NGP = IEL+1
C

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DUDX = 0.0
DUDY = 0.0
DVDX = 0.0
DVDY = 0.0
GAMADT = 0.0
C
C   INITIALIZE THE ARRAYS
C
DO 20 I = 1, NPE
DO 20 J = 1, NPE
S(I,J)=0.0
S01(I,J) = 0.0
S02(I,J) = 0.0
S01V1(I,J) = 0.0
S02V2(I,J) = 0.0
SV11(I,J) = 0.0
SV12(I,J) = 0.0
SV21(I,J) = 0.0
20 SV22(I,J) = 0.0
DO 30 I = 1,NN
DO 30 J = 1,NN
30 ELSTIF(I,J) = 0.0
C
C   DO-LOOPS ON NUMERICAL (GAUSS) QUADRATURE BEGIN HERE
C
DO 100 NI = 1,NGP
DO 100 NJ = 1,NGP
XI = GAUSS(NI,NGP)
ETA = GAUSS(NJ,NGP)
CALL SHAPE(NPE,XI,ETA,SF,GDSF,DET,ELXY)
CONST = DET*WT(NI,NGP)*WT(NJ,NGP)
V1 = 0.0
V2 = 0.0
UX = 0.0
UY = 0.0
VX = 0.0
VY = 0.0
DO 50 I = 1,NPE
L = 5*I - 4
V1 = VEL(L)*SF(I) + V1
V2 = VEL(L+1)*SF(I) + V2
UX = UX + VEL(L)*GDSF(1,I)
UY = UY + VEL(L)*GDSF(2,I)
VX = VX + VEL(L+1)*GDSF(1,I)
VY = VY + VEL(L+1)*GDSF(2,I)
DUDX = DUDX + VEL(L)*GDSF(1,I)
DUDY = DUDY + VEL(L)*GDSF(2,I)
DVDX = DVDX + VEL(L+1)*GDSF(1,I)
50 DVDY = DVDY + VEL(L+1)*GDSF(2,I)
C   SUM CONTRIBUTION OF SHAPE FUNCTION OVER THE NUMBER OF NODES IN THE
C   ELEMENT

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40 DO 80 I=1,NPE
   DO 80 J=1,NPE
      S(I,J) = CONST*SF(I)*SF(J) + S(I,J)
      S01(I,J) = CONST*SF(I)*GDSF(1,J) + S01(I,J)
      S02(I,J) = CONST*SF(I)*GDSF(2,J) + S02(I,J)
      S01V1(I,J) = CONST*V1*SF(I)*GDSF(1,J) + S01V1(I,J)
      S02V2(I,J) = CONST*V2*SF(I)*GDSF(2,J) + S02V2(I,J)
      SV11(I,J) = CONST*UX*SF(I)*SF(J) + SV11(I,J)
      SV12(I,J) = CONST*UY*SF(I)*SF(J) + SV12(I,J)
      SV21(I,J) = CONST*VX*SF(I)*SF(J) + SV21(I,J)
      SV22(I,J) = CONST*VY*SF(I)*SF(J) + SV22(I,J)
80 CONTINUE
100 CONTINUE
C   AVERAGE OVER THE NUMBER OF GAUSS INTEGRATION POINTS
      DUDX = DUDX/4.0
      DUDY = DUDY/4.0
      DVDX = DVDX/4.0
      DVDY = DVDY/4.0
C
C   CALCULATE THE FLUID VISCOSITY WITHIN SUBROUTINE VISC AS A FUNCTION
C   OF THE MAGNITUDE OF THE RATE OF DEFORMATION TENSOR
C
      CALL VISC(DUDX,DUDY,DVDX,DVDY,ITER,ITYPE,C4,C5,AK1,AMU,GAMADT)
      RATE = GAMADT
      CALL LAMBDA(RATE,AMBDA,IMODEL,TMCNST)
C*** DEFINE THE COEFFICIENTS FOR THE STOKES EQUATION HERE *****
111 II = 1
   DO 200 I=1,NPE
      JJ = 1
      DO 150 J=1,NPE
         ELSTIF(II,JJ) = -RHO*S01V1(I,J) - RHO*S02V2(I,J)
         ELSTIF(II,JJ+2)= S01(J,I)
         ELSTIF(II,JJ+3)= S02(J,I)
         ELSTIF(II+1,JJ+1)= -RHO*S01V1(I,J) - RHO*S02V2(I,J)
         ELSTIF(II+1,JJ+3)= S01(J,I)
         ELSTIF(II+1,JJ+4)= S02(J,I)
         ELSTIF(II+2,JJ) = 2.0*AMU*S01(I,J)
         ELSTIF(II+2,JJ+2) = S(I,J) + AMBDA*S01V1(I,J)+AMBDA*S02V2(I,J)
         *      - 2.0*SV11(I,J)*AMBDA
         ELSTIF(II+2,JJ+3) = -2.0*AMBDA*SV12(I,J)
         ELSTIF(II+3,JJ) = AMU*S02(I,J)
         ELSTIF(II+3,JJ+1) = AMU*S01(I,J)
         ELSTIF(II+3,JJ+2) = -AMBDA*SV21(I,J)
         ELSTIF(II+3,JJ+3) = S(I,J) + AMBDA*S01V1(I,J)+AMBDA*S02V2(I,J)
         *      -AMBDA*SV11(I,J) - AMBDA*SV22(I,J)
         ELSTIF(II+3,JJ+4) = -AMBDA*SV12(I,J)
         ELSTIF(II+4,JJ+1) = 2.0*AMU*S02(I,J)
         ELSTIF(II+4,JJ+3) = -2.0*AMBDA*SV21(I,J)
         ELSTIF(II+4,JJ+4) = S(I,J) + AMBDA*S01V1(I,J)+AMBDA*S02V2(I,J)
         *      - 2.0*AMBDA*SV22(I,J)
150 JJ = NDF*J+1

