MATHEMATICAL MODELING OF CONVERGING FLUID FLOW IN THE UNIAXIAL DIE OF THE FIXED BOUNDARY EXTRUSION-ORIENTATION-CRYSTALLIZATION PROCESS

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Master of Science

by
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CHAPTER I
INTRODUCTION

1.1 Background

The ability to impart controlled levels of alignment of molecules in films and fibers made from semicrystalline polymers such as polyethylene and polypropylene has been demonstrated by several groups of researchers employing several different techniques. Improvement in mechanical tensile properties such as the initial and secant moduli is reported as one of the benefits resulting from high levels of orientation in these polymer films and fibers (2-11). Even though the polymer industry has known for a number of years that the ultimate theoretical modulus of these common polymers, on the order of $10^2$ Giga Pascals, GPa, (1GPa=10$^9$ Pa=10$^{10}$dynes/cm$^2$) rivals that of steel, the conventional deformation processes of the industry such as hot drawing, rolling, cold drawing and extrusion have been inefficient at obtaining complete molecular alignment. As a consequence a semicrystalline polymer seldom exhibits a relative moduli which is more than one-tenth its theoretical value. Understandably then, a process which increases the relative moduli of these polymeric materials generates interest among those in the industry who desire to replace steel with lighter weight plastics in various areas of construction.

Southern and Porter were among the researchers who successfully produced highly oriented polymer fibers (3-10). Their process, solid
state extrusion, involved exerting an extremely high pressure, greater than 2000 atm (0.2 GPa), which caused the extrusion of a polymer from the chamber of an Instron capillary rheometer through a fiber die. Their transparent and highly oriented fibers exhibited extended chain crystals on the molecular level. Two disadvantages to their process, however, were the high pressures they were forced to use as well as the slow rates of formation of fiber their process displayed.

Wanting to duplicate Southern and Porter's successful production of highly oriented polymeric material but hoping to overcome the disadvantages of these researchers' process, Collier and his coworkers developed a process which employed specially designed and operated dies attached to the melt source, a single screw plasticating extruder (2, 11-14). Their process known as a Fixed Boundary Extrusion-Orientation-Crystallization (FBOC) process used moderate pressures, 2000-4000 psi (0.014-0.028 GPa). Although slightly higher extrusion rates were achieved, the slow rate of formation remained a problem.

1.2 Scope of the Investigation

Several different dies have been built and used by Collier and his students. Of concern for this investigation is the die which causes polymer molecules to be oriented in one direction, the machine direction. Known as the uniaxial die, this die extrudes the polymer in the form of ribbons. Figure 1 is a schematic sketch of this die showing its three sections: the reservoir section, the shaping section, and the land section. Only the converging shaping section is studied in this investigation.
The purpose of this investigation was to mathematically model the flow of a fluid in the shaping section of the current die. Due to the complexity of the partial differential equations generated in this model, a computer program was developed to solve these equations numerically. Using this program, the velocity profile as well as the profiles for shear and normal stresses may be generated for various operating conditions.
2.1 Crystalline Polymers in a Quiescent Environment

A crystalline material possesses a high degree of order in the atomic packing. In a quiescent environment polymer crystals grow from a melt or solution as thin sheets called lamellae. Typically, the lamella thickness is 100 to 500 Å (10^{-10}m) while its width extends into the micron (10^{-6}m) range (15). Each polymer molecule within the crystal is a long chain of atoms covalently bonded to each other. Since the polymer chain length is often many times longer than the lamella thickness, researchers have concluded that some form of chain folding is necessary to create the regularity in the lateral packing of the chains required by the unit cells of polymer crystals. Figure 2 depicts one model proposed for chain folding in single crystals of polymers (16).

When rapid crystallization rates are utilized, complex radial growths known as spherulites are developed. Internally, spherulites consist of chain folded lamellae of narrow width growing radially. The fibrous lamellae are parallel to the radius while the folded chains of the lamellae are normal to the radius.

In the melt crystallized system where two lamellae develop in very close proximity to each other, studies have shown that occasionally a chain, known as a tie molecule, becomes a part of two growing lamellae (15). Likewise two spherulites may be connected by a loose tie molecule.
Figure 2: Model of Chain Folding in Single Polymer Crystals
The existence of tie molecules connecting adjacent fibers of the spherulite as well as adjacent spherulites serves as a source of strength for the semicrystalline polymer. In high strength applications low modulus values not lack of strength, however, have kept polymers from being considered as replacements for metals (8). The low modulus values for semicrystalline polymers are a result of extensive chain folding in the lamellae fibers along with a lack of crystalline c-axis alignment. Continuity along the orientation axis is the necessary ingredient for producing high moduli materials (8). Loose tie molecules do not give this necessary continuity. Instead it is either stressed tie molecules or extended chain crystals which provide the required continuity. Consequently, a quiescent environment does not provide the proper conditions needed for producing orientation in semicrystalline polymers.

2.2 Crystalline Polymers in a Dynamic Environment

Orientation in polymers can be a result of the environment under which the polymer is crystallized or the environment to which the solid polymer is subjected after crystallization. Application of some sort of stress on the polymer is the common feature of these environments. Many industrial processes such as extrusion of films, spinning and drawing of fibers, calandering, and cold and hot drawing provide this essential feature which results in some degree of molecular orientation.

Many models have been introduced to describe the morphology of crystalline polymers crystallized under stress. Among these is the row structure model proposed by Keller and Machin who studied polymer samples which were products of flow induced crystallization from the
melt. Their model, shown in Figure 3, consists of a fibrillar nucleus
of extended chains parallel to the flow direction with folded chain
lamellae overgrown epitaxially on this nucleus (15, 18, 19). Similar
structures titled "shish-kebabs" have been obtained from supercooled
polymer solutions. Whether the polymer is crystallized from a melt or
solution, this model demands that the applied stress must incorporate
at least local elongational flow components (15). That is, a change in
velocity is required parallel to the flow direction. In addition, under
this type of stress, polymers are crystallized at a much faster rate.

Peterlin proposed a model for the structural changes caused by the
plastic deformation of the polymer during a drawing operation (20, 17).
Consider the extrudate structure, whether spherulitic or a row
structure of undeformed lamellae, as represented as a stack of chain
folded lamellae as shown in Figure 4 (20). Upon drawing these lamellae
break into blocks by the mechanism of shearing. The macroscopic fiber
becomes a bundle of microfibrils. Each microfibril, denoted by dashed
lines in Figure 5, consists of many extended chains resulting from the
chain unfolding during shear. In addition, a few taunt interfibrillar
tie molecules exist as a result of being tie molecules between lamellae
in the starting material. Both features, as indicated earlier,
contribute to the enhancement of mechanical properties such as modulus
value.

Other attempts to produce polymer samples with extended chain
domains were accomplished by Wunderlich and coworkers using pressure
induced crystallization (21-24). Their equipment was a closed pressure
bomb operating above a critical pressure. Commenting on the results of
Wunderlich's work, Collier and colleagues concluded that these extended
Figure 3: Effect of Stress on Development of Row Structures
Figure 4: Model of Transformation of a Stack of Parallel Lamellae
Figure 5: Model of Fibrous Structure Showing Microfibrils with Extended Chains (A) and Interfibrillar Tie Molecules (B).
chain domain could be a result of the melt being composed of slightly ordered regions that were randomly aligned with respect to each other (1, 25). Furthermore, they felt that oriented polymers have a directionally dependent compressibility with the higher compressibility perpendicular to the preferred orientation axis of the polymer. According to Collier and coworkers, a high melt pressure should enhance orientation within these slightly ordered regions further increasing the differences in the directional compressibility. Since chain alignment is the major resistance to crystallization, increasing the chain alignment or orientation by applying a high pressure should increase the crystallization rate as Wunderlich and coworkers found. Furthermore, the resultant crystalline domain should be and was an extended chain domain with the domains still randomly aligned with respect to each other.

As indicated in the first chapter, Southern and Porter have also been able to produce highly oriented polyethylene with extended chain crystals using a capillary rheometer (3-10). In their process high elongational rates occur in the region just proceeding the die. Due to the normal forces developed during elongational flow, the streamlines possibly take on a "wine glass stem" appearance as shown in Figure 6a (1). Chain alignment should increase as $\frac{\partial \nu}{\partial r}$ increases. This orientation is then retained through crystallization. Consequently, Figure 7 depicts the model these researchers feel best describes the morphology of the inner core of the fibers they have produced (6).

As indicated in Chapter I the need for a higher pressure than can be achieved in a commercial extruder is a major drawback to the solid state extrusion process. Consideration of the thermodynamics governing
Figure 6: Schematic Flow Behavior: (a) Southern and Porter’s Solid State Extrusion Process (b) Collier’s FBBOC Process
Figure 7: Extended Chain Model for Inner Core of Solid State Extrusion Strands
crystallization induced by flow might indicate the reason for this drawback. During crystallization, a first order transition, Gibbs free energy change, $\Delta F$, defined by equation 1, is equal to zero (1).

$$\Delta F = \Delta H - T \Delta S$$

(1)

$\Delta H$ = change in enthalpy  
$\Delta S$ = change in entropy  
$T$ = absolute temperature

Therefore, for fusion equation 1 becomes

$$0 = \Delta H_f - T M \Delta S_f$$

(2)

or

$$T M = \frac{\Delta H_f}{\Delta S_f}$$

(3)

Since entropy is a measure of the disorder in a polymer, as the chains align in the melt, the entropy decreases. The chain alignment increases as the velocity gradient in the direction of flow, $\frac{\partial u}{\partial r}$, increases. Consequently, the entropy is inversely proportional to $\frac{\partial u}{\partial r}$ and decreases with extensional strain. The relationship between the entropy of disordered melts and ordered melts and disordered crystalline states and ordered crystalline states is given as equation 4 in Figure 8 (12). Since equation 4 should hold, the entropy change from an oriented melt to an oriented crystalline state, $\Delta S_{ext}$, should be much smaller than the entropy change upon crystallization from a quiescent melt, $\Delta S_{quies}$, as equation 6 indicates.

$$\Delta S_{ext} < \Delta S_{quies}$$

(6)
Figure 8: Schematic representation of the relationship of entropies in a quiescent and extensional flow crystallizations

\[ S_1 \gg S_3 > S_2 > S_4 \]  

(4)
where
\[ \Delta S_{\text{ext}} = S_3 - S_4 \]
\[ \Delta S_{\text{quies}} = S_1 - S_2 \]

Assuming that the enthalpy change upon crystallization is relatively insensitive to flow conditions,

\[ \Delta H_{\text{ext}} \approx \Delta H_{\text{quies}} \quad (7) \]

Furthermore, reference to equation 3 shows that the melting point temperature is inversely proportional to the change of entropy. Coupling these two facts with equation 6 results in the conclusion that the melting point under flow conditions, \( T_{M_{\text{ext}}} \), is greater than the melting point characteristic of a quiescent atmospheric pressure crystallization as equation 8 indicates.

\[ T_{M_{\text{ext}}} > T_{M_{\text{quies}}} \quad (8) \]

If Southern and Porter used a temperature above \( T_{M_{\text{quies}}} \) but below the effective melting point under elongational flow, their sample probably begins to crystallize in the "wine glass stem" entrance to their die. As a consequence a high pressure would be necessary to push this crystallized sample into the die region.

In the Fixed Boundary Extrusion-Orientation-Crystallization (FBEOC) process developed by Collier and his students and studied in this investigation, elongational flow develops in the shaping section (see Figure 1) according to the following deformation rate tensor (25):
\[ \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

For their die this tensor represents an acceleration in the machine direction as indicated by the +1 and a shrinkage in the thickness direction as indicated by the -1. The third dimension, die width, remains constant as the diagonal zero indicates. Thus the flow becomes a two dimensional problem.

As in the solid state extrusion process, the streamlines of the viscoelastic polymer appear to take on the "wine glass stem" shape as shown in Figure 6B, Collier proposes that the chain alignment which results from the elongational flow may actually be the formation of a nematic "liquid crystal" or mesomorphic state within the polymer (25). A nematic "liquid crystal", as shown in Figure 9, is a state in which the polymer chains are axially aligned but chain ends and side groups are randomly placed. Unlike the solid state extrusion process the shaping section temperature is kept above the effective melting point of the flowing, oriented melt to inhibit crystallization until the land section (this section corresponds to the die in solid state extrusion). Then the orientation developed in the shaping section is retained by the crystallization in the land section. The model shown in Figure 7 depicts the extended chain morphology of this process as well. Collier also reports his samples had a fibrous structure similar to Peterlin's model (11).

Because the elongational flow of the shaping section appears to be extremely critical in determining the final morphology of the polymer
Figure 9: Nematic Liquid Crystalline Form
solid in this process, modeling of the flow in this section is important if a detailed study of what is happening to the material inside the die is to occur.
3.1 Basic Equations Encountered

The equations of continuity, motion, and energy are the starting equations for formulating fluid flow problems. Collectively they are known as the equations of change. Only the first two equations of change were encountered in the literature surveyed. Consequently, only these two equations are described below.

The first equation of change, the equation of continuity, is developed by applying the law of conservation of mass to a small volume element within the flowing fluid. This equation may be written as (21):

\[ \frac{\partial \rho}{\partial t} = - (\bar{v} \cdot \rho \bar{v}) \]  

(9)

where

- \( \rho \) = density
- \( t \) = time
- \( \bar{v} \) = velocity vector

The equation of continuity is tabulated in rectangular, cylindrical, and spherical coordinates in Table 3-1 (21).

The second equation of change which is encountered in literature detailing research on the converging flow of fluid is the equation of motion. This is a statement of conservation of momentum in a continuum and may be written as follows (21):
Table 3-1: The Equation of Continuity in Several Coordinate Systems

Rectangular coordinates \((x,y,z)\):

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v_x) + \frac{\partial}{\partial y} (\rho v_y) + \frac{\partial}{\partial z} (\rho v_z) = 0
\] (A)

Cylindrical coordinates \((r,\theta,z)\):

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (\rho r v_r) + \frac{1}{r} \frac{\partial}{\partial \theta} (\rho v_\theta) + \frac{\partial}{\partial z} (\rho v_z) = 0
\] (B)

Spherical coordinates \((r,\theta,\phi)\):

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (\rho r^2 v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\rho v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\rho v_\phi) = 0
\] (C)
\[
\frac{\partial \vec{v}}{\partial t} = -[\vec{v} \cdot \vec{\tau}] - \vec{v}p - [\vec{v} \cdot \vec{\tau}] + \rho \vec{g} \quad (10)
\]

where

\[\begin{align*}
\rho & = \text{pressure} \\
\vec{\tau} & = \text{stress tensor} \\
\vec{g} & = \text{body force vector}
\end{align*}\]

The equation of motion is a vector equation. Hence it represents three component equations. Equations A, B and C of Table 3-2, 3-3, 3-4 give the equations in rectangular, cylindrical, spherical coordinates respectively (21).

If a fluid is incompressible, that is, the fluid's density is constant, and the fluid follows Newton's law of viscosity, the stress tensor may be expressed as

\[
\vec{\tau} = -\mu \vec{\Delta} \quad (11)
\]

The symbol \( \Delta \) in the three main coordinate systems are given in Table 3-5. The coefficient of viscosity, \( \mu \), depends on both local pressure and temperature but not on \( \vec{\tau} \) or \( \vec{\Delta} \). Therefore, for an incompressible Newtonian fluid, the equation of motion becomes the famed Navier-Stokes equation. The component equations become equations D, E, and F in Tables 3-2, 3-3 and 3-4.

3.2 Fluid Dynamic Studies of Converging Flow

Hamel was one of the first researchers to consider the fluid dynamic problem of steady flow of an incompressible viscous fluid in a channel bounded by infinite non-parallel walls (22). This researcher used a cylindrical coordinate system. In addition, by neglecting inertia terms (terms on the left-hand side of equations D, E, F of Table 3-3)
Table 3-2: The Equation of Motion in Rectangular Coordinates $(x,y,z)$

In terms of $\tau$:

**x-component**
\[
\rho \left[ \frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right] = -\frac{\partial p}{\partial x} - \left[ \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right] + \rho g_x
\]  

**y-component**
\[
\rho \left[ \frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right] = -\frac{\partial p}{\partial y} - \left[ \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right] + \rho g_y
\]  

**z-component**
\[
\rho \left[ \frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right] = -\frac{\partial p}{\partial z} - \left[ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right] + \rho g_z
\]  

In terms of velocity gradients for a Newtonian fluid with constant $\rho$ and $\mu$:

**x-Component**
\[
\rho \left[ \frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right] = -\frac{\partial p}{\partial x} + \mu \left[ \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right] + \rho g_x
\]
Table 3-2: The Equation of Motion in Rectangular Coordinates \((x,y,z)\) Continued

\[ y\text{-component} \quad \rho \left[ \frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right] = -\frac{\partial p}{\partial y} \]  
\[ + \mu \left[ \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right] + \rho g_y \]  
\[ z\text{-component} \quad \rho \left[ \frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right] = -\frac{\partial p}{\partial z} \]  
\[ + \mu \left[ \frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right] + \rho g_z \]
Table 3-3: The Equation of Motion in Cylindrical Coordinates \((r, \theta, z)\)

In terms of \(\tau\):

\[
\begin{align*}
\text{r-component}^a & \quad \rho \left[ \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta^2}{r} + v_z \frac{\partial v_r}{\partial z} \right] = - \frac{\partial p}{\partial r} \tag{A} \\
- & \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \tau_{rr} \right) + \frac{1}{r} \frac{\partial \tau_{r\theta}}{\partial \theta} - \frac{\tau_{\theta\theta}}{r} + \frac{\partial \tau_{rz}}{\partial z} \right] + \rho g_r
\end{align*}
\]

\[
\begin{align*}
\text{\(\theta\)-component}^b & \quad \rho \left[ \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} + v_z \frac{\partial v_\theta}{\partial z} \right] = - \frac{1}{r} \frac{\partial p}{\partial \theta} \tag{B} \\
- & \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \tau_{r\theta} \right) + \frac{1}{r} \frac{\partial \tau_{\theta\theta}}{\partial \theta} + \frac{\partial \tau_{\theta z}}{\partial z} \right] + \rho g_\theta
\end{align*}
\]

\[
\begin{align*}
\text{z-component} & \quad \rho \left[ \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} \right] = - \frac{\partial p}{\partial z} \tag{C} \\
- & \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \tau_{\theta z} \right) + \frac{1}{r} \frac{\partial \tau_{\theta z}}{\partial \theta} + \frac{\partial \tau_{zz}}{\partial z} \right] + \rho g_z
\end{align*}
\]

In terms of velocity gradients for a Newtonian fluid with constant \(\rho\) and \(\mu\):

\[
\begin{align*}
\text{r-component}^a & \quad \rho \left[ \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta^2}{r} + v_z \frac{\partial v_r}{\partial z} \right] = - \frac{\partial p}{\partial r} \tag{D} \\
+ & \quad \frac{\mu}{r^2} \left[ \frac{\partial}{\partial r} \left( r \tau_{rr} \right) + \frac{1}{r} \frac{\partial^2 \tau_{r\theta}}{\partial \theta^2} - \frac{2 \tau_{\theta\theta}}{r^2} + \frac{\partial^2 \tau_{rz}}{\partial z^2} \right] + \rho g_r
\end{align*}
\]
Table 3-3: The Equation of Motion in Cylindrical Coordinates \((r, \theta, z)\)
Continued

\[
\begin{align*}
\text{\(\theta\)-component} & \quad \rho \left[ \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} + v_z \frac{\partial v_\theta}{\partial z} \right] = -\frac{1}{r} \frac{\partial p}{\partial \theta} \\
& \quad + \mu \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r \frac{\partial v_\theta}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial z^2} \right] + \rho g_\theta \tag{E} \\
\text{\(z\)-component} & \quad \rho \left[ \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} \right] = -\frac{\partial p}{\partial z} \\
& \quad + \mu \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_z}{\partial \theta^2} + \frac{1}{r^2} \frac{\partial^2 v_z}{\partial z^2} \right] + \rho g_z \tag{F}
\end{align*}
\]
Table 3-4: The Equation of Motion in Spherical Coordinates \((r, \theta, \phi)\)

