INFORMATION TO USERS

This reproduction was made from a copy of a document sent to us for microfilming. While the most advanced technology has been used to photograph and reproduce this document, the quality of the reproduction is heavily dependent upon the quality of the material submitted.

The following explanation of techniques is provided to help clarify markings or notations which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting through an image and duplicating adjacent pages to assure complete continuity.

2. When an image on the film is obliterated with a round black mark, it is an indication of either blurred copy because of movement during exposure, duplicate copy, or copyrighted materials that should not have been filmed. For blurred pages, a good image of the page can be found in the adjacent frame. If copyrighted materials were deleted, a target note will appear listing the pages in the adjacent frame.

3. When a map, drawing or chart, etc., is part of the material being photographed, a definite method of "sectioning" the material has been followed. It is customary to begin filming at the upper left hand corner of a large sheet and to continue from left to right in equal sections with small overlaps. If necessary, sectioning is continued again—beginning below the first row and continuing on until complete.

4. For illustrations that cannot be satisfactorily reproduced by xerographic means, photographic prints can be purchased at additional cost and inserted into your xerographic copy. These prints are available upon request from the Dissertations Customer Services Department.

5. Some pages in any document may have indistinct print. In all cases the best available copy has been filmed.
Huh, Jung Do

A NUMERICAL SIMULATION OF THE FLOW OF VISCOELASTIC MATERIALS IN THE DIE-ENTRY REGION

Rice University
Ph.D. 1985

University Microfilms International 300 N. Zeeb Road, Ann Arbor, MI 48106
RICE UNIVERSITY

A NUMERICAL SIMULATION OF THE FLOW OF
VISCOELASTIC MATERIALS IN THE DIE-ENTRY REGION

by

JUNG DO HUH

A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE

DOCTOR OF PHILOSOPHY

APPROVED, THESIS COMMITTEE:

L. V. McIntire, Head of Chemical Engineering, Chairman

J. D. Hellums, Dean of the School of Engineering

M. F. Wheeler, Professor of Mathematical Science

HOUSTON, TEXAS

APRIL, 1985
ABSTRACT

A NUMERICAL SIMULATION OF THE FLOW OF VISCOELASTIC MATERIALS IN THE DIE-ENTRY REGION

JUNG DO HUH

A major obstacle in the prediction of stress profiles in the viscoelastic flow of polymers is a mysterious breakdown of the numerical procedure, which occurs at relatively small values of the Deborah number. Numerous papers have been devoted to analyzing the reason for this failure, but the exact cause remains unclear. Amazingly, all constitutive equations attempted and all kinds of different numerical procedures employed have run into the very same problem.

We have investigated several currently popular constitutive models in a viscometric flow field and have found serious limitations in shear flows which may be the source of numerical problems. There is often a lack of appreciation for the computational uses of fluid models in the process of formulating constitutive equations. In the future, the use of the corotational time derivative, which appears to create this trouble, may be prohibited. Alternatively, it may be possible to avoid the limitation by adding a proper retardation time in constitutive models which use the corotational time derivative.

The well known upper convected Maxwell model does not exhibit limitation but it is believed that a different source of numerical instability may be inherently present. We have adopted the cylindrical axisymmetric 4:1 contraction channel (the die-entry region) to simulate this fluid using the mixed finite element method. The worrisome infinite elongational viscosity predicted by this model in steady
extensional flow, indeed, is responsible for the singular behavior of the stress solution field. The most difficult region for convergence, as might be expected, is found to be just after the reentrant corner.
ACKNOWLEDGMENTS

Paving the unknown, rocky, hard land forward has necessarily required buckets of sweat, thousand times of frustration and countless tormented days and nights. One person has stood tall and watched out the process with care and patience all the way to the end. Deepest appreciation goes to Author's advisor Professor Larry V. McIntire for his guidance and understanding in framing this thesis.

The author also admits that great teachings of two persons will be lingered in his dimming memory for years to come. They are the engineering dean J. D. Hellums and Professor M. F. Wheeler who have enlightened his ignorance and served on his oral examination committee.