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200 II = NDF*I+1
C
C   PENALTY TERMS
C
DO 300 NI = 1,IEL
DO 300 NJ = 1,IEL
XI = GAUSS(NI,IEL)
ETA = GAUSS(NJ,IEL)
CALL SHAPE(NPE,XI,ETA,SF,GDSF,DET,ELXY)
CONST = DET*WT(NI,IEL)*WT(NJ,IEL)
II = 1
DO 280 I = 1,NPE
JJ = 1
DO 260 J = 1,NPE
ELSTIF(II,JJ) = AK2*GDSF(1,I)*GDSF(1,J)*CONST + ELSTIF(II,JJ)
ELSTIF(II+1,JJ) = AK2*GDSF(2,I)*GDSF(1,J)*CONST + ELSTIF(II+1,JJ)
ELSTIF(II,JJ+1) = AK2*GDSF(1,I)*GDSF(2,J)*CONST + ELSTIF(II,JJ+1)
ELSTIF(II+1,JJ+1)=AK2*GDSF(2,I)*GDSF(2,J)*CONST+ELSTIF(II+1,JJ+1)
260 JJ = NDF*J +1
280 II=NDF*I + 1
300 CONTINUE
RETURN
END
SUBROUTINE STRESS(N,NPE,ELXY,W,AK1,GAMA,ITYPE,IEL,IMODEL,TMCNST)
C
C .....
C PURPOSE :
C -----
C SUBROUTINE TO COMPUTE THE GRADIENT OF SOLUTION AND
C STRESSES WITHIN EACH ELEMENT
C .....
C DEFINITION OF VARIABLES :
C 1 - INPUT ARGUMENTS :
C -----
C N - NUMBER OF THE ELEMENT FOR CURRENT CALCULATION
C NPE - NODES PER ELEMENT
C ELXY(4,2) - NODAL COORDINATES OF THE CURRENT ELEMENT
C           ELXY(I,1) - X COORDINATE  ELXY(I,2) - Y COORDINATE
C W(I,J) - ARRAY CONTAINS VELOCITY SOLUTION FOR EACH NODE IN
C          ELEMENT.  W(1,J) X-VELOCITY  W(2,J) Y-VELOCITY
C AK1 - ZERO SHEAR RATE VISCOSITY
C GAMA - PENALTY PARAMETER
C ITYPE - FLAG FOR TYPE OF VISCOSITY FUNCTION
C IEL - FLAG FOR TYPE OF ELEMENT.  IEL=1 BILINEAR QUADRATIC
C       ELEMENTS
C IMODEL - FLAG FOR THE TYPE OF CONSTITUTIVE EQUATION USED.
C TMCNST - FLUID TIME CONSTANT FOR THE UPPER CONVECTED MAXWELL
C          CONSTITUTIVE EQUATION.
C C4 - VISCOSITY CONSTANT - IF ITYPE=1, C4 = M FOR POWERLAW FLUID
C       IF ITYPE=2, C4 = LAMBDA FOR CARREAU MODEL.
C C5 - VISCOSITY CONSTANT - C5 = N EXPONENT FOR BOTH POWERLAW AND
C       CARREAU MODEL