In terms of \(\tau\):

\[
\text{r-component:} \quad \rho \left[ \frac{\partial v_r}{\partial t} + v_r \frac{\partial r}{\partial t} + v_\theta \frac{\partial v_r}{\partial r} + \frac{v_\phi}{r} \frac{\partial v_r}{\partial \phi} - \frac{v_\theta^2 + v_\phi^2}{r} \right]
\]

\[
= - \frac{\partial p}{\partial r} - \left[ \frac{1}{2} \frac{\partial}{\partial r} \left( r^2 \tau_r \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \tau_{\theta \theta} \sin \theta \right) \right] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi \phi} + \rho g_r \quad \text{(A)}
\]

\[
\text{\(\theta\)-component:} \quad \rho \left[ \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + v_\theta \frac{\partial v_\theta}{\partial \theta} + \frac{\mu_\phi}{r} \frac{\partial v_\theta}{\partial \phi} + \frac{v_\phi v_\theta}{r} - \frac{\mu_\phi^2 \cot \theta}{r} \right]
\]

\[
= - \frac{1}{r} \frac{\partial p}{\partial \theta} - \left[ \frac{1}{2} \frac{\partial}{\partial \theta} \left( r^2 \tau_{\theta \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \tau_{\theta \theta} \sin \theta \right) \right] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi \phi} + \rho g_\theta \quad \text{(B)}
\]

\[
\text{\(\phi\)-component:} \quad \rho \left[ \frac{\partial v_\phi}{\partial t} + v_r \frac{\partial v_\phi}{\partial r} + v_\phi \frac{\partial v_\phi}{\partial \phi} + \frac{v_\phi^2}{r} + \frac{\partial v_\theta}{\partial \phi} \cot \theta \right]
\]

\[
= - \frac{1}{r} \frac{\partial p}{\partial \phi} - \left[ \frac{1}{2} \frac{\partial}{\partial \phi} \left( r^2 \tau_\phi \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi \phi} \right] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi \phi} + \rho g_\phi \quad \text{(C)}
\]
Table 3-4: The Equation of Motion in Spherical Coordinates \((r, \theta, \phi)\)
Continued

In terms of velocity gradients for a Newtonian fluid with constant \(\rho\) and \(\mu\):\(^a\)

\[
\begin{align*}
\text{r-component} & \quad \rho \left[ \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_r}{\partial \phi} \right] \\
& = - \frac{\partial p}{\partial r} + \mu \left[ \nabla^2 v_r - \frac{2}{r^2} v_r - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} - \frac{2}{r^2} \frac{\partial v_\phi}{\partial \phi} \cot \theta \\
& \quad - \frac{2}{r^2 \sin \theta} \frac{\partial v_\phi}{\partial \phi} \right] + \rho g_r
\end{align*}
\]

\(\text{\(D\)}\)

\[
\begin{align*}
\text{\(\theta\)-component} & \quad \rho \left[ \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} \right] \\
& = - \frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left[ \nabla^2 v_\theta + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta}{r^2 \sin^2 \theta} \\
& \quad - \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial v_\phi}{\partial \phi} \right] + \rho g_\theta
\end{align*}
\]

\(\text{\(E\)}\)

\[
\begin{align*}
\text{\(\phi\)-component} & \quad \rho \left[ \frac{\partial v_\phi}{\partial t} + v_r \frac{\partial v_\phi}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\phi}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} \right] \\
& + \frac{v_\theta v_\phi}{r} \cot \theta \right] = - \frac{1}{r \sin \theta} \frac{\partial p}{\partial \phi} + \mu \left[ \nabla^2 v_\phi - \frac{v_\phi}{r^2 \sin^2 \theta} \\
& \quad + \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial v_\theta}{\partial \phi} \right] + \rho g_\phi
\end{align*}
\]

\(\text{\(F\)}\)

\(^a\)In these equations \(v^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)\)
Table 3-5: Components of the Rate-of-Deformation Tensor

**Cartesian Coordinates (x,y,z)**

\[
\begin{align*}
\Delta_{xx} &= 2 \frac{\partial \nu_x}{\partial x} \\
\Delta_{yy} &= 2 \frac{\partial \nu_y}{\partial y} \\
\Delta_{zz} &= 2 \frac{\partial \nu_z}{\partial z} \\
\Delta_{xy} &= \Delta_{yx} = \frac{\partial \nu_x}{\partial y} \\
\Delta_{xz} &= \Delta_{zx} = \frac{\partial \nu_x}{\partial z} + \frac{\partial \nu_z}{\partial x} \\
\Delta_{yz} &= \Delta_{zy} = \frac{\partial \nu_y}{\partial z} + \frac{\partial \nu_z}{\partial y}
\end{align*}
\]

**Cylindrical Coordinates (r,\theta,z)**

\[
\begin{align*}
\Delta_{rr} &= 2 \frac{\partial \nu_r}{\partial r} \\
\Delta_{\theta \theta} &= \Delta_{\theta r} = \Delta_{r \theta} = r \frac{\partial}{\partial r} \frac{\partial \nu_r}{\partial r} + \frac{1}{r} \frac{\partial \nu_r}{\partial \theta} \\
\Delta_{r \phi} = \Delta_{\phi r} &= \Delta_{\phi \phi} = \frac{\partial \nu_r}{\partial \phi} \\
\Delta_{\theta z} &= \Delta_{z \theta} = \frac{\partial \nu_z}{\partial \theta} + \frac{1}{r} \frac{\partial \nu_z}{\partial \phi} \\
\Delta_{z r} = \Delta_{r z} &= \frac{\partial \nu_z}{\partial r} + \frac{\partial \nu_r}{\partial z}
\end{align*}
\]

**Spherical Coordinates (r,\theta,\phi)**

\[
\begin{align*}
\Delta_{rr} &= 2 \frac{\partial \nu_r}{\partial r} \\
\Delta_{\theta \theta} &= \Delta_{\theta r} = \Delta_{r \theta} = r \frac{\partial}{\partial r} \frac{\partial \nu_r}{\partial r} + \frac{1}{r} \frac{\partial \nu_r}{\partial \theta} \\
\Delta_{\phi \phi} = \Delta_{\phi r} &= \Delta_{r \phi} = \frac{1}{\sin \theta} \frac{\partial^2 \nu_r}{\partial \phi \partial \theta} + \frac{1}{r} \frac{\partial \nu_r}{\partial \phi} \\
\Delta_{\theta \phi} &= \Delta_{\phi \theta} = \frac{\partial \nu_r}{\partial \theta} \\
\Delta_{\phi \theta} &= \Delta_{\theta \phi} = \frac{\partial \nu_r}{\partial \phi} \\
\Delta_{\phi \phi} &= \Delta_{\phi r} = \Delta_{r \phi} = \frac{1}{r \sin \theta} \frac{\partial \nu_r}{\partial \phi}
\end{align*}
\]
he derived a simple solution expressed in elliptic functions. Hamel's solution indicated that for an incompressible Newtonian fluid flow remained purely radial in the converging section.

For the researcher dealing with non-Newtonian fluids, studying and understanding the converging flow of these fluids becomes more complicated. For instance, if the assumption of a symmetrical shear stress tensor, \( \tilde{T} \), is made, the continuity equation and motion equation are then four equations containing ten unknown functions of position. The unknown functions are: pressure, three velocity components and six stress components. Six additional equations are required and are the component equations of the constitutive equation. The constitutive equation shows the relationship between the variables describing the state of stress and the variables describing the state of motion for the specific material being studied.

Several researchers have undertaken the study of the behavior of non-Newtonian fluids in a converging section. One researcher, P.N. Kaloni, considered the flow of an incompressible viscoelastic fluid in a channel bounded by infinite nonparallel walls (23). Because a viscoelastic fluid displays both viscous and elastic characteristics, this researcher used a constitutive equation developed by Oldroyd which accounts for both characteristics. This researcher also simplified his problem by neglecting the inertia terms of the motion equation. Unfortunately, even with this simplification the constitutive and motion equations were nonlinear. The author was able to linearize these equations using a technique proposed by Langlois. This technique is predicated on the assumption that the steady state of a slow flow field is a perturbation from the state of rest. In addition, the flow
variables are expandable in powers of a suitable small non-dimensional parameter which characterizes the amount of slowness of the flow. The first-order solution corresponds to the creeping flow of a Newtonian liquid. Kaloni found, however, a modification in the pressure distribution and stresses due to the presence of the elasticity of the fluid. In the second-order approximation some new features of the flow pattern emerged. Near the vertex of the converging section the usual radial flow was accomplished by a cross flow. Figure 10 shows an example of the type of flow pattern Kaloni's second-order approximation predicted for a channel angle of 45°. $\delta$ is a dimensionless radius.

Another researcher, Ramachar Yula, also studied the slow steady flow of a viscoelastic fluid in a converging section (24). The section of his study, however, was a cone. Like Kaloni this researcher used the constitutive equation developed by Oldroyd and Langlois' linearization technique. He found that the flow pattern was purely radial at large distances from the vertex. Unlike Kaloni this researcher did not neglect the inertial terms of the motion equation. As a result he discovered that in the vicinity of the vertex these terms have a strong influence on the flow causing circulatory flow even in the case of Newtonian liquids.

A third study of fluid flow in a converging section was undertaken by a pair of researchers (25). Unlike the previous researchers mentioned, these men carried out an experimental as well as a theoretical study of polystyrene melts flowing into a tapered slit die. The flow birefringence technique was used to measure stress-birefringent patterns while the technique of streak photography measured the local velocities of tracer particles suspended in the polymer. From these experiments,
Figure 10: Flow Patterns for a Viscoelastic Fluid in a Converging Channel
the researchers did not see any evidence of circulatory motion. This lack of apparent circulatory motion was attributed to the very slow motion of polymer melts even when the flow was accelerating. As a consequence, for their theoretical study, they assumed that the inertial terms of the equation of motion were negligible. For their constitutive equation, they modified a second-order fluid model suggested by another group of researchers. As part of their research, these men demonstrated that this model did represent a viscoelastic polymeric melt for a limited class of materials. When this constitutive model was employed, the theoretically predicted stress and velocity profile shapes compared favorably with the ones obtained experimentally. Furthermore, the magnitude of the theoretical and experimental stresses were comparable.
CHAPTER IV

CONVERGENCE OF A NEWTONIAN FLUID

4.1 The Coordinate System and Die Dimensions

The uniaxial ribbon die studied in this investigation has been previously shown in Figure 1. Because the cross-sectional area of the shaping section decreases as the fluid flows through it, cylindrical coordinates seemed the logical choice for a coordinate system. As shown in Figure 11, the z-axis lies along the imaginary line of convergence for the walls of the shaping section. The positive flow direction is opposite of the machine direction. The fluid, therefore, is flowing in the negative direction.

The dimensions of the shaping section of the die explored in this investigation are shown in Figure 12.

4.2 Equation of Change

In this analysis, the following assumptions concerning the fluid have been made:

1. The fluid is Newtonian.
2. The fluid is incompressible.
3. The fluid has reached a steady state condition.
4. The fluid is maintained isothermal.

The geometry of the uniaxial die allows several other simplifications. The shaping section is symmetrical around the \( \theta = 0^\circ \) axis. Hence only
Figure 11: The Coordinate System of the Die
Figure 12: Dimensions of the Shaping Section

- $0.1875''$
- $30^\circ$
- $r = 0.0864''$
- $R = 0.375''$
one-half of the shaping section must be mathematically modeled. Furthermore, the z-dimension remains constant throughout. The velocity in the z-direction, \( v_z \), is assumed to be equal to zero while any partial derivative with respect to z, \( \frac{\partial}{\partial z} \), also becomes zero.

Using these assumptions and simplifications, the equation of continuity (equation (B) of Table 3-1) reduces to the following:

\[
\frac{\partial v_r}{\partial r} + \frac{v_r}{r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} = 0
\]  

(12)

where \( v_r \) and \( v_\theta \) are the velocity components in the r and \( \theta \) directions.

As was indicated previously in Chapter III, assumptions (1) and (2) reduce the equation of motion to the Navier-Stokes equation. The component equations are equations D, E, and F of Table 3-3. The third assumption eliminates the partial derivatives with respect to time, \( \frac{\partial}{\partial t} \). Because \( v_z \) and \( \frac{\partial}{\partial z} \) are equal to zero, equation F is eliminated and equations D and E reduce to the following:

\[
\begin{align*}
\nu & \left( \frac{\partial^2 v_r}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} \right) \\
& + \nu \left( \frac{\partial^2 v_\theta}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} \right) = -\frac{\partial P}{\partial r} + \nu \left[ \frac{\partial^2 v_r}{\partial r^2} + \frac{1}{r \theta^2} \frac{\partial v_r}{\partial \theta} \right] \\
& + \nu \left[ \frac{\partial^2 v_\theta}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} - \frac{2}{r} \frac{\partial v_r}{\partial \theta} \right]
\end{align*}
\]

(13)

with \( P \), the pressure, \( \rho \), the fluid density, and \( \nu \), the kinematic viscosity of the fluid.
Before proceeding with the vorticity-stream function formulation of the problem, it would be advantageous to non-dimensionalize equations 12, 13, and 14. In order to non-dimensionalize, appropriate length and velocity scales must be chosen. For the two-dimensional flow under consideration here, an appropriate characteristic length, $R$, would be the radius measured from the origin to the entrance of the shaping section along the wall of the shaping section. In Figure 12, $R$ is this characteristic radius. An appropriate characteristic velocity, $\bar{V}$, would be the average velocity in the reservoir section. Defining the dimensionless variables

\[ r' = \frac{r}{R} \]  

\[ \nu' = \frac{\nu_r}{\bar{V}} \]  

\[ \theta' = \frac{\nu_\theta}{\bar{V}} \]  

\[ p' = \frac{p}{\rho \bar{V}^2} \]

equations 12, 13, and 14 become

\[ \frac{3 \nu_r'}{r} + \frac{\nu_r'}{r'} + \frac{1}{r} \frac{3 \nu_\theta'}{\theta'} = 0 \]  

\[ \nu_r' = \frac{3 \nu_r'}{r} + \frac{\nu_\theta'}{r'} \frac{\partial \nu_\theta'}{\partial r'} - \frac{\nu_\theta'}{r'} \theta' = -\frac{\partial p'}{\partial r'} + \frac{1}{\text{Re}} \left[ \frac{\nu_r'}{r'}^2 \right] \]  

\[ + \frac{1}{r'} \frac{\partial \nu_r'}{\partial r'} + \frac{3 \nu_r'}{r'} \frac{\partial \nu_r'}{\partial r'} + \frac{1}{r'} \frac{3 \nu_\theta'}{\partial r'}^2 - 2 \frac{\partial \nu_\theta'}{\partial \theta'} \]  

\[ + \frac{\partial^2 \nu_r'}{\partial r'^2} + \frac{\partial^2 \nu_r'}{\partial \theta'^2} - \frac{2}{r'} \frac{\partial \nu_\theta'}{\partial \theta'} \]
\begin{equation}
\nu_r \frac{\partial \psi_r}{\partial r} + \frac{\nu_\theta}{r} \frac{\partial \psi_\theta}{\partial \theta} + \nu_\theta \frac{\partial \psi_\theta}{\partial \theta} + \frac{\nu'_r}{r} \frac{\partial \psi'_r}{\partial \theta} + \frac{\nu'_\theta}{r} \frac{\partial \psi'_\theta}{\partial r} = - \frac{1}{r} \frac{\partial P'}{\partial \theta} + \frac{1}{\text{Re}} \left[ \frac{\partial^2 \nu'_r}{\partial r^2} + \frac{1}{r} \frac{\partial \nu'_r}{\partial r} \right] 
\end{equation}

where \( \text{Re} = \frac{\bar{V} R}{\nu} \) is the Reynolds number.

Equation 19 is satisfied by introducing the stream function \( \psi \).

\begin{align}
\nu'_r &= \frac{1}{r} \frac{\partial \psi}{\partial r} \\
\nu'_\theta &= - \frac{\partial \psi}{\partial r} 
\end{align}

Substituting equations 22 and 23 into equations 20 and 21 and eliminating \( P \) in these equations by cross differentiation gives the following equation:

\begin{equation}
\frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r} \frac{\partial^2 \psi}{\partial \theta^2} = \frac{1}{\text{Re}} \nabla^2 \psi 
\end{equation}

where

\begin{equation}
\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} 
\end{equation}

Equation 24 may be further simplified by using the vorticity relationship which is the curl of the velocity and is expressed in equation form as follows (28):

\begin{equation}
\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} = -\nabla^2 \psi \nabla \psi 
\end{equation}

with \( \nabla \) the vorticity symbol. Thus equation 24 becomes
Thus equation 26 and 27 are solved numerically to find the two unknowns, $\psi$ and $\gamma$.

Using equation 11, the dimensionalized stress equation may be expanded, giving

\[
\frac{1}{N_{Re}} \frac{\partial^2 \gamma}{\partial r^2} + \frac{1}{N_{Re}} \frac{\partial \gamma}{\partial r} \frac{\partial \gamma}{\partial \theta} + \frac{1}{r} \left( \frac{\partial \psi}{\partial r} \frac{\partial \psi}{\partial \theta} \right) + \left( \frac{1}{N_{Re}} - \frac{\partial \psi}{\partial \theta} \right) \frac{\partial \gamma}{\partial r} = 0 \tag{27}
\]

4.3 The Boundary Conditions for the Newtonian Problem

In order to develop a numerical scheme for solving equations 26 and 27 it is necessary to specify the value of $\psi$ along the boundaries of the flow domain. The values are easily found by integrating the inflow velocity.

Several simplifying assumptions are made. Because the geometry of the shaping section is best described using a cylindrical coordinate system, it is assumed that the inflow boundary of the shaping section is actually the dotted arc as shown in Figure 13. Furthermore, it is assumed that at the entrance there is simple planar Couette flow. The
equation for the velocity at the entrance is first given in rectangular coordinates. Once the various constants are identified, the equation is transformed to cylindrical coordinates.