In addition, Author's wife and children who have shared hardships and gone through troubled periods together must not be underestimated in their contribution to this work.

Finally, the Author wishes to thank Vicki Hester who has typed the whole material with accuracy and elegance.
TABLE OF CONTENTS

List of Tables..............................................................................viii
List of Figures..............................................................................ix

Chapter

I. INTRODUCTION.................................................................1

II. REVIEW..............................................................................4
   2.1 Numerical Methods and Topics.................................4
   2.2 Numerical Problems and Strategies.........................5
   2.3 Physics of Extrusion Die-Entry Problem...............10

III. MAXWELL-TYPE CONSTITUTIVE MODES......................14
   3.1 Derivation.................................................................14
   3.2 Definition of Material Functions in the
       Steady Simple Shear Flow........................................17
   3.3 Definition of the Material Function in
       Steady Simple Elongational Flow.............................19
   3.4 Material Functions of Maxwell Fluids.....................21

IV. LIMITATION OF THE STEADY VISCOMETRIC FLOW IN
    DIFFERENTIAL MODELS..................................................24
   4.1 ZFD Fluid...............................................................26
   4.2 Phan-Thien and Tanner Network Model...................32
   4.3 Giesekus Model........................................................38
   4.4 Leonov Model..........................................................42
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>V. SIMULATION OF THE EXTRUSION DIE-ENTRY</td>
<td>47</td>
</tr>
<tr>
<td>5.1 Problem Definition</td>
<td>47</td>
</tr>
<tr>
<td>5.2 Boundary Conditions</td>
<td>50</td>
</tr>
<tr>
<td>5.3 Galerkin Weak Solution Formulation--Mathematical Approach</td>
<td>53</td>
</tr>
<tr>
<td>5.4 Construction of System Residual Vector by the Mixed Finite Element Method</td>
<td>56</td>
</tr>
<tr>
<td>5.4.1 General Consideration</td>
<td>56</td>
</tr>
<tr>
<td>5.4.2 The Master Element and Shape Functions</td>
<td>62</td>
</tr>
<tr>
<td>5.4.3 Element Transformations</td>
<td>66</td>
</tr>
<tr>
<td>5.4.4 Integration by Gaussian Quadrature</td>
<td>69</td>
</tr>
<tr>
<td>5.4.5 Summary</td>
<td>70</td>
</tr>
<tr>
<td>5.5 Nonlinear Iteration Method</td>
<td>72</td>
</tr>
<tr>
<td>5.5.1 Successive Substitution Method with SOR</td>
<td>72</td>
</tr>
<tr>
<td>5.5.2 Newton-Raphson Method</td>
<td>73</td>
</tr>
<tr>
<td>5.5.3 Newton-Raphson with Continuation Method</td>
<td>73</td>
</tr>
<tr>
<td>5.5.4 Initial Value Approach</td>
<td>74</td>
</tr>
<tr>
<td>(1) Deborah number Marching Scheme--General Aspects</td>
<td>74</td>
</tr>
<tr>
<td>(2) Adams-Type Predictor-Corrector Multistep Method</td>
<td>77</td>
</tr>
<tr>
<td>(3) Local Error Control</td>
<td>80</td>
</tr>
<tr>
<td>(4) Stiff Problem</td>
<td>83</td>
</tr>
<tr>
<td>VI COMPUTATIONAL ASPECTS</td>
<td>88</td>
</tr>
<tr>
<td>6.1 Generation of the Starting Vector in the Initial Value Problem</td>
<td>88</td>
</tr>
<tr>
<td>6.2 Computational Technique and Parameter Specification</td>
<td>92</td>
</tr>
<tr>
<td>Chapter</td>
<td>Section</td>
</tr>
<tr>
<td>---------</td>
<td>-------------------------------------------------------------------------</td>
</tr>
<tr>
<td>VII</td>
<td>COMPUTATIONAL RESULTS</td>
</tr>
<tr>
<td></td>
<td>7.1 The cause of the numerical failure of the upper convected Maxwell model</td>
</tr>
<tr>
<td></td>