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C      RHO - FLUID DENSITY
C
C      2 - OUTPUT ARGUMENTS :
C      -----
C      P - HYDROSTATIC PRESSURE CALCULATED AT THE CENTER OF EACH
C      ÉLEMENT.
C      GAMADT - MAGNITUDE OF THE RATE OF DEFORMATION TENSOR.
C      AMU - VALUE OF THE VISCOSITY AT THE NODE CENTER
C      AMBDA - VALUE OF THE FLUID TIME CONSTANT FOR MAXWELL TYPE FLUIDS
C      EPSDOT - EXTENSIONAL GRADIENT - DIAGONOL TERMS OF THE RATE OF
C      DEFORMATION TENSOR
C
C      3 - INTERNAL VARIABLES :
C      -----
C      UX - DERIVATIVE OF THE VELOCITY FIELD X-VELOCITY / X DIRECTION
C      UY - X-VELOCITY / Y DIRECTION
C      VX - Y-VELOCITY / X DIRECTION
C      VY - Y-VELOCITY / Y DIRECTION
C      XI, ETA - COORDINATES AT THE CENTER OF EACH ELEMENT
C      GRAD - GRADIENT OF THE VELCOITY FIELD
C
C      4 - SUBROUTINES CALLED :
C      -----
C      SHAPE - CALCULATION OF TRIAL FUNCTIONS
C      VISC - VISCOSITY CALCULATION
C      LAMBDA - TIME CONSTANT CALCULATION
C
C.....
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION SF(9),GDSF(2,9),ELXY(4,2),W(2,9)
      COMMON/VIS/C4,C5,AMBDA,RHO,ITER
      UX=0.0
      UY=0.0
      VX=0.0
      VY=0.0
      GRAD = 0.0
C
C      .....
C      CACULATION OF STRESSES/GRADIENT OF SOLUTION AT THE
C      CENTER OF THE QUADRILATERAL ELEMENTS
C      .....
C
100 XI = 0.0
      ETA = 0.0
      CALL SHAPE(NPE,XI,ETA,SF,GDSF,DET,ELXY)
C      CALCULATE VELOCITY GRADIENTS AT THE CENTER OF THE ISOPARAMETRIC
C      ELEMENT. USED TO CALCULATE THE SHEAR RATE FOR VISCOSITY AND
C      TIME CONSTANT SUBROUTINES.
      DO 110 I=1,NPE
      UX=UX + W(1,I)*GDSF(1,I)
      UY=UY + W(1,I)*GDSF(2,I)