The non-dimensional equation for the velocity at the entrance of the shaping section can be written as

$$v_x' = D \left( y' - A \right). \quad (31)$$

With $v_x'$ the dimensionless velocity component in the x-direction and D and A constants. The constant, A, is found at the wall since $v_x'$ is zero at this point. The value of $y'$ at the wall is

$$y'_{\text{wall}} = \frac{y_{\text{wall}}}{R} = \frac{0.1875}{0.375} = 0.5 \quad (32)$$

Hence A must be 0.25. Since the direction of the flow was established as the negative direction, the velocities calculated by equation 31 must be negative. This means the average velocity is negative as well. Furthermore, since the velocity was non-dimensionalized by the average inflow velocity, the average of equation 31 should be equal to negative unity. Using the equation defining the average velocity (26),

$$\overline{v} = \frac{1}{s_{\text{Max}}} \int_0^{s_{\text{Max}}} v_x' dS' \quad (33)$$

with $S'$ the dimensionless cross-sectional area of the reservoir and $s_{\text{Max}}$ the maximum S' value, constant D may be found. Substituting equation 31 into equation 33 and replacing 0.25 for A and $\frac{s'}{Z}$ for $y'$ the following equation,
\[-1 = \frac{1}{S_{\text{Max}}} \int_{0}^{S'_{\text{Max}}} D \left( \frac{S'}{z'} \right)^2 - 0.25 \, \text{d}S' \]  

(34)

with \( z' \) the dimensionless constant die width results. For this die \( z' \) equals 1.333 and \( S'_{\text{Max}} \) equals 0.666. After performing the necessary integration, constant \( D \) is found to be 6.0. Therefore, equation 31 may be written as

\[ v_x' = 6.0 \left[ y'^2 - 0.25 \right]. \]  

(35)

To transform equation 35 to cylindrical coordinates, the following transformations are employed (21)

\[ y' = r' \sin \theta' \]  

(36)

and

\[ v_r' = v_x' \cos \theta' + v_y' \sin \theta' \]  

(37)

But for simple planar Couette flow, \( v_y' \) equals zero. Therefore, with the proper substitutions, equation 37 may be written as

\[ v_r' = 6.0 \left[ r'^2 \sin^2 \theta' - 0.25 \right] \cos \theta' \]  

(38)

Substituting equation 38 into equation 22 and integrating the stream function at the entrance to the flow domain can be written as

\[ \psi = 2.0 \, r'^3 \sin^3 \theta - 1.5r' \sin \theta \text{ at } r' = 1.0 \]  

(39)

Other boundary conditions for \( \psi \) become

\[ \psi = -0.5 \quad \text{at } \theta = 30^\circ \]  

(40)
\[ \psi = 0 \quad \text{at} \quad \theta' = 0^\circ \] \hspace{1cm} (41)

The boundary conditions for \( \int \) at \( r' = 1.0 \) are found by applying equation 26 to equation 39. The resulting expression for finding the vorticity values along the entrance boundary is

\[ \int = -12.0 \, r' \sin \theta \quad \text{at} \quad r' = 1.0. \] \hspace{1cm} (42)

In addition,

\[ \int = 0 \quad \text{at} \quad \theta' = 0^\circ \] \hspace{1cm} (43)

For this investigation the boundary condition of \( \psi \) along the wall of the shaping section is assumed to be a constant value as given in equation 40. Since \( \theta' \) has a constant value of \( 30^\circ \) along the entire length of the wall, \( \psi \) can be a constant value only if \( \psi \) is a function of \( \theta' \) not \( r' \) along the wall. Hence, at the wall \( \frac{\partial \psi}{\partial r} \), and \( \frac{\partial^2 \psi}{\partial r^2} \) are both equal to 0. Combining this information with equation 26, the boundary condition for \( \int \) along the wall is given as

\[ \int = -\frac{1}{r'} \, \frac{\partial^2 \psi}{\partial \theta'^2} \quad \text{at} \quad \theta' = 30^\circ. \] \hspace{1cm} (44)

With the specification of the boundary conditions for the stream function and vorticity, a well-posed problem has been formulated and the system of differential equations, equations 26 and 27, can now be numerically modeled.

4.4 Numerical Modeling of the Newtonian Equations

One of the most commonly used techniques for solving a Poisson equation, such as the stream function equation, is an iterative method
consisting of an inner and outer iteration. Several researchers, Greenspan (29) and Chen (28), have used this method to study the flow patterns of fluids in curved tubes. Equations 26 and 27 become a pair of linear equations when a finite difference approximation is applied to each. Each of these equations is solved by an inner iteration scheme based on the successive over-relaxation method (SOR) (27). This method was designed so that the system of linear equations has a nonnegative coefficient matrix whose diagonal elements are the dominating ones (28). This trait gives the system good stability. Furthermore, this method causes swift convergence due to a careful selection of a parameter of the system known as the over-relaxation factor. This factor helps diminish the dominant eigenvalue of the coefficient matrix (28). The outer iteration is simply a numerical search for the values of $\psi$ and $\mathcal{A}$ which solve equations 26 and 27 simultaneously. The success of this search depends on a good selection of the initial guess for $\mathcal{A}$ and $\psi$. A parameter known as a smoothing factor is used to decrease the size of the step of each search (28).

Chen's pictorial representation of the inner-outer iterative method as shown in Figure 14 describes this method very well (28). He assumes the superscripts in parentheses represent the number of inner iterations while the superscripts in the brackets represent the number of outer iterations. The variables $\psi^{[o]}$ and $\mathcal{A}^{[o]}$ represent the starting values of $\psi$ and $\mathcal{A}$. Each outer iteration lie between two vertical dotted lines. Each inner iteration loop proceeds from left to right between these two lines. Within each outer iteration, the $\psi$ inner iteration loop is always completed before the $\mathcal{A}$ inner iteration loop. The final value of each inner iteration loop becomes the starting
Figure 14: W.R. Chen's Representation of the Inner-Outer Iterative Method
value of the next outer iteration as shown in Figure 14. Each inner iteration loop is terminated when

\[ \psi^{(k-1)} - \psi^{(k)} \leq e_\psi \text{ for } \psi \]  

(45)

or

\[ \bigcap^{(k-1)} - \bigcap^{(k)} \leq e_\bigcap \text{ for } \bigcap \]  

(46)

where \( e_\psi \) and \( e_\bigcap \) are the errors of convergence. The outer iterations proceed until

\[ \psi^{[n-1]} - \psi^{[n]} \leq e_\psi \]  

(47)

and

\[ \bigcap^{[n-1]} - \bigcap^{[n]} \leq e_\bigcap \]

The values \( \psi^{[n]} \) and \( \bigcap^{[n]} \) become the solution to equations 26 and 27. For this investigation \( e_\psi \) is selected as \( 1 \times 10^{-3} \) while \( e_\bigcap \) is selected as \( 4 \times 10^{-2} \). These were the same errors of convergence suggested by Gatski in his study of the flow of Newtonian and non-Newtonian fluids through a contraction (30).

4.4-1 The Finite Difference Grid

The portion of the shaping section mathematically modeled in this investigation is divided into a cylindrical computational grid consisting of thirty spaces in the \( \theta' \)-direction and sixty spaces in the \( r' \)-direction. Two subscripts \( i,j \) corresponding to the \( r' \) and \( \theta' \) coordinates respectively are attached to each variable, e.g., \( \psi_{i,j} \) and \( \bigcap_{i,j} \). Due to the geometrical symmetry of the shaping section around the \( \theta \) equals \( 0^\circ \) line, only the portion of the section from this line to the wall is
included in the model. Figure 15 shows the grid. Figure 16 indicates the location of the two variables \( \psi_{i,j} \) and \( \psi_{i,j} \), on a typical grid cell.

### 4.4.2 The Inner Iteration

As was explained previously using Figure 14, two inner iteration loops are necessary to solve equations 26 and 27 for \( \psi \) and \( \psi \). The iteration for \( \psi \) consists of using the following finite difference approximations for the respective derivatives in equation 26.

\[
\frac{\partial^2 \psi}{\partial r^2} = \frac{\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}}{\Delta r^2}
\]

\[
\frac{\partial^2 \psi}{\partial \theta^2} = \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{\Delta \theta^2}
\]

\[
\frac{\partial \psi}{\partial r} = \frac{\psi_{i+1,j} - \psi_{i,j}}{\Delta r}
\]

Substituting equation 48 through 49 into equation 26 and solving for \( \psi_{i,j} \) gives the following result

\[
\psi_{i,j} = A_1 \psi_{i,j} + A_2 \psi_{i,j-1} + A_3 \psi_{i-1,j} + A_4 \psi_{i+1,j} + A_2 \psi_{i,j+1}
\]

where the \( A_1 \) 's are

\[
A_1 = \frac{1}{\Delta r^2 + \frac{2}{r^2} + \frac{1}{(\Delta \theta)^2} + \frac{1}{r' \Delta r}}
\]
Figure 15: Cylindrical Grid System
Figure 16: Location of the Variables in a Typical Grid Cell
As can be seen, any values of the kth iteration which have already been calculated (i.e. $\psi_{i,j-1}$) are used in the calculation of the $\psi_{i,j}$ value. To speed convergence further, the SOR method takes this value of $\psi_{i,j}$ and subtracts the $\psi_{i,j}$ value of the (k-1)th iteration. This difference is multiplied by an over-relaxation parameter, $W_\psi$, and added to the $\psi^{(k)}_{i,j}$ value. The process is summarized in equation 56.

$$
\psi^{(k)}_{i,j} = W_\psi \left[ \psi_{i,j} - \psi^{(k-1)}_{i,j} \right] + \psi^{(k-1)}_{i,j} 
$$

(Equation 56)

To calculate $\nabla$, the finite difference approximations for the second order derivatives of $\nabla$ are the same as those given for $\psi$ (equations 48 and 49). The first order derivative approximations, however, are given as follows

$$
\frac{\partial \psi}{\partial r} = \frac{\psi_{i+1,j} - \psi_{i-1,j}}{2\Delta r} 
$$

(57)

$$
\frac{\partial \psi}{\partial \theta} = \frac{\psi_{i,j+1} - \psi_{i,j-1}}{2\Delta \theta} 
$$

(58)
Substituting the proper finite difference approximations into equation 27 results in four equations to calculate $\mathcal{E}_{i,j}$ depending on the value of $\mathcal{E}$ and $\mathcal{V}$.

\[
\frac{\partial \mathcal{E}}{\partial r} = \begin{cases} 
\frac{n_{i+1,j} - n_{i,j}}{2\Delta r} & \mathcal{E} \geq 0 \\
\frac{n_{i,j} - n_{i-1,j}}{2\Delta r} & \mathcal{E} < 0
\end{cases}
\]  

(59)

\[
\frac{\partial \mathcal{V}}{\partial \theta} = \begin{cases} 
\frac{n_{i,j+1} - n_{i,j}}{2\Delta \theta} & \mathcal{V} \geq 0 \\
\frac{n_{i,j} - n_{i,j-1}}{2\Delta \theta} & \mathcal{V} < 0
\end{cases}
\]  

(60)

with

\[
\mathcal{E} = 2\Delta \theta' - N_R e (\psi_{i,j+1} - \psi_{i,j-1})
\]  

(63)

\[
\mathcal{V} = \psi_{i+1,j} - \psi_{i-1,j}
\]  

(64)

Substituting the proper finite difference approximations into equation 27 results in four equations to calculate $n_{i,j}$ depending on the value of $\mathcal{E}$ and $\mathcal{V}$.

\[
\mathcal{E}_{i,j} = A_5 n_{i+1,j}^{(k-1)} + A_8 n_{i-1,j}^{(k)} + A_6 n_{i,j+1}^{(k-1)}
\]  

(65)

\[
+ A_7 n_{i,j-1}^{(k)} \quad (\mathcal{E} \geq 0, \mathcal{V} > 0)
\]

\[
\mathcal{E}_{i,j} = A_5 n_{i+1,j}^{(k-1)} + A_8 n_{i-1,j}^{(k)} + A_7 n_{i,j+1}^{(k-1)}
\]  

(66)

\[
+ A_6 n_{i,j-1}^{(k)} \quad (\mathcal{E} \geq 0, \mathcal{V} < 0)
\]
\( \nabla_{i,j} = A_8 \nabla_{i+1,j}^{(k-1)} + A_5 \nabla_{i-1,j}^{(k)} + A_6 \nabla_{i,j+1}^{(k-1)} + A_7 \nabla_{i,j-1}^{(k)} \quad (\delta < 0, \gamma \geq 0) \)  

(67)  

\( \nabla_{i,j} = A_8 \nabla_{i+1,j}^{(k-1)} + A_5 \nabla_{i-1,j}^{(k)} + A_7 \nabla_{i,j+1}^{(k-1)} + A_6 \nabla_{i,j-1}^{(k)} \quad (\delta < 0, \gamma < 0) \)  

(68)  

with

\[
A_9 = \left[ \frac{1}{2} \frac{2}{N_{Re} \Delta r^2} + \frac{2}{N_{Re} r^2 \Delta \theta^2} + \frac{|\delta|}{2N_{Re} r \Delta \theta \Delta r} \right]  
+ \frac{1}{2} \frac{|\delta|}{r^2 \Delta \theta \Delta r}  
\]  

(69)  

\[
A_5 = A_9 \left[ \frac{1}{N_{Re} \Delta r^2} + \frac{|\delta|}{2N_{Re} r \Delta r \Delta \theta} \right]  
\]  

(70)  

\[
A_6 = A_9 \left[ \frac{1}{N_{Re} r^2 \Delta \theta^2} + \frac{|\delta|}{2r \Delta r \Delta \theta} \right]  
\]  

(71)  

\[
A_7 = A_9 \left[ \frac{1}{N_{Re} r^2 \Delta \theta^2} \right]  
\]  

(72)  

\[
A_8 = A_9 \left[ \frac{1}{N_{Re} \Delta r^2} \right]  
\]  

(73)  

Equation 74 is then employed to get the final \( \nabla_{i,j}^{(k)} \) value via the SOR method.
From equation 63, 64, 65, or 66 with \( w_n \) the over-relaxation parameter of \( \cap \).

### 4.4.3 The Outer Iteration

The outer iteration begins with the initialization of all the values of \( \psi[0] \) and \( \cap[0] \). On the boundaries of the flow domain the \( \psi[0] \) values are defined by equations 39 through 41 while the \( \cap[0] \) values are defined by equations 42 and 43. All other \( \psi[0] \) and \( \cap[0] \) points are set equal to zero.

The outer iteration continues with \( \psi^{(0)} \) being set equal to \( \psi[0] \). The \( \psi^{(k)} \) sequence is then generated using equation 56 until the convergence criterion, equation 45, is satisfied. Upon satisfaction of this criterion, \( \psi_i^1 \) values are determined by the smoothing formula

\[
\psi_i^1 = \beta \psi_i^0 + (1 - \beta) \psi_i^{(k)}
\]

As the next step in the procedure, the boundary condition for \( \theta = 30^\circ \) is defined by a difference approximation suggested by Gatski (30).

\[
\cap[1] = \frac{2}{r^2} \frac{\psi_{i,J}^1 - \psi_{i,J-1}^1}{2 \Delta \theta}
\]

In this investigation, \( J \) is the boundary node and is equal to 31. The sequence \( \cap^{(k)} \) is generated from equation 74 until the convergence criterion of equation 46 is met. The \( \cap_i^1 \) values are calculated.
using the following equation

\[ \nabla_{i,j}^{[1]} = \beta \nabla_{i,j}^{[0]} + (1 - \beta) \nabla_{i,j}^{(k)} \]  

(77)

where \( \beta \) is the smoothing factor.

The \( n \)th outer iteration is a repeat of the first outer iteration with \( \psi^{(0)} \) first set equal to \( \psi^{[n-1]} \) as shown in Figure 14. The procedure continues with \( \psi^{[0]} \) and \( \nabla_{i,j}^{[0]} \) replaced by \( \psi^{[n-1]} \) and \( \nabla_{i,j}^{[n-1]} \) and \( \psi^{[1]} \) and \( \nabla_{i,j}^{[1]} \) replaced by \( \psi^{[n]} \) and \( \nabla_{i,j}^{[n]} \) for \( N=1,2,3 \ldots \) in equations 75, 76 and 77.

The outer iteration is completed when the convergence criteria of equation 47 are met.

4.4-4 The Velocity and Stress Values

The equation for finding the velocity in the \( r' \)-direction, equation 22, is rewritten in the form of a finite difference approximation equation using equation 58. As a consequence the values of \( v_{r'} \) at the interior points of the grid are calculated by equation 78.

\[ v_{r'}_{i,j} = \frac{\psi_{i,j+1} - \psi_{i,j-1}}{2 \Delta \theta_{r'}} \]  

(78)

The value of \( v_{r'} \) along the wall of the shaping section is assumed to be zero.

In the same manner the shear stress equation, equation 28 is written using finite difference approximations for the first and second order derivatives of \( \psi \). Equation 79 is the result.
Finally, the normal stress difference, \( \alpha' \), is equal to \( \tau_{rr}' - \tau_{\theta\theta}' \) or \( 2\tau_{rr}' \) since \( \tau_{\theta\theta}' \) equals \( -\tau_{rr}' \). An additional finite difference approximation must be defined for \( \frac{\partial^2 \psi}{\partial r \partial \theta} \) (27).

\[
\frac{\partial^2 \psi}{\partial r \partial \theta} = \frac{\psi_{i+1,j+1} - \psi_{i+1,j-1} - \psi_{i-1,j+1} + \psi_{i-1,j-1}}{4 \Delta r \Delta \theta} \tag{80}
\]

Incorporating this with the approximation for \( \frac{\partial \psi}{\partial \theta} \) (equation 58), an equation for \( \alpha' \) may be written using equation 29.

\[
\alpha'_{i,j} = \frac{-4}{N_{Re}} \left[ \frac{\psi_{i,j+1} - \psi_{i,j-1}}{2 \Delta \theta'} \right]^{\frac{1}{2}} \tag{81}
\]

As can be seen, the \( r' \)-direction velocity, shear stress, and normal stress all depend on the values of \( \psi \). Hence they are not part of the iteration scheme but may be calculated after the iteration scheme is completed.

4.5 The Results

The FORTRAN IV program which uses this inner-outer iteration technique to solve equation 26 and 27 is given in Appendix A. The flow
The chart used for this program is given in Figure 17 and the variables of the program are explained in Table 4-6.

The average velocity, $\bar{V}$, and characteristic radius, $R$, used in this investigation were taken from Chang's thesis (12).

\[ \bar{V} = 0.032 \, \text{cm/s} \]
\[ R = 0.95 \, \text{cm} \]

The value for the kinematic viscosity came from the literature (31).

\[ \nu = 2.67 \times 10^5 \, \text{s/cm}^2 \]

Hence the Reynolds number became $1.14 \times 10^{-7}$. The grid sizes were chosen to be the following:

\[ \Delta r' = \frac{0.7696}{60} \]
\[ \Delta \theta' = \pi/180 \]

In addition, the following over-relaxation parameters and smoothing factors were selected. Computational tests determined that these were the optimum values for this model.

\[ W_\psi = 1.8 \]
\[ W_\omega = 1.5 \]
\[ \beta_\psi = 0.1 \]
\[ \beta_\omega = 0.1 \]

The numerical calculations were completed on the IBM 370/158 computer located at the Ohio University Computer Center.

A contour plot of the stream function is shown in Figure 18. Since the motion is steady the streamlines represent the paths (streaklines) that tracer elements would follow if injected into the flow. At the
Figure 17: Flow Chart for the Newtonian Program
Table 4-6: Text and FORTRAN Program Variables

<table>
<thead>
<tr>
<th>Text Variable</th>
<th>FORTRAN Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\psi, \psi^{(k)}, \psi^{[n]}$</td>
<td>SI, SI1, SI2</td>
</tr>
<tr>
<td>$\chi, \chi^{(k)}, \chi^{[n]}$</td>
<td>ETA, ETA1, ETA2</td>
</tr>
<tr>
<td>$\nu_r$</td>
<td>VR</td>
</tr>
<tr>
<td>$\tau_{r\theta}$</td>
<td>SHEAR</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>TDIFF</td>
</tr>
<tr>
<td>$N_{Re}$</td>
<td>REN</td>
</tr>
<tr>
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<td>WSI</td>
</tr>
<tr>
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<td>WETA</td>
</tr>
<tr>
<td>$\beta_\psi$</td>
<td>XSI</td>
</tr>
<tr>
<td>$\beta_\chi$</td>
<td>XETA</td>
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</tr>
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<td>ERRORE</td>
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</tr>
<tr>
<td>$\Delta \theta'$</td>
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</tr>
<tr>
<td>$\delta$</td>
<td>DELTA</td>
</tr>
<tr>
<td>$\gamma$</td>
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<td>AK8</td>
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<tr>
<td>$A_9$</td>
<td>AK9</td>
</tr>
</tbody>
</table>
Figure 18: Stream Function Contour Lines for a Newtonian Fluid in the Flow Domain
entrance of the shaping section the streamlines appear to correspond to lines which radiate from the point of intersection of the nonparallel walls of the shaping section. Toward the exit of the section, however, the lines begin to bend toward the centerline. This bend may be attributed to the development of secondary flow within the converging flow field as the vertex of the converging section is approached. Similar results have been reported in the literature when the inertial terms of the equation of motion are included in the mathematical study of the flow as was the case in this investigation.