<td>7.2 Physics of the Maxwell Fluid in the Contraction Channel</td>
</tr>
<tr>
<td>VIII</td>
<td>CONCLUDING REMARKS</td>
</tr>
<tr>
<td></td>
<td>BIBLIOGRAPHY</td>
</tr>
<tr>
<td>Table Number</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>1</td>
<td>Summary of the Die-Entry Computation of Viscoelastic Fluids</td>
</tr>
<tr>
<td>2</td>
<td>Material Functions of Maxwell Fluids in Steady Simple Flows</td>
</tr>
<tr>
<td>3</td>
<td>Special Cases of Phan-Thien and Tanner Model</td>
</tr>
<tr>
<td>4</td>
<td>Special Cases of Giesekus Model</td>
</tr>
<tr>
<td>5</td>
<td>Limitation of Differential Models</td>
</tr>
<tr>
<td>6</td>
<td>Viscometric Flow Profiles of the Phan-Thien Model for a Cylindrical Axisymmetric Channel</td>
</tr>
<tr>
<td>7</td>
<td>Comparison between the STEP-Newton and the RK-Newton</td>
</tr>
<tr>
<td>8</td>
<td>Numerical Performance of the RK-Newton</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure Number</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A Spring-Dashpot Mechanical Model of a Viscoelastic Fluid</td>
<td>14</td>
</tr>
<tr>
<td>2</td>
<td>Material Functions for Six Limits of the Giesekus Model</td>
<td>40</td>
</tr>
<tr>
<td>3</td>
<td>Schematic Diagram of the Axisymmetric Die-Entry Region</td>
<td>47</td>
</tr>
<tr>
<td>4</td>
<td>Formulation of the Finite Element Meshes near the Contraction Region</td>
<td>57</td>
</tr>
<tr>
<td>5</td>
<td>Master Element, Node Numbering and Shape Function for 4-, 9- and 8-node Quadrilateral Finite Elements</td>
<td>65</td>
</tr>
<tr>
<td>6</td>
<td>Contour Lines for Plotting Variables in the Given Geometry</td>
<td>106</td>
</tr>
<tr>
<td>7</td>
<td>Axial Normal Stress Fields with Changes of the Deborah Number on the Centerline</td>
<td>107</td>
</tr>
<tr>
<td>8</td>
<td>Radial Stress Distribution along Contour Lines near the Die-Entry Region</td>
<td>108</td>
</tr>
<tr>
<td>9</td>
<td>Shear Stress Distribution along Contour Lines near the Die-Entry Region</td>
<td>110</td>
</tr>
<tr>
<td>10</td>
<td>Axial Stress Distribution along Contour Lines near the Die-Entry Region</td>
<td>112</td>
</tr>
<tr>
<td>11</td>
<td>Angular Stress Distribution along Contour Lines near the Die-Entry Region</td>
<td>114</td>
</tr>
<tr>
<td>12</td>
<td>Pressure Distribution along Contour Lines near the Die-Entry Region</td>
<td>115</td>
</tr>
<tr>
<td>13</td>
<td>Radial Velocity along Contour Lines near the Die-Entry Region</td>
<td>118</td>
</tr>
<tr>
<td>14</td>
<td>Axial Velocity along Contour Lines near the Die-Entry Region</td>
<td>119</td>
</tr>
</tbody>
</table>
I. INTRODUCTION

Non-Newtonian fluids include the whole spectrum of the materials located between one extreme end of a Hookean elastic solid, which has a perfect memory of the past deformation and the other extreme end of a Newtonian viscous liquid which constantly deforms its shape with time when it is subjected to a shear force. By definition, any fluid that does not exhibit linear shear stress - shear rate constitutive behavior may be called a non-Newtonian fluid. Such fluids may or may not possess elasticity (memory). Examples of non-Newtonian fluids are abundant, i.e. toothpaste, paints, oils, blood, printing inks, etc.

A class of non-Newtonian fluids of our particular interest is the viscoelastic material, which exhibits partially elastic properties as well as partially those of Newtonian viscous liquids. Thus, this material possesses some memory effect. It "remembers" recent deformations most clearly, but this memory is fading with the passage of time. The most important examples of the viscoelastic materials are industrially polymer melts and solutions associated with the synthetic fiber and plastic industries.