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      VX=VX + W(2,I)*GDSF(1,I)
110 VY=VY + W(2,I)*GDSF(2,I)
C
C   PRESSURE COMPUTATION FOR THE STOKES FLOW (PENALTY METHOD)
C
      GRAD = UX+VY
      EPSDOT = DSQRT(2.0*UX**2 + 2.0*VY**2)
      P = GAMA*GRAD
C   PRINT OUT THE VISCOSITY AND THE TIME CONSTANT LAMBDA AT THE CENTER
C   OF EACH ELEMENT.
      CALL VISC(UX,UY,VX,VY,ITER,ITYPE,C4,C5,AK1,AMU,GAMADT)
      RATE = GAMADT
      CALL LAMBDA(RATE,AMBDA,IMODEL,TMCNST)
170 WRITE(6, 4) N,P,GAMADT,AMU,AMBDA,EPSDOT
      4 FORMAT(5X,I5,5(4X,E13.6))
      RETURN
      END
      SUBROUTINE STREAM(NNM,PSINIT,NEM,NPE,NDF,NBW)
C.....
C   PURPOSE :
C   -----
C   CALCULATION OF THE STREAMLINES FROM THE VELOCITY SOLUTION
C   A SINGLE VALUE OF THE STREAM FUNCTION (PSINIT) IS SPECIFIED AT ONE
C   NODE IN THE MESH.
C.....
C   DEFINITION OF VARIABLES :
C   1 - INPUT ARGUMENTS :
C   -----
C   NNM - NUMBER OF NODES IN THE MESH
C   PSIINIT - INITIAL VALUE OF THE STREAM FUNCTION SPECIFIED AT NODE 1
C   NEM - NUMBER OF ELEMENTS IN THE MESH
C   NPE - NODES PER ELEMENT
C   NDF - NUMBER OF DEGREES OF FREEDOM PER NODE
C   NBW - VALUE OF THE TOTAL BAND WIDTH
C   X(NNM),Y(NNM) - COORDINATES OF THE NODES IN THE MESH
C   NOD(NNM,9) - BOOLEAN CONNECTIVITY MATRIX
C   GSTIF(NNM,NBW) - GLOBAL STIFFNESS MATRIX
C
C   2 - OUTPUT ARGUMENTS :
C   -----
C   PSI(NNM) - VALUE OF STREAM FUNCTION AT NODE I
C
C   3 - INTERNAL VARIABLES :
C   DELPSI(NPE) - CHANGE IN PSI ALONG A ELEMENT BOUNDARY
C   DNX,DNY - NORMAL VECTORS ALONG EACH SIDE OF THE ELEMENT USED
C             IN CALCULATING THE CHANGE IN PSI
C   U(4),V(4) - VALUES OF THE X AND Y VELOCITY FOR EACH NODE IN AN
C               ELEMENT
C

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C.....
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/MSH/X(120),Y(120),DX(21),DY(21),NOD(120,9)
      COMMON/STR/GSTIF(595,90)
      DIMENSION DELPSI(4),U(4),V(4),PSI(120)
C    INITIALIZE STREAM FUNCTIONS
      DO 10 J=1,NNM
        PSI(J) = 0.0
10    CONTINUE
C    INITIAL VALUE OF PSI AT LOCAL NODE 1 ON ELEMENT 1
      PSI(1) = PSINIT
C    DO LOOP OVER NUMBER OF ELEMENTS
C
      DO 20 N = 1,NEM
C    INITIALIZE VALUES OF DELTA PSI
        DO 50 M = 1,4
          DELPSI(M) = 0.0
50    CONTINUE
C    CALCULATE CORRESPONDENCE BETWEEN GLOBAL VELOCITY SOLUTION AND
C    LOCAL NODE NUMBERS
        DO 30 K = 1,NPE
          NI = NOD(N,K)
          LI = NI*NDF - 4
          U(K) = GSTIF(LI,NBW)
          V(K) = GSTIF(LI+1,NBW)
30    CONTINUE
C    CALCULATE THE CHANGE IN PSI ALONG INTEGRATION PATHS WHICH
C    CORRESPOND TO BOUNDARY SIDES
        DO 40 J = 1,3
          IM1 = NOD(N,J)
          IM2 = NOD(N,J+1)
C    DL IS THE INTEGRATION PATH LENGTH FOR THE NUMERICAL INTEGRATION
          DL = DSQRT(((X(IM2)-X(IM1))/2.0)**2 + ((Y(IM2)-Y(IM1))/2.0)**2)
C    DNX, AND DNY ARE THE NORMAL VECTORS ALONG THE BOUNDARIES OF EACH
C    ELEMENT.
          DNX = (Y(IM2) - Y(IM1))/(2.0*DL)
          DNY = -1.0*(X(IM2) - X(IM1))/(2.0*DL)
          DELPSI(J) = DNX*(U(J+1) + U(J)) + DNY*(V(J+1) + V(J))
          PSI(IM2) = PSI(IM1) + DELPSI(J)
40    CONTINUE
C    CALCUALTE VALUES OF PSI AT EACH NODE
60    CONTINUE
20    CONTINUE
C    PRINT OUT VALUES OF NODAL COORDINATES AND VALUE OF THE STREAM
C    FUNCTION
        WRITE(6,70)
70    FORMAT(///,3X,'OUTPUT OF VALUES OF THE STREAM FUNCTION',//)
        WRITE(6,80)
80    FORMAT(5X,'NODE',4X,'X COORDINATE',4X,'Y COORDINATE',4X,
      * 'STREAM FUNCTION',///)
        DO 90 MM = 1,NNM

```