Figure 19 is a plot of the contours of constant velocity in the r'-direction. As was indicated earlier, elongational flow is produced in the shaping section by decreasing the thickness of the die while accelerating the flow in the machine direction. Hence it is obvious that the relative magnitude of the constant velocity lines should increase as the exit of the shaping section is approached.

Figure 20 and 21 show the shear stress and normal stress difference contour lines respectively. Further comment on these results will be undertaken in the final section of Chapter V after the corresponding plots for the Non-Newtonian fluid have been presented. All values in Figure 20 have been multiplied by $1 \times 10^{-8}$ while those in Figure 21 have been multiplied by $1 \times 10^{-9}$. 
Figure 19: Constant $v_r$ Contour for a Newtonian Fluid in the Flow Domain
Figure 20: Constant $\tau_{r\theta}'$ Contours for a Newtonian Fluid in the Flow Domain
Figure 21: Constant $\tau'_{rr} - \tau'_{\theta\theta}$ Contours for a Newtonian Fluid in the Flow Domain
CHAPTER V

CONVERGENCE OF A NON-NEWTONIAN FLUID

5.1 The Constitutive Equation

The assumptions concerning the fluid for this portion of the investigation are almost identical to those given at the commencement of Section 4.2. The assumptions for this chapter are given as

1. The fluid is non-Newtonian.
2. The fluid is incompressible.
3. The fluid has reached a steady state condition.
4. The fluid is maintained isothermal.

Only assumption (1) has changed. With this alteration the expression for employed when studying a Newtonian fluid (see equation 11) is no longer valid. Instead for the simple non-Newtonian fluid studied in this investigation, the relationship for may be given as

\[ \vec{\tau} = \eta \vec{\Delta} \]  \hspace{1cm} (82)

where \( \eta \), a scalar, is a function of \( \vec{\Delta} \) (or a function of \( \vec{\tau} \)) as well as of temperature and pressure. For \( \eta \) to be a scalar function of \( \vec{\Delta} \) it must depend only on the "invariants" of \( \vec{\Delta} \). As Bird defines them, "the invariants are those special combinations of the components of \( \vec{\Delta} \) that transform as scalars under a rotation of the coordinate system" (21). Hence

\[ I_1 = (\vec{\Delta} : \vec{\Delta}) = \Sigma_i \Delta_{ii} \]  \hspace{1cm} (83)

66
\[ I_2 = \langle \vec{\alpha} \cdot \vec{\alpha} \rangle = \varepsilon_{i} \varepsilon_{j} \Delta_{ij} \Delta_{ij} \tag{84} \]

\[ I_3 = \text{det} \vec{\alpha} = \varepsilon_{i} \varepsilon_{j} \varepsilon_{k} \varepsilon_{ijk} \Delta_{ij} \Delta_{jk} \tag{85} \]

For an incompressible fluid, \( I_1 \) equals zero. In addition, \( I_3 \) is ordinarily assumed to be relatively unimportant in most flow situations. Hence for this investigation it is assumed that \( \eta \) depends only on the second invariant.

The Ostwalt-de Waele model, more commonly known as the power law, was used as the empirical expression for \( \bar{r} \). As a consequence, equation 82 becomes

\[ \bar{r} = - \left\{ M \left| \sqrt{\frac{\varepsilon_{i} \varepsilon_{j}}{\Delta_{ij} \Delta_{ij}}} \right|^{N-1} \right\} \bar{\alpha} \tag{86} \]

The parameters \( M \) and \( N \) vary not only from material to material but also from operating conditions to operating conditions for the same material. And of course the expression in the braces is equal to \( \eta \).

Employing the assumption that the fluid is incompressible and the \( z \)-axis is the neutral axis, the expression \( \frac{1}{2} (\vec{\alpha} \cdot \vec{\alpha}) \) becomes

\[ \frac{1}{2} (\vec{\alpha} \cdot \vec{\alpha}) = 2 \left[ \frac{\partial v}{\partial r} \right]^{2} + \left( \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{v}{r} \right)^{2} + \]

\[ \left[ \frac{-\nu \partial \theta}{r} + \frac{\partial \theta}{\partial r} + \frac{1}{r} \frac{\partial \theta}{\partial \theta} \right]^{2} \tag{87} \]

The parameter \( M \) has the dimensions of

\[ \frac{\text{Mass}}{(\text{Length})^{2} \cdot (\text{Time})^{2-N}} \tag{88} \]
Therefore, if \( v_r, v_\theta, \) and \( r \) are replaced by equations 15 through 18, the result is the following:

\[
\eta = \frac{MV}{R^{N-1}} \left[ \sqrt{2 \left[ \frac{\partial v_r'}{\partial r'} \right]^2 + \left( \frac{1}{r'} \frac{\partial v_r'}{\partial \theta'} + \frac{v_r'}{r'} \right)^2} + \left( -\frac{v_\theta'}{r'} + \frac{\partial v_\theta'}{\partial r'} \right)^2 \right]^{N-1}
\]

(89)

As should be the case, \( \eta \) has viscosity dimensions \( \frac{\text{Mass}}{\text{Length} \cdot \text{Time}} \).

5.2 Equations of Change

Because the equation of continuity is a mass balance equation, it does not change when a non-Newtonian fluid is considered. Hence equation 19 still applies.

When dealing with an incompressible non-Newtonian fluid, the component equations of motion are equations A, B, and C of Table 3-3. Once again equation C is eliminated because the z-axis is neutral. In addition, the assumption of steady state eliminates the partial derivatives with respect to time. The result is the following pair of equations:

\[
\rho \left( v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta'^2}{r} \right) = -\frac{\partial \rho}{\partial r} - \left( \frac{1}{r} \frac{\partial \tau_{rr}}{\partial r} \right) + \frac{1}{r} \frac{\partial \tau_{r\theta}}{\partial \theta} - \frac{\tau_{r\theta}}{r}
\]

(90)

\[
\rho \left( v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} \right) = \frac{1}{r} \frac{\partial \rho}{\partial \theta} - \left( \frac{1}{r^2} \frac{\partial \tau_{r\theta}}{\partial r} \right) + \frac{1}{r} \frac{\partial \tau_{\theta\theta}}{\partial \theta}
\]

(91)
The component equations for $\tau$ are the following:

$$\tau_{rr} = -\eta \Delta_{rr} = -\eta \left[ 2 \frac{\partial \nu_r}{\partial r} \right]$$  \hspace{1cm} (92)

$$\tau_{\theta\theta} = -\eta \Delta_{\theta\theta} = -\eta \left[ 2 \left( \frac{1}{r} \frac{\partial \nu_\theta}{\partial \theta} + \frac{\nu_\theta}{r} \right) \right]$$  \hspace{1cm} (93)

$$\tau_{r\theta} = -\eta \Delta_{r\theta} = -\eta \left[ \frac{\nu_\theta}{r} + \frac{\partial \nu_\theta}{\partial r} + \frac{1}{r} \frac{\partial \nu_r}{\partial \theta} \right]$$  \hspace{1cm} (94)

If the partial derivative with respect to $r$ or to $\theta$ is taken of any of these three equations, the chain rule must be applied since $\eta$ is no longer a constant scalar. Therefore,

$$\frac{\partial \tau_{rr}}{\partial r} = -\eta \frac{\partial \Delta_{rr}}{\partial r} - \Delta_{rr} \frac{\partial \eta}{\partial r}$$  \hspace{1cm} (95)

$$\frac{\partial \tau_{rr}}{\partial \theta} = -\eta \frac{\partial \Delta_{rr}}{\partial \theta} - \Delta_{rr} \frac{\partial \eta}{\partial \theta}$$  \hspace{1cm} (96)

If a similar exercise were done for $\tau_{\theta\theta}$ and $\tau_{r\theta}$ and the results were substituted into equations 87 and 88, the result would be a pseudo Navier-Stokes equation with the constant $\mu$ replaced by the scalar function $\eta$. In addition, there would be extra terms since the partial derivatives of $\eta$ with respect to $r$ and $\theta$ are not equal to zero. The following two equations are the result.

$$\nu_r \frac{\partial \nu_r}{\partial r} + \frac{\nu_\theta}{r} \frac{\partial \nu_r}{\partial \theta} - \frac{\nu_\theta^2}{r} = -\frac{\partial p}{\partial r} + \frac{\eta}{R} \left[ \frac{-\nu_r}{r^2} + \frac{1}{r} \frac{\partial \nu_r}{\partial r} + \frac{\partial^2 \nu_r}{\partial r^2} \right. \left. + \frac{1}{r^2} \frac{\partial^2 \nu_r}{\partial \theta^2} - 2 \frac{\partial \nu_\theta}{\partial \theta} \right] + \left( \text{Extra } \frac{\partial \eta}{\partial r} \text{ or } \frac{\partial \eta}{\partial \theta} \text{ terms} \right)$$  \hspace{1cm} (97)
If equations 15 through 18 are now used to dimensionalize $v_r$, $v_\theta$, $r$ and $P$, after which $v_r$ and $v_\theta$ are replaced by equations 22 and 23 and $P$ is eliminated by cross-differentiation, the following equation results.

\[
\frac{1}{r^2} \frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r^2} \frac{\partial^2 \psi}{\partial r \partial \theta'} - \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} = \frac{1}{N(\eta)} \frac{V^4}{\rho V R} + \frac{\text{DTOT}}{\rho V R}
\]  

(99)

Details for deriving equation 99 are given in Appendix D. $N^{(n)}_{Re}$ is a Reynolds number equal to $\frac{q \nu R}{\nu}$. The value of $N^{(n)}_{Re}$ changes as $\eta$ changes. Furthermore, with equations 22 and 23 substituted for $v_r$ and $v_\theta$, equation 89 becomes

\[
n = \frac{M}{V} \frac{N-1}{R^{N-1}} \sqrt{4 \left( \frac{-1}{r} \frac{1}{\theta} \frac{\partial \psi}{\partial \theta'} + \frac{1}{r} \frac{\partial^2 \psi}{\partial \theta^2} \right)^2 + \left( \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} \right)^2}
\]  

(100) 

DTOT is the summation of all the extra terms and is equal to the following:

\[
\text{DTOT} = \left[ -2 \frac{\Delta' r \theta}{\partial \theta'} - \frac{2 \Delta' r r}{r^2} - 2 \frac{\Delta' r r}{r \partial r} \right] \frac{\partial n}{\partial r} + \left[ 2 \frac{\Delta' r \theta}{\partial \theta'} \right]
\]  

(101) 

\[
-2 \frac{\Delta' r r}{r \partial \theta'} + 3 \Delta' \frac{r \theta}{r} \right] \frac{\partial n}{\partial r'} - \frac{\Delta' r \theta}{r^2} \frac{\partial^2 n}{\partial \theta^2} - 2 \frac{\Delta' r \theta}{r \partial r} \frac{\partial^2 n}{\partial r \partial \theta}
\]  

where
\[ \Delta'_{rr} = 2 \left[ \frac{-1}{r}, 3 \frac{\partial \psi}{\partial \theta} \right] + \frac{2}{r'} \frac{\partial^2 \psi}{\partial \theta' \partial r'} \]  
(102) \[ \Delta'_{r \theta} = -\Delta'_{rr} \]  
(103) \[ \Delta'_{r \theta} = \frac{1}{r'} \frac{\partial \psi}{\partial r'} - \frac{3}{r^2} \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta'^2} \]  
(104)

Finally, replacement of \( \nabla^2 \psi \) in equation 99 with the equivalent \(- \nabla \) yields an equation very similar to equation 27.

\[ \frac{1}{N(\eta)} \frac{\partial \nabla}{\partial r^2} + \frac{1}{N(\eta)} \frac{1}{r^2} \frac{\partial \nabla}{\partial \theta'^2} + \frac{1}{r'} \left[ \frac{\partial \psi}{\partial r'} - \frac{\partial \nabla}{\partial \theta'} \right] = \frac{\varepsilon \psi}{\varepsilon \theta'} \]  
(105) \[ + \left( \frac{\partial \psi}{\partial r'} - \frac{\partial \nabla}{\partial \theta'} \right) \frac{\partial \nabla}{\partial r'} \]  

Hence equation 105 and equation 26 are the two equations which are now solved numerically to find \( \psi \) and \( \nabla \) for a non-Newtonian flow domain.

Dimensionalizing equations 92 through 94 and substituting equation 22 and 23 for \( v_r' \) and \( v_{\theta}' \) respectively yields stress equations in terms of the stream function.

\[ \tau'_{r \theta} = -\frac{n}{\varepsilon \psi} \frac{\Delta'_{rr}}{\varepsilon RV} = -\frac{n}{\varepsilon RV} \left[ \frac{1}{r'} \frac{\partial \psi}{\partial r'} - \frac{3}{r^2} \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta'^2} \right] \]  
(106)

\[ \tau'_{rr} = -\frac{n}{\varepsilon RV} \left[ \frac{-2}{r'^2} \frac{\partial \psi}{\partial \theta'} + \frac{2}{r'} \frac{\partial \psi}{\partial \theta' \partial r'} \right] \]  
(107)

\[ \tau'_{\theta \theta} = \frac{n}{\varepsilon RV} \left[ \frac{\Delta'_{rr}}{\varepsilon RV} \right] \]  
(108)

with \( n \) given by equation 100. An equivalent expression for \( n \) in terms of \( \Delta'_{rr} \) and \( \Delta'_{r \theta} \) may also be given if equations 102 through 104 are
employed in conjunction with equation 100. This expression should aid in understanding the derivation of the stress boundary conditions.

\[
n = \frac{MV^{N-1}}{R^{N-1}} \sqrt{4 \frac{\Delta r r}{rr} + \frac{\Delta r \theta}{r \theta}}^{N-1} \tag{109}
\]

5.3 The Boundary Conditions for the Non-Newtonian Problem

The power law parameters, \( M \) and \( N \), were taken from the literature for low density polyethylene at 190°C (32).

\[
N = \frac{1}{3}
\]

\[
M = 1.62 \times 10^7 \frac{g}{\text{cm}^5 \text{s}^{5/3}}
\]

As was explained in Section 4.3, the flow at the entrance to the shaping section is assumed to be simple planar Couette flow. For a power law fluid the equation for velocity which corresponds to equation 31 may be written as

\[
\nu_x' = E \left[ y' \left( \frac{1}{N} + 1 \right) - B \right] \tag{110}
\]

with \( E \) and \( B \) constants and \( N \) equal to 1/3 (32). Employing the same analysis techniques to find \( B \) and \( E \) as were used to find \( A \) and \( D \) in equation 31 gives the following velocity equation,

\[
\nu_x' = 20.0 \left( y' \left( \frac{4}{N} - 0.0625 \right) \right) \tag{111}
\]

Transforming to cylindrical coordinates yields

\[
\nu_r' = 20.0 \left[ \frac{r' \sin \theta'}{N} \left( \frac{4}{N} - 0.0625 \right) \right] \cos \theta'. \tag{112}
\]

The corresponding stream function equation at the entrance becomes
\[ \psi = 4.0 \ r' \sin^5 \theta' - 1.25 \ r' \sin \theta' \text{ at } r' = 1.0 \quad (113) \]

Other boundary conditions for \( \psi \) are

\[ \psi = -0.5 \quad \text{at } \theta' = 30^\circ \quad (114) \]

\[ \psi = 0 \quad \text{at } \theta' = 0^\circ \quad (115) \]

The boundary condition equation for \( \psi \) at \( r' = 1.0 \) is again found by applying equation 26 to equation 113 and is given as follows,

\[ \psi = -80 \ r' \sin^3 \theta' \text{ at } r' = 1.0 \quad (116) \]

The boundary conditions for \( \psi \) at \( \theta' = 0^\circ \) and \( 30^\circ \) remain the same as those given for the Newtonian case.

\[ \psi = 0 \quad \text{at } \theta = 0^\circ \quad (117) \]

\[ \psi = \frac{1}{r'^2} \frac{\partial^2 \psi}{\partial \theta'^2} \text{ at } \theta = 30^\circ \quad (118) \]

The boundary condition for the shear stress at the entrance to the shaping section is found by taking the appropriate partial derivatives of \( \psi \) (equation 113) specified by equation 106. The resulting equation is

\[ \tau'_{r\theta} = \left. \left[ K \ 80.0 \ r' \sin^3 \theta' \right]^{N-1} \right|_{r=1.0} + 80 \ r' \sin^3 \theta' \]  

\[ \tau'_{r\theta} = -160 \ r' \sin^5 \theta' \text{ at } r = 1.0 \quad (119) \]

where \( K \) is equal to \( M \frac{V}{R} \). Using the same technique, the equation for \( \tau_{rr} \) is
In addition, we have

\[ \tau'_r = - \tau'_r \]

at \( r' = 1.0 \) \hspace{1cm} (121)

Note that these boundary equations may always be split into the \( \eta \) boundary term (in the braces) and the \( \Delta_{ij} \) term (in the brackets).