Steady shear behavior of these viscoelastic fluids in simple geometries is well characterized by experimentally measuring the characteristic material functions, such as shear viscosity and the first and the second normal stress differences as functions of shear rate. However, when complex geometries are involved, it is impossible or if possible, it is hard to measure material functions properly or even to know what material functions to measure. This is because elongational flow in addition to shear usually plays an important role, so that flow
behavior is much more complicated. In an attempt to resolve this problem, theoreticians have initially resorted to a crude prediction by using generalized Newtonian or simple explicit-type models like the second order fluid, for stress simulations. These usually did not agree, even qualitatively, with experimental data for polymer melts in complex flows. Recently, development of high speed computers and demand for better predictions of flow characteristics have allowed the use of nonlinear implicit-type of constitutive models in simulation in complex geometries. Unfortunately, this task is seemingly limited by the lack of proper models developed to agree with experimental data reasonably well in shear and elongational tests as well as by numerical difficulties involved in simulation. It is mentioned that all work with implicit-type models thus far has dealt with isothermal incompressible flows only. Essentially no nonisothermal work has appeared in the reviewed published literature.

Presently, a central issue in numerical simulation of viscoelastic fluids is the feasibility of the calculations of stress, velocity and pressure distributions in flows with elongationed components as well as shear components. In other words, numerical convergence up to a high value of the Weissenberg (or Deborah) number is constantly sought by researchers for these flows because of the practical interest of the polymer processing industry. Here they often meet such complex flows, for instance, in melt spinning, film blowing, injection molding, extrusion, etc. In spite of much effort, consistent numerical failure at relatively low Weissenberg numbers has raised serious problems and controversy among researchers about a method for computer successful
implementation. In addition it has become a very cumbersome obstacle for progress in theoretical study in this field. Active investigations are currently going on to pinpoint the exact cause of the numerical failures. Recently, Crochet, Davies and Walters [23] have pointed out several possible reasons which might be responsible for or contribute to failure. They are, 1. choice of rheological model; 2. stress evaluation; 3. mesh refinement near abrupt geometry changes; 4. re-entrance corner strategies; 5. bifurcation of the solution field; 6. interaction between discretization error and nonlinear iteration; and 7. algorithms.
II. REVIEW

2.1 Numerical Methods and Topics.

There have been two different numerical procedures commonly used in the computation of viscoelastic flows. One is the finite difference method, which has been popular for a long time, and the other is the finite element method which emerged around 1970 in fluid mechanics. The finite element method, which is employed here, is gaining popularity because it can handle boundary conditions relatively easily, even in complex geometries, when compared to the finite difference method.

One of the finite element methods, known as a mixed finite element or a primitive variable method, was first introduced in non-Newtonian fluid mechanics by Kawahara and Takeuchi [37] in 1977. Since then, Brown and Armstrong at MIT [2, 50, 70], Finlayson at U. of Washington in Seattle [11, 12, 33, 34, 36, 49, 65], Crochet and Keunings at Catholic University at Louvain in Belgium [18, 19, 20, 21, 22, 38, 39], and Tanner at U. of Sydney in Australia [7, 9, 60] have been actively engaged in research efforts using this method. This method has been implemented with the rate type of differential constitutive models only.

There is another finite element procedure, known as a particle tracking method, which has been devised to handle integral types of constitutive models. Casewell at Brown University [10, 66], Malkus and Bernstein at IIT [3, 47, 48], Winter at U. of Massachusetts [68, 69], and Macosko and Scriven at U. of Minnesota [51] belong to the group favoring this class of algorithms.

Headed by Davies and Walters at the University College of Wales in Great Britain [13, 14, 17, 25, 52, 53], there is also a finite
difference group which has studied computations with both differential and integral models. Leal at Caltech [41, 61] and Townsend at U. of Swansea in Great Britain [57, 58, 62, 63, 64] also can be identified with this group. However, this method faces very tough boundary condition problems when the geometry of the flow boundaries becomes complex.