```

        WRITE(6,100) MM,X(MM),Y(MM),PSI(MM)
100    FORMAT(6X,I4,3X,3E15.5)
90    CONTINUE
        RETURN
        END
        SUBROUTINE VISC(DUDX,DUDY,DVDX,DVDY,ITER,ITYPE,ETAM,ETAN,AK1,AMU,
*          GAMADT)
C.....
C    PURPOSE :
C    -----
C    CALCULATION OF THE VISCOSITY AS A FUNCTION OF THE MAGNITUDE OF
C    THE RATE OF DEFORMATION TENSOR. TWO CHOICES FOR THE GENERALIZED
C    NEWTONIAN VISCOSITY FUNCTION (POWERLAW FLUID AND CARREAU MODEL)
C
C    AVERAGE THE VELOCITY GRADIENTS OVER THE NUMBER OF GAUSS POINTS
C    USED IN THE NUMERICAL INTEGRATION
C.....
C    DEFINITION OF VARIABLES :
C    1 - INPUT ARGUMENTS :
C    -----
C        DUDX - DERIVATIVE OF X-VELOCITY WITH RESPECT TO X-DIRECTION
C               AVERAGED OVER 4 GAUSS INTEGRATION POINTS ON EACH ELEMENT
C        DUDY - D X-VEL / D Y
C        DVDX - D V-VEL / D X
C        DVDY - D V-VEL / D Y
C        ITER - ITERATION NUMBER FOR NON-LINEAR ITERATION
C        ITYPE - FLAG FOR THE TYPE OF VISCOSITY FUNCTION REQUESTED
C        ETAM - VISCOSITY CONSTANT = M OF POWERLAW FLUID
C               = LAMBDA OF CARREAU MODEL FUNCTION
C        ETAN - EXPONENT N FOR BOTH THE POWERLAW AND THE CARREAU MODEL
C        AK1 - NEWTONIAN ZERO SHEAR RATE VISCOSITY
C
C    2 - OUTPUT ARGUMENTS :
C    -----
C        AMU - VALUE OF THE VISCOSITY
C        GAMADT - MAGNITUDE OF THE RATE OF DEFORMATION TENSOR
C.....
        IMPLICIT REAL*8(A-H,O-Z)
C    CALCULATION OF THE MAGNITUDE OF THE RATE OF DEFORMATION TENSOR
        GAMADT = DSQRT(2.0*DUDX**2 + 2.0*DVDY**2 + (DVDX + DUDY)**2)
C    FIRST ITERATION OF ALL VISCOSITY MODELS ASSUMES NEWTONIAN BEHAVIOR
        IF (ITER.EQ.1) AMU = AK1
        IF (ITER.EQ.1) GOTO 40
        GOTO (10,20,30), ITYPE+1
C    NEWTONIAN FLUID
10    AMU = AK1
        GOTO 40
C    POWERLAW MODEL FUNCTION
20    AMU = ETAM*(GAMADT)**(ETAN-1.0)

```



```
      GOTO 40
C      CARREAU MODEL FUNCTION
30      AMJ = AK1*(1.0+(ETAM*GAMADT)**2)**((ETAN-1.0)/2.0)
40      RETURN
      END
```

**The vita has been removed from
the scanned document**