According to Gatski, the symmetry of the shaping section dictates that \( \Delta'_{ij} \) (the term in brackets in equation 106) be zero at the centerline (30). Therefore,

\[ \tau'_{r\theta} = 0 \]

at \( \theta = 0^\circ \) \hspace{1cm} (122)

If \( \Delta'_{r\theta} \) is zero at the centerline, \( \eta \) is given by

\[ \eta = K \left| 2\Delta'_{rr} \right|^{N-1} = K \left| \frac{-4}{r'^2} \frac{\partial \psi}{\partial \theta'} + \frac{4}{r'} \frac{\partial^2 \psi}{\partial \theta' \partial r'} \right|^{N-1} \]

at \( \theta = 0^\circ \) \hspace{1cm} (123)

As a result, the expressions for the normal stresses along the centerline are

\[ \tau'_r = - \frac{1}{\rho_{RV}} \left\{ \begin{array}{c} \frac{-2}{r'^2} \frac{\partial \psi}{\partial \theta'} + \frac{2}{r'} \frac{\partial^2 \psi}{\partial \theta' \partial r'} \end{array} \right\}^{N-1} \]

\[ \left[ \frac{-2}{r'^2} \frac{\partial \psi}{\partial \theta'} + \frac{2}{r'} \frac{\partial^2 \psi}{\partial \theta' \partial r'} \right] \]

at \( \theta = 0^\circ \) \hspace{1cm} (124)
At the wall \( v_r \) is zero at each \( r' \) value. Thus there is no change of \( v_r \) with respect to \( r \) along the entire length of the wall. Therefore, \( \Delta_{rr} \) which is equal to \( 2\frac{\partial v_r}{\partial r} \) (see Table 3-5) is zero along the wall. The results are

\[
\tau_{rr}' = -n\frac{\Delta_{rr}'}{RV} = 0 \quad \text{at } \theta = 30^\circ \tag{125}
\]

\[
\tau_{rr}' = -\tau_{rr}' = 0 \quad \text{at } \theta = 30^\circ \tag{126}
\]

In addition, along the wall \( \psi \) is a constant value and does not change with respect to \( r \). Hence along the wall, \( \frac{\partial \psi}{\partial r} \) and \( \frac{\partial^2 \psi}{\partial r^2} \) are zero and \( \Delta_{r\theta}' \) reduces to

\[
\Delta_{r\theta}' = \frac{1}{r'2} \frac{\partial^2 \psi}{\partial \theta'2} \quad \text{at } r = 30^\circ \tag{127}
\]

Furthermore, using the same reasoning

\[
n = K \left[ \frac{1}{r'2} \frac{\partial^2 \psi}{\partial \theta'2} \right]^{N-1} \quad \text{at } r = 30^\circ. \tag{128}
\]

Combining equation 127 and 128, \( \tau_{r\theta}' \) may be written as

\[
\tau_{r\theta}' = -\frac{1}{\varphi RV} \left\{ n \left[ \frac{1}{r'2} \frac{\partial^2 \psi}{\partial \theta'2} \right]^{N-1} \right\} \frac{1}{r'2} \frac{\partial^2 \psi}{\partial \theta'2} \quad \text{at } \theta' = 30^\circ \tag{129}
\]

Table 5-7 summarizes the assumed boundary conditions for the non-Newtonian problem.
Table 5-7: Summary of the Boundary Conditions for the Non-Newtonian Fluid Problems

<table>
<thead>
<tr>
<th></th>
<th>At $r' = 1.0$</th>
<th>At $\theta' = 0^\circ$</th>
<th>At $\theta' = 30^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\psi$</td>
<td>$4r' r^5 \sin^5 \theta' - 1.25 r' \sin \theta'$</td>
<td>0</td>
<td>-0.5</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>$-80.0 r'^3 \sin^3 \theta'$</td>
<td>0</td>
<td>$-\frac{1}{r'^2} \frac{\partial^2 \psi}{\partial \theta'^2}$</td>
</tr>
<tr>
<td>$\tau_{r\theta}'$</td>
<td>$-k' \left</td>
<td>80.0 r'^3 \sin^3 \theta' \right</td>
<td>^{N-1}$</td>
</tr>
<tr>
<td>$\tau_{rr}'$</td>
<td>$-k' \left</td>
<td>80.0 r'^3 \sin^3 \theta' \right</td>
<td>^{N-1}$</td>
</tr>
<tr>
<td>$\tau_{\theta\theta}'$</td>
<td>$-\tau_{rr}'$</td>
<td>$-\tau_{rr}'$</td>
<td>0</td>
</tr>
<tr>
<td>$\Delta_{r\theta}'$</td>
<td>$-160.0 r'^3 \sin^5 \theta' + 80.0 r'^3 \sin^3 \theta$</td>
<td>0</td>
<td>$\frac{1}{r'^2} \frac{\partial^2 \psi}{\partial \theta'^2}$</td>
</tr>
<tr>
<td>$\Delta_{rr}'$</td>
<td>$160.0 r'^3 \sin^4 \theta' \cos \theta'$</td>
<td>$-\frac{2}{r'} \frac{\partial \psi}{\partial \theta'} + \frac{2}{r'^2} \frac{\partial^2 \psi}{\partial \theta' \partial r'}$</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 5-7, Continued

<table>
<thead>
<tr>
<th>At $r' = 1.0$</th>
<th>At $\theta' = 0^\circ$</th>
<th>At $\theta' = 30^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta$</td>
<td>$-K \left</td>
<td>80.0 \ r'^3 \sin^3 \theta' \right</td>
</tr>
</tbody>
</table>

NOTE: $K' = \frac{K}{\varphi RV}$
5.4 Numerical Modeling of the Non-Newtonian Equations

The technique for numerically solving equations 26 and 105 is almost the same as the one described in Section 4.4 and represented by Figure 14. Each outer iteration contains a \( \psi \) inner iteration loop and a \( \int \) inner iteration. The one difference occurs due to the extra term (DTOT) in equation 105. Since each term of DTOT involves \( \eta, \Delta'_r, \) or \( \Delta'_{r\theta} \) or some partial derivative of these three variables, first \( \eta, \Delta'_r \) and \( \Delta'_{r\theta} \) are found for all points on the finite difference grid. Since, however, \( \eta, \Delta'_r, \) and \( \Delta'_{r\theta} \) depend only on \( \psi \) not on \( \int \) (see equations 100, 102, and 104), these values may be calculated prior to the commencement of the \( \int \) inner iteration loop. Equations 48, 49, 57, 58, and 80 are the finite difference approximations of the \( \psi \) derivatives used to develop expressions for \( \eta, \Delta'_r, \) and \( \Delta'_{r\theta} \) at the interior points of the finite difference grid.

\[
\eta_{i,j}^{[n]} = k \left[ 4(C_2 - C_1)^2 + (C_3 - C_4 + C_5)^2 \right]^{1/2} \left[ \frac{1}{N-1} \right] \quad (130)
\]

\[
\Delta'_{rr}^{[n]} = 2(C_2 - C_1) \quad (131)
\]

\[
\Delta'_{r\theta}^{[n]} = (C_3 - C_4 + C_5) \quad (132)
\]

where

\[
C_1 = \frac{\psi_{i,j+1}^{[n]} - \psi_{i,j-1}^{[n]}}{2 \, r^2 \, \Delta \theta} \quad (133)
\]
Finding \( n \) and \( \Delta'_{rr} \) at the centerline involves redefining the finite difference approximation for \( \frac{\partial \psi}{\partial \theta'} \) and \( \frac{\partial^2 \psi}{\partial r' \partial \theta'} \).

At \( \theta' \) equals 0°

\[
\frac{\partial \psi}{\partial \theta'} = \frac{\psi_{i,J+1} - \psi_{i,J}}{\Delta \theta}
\]

\[
\frac{\partial^2 \psi}{\partial r' \partial \theta'} = \frac{\psi_{i+1,J+1} - \psi_{i,J+1} - \psi_{i+1,J} + \psi_{i,J}}{\Delta r' \Delta \theta'}
\]

with \( J = 1 \). Hence at the centerline

\[
\eta_{i,1}^{[n]} = k \left| 4(B_{1} - B_{2}) \right|^{N-1}
\]

\[
\Delta'_{rr,1}^{[n]} = 2(B_{1} - B_{2})
\]

where

\[
B_{1} = \frac{\psi_{i+1,2} - \psi_{i+1,1} + \psi_{i,1}}{r' \Delta \theta' \Delta r'}
\]
At the wall $\eta$ and $\Delta_{r\theta}'$ expressions may be developed using equation 144 as the finite difference approximation for $\frac{\partial^2 \psi}{\partial (\theta')^2}$.

$$\frac{\partial^2 \psi}{\partial (\theta')^2} = 2 \left[ \frac{\psi_{i,J-1} - \psi_{i,J}}{(\Delta \theta')^2} \right]$$

Hence at $\theta'$ equals 30°, $J=31$ and

$$\eta = K \left| \begin{array}{c} B_3 \end{array} \right| ^{N-1}$$

$$\Delta_{r\theta}' = B_3$$

where

$$B_3 = 2 \left[ \begin{array}{cc} \psi[n] & \psi[n] \\ \frac{i,30}{i,31} & \frac{r^2 \Delta \theta'}{2} \end{array} \right]$$

Once the interior and boundary values for $\eta$, $\Delta_{rr}'$ and $\Delta_{r\theta}'$ are found, DTOT may be found for the nth outer iteration. Since DTOT does not depend on $\bigwedge$, it remains constant as the inner iteration loop of $\bigwedge$ is carried out. Hence, equation 101 in finite difference form becomes

$$\text{DTOT}[n] = \left[ \frac{\Delta[n]}{r^2 \Delta \theta'} \frac{- \Delta[n]}{r^2 i,j+1} \frac{-2 \Delta[n]}{r^2 i,j} \right]$$

$$+ \left[ \frac{\Delta'[n]}{r^2 \Delta \theta'} \frac{- \Delta'[n]}{r^2 i+1,j} \frac{\eta[n]}{2 \Delta \theta'} \right]$$
\[
\left[ \frac{3}{r'^2} \frac{\Delta \theta}{r'^2} \frac{\Delta [n]}{r'^2} - \frac{\Delta \theta}{r'^2} \frac{\Delta [n]}{r'^2} \frac{\Delta [n]}{r'^2} \right]
\]

\[
\left( \frac{\eta_{i+1,j} - \eta_{i-1,j}}{2\Delta r'^2} \right) - \frac{\Delta \theta}{r'^2} \left( \frac{\eta_{i,j+1} - 2\eta_{i,j} + \eta_{i,j-1}}{\Delta \theta'^2} \right)
\]

\[
- \frac{2\Delta \eta_{i+1,j+1} - \eta_{i-1,j+1} - \eta_{i+1,j-1} + \eta_{i-1,j-1}}{4\Delta r'^2 \Delta \theta'^2}
\]

\[ (148) \]

5.5 Results

The FORTRAN IV program which solves equations 26 and 105 using the inner-outer iteration technique is given in Appendix B. The flow chart used to write this program for the non-Newtonian problem is given in Figure 22. Any additional variable not explained in Table 4-6 are given in Table 5-8.

The average velocity, characteristic radius, over-relaxation parameters, smoothing factors, and grid sizes are the same as those given in Section 4.5. The density used for the non-Newtonian problem is

\[ \rho = 0.86 \text{ g/cm}^3 \]

Figure 23 gives the stream function contour lines for a non-Newtonian fluid. Close scrutiny of Figure 23 and Figure 20 reveals that the plot of stream lines remains the same for the flow of a Newtonian fluid as compared to the flow of a power law fluid in this domain. A reason for this can be seen when equation 26 is examined. The stream function, \( \psi \), is only affected by changes in viscosity through the vorticity term. Hence if the vorticity term is not the dominant term, the stream function
Figure 22: Flow Chart for the Non-Newtonian Problem
Table 5-8: Additional Text and FORTRAN Program Variables

<table>
<thead>
<tr>
<th>Text Variable</th>
<th>FORTRAN Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \phi )</td>
<td>RHO</td>
</tr>
<tr>
<td>( \overline{V} )</td>
<td>VEL</td>
</tr>
<tr>
<td>R</td>
<td>RR</td>
</tr>
<tr>
<td>m</td>
<td>AN</td>
</tr>
<tr>
<td>n</td>
<td>AM</td>
</tr>
<tr>
<td>n</td>
<td>ANU</td>
</tr>
<tr>
<td>( \Delta'_{rr} )</td>
<td>TAURR</td>
</tr>
<tr>
<td>( \Delta'_{\theta\theta} )</td>
<td>TAUTT</td>
</tr>
<tr>
<td>( \Delta'_{r\theta} )</td>
<td>TAURT</td>
</tr>
<tr>
<td>( C_1 )</td>
<td>C1</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>C2</td>
</tr>
<tr>
<td>( C_3 )</td>
<td>C3</td>
</tr>
<tr>
<td>( C_4 )</td>
<td>C4</td>
</tr>
<tr>
<td>( C_5 )</td>
<td>C5</td>
</tr>
<tr>
<td>DTOT</td>
<td>TOTAL</td>
</tr>
</tbody>
</table>
Figure 23: Stream Function Contour Lines for a Non-Newtonian Fluid in the Flow Domain
will be relatively unaffected by changes in viscosity. This means that the stream function equation (equation 26) and the vorticity equation (equation 27 or 105) are weakly coupled in this investigation.

Figure 24 is a plot of the contours of constant velocity in the r-direction. Since \( v'_r \) depends only on \( \psi \) as given in equation 22 and the stream lines remain the same whether a Newtonian or power law fluid is flowing in this domain, then the constant \( v'_r \) contours will not vary. Such is the case if Figure 21 and 24 are compared.

The stresses, however, are influenced by changes in viscosity. Figure 25 shows the constant shear stress lines. All stresses indicated on Figure 25 have been multiplied by \( 1 \times 10^{-8} \). Hence the order of magnitude of the shear stresses is the same for both the Newtonian and power law case. Figure 26 compares the location and shape of several constant shear stress lines of the Newtonian fluid (the solid lines) with those of the non-Newtonian fluid (the dashed lines).

Figure 27 is a plot of the constant normal stress difference lines for the power law fluid. All values shown on Figure 27 have been multiplied by \( 1 \times 10^{-9} \). Again it can be seen that a viscosity which depends on \( \Delta_{rr} \) and \( \Delta_{\theta\theta} \) changes the shape and location of the various normal stress difference lines from those shown in Figure 21. Figure 28 compares the location and shape of several constant shear stress lines of the Newtonian fluid (the solid lines) with those of the non-Newtonian fluid (the dashed lines).
Figure 24: Constant $v'_r$ Contours for a Non-Newtonian Fluid in the Flow Domain
Figure 25: Constant $\tau'_r$ Contours for a Non-Newtonian Fluid in the Flow Domain
Figure 26: Comparison of the Location and Shape of Constant $\tau'_{r\theta}$ Contour Lines from Figure 20 and 25.
Figure 27: Constant $\tau_{rr} - \tau_{\theta\theta}$ Contours for a Non-Newtonian Fluid in the Flow Domain
Figure 28: Comparison of the Location and Shape of the Constant $\tau'_{rr} - \tau'_{\theta\theta}$ Contour Lines from Figure 21 and 27.
CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

The purpose of this study was to investigate the flow of a Newtonian and a non-Newtonian fluid in a two-dimensional contraction. This was done by numerically modeling the equations governing the flow. The power-law model was used as the constitutive equation for the non-Newtonian fluid. The problem was formulated in terms of the vorticity and stream function because of the two dimensionality of the problem. In addition, the flow was assumed to be steady thus eliminating, for the most part, any time dependent numerical instabilities which might arise. Contour plots of the different flow variables such as stream function, velocity, and stresses were made. With these contour plots consistent pictures of the Newtonian flow and non-Newtonian were formed and compared.

Upon completion of this investigation, the following recommendations are made about future areas of study.

1. As Figure 18 and 23 showed, circulatory flow appears to be forming toward the exit of the shaping section. In the future mathematical modeling of the uniaxial die should include not only the shaping section but also the early portions of the land section in the flow domain. Extension of the flow domain would determine the seriousness of the circulation at the exit of the shaping section.
2. A constitutive model which includes the elastic as well as viscous effects of a polymer melt should be tried in a future mathematical modeling study. Whatever constitutive equation is chosen should be tested to ensure that it does represent the viscoelastic polymeric melt under the operating conditions being studied. This can be shown by placing the constitutive model into the equation of motion for a simple laminar shearing flow situation. If the proper constitutive equation has been chosen, the results of this operation should compare well with the rheogoniometer data obtained for this particular polymer melt at the operating conditions being studied. Thus using rheogonimeter data, the parameters of the constitutive equation at different operating conditions may be found.

3. A current study being carried out by a student at the Ohio University Polymer Research Laboratory involves the experimental determination, via the technique of stress-birefringence, of shear stresses and the first normal stress difference in the shaping section of the die studied in this investigation. A comparison between the experimental data and theoretical data on the flow patterns should be made until a proper constitutive equation is found.

4. Once a proper constitutive equation is established, the model developed in this investigation should be modified to employ this constitutive equation in the non-Newtonian solution. The model should then be used to study flow patterns of the polymeric melt through contracting shaping sections which have
walls with geometries different from the die explored by this investigation. Hopefully, this mathematical model could be used to eliminate unreasonable designs thus avoiding the costly exercise of building and testing every die proposed. In addition, this model should allow the researcher to study the effects of changing various dimensions of the die, ie. the shaping section length or thickness, on the flow patterns of the polymeric melt. Hence this model should be used as an aid in designing the die which provides the least resistance to flow in the shaping section, the critical portion of the Fixed Boundary Extrusion-Orientation-Crystallization process.

5. Furthermore, in this investigation the z-direction is assumed to be a neutral direction. Actually, the z-direction may be contributing to any secondary flow along the walls of the shaping section. A future study should eliminate this assumption from the model.

6. Finally, further work is needed to properly define the boundary conditions at θ=0°. Those used in this investigation result in a discontinuity in the velocity contours.
REFERENCES


NOMENCLATURE

Superscript \((k)\) = \(K^{\text{th}}\) inner iteration

Superscript \(\left[n\right]\) = \(N^{\text{th}}\) outer iteration

\(A\) = Constant in equation (31)

\(A_1, A_2, A_3 \ldots A_9\) = Constants in equation (51) through (55) and (65) through (73)

\(B\) = Constant in equation (106)

\(B_1, B_2, B_3\) = Variables in equations (131) through (135)

\(C_1, C_2, C_3, C_4, C_5\) = Variables in equations (128) through (130)

\(D\) = Constant in equation (31)

\(D_{\text{TOT}}\) = Variable of equation (101) and (105)

\(e_\psi, e_\zeta\) = Errors of convergence

\(\Delta F\) = Change in free energy

\(g_r, g_\theta, g_z\) = Gravitational acceleration components in the cylindrical coordinate system

\(g_x, g_y, g_z\) = Gravitational acceleration components in the rectangular coordinate system

\(g_r, g_\theta, g_\phi\) = Gravitational acceleration components in the spherical coordinate system

\(\Delta H\) = Change in enthalpy

\(\Delta H_{\text{ext}}\) = Change in enthalpy from an oriented melt to an oriented crystalline state
\( \Delta H_f \) = Change in enthalpy upon fusion

\( \Delta H_{\text{quies}} \) = Change in enthalpy from a quiescent melt to a disordered crystalline state

\( I_1, I_2, I_3 \) = Three invariants defined in equations (83) through (85)

\( K \) = Constant in equation (118)

\( M \) = Power law parameter

\( N \) = Power law parameter

\( N_{\text{Re}} \) = Reynold's number for the Newtonian problem

\( N_{\text{Re}}(\eta) \) = Reynold's number for the non-Newtonian problem

\( P \) = Pressure

\( P' \) = Dimensionless pressure

\( R \) = Characteristic radius

\( r \) = Coordinate direction in the cylindrical and spherical coordinate systems

\( r' \) = Dimensionless coordinate direction

\( R \) = Die dimension in Figure (12)

\( r \) = Die dimension in Figure (12)

\( \Delta r' \) = Dimensionless grid size in the r-direction

\( \Delta S \) = Change in entropy

\( \Delta S_{\text{ext}} \) = Change in entropy from an oriented melt to an oriented crystalline state
\[ \Delta S_f = \text{Change in entropy upon fusion} \]
\[ \Delta S_{\text{quies}} = \text{Change in entropy from a quiescent melt to a disordered crystalline state} \]
\[ S_1 = \text{Entropy of the disordered melt} \]
\[ S_2 = \text{Entropy of the disordered crystalline state} \]
\[ S_3 = \text{Entropy of the ordered melt} \]
\[ S_4 = \text{Entropy of the oriented crystalline state} \]
\[ S = \text{Cross-sectional area} \]
\[ S' = \text{Dimensionless cross-sectional area} \]
\[ S_{\text{max}} = \text{Maximum cross-sectional area} \]
\[ S'_{\text{max}} = \text{Dimensionless maximum cross-sectional area} \]
\[ t = \text{Time} \]
\[ T = \text{Absolute temperature} \]
\[ T_M = \text{Melting point temperature} \]
\[ T_{M_{\text{ext}}} = \text{Effective melting point under elongational flow} \]
\[ T_{M_{\text{quies}}} = \text{Effective melting point of quiescent atmospheric pressure crystallization} \]
\[ \bar{V} = \text{Average velocity} \]
\[ \vec{v} = \text{Velocity vector} \]
\[ v_r, v_\theta, v_z = \text{Three velocity components in the cylindrical coordinate system} \]
\( v'_r, v'_\theta, v'_z \) = Three dimensionless velocity components in the cylindrical coordinate system