Geometries used for numerical study in this area are ever expanding. Most attention has been given to the extrusion die-entry [14, 17, 19, 24, 25, 39, 50, 66, 70] and exit problems [7, 10, 12, 16, 20, 21, 22, 32, 60, 65, 69], but simulations of wirecoating dies [9], injection-molding [29], melt spinning [38, 47], parallel squeezing [42, 43, 49], pressure hole [33, 34, 57, 62], bubble growth and collapse [51], journal bearing [2], and flow through rotating spheres and disks [4, 18, 41, 61, 63, 67] have also appeared.

2.2 Numerical Problems and Strategies.

Our attempt to investigate elastic flow behavior centers on the die-entry problem, in which when a flow undergoes a sudden contraction, during which strong elasticity effects can be revealed. A survey of the numerical work done for this problem is shown in Table 1.
Table 1. Summary of the die-entry computation of viscoelastic fluids.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Reference</th>
<th>Constitutive equation</th>
<th>Numerical method</th>
<th>Range of Deborah number convergence</th>
</tr>
</thead>
<tbody>
<tr>
<td>planar contraction</td>
<td>1. Davies et al. [24] (1979)</td>
<td>Oldroyd</td>
<td>finite difference stream function/ vorticity. Successive approximation for stresses.</td>
<td>$0 \leq De \leq 2.8$</td>
</tr>
<tr>
<td></td>
<td>2. Crochet and Bezy [19] (1979)</td>
<td>Phan-Thien and Tanner</td>
<td>mixed finite element</td>
<td>$0 \leq De \leq 0.9$</td>
</tr>
<tr>
<td></td>
<td>3. Court et al. [17] (1981)</td>
<td>upper connected Maxwell (integral model)</td>
<td>same as 1.</td>
<td>$0 \leq De \leq 2.8$</td>
</tr>
<tr>
<td></td>
<td>4. Mendelson et al. [50] (1982)</td>
<td>upper connected Maxwell</td>
<td>mixed finite element</td>
<td>$0 \leq De \leq 0.8$</td>
</tr>
<tr>
<td></td>
<td>5. Davies et al. [25] (1984)</td>
<td>upper connected Maxwell</td>
<td>finite difference Picard iteration with SOR mixed finite element Newton-Raphson</td>
<td>$0 \leq De \leq 3.9$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0 \leq De \leq 6.0$</td>
</tr>
</tbody>
</table>
Table 1. (continued)

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Reference</th>
<th>Constitutive equation</th>
<th>Numerical method</th>
<th>Range of Deborah number convergence</th>
</tr>
</thead>
<tbody>
<tr>
<td>axisymmetric contraction</td>
<td>1. Crochet and Bezy [19], (1979)</td>
<td>Phan-Thien and Tanner</td>
<td>mixed finite element Newton-Raphson method</td>
<td>$0 \leq De \leq 1.15$</td>
</tr>
<tr>
<td></td>
<td>2. Viriyayuthakorn et al. [66] (1980)</td>
<td>upper convected Maxwell (integral form)</td>
<td>finite element particle tracking method successive approximation</td>
<td>$0 \leq De \leq 3.0$</td>
</tr>
<tr>
<td></td>
<td>3. Keunning et al. [39] (1984)</td>
<td>Phan-Thien and Tanner with retardation</td>
<td>mixed finite element Newton-Raphson</td>
<td>$0 \leq De \leq 1.75$</td>
</tr>
<tr>
<td></td>
<td>4. Davies et al. [25] (1984)</td>
<td>upper convected Maxwell</td>
<td>mixed finite element Newton-Raphson</td>
<td>$0 \leq De \leq 5.0$</td>
</tr>
<tr>
<td></td>
<td>5. Yeh et al. [70] (1984)</td>
<td>upper convected Maxwell</td>
<td>mixed finite element Newton-Raphson with continuation method</td>
<td>$0 &gt; De &gt; 0.86$</td>
</tr>
</tbody>
</table>
As mentioned, it is noted that either a finite difference or finite element method fails to converge at a low Deborah number for all the work listed. Also the differential constitutive models employed for most of these papers are the upper convected Maxwell or similar models, except for the work of Crochet and Keunings [39] who have used the Phan-Thien and Tanner model [54] with the retardation term. The Deborah number convergence range listed in the table is somewhat arbitrary because different contraction ratios and upstream entry conditions according to each problem may have been used. It does however serve the purpose of showing a low Deborah number limit of convergence.