\( v'_x, v'_y, v'_z \) = Three velocity components in the rectangular coordinate system

\( v'_r, v'_\theta, v'_\phi \) = Three dimensionless velocity components in the spherical coordinate system

\( W, W_\psi, W_\wedge \) = Over-relaxation parameters

\( x \) = Coordinate direction in the rectangular coordinate system

\( y \) = Coordinate direction in the rectangular coordinate system

\( y'_w \) = Dimensionless coordinate direction

\( y'_w \) = Dimensionless Y-coordinate at the wall of the die

\( z \) = Coordinate direction in the cylindrical and rectangular coordinate system

GREEK SYMBOLS

\( \alpha' \) = Dimensionless normal stress difference

\( \beta_\psi, \beta_\wedge \) = Smoothing factors

\( \delta_{ij} \) = Rate of deformation tensor symbols
\[ \tau_{rr}, \tau_{\theta\theta}, \tau_{r\theta} \]

= Dimensionless components in the cylindrical coordinate system

\[ \tau_{xx}', \tau_{yy}', \tau_{zz}' \]

= Stress components in the rectangular coordinate system

\[ \tau_{xy}', \tau_{xz}', \tau_{yz} \]

= Stress components in the spherical coordinate system

\[ \tau_{rr}', \tau_{\theta\theta}', \tau_{\phi\phi}' \]

= Stress components in the spherical coordinate system

\[ \tau_{r\theta}', \tau_{r\phi}', \tau_{\theta\phi} \]

= Coordinate direction in the cylindrical and spherical coordinate system

\[ \theta \]

= Dimensionless coordinate direction

\[ \Delta \theta' \]

= Dimensionless grid size in the \( \theta \)-direction

**MATHEMATICAL OPERATORS**

\[ \bar{\nabla} \]

= "del" operator

\[ \text{det} \]

= Determinant

\[ \bar{\nabla}^2 \]

= Laplacian operator

\[ \cdot \]

= Dot product

\[ :) \]

= Double dot product

**EXPRESSION SYMBOLS**

\[ \{ \} \]

= Braces

\[ [\ ] \]

= Brackets
APPENDIX A

FORTRAN IV PROGRAM FOR

SOLVING NEWTONIAN FLOW PROBLEM
C*******************************************************************************
C PROGRAM FOR CALCULATING AND PLOTTING THE STREAM
C FUNCTIONS, VELOCITY, AND STRESS DIFFERENCES IN
C THE AXIAL DIE OF THE FIXED BOUNDARY EXTRUSION
C ORIENTATION CRYSTALLIZATION PROCESS AT OHIO
C UNIVERSITY.
C
C THIS PROGRAM IS FOR A NEWTONIAN FLUID.
C*******************************************************************************
C DESCRIPTION
C THE SYSTEM EQUATIONS CONSIST OF TWO ELLIPICAL
C PARTIAL DIFFERENTIAL EQUATIONS. EACH EQUATION
C IS SOLVED BY AN ITERATIVE SCHEME CALLED
C SUCCESSIVE OVER-RELAXATION (SOR) WHICH CONSTITUTES
C THE INNER ITERATION. THE OUTER ITERATION IS THE
C SCHEME TO SOLVE THREE EQUATIONS SIMULTANEOUSLY.
C*******************************************************************************
C DIRECTIONS
C FOR THE DIE WHICH IS MODELED IN THIS PROGRAM SEE
C LINDA NIKROO'S THESIS, CHAPTER 4-PART 1. IF A
C DIFFERENT DIE IS TO BE MODELED, THE BOUNDARY
C CONDITIONS MUST BE MODIFIED. SEE PART 4.3 OF
C THIS SAME THESIS.
C*******************************************************************************
C DEFINITION OF VARIABLES
C SI,S1, S12: DIMENSIONLESS STREAM FUNCTIONS
C ETA, ETA1, ETA2: DIMENSIONLESS VORTICITY
C WS1, WETA: OVER-RELAXATION FACTOR FOR SI AND
C ETA RESPECTIVELY
C XS1, XETA: SMOOTHING FACTOR FOR SI AND ETA
C RESPECTIVELY
C ERPS, ERPO: ACCURACY FOR SI AND ETA
C DELR: INCREMENT IN R-DIRECTION
C DELT: INCREMENT IN THE-ETA-DIRECTION
C I: SUBSCRIPT IN R-DIRECTION
C J: SUBSCRIPT IN THE-ETA-DIRECTION
C REN: REYNOLDS NUMBER
C VR: DIMENSIONLESS VELOCITY IN THE R-DIRECTION
C TDIFF: DIMENSIONLESS NORMAL STRESS DIFFERENCE
C TSH: DIMENSIONLESS SHEAR STRESS
C*******************************************************************************
C----MAIN PROGRAM
C*******************************************************************************
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION SI(61,31), S11(61,31), S12(61,31)
DIMENSION ETA1(61,31), ETA2(61,31)
DIMENSION VR(61,31), SHEAR(61,31), TDIFF(61,31)
READ(5,1) REN
1 FORMAT(E13.4)
C INITIALIZE THE DIMENSION VARIABLES
DO 2 I=1,61
  DO 2 J=1,31
       SI(I,J)=0.0E00
 2 CONTINUE
C SET THE CONSTANTS
READ(5,3) WSL, WETA, XSI, ETA
3 FORMAT(*E10.4)
DELR = 0.7696/60.0
DELT1 = 3.14156/180.0
R = 1.0E00
ERRORS = 1.0E-03
ERROR = 4.0E-02

C***********************************************************************
C SET THE BOUNDARY CONDITIONS OF SI AND ETA
C***********************************************************************
I = 1
DO 4 J = 1, 31
SI(I,J) = -6.0*SI*(0.25*DSIN(DFLOAT(J-1)*3.14156/180.)-R**2)*
> (DSIN(DFLOAT(J-1)*3.14156/180.))**3/3.0)
ETA(I,J) = -12.0*R*(DSIN(DFLOAT(J-1)*3.14156/180.0))
V4(I,J) = 6.0*(R**2)*(DSIN(DFLOAT(J-1)*3.14156/180.0)**2)-0.25)*
> DCOS(DFLOAT(J-1)*3.14156/180.)
TIPF(I,J) = (-2./REN)*(24.0*R*DSIN(DFLOAT(J-1)*3.14156/180.0)**
> 2).*DCOS(DFLOAT(J-1)*3.14156/180.)
SHEAR(I,J) = -(1./REN)*(-24.0*R*DSIN(DFLOAT(J-1)*3.14156/180.0)**
> 3)*2.*R*DSIN(DFLOAT(J-1)*3.14156/180.)

4 CONTINUE
J = 31
DO 5 I = 1, 61
SI(I,J) = -6.0*SI*(0.25*DSIN(DFLOAT(J-1)*3.14156/180.)-R**2)*
> (DSIN(DFLOAT(J-1)*3.14156/180.))**3/3.0)

5 CONTINUE

C***********************************************************************
C SOLVE THE SYSTEM OF EQUATIONS (OUTER ITERATION)
C***********************************************************************
DO 25 NI = 1, 40
C***********************************************************************
C SOLVE SI(I,J) BY SCR (INNER ITERATION)
C***********************************************************************
DO 6 NSI = 1, 300
NSIAX = NSI
WRITE(6,6) NSI
6 FORMAT(*,NSIAX=13)
DO 7 J = 2, 60
R = 1.0*DFLOAT(I-1)*DELR
DO 7 J = 2, 60
AK1 = 1./2./DELR**2+2./((R*B**2*DELT1**2))**1./((R*B))
AK2 = AK1*(1./((R*B**2*DELT1**2))
AK3 = AK1*(1./((R*B))
AK4 = AK1*(1./((R*B))
SI(I,J) = SI(I,J)
SI(I,J) = AK1*ETA(I,J)+AK2*SI(I,J-1)+AK3*SI(I-1,J)+AK4*SI(I,J+1)
> AK4*SI(I+1,J)
7 SI(I,J) = SI(I,J)+WSI*SI(I,J-SI(I,J))
CALL CONV(I,SI,SI1,ERRORS,ERRNEW)
IF (ERREME EQ 1.0E33) GO TO 37
IF (111,0.0) GO TO 9
3 CONTINUE
GO TO 37
9 DO 10 I=2,50
DO 10 J=2,30
10 SI(I,J) = XS*I*SI2(I,J)*(1-XSI)*SI(I,J)
C
WRITE(6,11) NSEA
11 FORMAT('SI(I,J) AFTER ',I4,' ITERATIONS',//)
DO 12 I=1,61,10
12 WRITE(6,13) (SI(I,J),J=1,31)
13 FORMAT(110E12.4,/,)
CALL CCNV(I!,Sfr,ERRORS,ERREME)
IS1 = 11
DO 14 I=2,60
DO 14 J=2,30
14 SI2(I,J) = SI(I,J)
C
SOLVE ETA BY SCR (INNER ITERATION)
C
DO 15 I=2,60
R = 1.-DFLOAT(I-1)*DELR
ETA(I,31) = 2.*(SI(I,31)-SI(I,30))/(R*DELM*2)
ETA(I,31) = XETA*ETA2(I,31)+(1.-XETA)*ETA(I,31)
15 ETA2(I,31) = ETA(I,31)
DO 22 NET=1,200
NETA = NETA
WRITE(6,16) NETA
16 FORMAT(' NETA = ',I4)
DO 21 I=2,30
R = 1.-DFLOAT(I-1)*DELR
DO 21 J=2,30
111 = I
JJJ = J
DELTA = 2.0*DELM*REN*(SI(I,J+1)-SI(I,J-1))
GAMMA = SI(I+1,J)-SI(I-1,J)
AKP = A./12./(DELM*2*REN)+2.0/(R*DELM*2*REN)+DABS(DELTA)/
    (2.*R*DELM*REN)+DABS(GAMMA)/(2.*R*DELM*REN)
AKS = AKP*(1./(R*DELM*2*REN)+DABS(DELTA)/(2.*R*DELM*REN)+DABS(GAMMA)/(2.*R*DELM*REN))
AKG = AKP*(1./(R*DELM*2*REN)+DABS(GAMMA)/(2.*R*DELM*REN))
AKS = AKG*(1./(R*DELM*2*REN))
ETA(I,J) = ETA(I,J)
    IF (DELTA.GE.0.0E00 AND GAMMA.GE.0.0E00) GO TO 17
    IF (DELTA.LE.0.0E00 AND GAMMA.LE.0.0E00) GO TO 19
    IF (DELTA.LE.0.0E00 AND GAMMA.GE.0.0E00) GO TO 19
    IF (DELTA.GE.0.0E00 AND GAMMA.LE.0.0E00) GO TO 20
17 ETA(I,J) = AK7*ETA(I,J-1)+AKS*ETA(I,J-1)+AKS*ETA(I>+1,J)
    GO TO 21
18 ETA(I,J) = AK6*ETA(I,J-1)+AKS*ETA(I,J-1)+AKS*ETA(I>+1,J)
    GO TO 21
19 ETA(I,J) = AK7*ETA(I,J-1)+AKS*ETA(I,J-1)+AK6*ETA(I,J+1)+AKS*ETA(I>+1,J)
    GO TO 21
GO TO 21  
20 ETA(I,J) = AK6*ETA(I,J-1)+AK5*ETA(I-1,J)+AK7*ETA(I,J+1)+AK8*ETA(I,J)  
21 ETA(I,J) = ETA(I,J)+ETA*(ETA(I,J)-ETA(I,J))  
   CALL CONV(1,ETA,ETA1,ERROR,ERRNEW)
   IF(ENERNEW.GT.1.0E03) GO TO 37
   IF(ETA.EQ.0.1) GO TO 23
22 CONTINUE
   GO TO 37
23 DO 24 I=2,60
   DO 24 J=2,30
24 ETA(I,J) = XETA*ZETA2(I,J)+(-XETA)*ETA(I,J)
   CALL CONV(L2,ETA,ETA,ERROR,ERRNEW)
   IF(E21.EQ.1.GT.1.0E0)
   CONTINUE
25 DO 26 I=1,60
   DO 26 J=1,30
26 ETA(I,J) = ETA(1,J)
27 DO 26 I=1,30
   ETA = ETA
   DO 26 J=1,30
28 ETA2(I,J) = ETA(I,J)
   IF(IS1.EQ.1.AND.ETA.EQ.1) GO TO 29
29 CONTINUE
30 DO 31 I=2,60
   R = 1.0-OFLOAT(I-1)*DELTH
   DO 31 J=2,30
31 VR(I,J) = (SI(I,J+1)-SI(I,J-1))/(2.*R*DELTH)
   C1 = (SI(I,J+1)-SI(I,J-1))/(2.*R*DELTH)
   C2 = (SI(I+1,J+1)-SI(I+1,J-1)-SI(I-1,J+1)+SI(I-1,J-1))/(4.*R*DELTH)
   C3 = (SI(I+1,J)-SI(I-1,J))/(2.*R*DELTH)
   C4 = (SI(I+1,J)-2.*SI(I,J)+SI(I-1,J))/DELTH**2
   C5 = (SI(I+1,J)-2.*SI(I,J)+SI(I-1,J))/DELTH**2
   TOFF(I,J) = (-2.*REN)*(-2.*C1+C2+C2)
   SHERE(I,J) = -(1./REN)*(C3-C4+C5)
31 CONTINUE
C***********************************************************************
C WRITE THE SI VALUES
C***********************************************************************
   WRITE(6,32)
32 FORMAT(///,30X,'SI VALUES',///)
   CALL WRITE(SI)
C***********************************************************************
C WRITE THE ETA VALUES
C***********************************************************************
   WRITE(6,33)
33 FORMAT(///,30X,'ETA VALUES',///)
   CALL WRITE(ETA)
C***********************************************************************
C WRITE THE VR VALUES
C***********************************************************************
   WRITE(6,34)
34 FORMAT(///,30X,'VR VALUES',///)
   CALL WRITE(VR)
C***********************************************************************
C WRITE THE SHEAR VALUES
C***********************************************************************
C***************************
WRITE(6,35)
35 FORMAT(///,30X,'SHEAR VALUES',///)
CALL WRITE(SHEAR)

C***************************
WRITE THE TDIFF VALUES
C***************************
WRITE(6,36)
36 FORMAT(///,30X,'TDIFF VALUES',///)
CALL WRITE(TDIFF)
CALL PUNCH(3,S1)
CALL PUNCH(7,VR)
CALL PUNCH(8,SHEAR)
CALL PUNCH(9,TDIFF)
37 STOP
END
The listing for the subroutine PUNCH is given in Appendix C
APPENDIX B

FORTRAN IV PROGRAM FOR
SOLVING NON-NEWTONIAN FLOW PROBLEM
PROGRAM FOR CALCULATING AND PLOTTING THE STREAM
FUNCTIONS, VELOCITY, AND STRESS DIFFERENCES IN
THE UNIAXIAL DIE OF THE FIXED BOUNDARY EXTRUSION
ORIENTATION CRYSTALLIZATION PROCESS AT OHIO
UNIVERSITY.

THIS PROGRAM IS FOR A POWER LAW FLUID.

DESCRIPTION
THE SYSTEM EQUATIONS CONSIST OF TWO ELLIPTICAL
PARTIAL DIFFERENTIAL EQUATIONS. EACH EQUATION
IS SOLVED BY AN ITERATIVE SCHEME CALLED
SUCCESSIVE OVER-RELAXATION (SOR) WHICH CONSTITUTES
THE INNER ITERATION. THE OUTER ITERATION IS THE
SCHEME TO SOLVE THREE EQUATIONS SIMULTANEOUSLY.

DIRECTIONS
FOR THE DIE WHICH IS MODELED IN THIS PROGRAM SEE
LINDA ANKROM'S THESIS, CHAPTER 4-PART I. IF A
DIFFERENT DIE IS TO BE MODELED, THE CONSTANTS IN THE
BOUNDARY CONDITIONS MUST BE CHANGED. SEE THE SAME
THESIS, PART 5.2. IN ADDITION,
IF THE POWER LAW EXPONENT IS NOT 1/3, THE EXPONENTS
IN THE BOUNDARY CONDITIONS WILL CHANGE. SEE CHAPTER
5 OF THE SAME THESIS FOR DETAILS.

DEFINITIONS OF VARIABLES
SI, SII, SII: DIMENSIONLESS STREAM FUNCTIONS
ETA, ETA1, ETA2: DIMENSIONLESS VORTICITY
WSI, WETA: OVER-RELAXATION FACTOR SI AND
ETA RESPECTIVELY
XS1, XETA: SMOOTHING FACTOR FOR SI AND ETA
ERRORS, ERRONE: ACCURACY FOR SI AND ETA
DELR: INCREMENT IN THE R-DIRECTION
DELT: INCREMENT IN THE THETA-DIRECTION
II: SUBSCRIPT IN THE R-DIRECTION
J: SUBSCRIPT IN THE THETA-DIRECTION
RH0: DENSITY
VEL: AVERAGE VELOCITY AT ENTRANCE TO SHAPING SECTION
RR: RADIUS FROM VERTEX TO ENTRANCE OF SHAPING SECTION
ALONG THE WALL OF THE SHAPING SECTION
X%: POWER LAW EXPOSURE
AM: POWER LAW CONSTANT
VR: DIMENSIONLESS VELOCITY IN THE R-DIRECTION
TOIFF: DIMENSIONLESS NORMAL STRESS DIFFERENCE
SHEAR: DIMENSIONLESS SHEAR STRESS
ANU: NON-NEWTONIAN VISCOSITY. THIS IS A SCALAR
WHICH IS A FUNCTION OF THE 'RATE OF DEFORMATION
TENSOR.'
IMPLICIT REAL*8(A-H,O-Z)
COMMON SI(51,31),SI1(61,31),SI2(61,31)
COMMON ETA(51,31),ETA1(61,31),ETA2(61,31)
COMMON ANU(61,31),TAUUR(61,31)
COMMON TAUT(61,31),TAUUR(61,31)
COMMON TOIFF(61,31),VRI(61,31),SHEAR(61,31)
COMMON RHO,VEL,R,AN,AM,DELT,H,DEL.R
READ(5,1) RHO,VEL,RR,AN,AM
1 FORMAT(5E10.4)
C INITIALIZE THE DIMENSION VARIABLES
DO 2 I=1,51
   DO 2 J=1,31
      ANU(I,J) = 0.0E00
      TAUR(I,J) = 0.0E00
      TAUT(I,J) = 0.0E00
      TOIFF(I,J) = 0.0E00
      VRI(I,J) = 0.0E00
      SHEAR(I,J) = 0.0E00
      SI(I,J) = 0.0E00
      SI1(I,J) = 0.0E00
      SI2(I,J) = 0.0E00
      ETA(I,J) = 0.0E00
      ETA1(I,J) = 0.0E00
      ETA2(I,J) = 0.0E00
   2 CONTINUE
C SET THE CONSTANTS
READ(5,3) WS1,ETA,XSI,XETB
C**-----------------------------------------------
3 FORMAT(4E14.4)
   DELR = 0.7696/60.0
   DELTH = 3.14156/180.
   R = 1.0E00
   ERRORS = 1.E-03
   ERRONE = 4.E-02
C******************************************************************************
C SET THE BOUNDARY CONDITIONS OF SI AND ETA
C******************************************************************************
I = 1
DO 4 J=1,31
   SI(I,J) = -20.0*R*(0.0625*DSIN(DFLOAT(J-1)+3.14156/180.0)-R**4*
      (DSIN(DFLOAT(J-1)+3.14156/180.0)**5/5.0))**3
   ETA(I,J) = -80.0*R**3*(DSIN(DFLOAT(J-1)+3.14156/180.0)**3
4 CONTINUE
DO 5 J=2,31
   FFOTT = 80.0*R**3*DSIN(DFLOAT(J-1)+3.14156/180.0)**3
   ANU(I,J) = AM*(((VEL/R)*DA5S(FFOTT))**((AN-1.))
5 CONTINUE
DO 6 J=1,31
   TAUUR(I,J) = 160.0*R**3*DSIN(DFLOAT(J-1)+3.14156/180.0)**3
      (DCOS(DFLOAT(J-1)+3.14156/180.0))**3
   TAUUR(I,J) = -TAUR(I,J)
   TAUU1(I,J) = (-160.0*R**3*DSIN(DFLOAT(J-1)+3.14156/180.0)**3
      (DCOS(DFLOAT(J-1)+3.14156/180.0))**3
   VRI(I,J) = 20.0*DSIN(DFLOAT(J-1)+3.14156/180.0)**3
      (DCOS(DFLOAT(J-1)+3.14156/180.0))**3
   TOIFF(I,J) = (2.*ANU(I,J)/(VEL*RHO*RR))*TAUR(I,J)
   SHEAR(I,J) = (2.*ANU(I,J)/(VEL*RHO*RR))*TAUR(I,J)
6 CONTINUE
J = 31
DO 7 I=1,61
\[
S_i(i,j) = (-20.0 \cdot R \cdot (0.0625 \cdot S\sin(D\text{FLOAT}(J-1) \cdot 3.14156/180.) - R^2) \\
(D\sin(D\text{FLOAT}(J-1) \cdot 3.14156/180.)) \cdot 5/5.0)
\]

C SOLVE THE SYSTEM OF EQUATIONS (OUTER ITERATION)

C*******************************
DO 31 N=1,40
C**** SOLVE S1(l,J) BY SOR (INNER ITERATION)
DO 10 NSI=1,200
NSIA = NSI
WRITE(6,0) NSI
9 FORMAT('NSI = ',I3)
DO 9 I=2,60
R = 1.0-DFLOAT(I-1)*DELR
DO 9 J=2,30
AK1 = 1.0/(2.0/DELR)**2+2./((R**2+DELTH)**2+1./R**DELR)
AK2 = AK1*(1.0/DELT)**2
AK3 = AK1*(1.0/DELR)**2
AK4 = AK1*(1.0/DELR)**2
SI(i,j) = SI(i,j)
SI(i,j) = AK1*TAU(i,j)+AK2*SI(i-1,j)+AK3*SI(i-1,j+1)+AK4*S1(i,j+1)
> AK4*SI(i,j+1)
9 SI(i,j) = SI1(i,j)+SI11*(SI(i,j)-SI(i,j))
CALL CONV(1,SI,SI1,ERRORS,ERRORNEW)
IF(IDERROR.GT.1.E03) GO TO 30
IF(IDERROR.EQ.1) GC TO 30
10 CONTINUE
GO TO 30
11 DO 12 I=2,60
DO 12 J=2,30
12 SI(i,j) = XI*SI*S12(i,j)+(1.-XI)*SI(i,j)
C
C WRITE(6,13) NSIA
13 FORMAT('SI(i,j) AFTER 1.14.*ITERATIONS*//')
DO 14 I=1,61,10
14 WRITE(6,15) SI(i,j),J=1,31
15 FORMAT(4(10E12.4,//))
C
C CALL CONV(1,SI,SI2,ERRORS,ERRORNEW)
SI = 11
DO 16 I=2,60
DO 16 J=2,30
16 SI2(i,j) = SI(i,j)
C*******************************
C**** SOLVE ETA BY SOR (INNER ITERATION)
C*******************************
DO 17 I=2,60
R = 1.0-DFLOAT(I-1)*DELR
ETA(i,31) = 2.*(SI(i,31)-SI(i,30))/(R*DELT)**2
ETA(i,31) = ETA(i,31)
TAUR(i,31) = -ETA(i,31)
ANU(i,31) = ANU(((VEL/R)*DABS(-ETA(i,31)))*((AN-1.1))
TAURR(i,1) = 2.*(SI(i,1)-SI(i,2))/DELT*(SI(i,1)-SI(i,2)-SI(i+1)+1.1))
> SI(i+1,1)+SI1(i+1,1))/(DELT**DELR))
TAUT(i,1) = -TAURR(i,1)
ANU(i,1) = ANU(((VEL/R)*DABS(-TAURR(i,1)))*((AN-1.1))
ETA(i,31) = XETA*ETA2(i,31)+(1.-XETA)*ETA(i,31)
17 CONTINUE
17 ETA2(I,J) = ETA(I,J)  
DO 24 NETA=1,200  
NETAS = NETA  
WRITE(6,13) NETA  
13 FORMAT(* NETA = *,14)  
DO 23 I=2,60  
3 = 1.0-DFLOAT(I-1)+DERL  
DO 23 J=2,30  
11 I = J  
JJJ = J  
CALL POWER(TOTAL)  
12 DERL = 2.0#DELT#-REN#(5(I,J+1)-5(I,J-1))  
GAMMA = S(I+1,J)-S(I-1,J)  
AK9 = 1./2./(DERL**2*REN)+2.0/(R**2*DELT**2*REN)+DA35(FELTA)/  
> (2.0*R#REN#DEL#DEL#)+DABS(GAMMA)/(2.*R#DEL#DEL#)  
AK5 = AK9*(1./(DEL**2#REN)+DABS(DELTA)/(2.*REN#DEL#DEL#))  
AK6 = AK9*(1./(R**2#DEL**2#REN)+DABS(GAMMA)/(2.*R#DEL#DEL#))  
AK7 = AK9*(1./(R**2#DELT**2#REN))  
AK8 = AK9*(1.0/(DEL**2#REN))  
ETA(I,J) = ETA(I,J)  
18 IF(DERL.GE.0.00000000000001) Go to 19  
IF(DERL.GE.0.00000000000001) Go to 20  
IF(DERL.GE.0.00000000000001) Go to 21  
IF(DERL.GE.0.00000000000001) Go to 22  
19 ETA(I,J) = AK7*ETA(I,J-1)+AK8*ETA(I-1,J)+AK6*ETA(I+1,J)+AK5*ETA(I-1,J)+AK9*TOTAL  
Go to 23  
20 ETA(I,J) = AK6*ETA(I,J-1)+AK8*ETA(I-1,J)+AK7*ETA(I+1,J)+AK9*TOTAL  
Go to 23  
21 ETA(I,J) = AK7*ETA(I,J-1)+AK8*ETA(I-1,J)+AK6*ETA(I+1,J)+AK9*TOTAL  
Go to 23  
22 ETA(I,J) = AK6*ETA(I,J-1)+AK8*ETA(I-1,J)+AK7*ETA(I+1,J)+AK9*TOTAL  
Go to 23  
23 ETA(I,J) = ETA(I,J+1)+META*ETA(I,J-1)+ETA(I,J+1)+AK9*TOTAL  
CALL CONV(I,J,ETA,ETA1,ERRORF,ERRORW)  
IF(ERRORW.GT.1.0E03) Go to 38  
IF(I.EQ.1) Go to 25  
24 CONTINUE  
Go to 38  
25 DO 26 I=2,60  
26 DO 26 J=2,30  
26 ETA(I,J) = X*ETA+ETA2(I,J)+1.0-X*ETA)*ETA(I,J)  
C  
C  
C  
WRITE(6,27) NETA  
27 FORMAT(* ETA(I,J) AFTER *,14,ITERATIONS*,/)  
DO 29 I=1,61,10  
29 FORMAT(14(I2.4,/,))  
CALL CONV(I,J,ETA,ETA2,ERRORF,ERRORW)  
IETA = I  
DO 30 I=2,60  
30 DO 30 J=2,30  
30 ETA2(I,J) = ETA(I,J)  
IF(ISTEMP.EQ.1 AND IETA.EQ.1) Go to 32  
31 CONTINUE  
C**********************************************************************
C      WRITE THE SI VALUES
C*****************************************************************************
  32 WRITE(6,33)
      FORMAT(///,5D10,'SI VALUES',///)
      CALL WRITE(SI)
C      WRITE THE ETA VALUES
C*****************************************************************************
  34 WRITE(6,34)
      FORMAT(///,5D10,'ETA VALUES',///)
      CALL WRITE(ETA)
C      WRITE THE VR VALUES
C*****************************************************************************
  35 WRITE(6,35)
      FORMAT(///,5D10,'VR VALUES',///)
      CALL WRITE(VR)
C      WRITE THE SHEAR VALUES
C*****************************************************************************
  36 WRITE(6,36)
      FORMAT(///,5D10,'SHEAR VALUES',///)
      CALL WRITE(SHEAR)
C      WRITE THE TDIFF VALUES
C*****************************************************************************
  37 WRITE(6,37)
      FORMAT(///,5D10,'TDIFF VALUES',///)
      CALL WRITE(TDIFF)
      CALL PUNCH(3,SI)
      CALL PUNCH(7,VR)
      CALL PUNCH(8,ETA)
      CALL PUNCH(9,TDIFF)
  38 STOP
END
SUBROUTINES

SUBROUTINE POWER(TOTAL,REN,[P,JP,[I,J])
C***************************************************************************
C SUBROUTINE FOR FINDING EXTRA POWER LAW TERMS
C AND VR.TDIFF.I AND SHEAR
C***************************************************************************
IMPLICIT REAL*8(A-H,O-Z)
COMMON SI(61,31),SI(61,31),SIL(61,31)
COMMON ETA(61,31),ETA(61,31),ETA(61,31)
COMMON ANU(61,31),TAURR(61,31)
COMMON TAU potrà(61,31),TAURR(61,31)
COMMON TDIFF(61,31),VR(61,31),SHEAR(61,31)
COMMON RHO,VEL,RR,AN,AM,DELTH,DELR,R
Jordan = JP
JPP = JP
C1 = (SI(1*I+1,J)+SI(1*I,J-1))/2.**62*6DELTH
C2 = (SI(1*I+1,2+1+1,J)+SI(1*I,J-1)+SI(1*I,J-1))/4.**6R*DELR
C3 = (SI(1*I+1,2+1+1,J)+SI(1*I,J-1)+SI(1*I,J-1))/6DELTH**2**2
ANU(I,J) = AM**((VEL/RR)*DABS((4.**((C2-C1))**2)+(C3-C4+C5)**2)**
0.5)***(AN-I,J)
REN = (RHO*VEL*RR)/ANU(I,J)
TAUQR(I,J) = -2.*C1+2.*C2
TAUTR(I,J) = -TAURR(I,J)
TAURR(I,J) = C3-C4+C5
VR(I,J) = (SI(1*I+1,J)-SI(1*I,J-1))/2.**6R*DELR
TDIFF(I,J) = -(2./REN)*TAURR(I,J)
SHEAR(I,J) = -(1./REN)*TAURR(I,J)
T1 = ((ANU(I,J+1)-ANU(I,J-1))*TAURR(I,J)-TAURR(I,J-1))/2.*
6DELTH**2
T2 = TAUQR(I,J)*ANU(I,J+1)-2.*ANU(I,J)+ANU(I,J-1))/6DELTH**2
T3 = ((ANU(I,J)-ANU(I,J-1))/2.*TAURR(I,J)-TAURR(I,J-1))/2.*
6DELTH**2
T4 = (TAURR(I,J)*ANU(I,J)-2.*ANU(I,J)-ANU(I,J))/(2.*DELTH)
T5 = ((TAURR(I,J)-TAURR(I,J))*ANU(I,J-1))/2.*DELTH
T6 = (TAURR(I,J)*ANU(I,J+1)-ANU(I,J-1))/2.*DELTH
T7 = (ANU(I,J)-ANU(I,J-1))*(TAURR(I,J+1)-TAURR(I,J-1))/4.*
6DELTH
T8 = (ANU(I,J+1)-ANU(I,J-1))*(TAURR(I,J+1)-TAURR(I,J-1))/4.*
6DELTH
T9 = (TAURR(I,J)*ANU(I,J+1)-ANU(I,J-1)-ANU(I,J+1))/4.*
6DELTH
T10 = ((ANU(I,J)-ANU(I,J-1))*TAURR(I,J+1)-TAURR(I,J))/4.*
6DELTH
T11 = ((ANU(I,J+1)-ANU(I,J-1))*TAURR(I,J+1)-TAURR(I,J))/4.*
6DELTH
T12 = (TAURR(I,J)*ANU(I,J+1)-ANU(I,J-1)-ANU(I,J+1))/4.*
6DELTH
T13 = (((RHO*VEL*RR)**(1.1/R)**2*(T1+T2)*T3*T4*(1.1/R)**2)*T5*
(1.1/R)**2*(T7+T9))*(1.1/R)*(T10+T11+T12))
RETURN
END
The listing for the subroutine PUNCH is given in Appendix C.
APPENDIX C

DIRECTIONS FOR PLOTTING THE RESULTS USING

THE OHIO UNIVERSITY DEPARTMENT OF

CHEMICAL ENGINEERING'S

CHEMSTR MACHINE
The 2-Dimensional Plotting Program (TWOD) used to plot the constant contour lines of the variables studied in this investigation actually consists of three (3) main programs and six (6) subroutines. The names of the main programs with their respective filetype and filemode are

1. GRID FORTRAN C
2. MAP1 FORTRAN C
3. PLOT1 FORTRAN C

The information for the subroutines appears below.

1. CONT1 FORTRAN C
2. FIND1 FORTRAN C
3. LABL1 FORTRAN C
4. OUT1 FORTRAN C
5. SWIFT1 FORTRAN C
6. SWITCH1 FORTRAN C

These programs and subroutines are currently stored on the Chemical Engineering tape, No. CC5481. The tape is loaded with CMS tape dump format. These programs were originally located on the CHEMSTR machine.

The graphics output file is generated on Tektronix/ADM3A graphic terminals or the Anderson-Jacobson type AJ832 terminals depending on which graphics library is called during the execution of TWOD. The method for calling the graphics library will be detailed later.

A data file for each of the three main programs (GRID, MAP1, and PLOT 1) must be set up. This appendix describes how this is to be accomplished. It is assumed the reader will be creating his data files via a terminal rather than via cards.

The PLOT1 data file remained the same for the plotting of the four variables from the Newtonian program (Appendix A) and the four variables
from the non-Newtonian program (Appendix B). To create this data file, type

```
FEDIT PLOT1 DATA
```

The computer will respond with

- NEW FILE

To gain access to the mode where the data may be entered, type

```
INPUT
```

When the ready signal (●) is received, begin entering data in the following manner:

<table>
<thead>
<tr>
<th>Line</th>
<th>Column</th>
<th>Data Entry</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-10</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>0.12</td>
<td>For plotting in cylindrical coordinates, these cards should appear as shown.</td>
</tr>
<tr>
<td>2</td>
<td>Blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1-10</td>
<td>-1.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>1.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>12-30</td>
<td>-1.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>1.</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1-10</td>
<td>0.7</td>
<td>This indicates a Tektronix terminal is to be used to plot the output. If the Anderson-Jacobson terminal is to be used, this data entry should be 0.95</td>
</tr>
</tbody>
</table>

Hit the RETURN key twice. Now type FILE.

At this point the reader has a choice as to the manner by which he proceeds.
1. He may decide to continue his exploration of the two-dimensional plotting program using the eight data files (four resulting from the Newtonian program and four resulting from the non-Newtonian program) for the GRID program already created by this investigation.

2. He may create his own data files for the GRID program by running the Newtonian and non-Newtonian programs of Appendix A and B respectively.

If the first option is pursued it becomes necessary to know the FILE NAME, FILE TYPE, and FILE MODE of each of the files. This information is given below with the variable to which each file corresponds.

### Newtonian Program

<table>
<thead>
<tr>
<th>File Name</th>
<th>File Type</th>
<th>File Mode</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>2C1A</td>
<td>DATA</td>
<td>E</td>
<td>SI</td>
</tr>
<tr>
<td>2C2A</td>
<td>DATA</td>
<td>E</td>
<td>VR</td>
</tr>
<tr>
<td>2C3A</td>
<td>DATA</td>
<td>E</td>
<td>SHEAR</td>
</tr>
<tr>
<td>2C4A</td>
<td>DATA</td>
<td>E</td>
<td>TDIFF</td>
</tr>
</tbody>
</table>

### Non-Newtonian Program

<table>
<thead>
<tr>
<th>File Name</th>
<th>File Type</th>
<th>File Mode</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>4A1A</td>
<td>DATA</td>
<td>E</td>
<td>SI</td>
</tr>
<tr>
<td>4A2A</td>
<td>DATA</td>
<td>E</td>
<td>VR</td>
</tr>
<tr>
<td>4A3A</td>
<td>DATA</td>
<td>E</td>
<td>SHEAR</td>
</tr>
<tr>
<td>4A4A</td>
<td>DATA</td>
<td>E</td>
<td>TDIFF</td>
</tr>
</tbody>
</table>
The appropriate disk must be accessed before these files may be used and a temporary disk established. This may be done by typing the following commands:

```
ACCESS 206 E
DEF T3350 150 3
FORMAT 150 A
```

The computer will respond by asking if all files should be erased. The reader types

`YES`

The computer will then respond with

```
ENTER DISK LABEL
```

Type in respond

`TDISK`

Computer will tell the reader that it is formatting 150 A. A ready message will appear. The reader should now UNPACK all the data files from disk E to the temporary disk A. This may be done for each file by typing

```
UNPACK filename DATA E
```

Now the files are ready to be used by the GRID program of TWOD.

If, on the other hand, the reader chooses the other option (creating the data files by running the Newtonian and non-Newtonian programs), the following steps must be followed.

**STEP 1.** The programs incorporate a subroutine called PUNCH. This subroutine creates individual data files for each four variables plotted. Each card of the data file consists of an $r$ value, $\theta$ value, and the appropriate variable value
at this specified \( r \) and \( \theta \) location. The listing of the
PUNCH subroutine appears below.

```plaintext
SUBROUTINE PUNCH (10, AO)
C********************************************************************************
**R**
********************************************************************************
Subroutine for creating a file for plotting
SI, VR, TDIFF, and SHEAR
********************************************************************************
NOTE
3 is the file for SI
7 is the file for VR
8 is the file for SHEAR
9 is the file for TDIFF
********************************************************************************
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION AO(61,31)
DO 2 I = 1, 60, 1
   R = (DFLOAT (61-I)*0.0128267 + 0.2304)*30.
DO 2 J = 1, 31, 1
   TH = DFLOAT (J-1)
   WRITE (10, 1) R, TH, AO(I,J)
1 FORMAT (3E15.4)
2 CONTINUE
3 RETURN
END
```

Before running either the Newtonian or non-Newtonian programs, these
commands must be given:

FILE 5 DISK FILE 6 TERMINAL

FILE 3 DISK FILE 7 DISK FILE 8 DISK FILE 9 DISK LOAD

START
The first filename in the parentheses (the 2C names) are specified if the Newtonian program is to be run while the second filename is indicated if the non-Newtonian program is to be run.

**STEP 2.** In each of the above data files the plotted variable is in E15.4 format. The format specified for this variable in the GRID program of TWOD is the F10.6 format. Hence a program called CHANGE is run using each data file to change the plotted variables to the proper format. The CHANGE program is given below. The symbol $A$ is the r-value, $B$ is the $\theta$-value, and $C$ is the value of the variable to be plotted at this particular $r$ and $\theta$ location.

```plaintext
DO 3 I=1,1860
READ (5, 1) A, B, C
1 FORMAT(3E15.4)

C***********************************************************
| This program changes the format of the data from an |
| E format to an F format. Furthermore, this program    |
| changes the magnitude of the data so that it is      |
| within the specified F10.6 format of the TWOD program.|
|***********************************************************

C = C*1.
WRITE (7,2) A, B, C
2 FORMAT(3F10.6)
3 CONTINUE
STOP
END
```

Note the underscored line. This line is used to scale down the value of the plotted variables which are too large to fit in a F10.6 format. The proper lines for running this program with each of the data files are
To alter the underscore line, type

FEDIT CHANGE FORTRAN

The computer responds with

- FEDIT
- 

Type

\[ /C = C^* \]

The computer will type the underscored line. To change this line to the one needed for data file 2C2 or 4A2, type

CHANGE/*1./*0.1

The computer will type the changed line. Then type

FILE

To compile the program, type FORTG CHANGE FORTRAN .

When the CHANGE program is to be run for each of the data files, these commands should be given:

FILE 5 DISK \( \{ \begin{array}{c}
2C1 \\
2C2 \\
2C3 \\
2C4 \\
\end{array} \) \) or \( \{ \begin{array}{c}
4A1 \\
4A2 \\
4A3 \\
4A4 \\
\end{array} \) \)

DATA (LRECL 80 RECFMF BLOCK 80

GLOB

FILE 6 TERMINAL
Only one option in each set of parentheses should be selected. Note that when 2C1 is specified 2C1A should be specified when 2C2 is specified, 2C2A should be specified, and so forth.

STEP 3. Once each data file has been run through the CHANGE program, the following line is added to the top of each data file. To accomplish this, type

\[
\text{FEDIT filename DATA}
\]

The computer responds with

\*FEDIT

Type

\*INPUT

Now input the following line of data.

<table>
<thead>
<tr>
<th>Column</th>
<th>Data Entry</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>10.</td>
<td>Width in inches of r-axis</td>
</tr>
<tr>
<td>11-20</td>
<td>3.</td>
<td>Number of divisions per inch along the r or ( \theta )-axis</td>
</tr>
<tr>
<td>21-30</td>
<td>0.</td>
<td>Minimum r-axis value</td>
</tr>
<tr>
<td>31-40</td>
<td>30.*</td>
<td>Maximum r-axis value</td>
</tr>
<tr>
<td>41-50</td>
<td>0.</td>
<td>Minimum ( \theta )-axis value (in degrees)</td>
</tr>
<tr>
<td>51-60</td>
<td>30.</td>
<td>Maximum ( \theta )-axis value (in degrees)</td>
</tr>
</tbody>
</table>

*NOTE: All the r-values were multiplied by 30 in the PUNCH subroutine to put them in the same range as the \( \theta \)-values.*
Hit the RETURN key twice.

Now type FILE.

Data files must now be created for the MAP1 program of TWOD before plotting the results of either the Newtonian or non-Newtonian program. First create a data file for plotting the Newtonian SI values. Type

FEDIT M2C1 DATA

The computer responds

• FEDIT

•

Type

INPUT

Enter the following data appropriately.

<table>
<thead>
<tr>
<th>Line No.</th>
<th>Column</th>
<th>Format</th>
<th>Data Entry</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-10</td>
<td>G10.0</td>
<td>10.0</td>
<td>No. of contours to be plotted</td>
</tr>
<tr>
<td>11-20</td>
<td>G10.0</td>
<td></td>
<td>-.10</td>
<td>Starting contour value</td>
</tr>
<tr>
<td>21-30</td>
<td>G10.0</td>
<td></td>
<td>-.04</td>
<td>Contour interval</td>
</tr>
</tbody>
</table>

After entering the data, hit the RETURN Key twice. Then type FILE.

The same procedure should be followed to create the other data files for the MAP1 program. Table C-1 gives the appropriate information.

Because this program was originally written to plot in rectangular coordinates, one line has to be added to the PLOT1 program to be able to plot in cylindrical. Type

FEDIT PLOT1 FORTRAN

The computer responds with

• FEDIT

•
Table C-1: Creating Data Files for the MAP1 Program

**STEP 1**

<table>
<thead>
<tr>
<th>Newtonian Plots</th>
<th>Non-Newtonian Plots</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Variables</strong></td>
<td><strong>Variables</strong></td>
</tr>
<tr>
<td>VR</td>
<td>SI</td>
</tr>
<tr>
<td>SHEAR</td>
<td>VR</td>
</tr>
<tr>
<td>TDIFF</td>
<td>SHEAR</td>
</tr>
<tr>
<td></td>
<td>TDIFF</td>
</tr>
<tr>
<td><strong>File Name</strong></td>
<td><strong>File Name</strong></td>
</tr>
<tr>
<td>M2C2</td>
<td>M4A1</td>
</tr>
<tr>
<td>M2C3</td>
<td>M4A2</td>
</tr>
<tr>
<td>M2C4</td>
<td>M4A3</td>
</tr>
<tr>
<td></td>
<td>M4A4</td>
</tr>
<tr>
<td><strong>File Type</strong></td>
<td><strong>File Type</strong></td>
</tr>
<tr>
<td>DATA</td>
<td>DATA</td>
</tr>
<tr>
<td>DATA</td>
<td>DATA</td>
</tr>
<tr>
<td>DATA</td>
<td>DATA</td>
</tr>
</tbody>
</table>

**STEP 2**

<table>
<thead>
<tr>
<th>Newtonian Plots</th>
<th>Non-Newtonian Plots</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Variable</strong></td>
<td><strong>Variable</strong></td>
</tr>
<tr>
<td>VR</td>
<td>SI</td>
</tr>
<tr>
<td>SHEAR</td>
<td>VR</td>
</tr>
<tr>
<td>TDIFF</td>
<td>SHEAR</td>
</tr>
<tr>
<td></td>
<td>TDIFF</td>
</tr>
<tr>
<td><strong>First 10</strong></td>
<td><strong>First 10</strong></td>
</tr>
<tr>
<td><strong>Columns</strong></td>
<td><strong>Columns</strong></td>
</tr>
<tr>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>-0.10</td>
<td>-0.10</td>
</tr>
<tr>
<td>-0.04</td>
<td>-0.04</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Second 10</strong></td>
<td><strong>Second 10</strong></td>
</tr>
<tr>
<td><strong>Columns</strong></td>
<td><strong>Columns</strong></td>
</tr>
<tr>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>-0.15</td>
<td>-0.15</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Third 10</strong></td>
<td><strong>Third 10</strong></td>
</tr>
<tr>
<td><strong>Columns</strong></td>
<td><strong>Columns</strong></td>
</tr>
<tr>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>0.30</td>
<td>0.30</td>
</tr>
<tr>
<td>-0.10</td>
<td>-0.10</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Now check to see if the necessary line is there by typing

/ CALL POLTRN(0.,-30.,0.)

If the computer responds by typing this line, type QUIT to leave the
FEDIT mode. If, however, the computer types

- NOT FOUND
- EOF

the reader should type

TOP

The reader should then type

/ CALL PLOTS(6,830,7)

The computer will type this line. After the ready signal appears, type

INPUT

Now type the following line beginning in the seventh column.

CALL POLTRN(0.,-30,0.)

The middle number may be changed depending on the wall angle of the
shaping section. To leave the INPUT mode, hit the RETURN key twice.

Now type FILE. Next type

FORTG PLOT1 FORTRAN.

The computer will ask one questions. To answer just hit the RETURN key.

Once the data files are filed, the three programs (GRID, PLOT1,
MAP1) are executed from CMS by typing TWOD. This command is an EXEC
file built such that it is interactive with the user at execution of each
main program. The EXEC file asks for the following files:

a. DATA FILE NAME FOR GRID? 2C1A
b. DATA FILE NAME FOR MAP1? M2C1
c. DATA FILE NAME FOR PLOTL? P1
d. OUTPUT FILE NAME FOR PLOT FILE? 2C1
e. GRAPHICS LIBRARY TO BE USED? TEKTRNX

The underlined items are the responses when the Newtonian SI variables are to be plotted. If the reader uses the Anderson-Jacobson plotter, question (e) is answered with AJPLOTR.

The output file is stored on the disk with the file name given as an answer to question (d) and the file type 'PLOT' if the Tektronix graphics library is used or 'AJPLOT' if the Anderson-Jacobson graphics library is used. Plot file types are generated for this program with the command:

```
PLOT filename PLOT filemode
```

AJPLOT filetypes can be generated with the command:

```
AJ832TYP filename AJPLOT filemode.
```

It should be noted by the user of this Appendix information, that some of the computer commands indicated are very specific to Ohio University and the Chemical Engineering Department's CHEMSTR machine. These specific commands are UNPACK, FEDIT, FORTG, GLOB, and AJ832TYP.
APPENDIX D

DERIVATION OF EQUATION 99
The derivation of equation 99 begins with equations 90 and 91. These equations are dimensionalized using equations 15 through 18. The result is

\[
\frac{v'_r}{r'} \frac{\partial v'_r}{\partial r'} + \frac{v'_\theta}{r'} \frac{\partial v'_\theta}{\partial r'} - \frac{v'_\theta}{r'}^2 = -\frac{\partial p'}{\partial r'} + \left[ \frac{\partial^2 \tau'_r}{\partial r' \partial r'} + \frac{\tau'_r}{r'} \right]
+ \frac{1}{r'} \frac{\partial \tau'}{\partial \theta'} - \frac{\tau'}{r'} \frac{\partial \theta'}{r'} \right]
(D-1)
\]

\[
\frac{v'_r}{r'} \frac{\partial v'_\theta}{\partial r'} + \frac{v'_\theta}{r'} \frac{\partial v'_\theta}{\partial r'} + \frac{v'_r}{r'} \frac{\partial v'_r}{\partial \theta'} = - \frac{1}{r'} \frac{\partial p'}{\partial \theta'} + \left[ \frac{\partial^2 \tau'_r}{\partial r' \partial \theta'} + \frac{2 \tau'_r}{r'} \right]
+ \frac{1}{r'} \frac{\partial \tau'}{\partial \theta'} \right]
(D-2)
\]

Differentiating equation D-1 by \( \theta' \) gives

\[
\frac{v'_r}{r'} \frac{\partial^2 v'_r}{\partial r' \partial \theta'} + \frac{v'_r}{r'} \frac{\partial v'_r}{\partial r'} + \frac{v'_\theta}{r'} \frac{\partial^2 v'_\theta}{\partial r' \partial \theta'} + \frac{1}{r'} \frac{\partial v'_r}{\partial r'} \frac{\partial v'_\theta}{\partial \theta'} + \frac{1}{r'} \frac{\partial v'_\theta}{\partial \theta'} \frac{\partial v'_r}{\partial r'} - \frac{2}{r'} \frac{\partial v'_r}{\partial \theta'} \frac{\partial v'_\theta}{\partial \theta'}
= - \frac{\partial^2 p'}{\partial r' \partial \theta'} - \left[ \frac{\partial^2 \tau'_r}{\partial r' \partial \theta'} + \frac{1}{r'} \frac{\partial \tau'_r}{\partial \theta'} + \frac{1}{r'} \frac{\partial^2 \tau'_r}{\partial \theta' \partial \theta'} - \frac{1}{r'} \frac{\partial \tau'_r}{\partial \theta'} \right]
(D-3)
\]

Solving for \(-\frac{\partial^2 p'}{\partial r' \partial \theta'}\) yields

\[
-\frac{\partial^2 p'}{\partial r' \partial \theta'} = \frac{v'_r}{r'} \frac{\partial^2 v'_r}{\partial r' \partial \theta'} + \frac{v'_r}{r'} \frac{\partial v'_r}{\partial r'} + \frac{v'_\theta}{r'} \frac{\partial^2 v'_\theta}{\partial r' \partial \theta'} + \frac{1}{r'} \frac{\partial v'_r}{\partial r'} \frac{\partial v'_\theta}{\partial \theta'} + \frac{1}{r'} \frac{\partial v'_\theta}{\partial \theta'} \frac{\partial v'_r}{\partial r'} - \frac{2 v'_r v'_\theta}{r'} \frac{\partial v'_r}{\partial \theta'} \frac{\partial v'_\theta}{\partial \theta'}
+ \left[ \frac{\partial^2 \tau'_r}{\partial r' \partial \theta'} + \frac{1}{r'} \frac{\partial \tau'_r}{\partial \theta'} + \frac{1}{r'} \frac{\partial^2 \tau'_r}{\partial \theta' \partial \theta'} - \frac{1}{r'} \frac{\partial \tau'_r}{\partial \theta'} \right]
(D-4)
\]

In the same manner equation D-2 is differentiated by \( r \).
Solving for \( \frac{1}{r} \frac{\partial \rho'}{\partial \theta} \) in equation D-2 yields

\[
\frac{1}{r} \frac{\partial \rho'}{\partial \theta} = -\frac{v_r}{r^2} + \frac{v_\theta}{r^2} \frac{\partial v'}{\partial r} - \frac{v_r'}{r^2} + \left[ \frac{\partial^2 v'}{\partial r^2} - \frac{2}{r^2} + \frac{2}{r^2} \frac{\partial r}{\partial r} - \frac{1}{r^2} \frac{\partial \rho'}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 \rho'}{\partial \theta^2} \right] \tag{D-5}
\]

Substituting equations D-4 and D-6 into equation D-5 gives the following:

\[
\frac{v_r}{r^2} + \frac{\partial^2 v'}{\partial r^2} - \frac{v_\theta}{r^2} \frac{\partial v'}{\partial \theta} + \frac{1}{r^2} \frac{\partial v'}{\partial r} + \frac{v_r'}{r^2} + \frac{\partial v'}{\partial \theta} + \left[ \frac{v_r}{r^2} + \frac{v_\theta}{r^2} + \frac{v_r'}{r^2} \right] \tag{D-6}
\]
The velocity terms are all grouped on the left-hand side of the equation. Rather than rewriting them, they are called "VELOCITY TERMS".

\[
\begin{align*}
\text{VELOCITY TERMS} & = \frac{1}{r^1} \frac{\partial^2 \tau_{rr}'}{\partial r^1 \partial r^1} + \frac{1}{r^2} \frac{\partial \tau_{rr}'}{\partial r^2} + \frac{1}{r^1} \frac{\partial \tau_{rr}'}{\partial r^1} - \frac{3}{r'} \frac{\partial \tau_{r\theta'}}{\partial r'} \\
& - \frac{1}{r^2} \frac{\partial^2 \tau_{r\theta'}}{\partial r^2 \partial r^1} - \frac{3}{r'} \frac{\partial \tau_{r\theta'}}{\partial r'}
\end{align*}
\]

(D-8)

Replacing \( \tau_{r\theta'} \) by \( \tau_{rr'} \) yields

\[
\begin{align*}
\text{VELOCITY TERMS} & = \frac{2}{r^1} \frac{\partial^2 \tau_{rr}'}{\partial r^1 \partial r^1} + \frac{2}{r^2} \frac{\partial \tau_{rr}'}{\partial r^2} + \frac{1}{r^1} \frac{\partial \tau_{rr}'}{\partial r^1} - \frac{3}{r'} \frac{\partial \tau_{r\theta'}}{\partial r'} \\
& - \frac{3}{r^2} \frac{\partial^2 \tau_{r\theta'}}{\partial r^2 \partial r^1}
\end{align*}
\]

(D-9)

Taking the first derivative of equation 106 with respect to \( r \) and \( r' \), and the first derivative of equation 107 with respect to \( \theta \) gives

\[
\frac{\partial \tau_{r\theta'}}{\partial r'} = -\frac{1}{\rho_{RV}} \left[ \eta \frac{\partial \Delta'}{\partial r'} + \Delta' \frac{\partial \eta}{\partial r'} \right]
\]

(D-10)
Taking the second derivative of equation D-10 with respect to $r$, the second derivative of equation D-11 with respect to $\theta$, and the second derivative of equation D-12 with respect to $r$ gives

$$\frac{\partial^2 \tau_{rr}'}{\partial r'^2} = -\frac{1}{\varphi_{RV}} \left[ n \frac{\partial^2 \Delta_{rr}'}{\partial r'^2} + 2 \Delta_{rr} \frac{\partial^2 \Delta_{rr}'}{\partial r'^2} + \Delta_{rr} \frac{\partial^2 \eta}{\partial \theta'^2} \right] \quad (D-13)$$

$$\frac{\partial^2 \tau_{r\theta}'}{\partial \theta'^2} = -\frac{1}{\varphi_{RV}} \left[ n \frac{\partial^2 \Delta_{r\theta}'}{\partial \theta'^2} + 2 \Delta_{r\theta} \frac{\partial^2 \Delta_{r\theta}'}{\partial \theta'^2} + \Delta_{r\theta} \frac{\partial^2 \eta}{\partial \theta'^2} \right] \quad (D-14)$$

$$\frac{\partial^2 \tau_{rr}''}{\partial r'^2 \partial \theta'} = -\frac{1}{\varphi_{RV}} \left[ n \frac{\partial^2 \Delta_{rr}'}{\partial r'^2 \partial \theta'} + \Delta_{rr} \frac{\partial^2 \eta}{\partial r'^2} + \Delta_{rr} \frac{\partial \eta}{\partial r'^2} \right]$$

Replacing the first and second derivative terms in equation D-9 by the appropriate equations (D-10 through D-15) gives

$$\text{VELOCITY TERMS} = \frac{n}{\varphi_{RV}} \left[ \frac{2 \Delta_{rr}'}{r'} \frac{\partial^2 \Delta_{rr}'}{\partial r'^2} + \frac{1}{r} \Delta_{rr} \frac{\partial^2 \Delta_{rr}'}{\partial \theta'^2} + \frac{1}{r'^2} \frac{\partial^2 \Delta_{r\theta}'}{\partial \theta'^2} + \frac{3}{r'} \frac{\partial \Delta_{rr}'}{\partial r'} + \frac{2}{r'^2} \frac{\partial \Delta_{rr}'}{\partial \theta'} + 2 \Delta_{rr} \frac{\partial^2 \eta}{\partial r'^2} + \frac{2 \Delta_{r\theta}'}{r'} \frac{\partial \eta}{\partial r'} \right]$$

$$+ \left( \frac{2 \Delta_{rr}'}{r'} - \frac{2 \Delta_{rr}}{r \partial \theta'} + \frac{3}{r'} \frac{\partial \Delta_{rr}'}{\partial r'} \right) \frac{\partial \eta}{\partial r'} - \frac{\Delta_{r\theta}'}{r'^2} \frac{\partial \eta}{\partial \theta'^2} - \frac{2}{r'} \Delta_{rr} \frac{\partial \eta}{\partial r'^2} - \frac{2}{r'^2} \Delta_{rr} \frac{\partial \eta}{\partial \theta'^2} \right] \quad (D-16)$$
The terms in braces in equation D-16 becomes the variable DTOT in equation 99 of the text. If, in addition, equations 22 and 23 are used as replacements for \( v_r' \) and \( v_\theta' \) respectively (in the VELOCITY TERMS portion) and equations 102 and 104 are substituted for \( \Delta_{rr}' \) and \( \Delta_{r\theta}' \) in the bracketed portion of D-16, the underlined portion of equation D-16 reduces to

\[
\frac{1}{r'} \frac{\partial \psi}{\partial \theta'} \frac{\partial^2 \psi}{\partial r'^2} - \frac{1}{r'} \frac{\partial \psi}{\partial r'} \frac{\partial^2 \psi}{\partial \theta'^2} = \frac{1}{N(\eta)} \frac{\partial^4 \psi}{\partial r^4} \tag{D-17}
\]

the other terms of equation 99. Complete details of this derivation may be found in reference (22).