Another important point to be mentioned is that the researchers listed are oriented towards solving the discretized set of nonlinear equations with successive substitution or Newton-Raphson method, at a particular Deborah number instead of focusing on how one can devise a Deborah number marching scheme. A totally different perspective may be gained in handling the set of nonlinear equations by recognizing that the whole problem is essentially the same as an initial value problem with respect to the Deborah number. One can therefore set up a marching scheme by imbedding a Deborah number parameter into the discretized nonlinear set of equations. Then, this is solved by the multi-step, Adams-Bashforth and Adams-Morton predictor-corrector with an automatic step-size control, and the initial four steps required are constructed by the fourth order, one step, Runge-Kutta method [56]. At each incremental level, the Newton-Raphson iteration is adopted to improve the crude solutions further. This scheme has turned out to be a very powerful tool in advancing a Deborah number so that it can save a good
amount of computing time.

The simplest, first order, Deborah number marching scheme (explicit forward difference or Euler method) has been used by Mendelson et al. [50], without recognition by the name of the continuation method which has been often used in beam loading problems by solid mechanics researchers. Unless the step-size remains inefficiently small, as widely known, this Euler method is inaccurate and unstable in its numerical performance.

A further aspect of implementing this marching scheme is the consideration of boundary conditions. As in the transient problem, the boundary conditions are constantly changing with each level of Deborah number incrementation, since the variables at the boundary are functions of a Deborah parameter. An effective boundary condition strategy is going to be presented here, using the viscometric flow profile of the Thien-Tanner model and a material balance between the upstream and the downstream cross sections of the contraction geometry. Because the inlet and the outlet boundary conditions are derived from the fully developed flow profiles, sufficiently long upstream and downstream channels must be provided unless one may use an infinite element to meet this situation.

The works of Mendelson et al. [50] and Viriyayuthakorn et al. [66] strongly suggest that numerical failure occurs due to the very intensive pressure and stress singularity present near the re-entrant corner and indicate that extremely refined meshes around that corner are essential for the viscoelastic flow simulation. Davies et al., Yeh et al. and Crochet et al. [25, 70, 39] have studied the effect of mesh
refinement near the re-entrant corner. They have found that finer meshes near the corner have given more accurate results, but numerical breakdown has arrived at a lesser Deborah number than that seen using the cruder meshes. It has been wondered at this point if the degree of singularity may be too strong even for the finest meshes, or if the essential problem is not the corner singularity itself. However, evidence has shown that there is some mesh dependence of the convergence limit.

Modifying meshes which have been used first by Viriyayuthakorn and Casewell [66], we employ streamline oriented, moderately refined meshes for the transition flow section and generate grids automatically for the straight channels of the upstream and the downstream. Also we smooth out the tip of the re-entrant corner slightly by using isoparametric shape functions to reduce the singularity.

The whole finite element code presented has been built by the authors on the basis of an unsymmetric frontal solver, which is the work of Hood [31]. We found that this frontal solver is very effective in reducing the array storage requirement of the program which is a critical factor for a limited computational facility such as exists at Rice.

2.3 Physics of Extrusion Die-entry Problem.

Now, let us briefly review some physical aspects of the die-entry problem reported in several recent papers. These have been produced solely as simulation results. The magnitude of the corner vortex (or secondary flow), the extra entry pressure loss, and the overshoot of
velocity, stress and pressure near the corner with increase of the Deborah number are of principal interest. Perera and Walters [53] were the first to investigate the corner vortex growth with increasing elasticity, which should be different from the viscous Newtonian vortex. However, their work has failed to show vortex growth due to numerical divergence. The same unresolved conclusion has been made by Crochet and Bezy [19].

It is known that the growth rate of the vortex is heavily dependent on the constitutive model. For instance, the upper convected Maxwell model is believed to have a very slow growth rate; that is, its vortex size is not very different from the viscous vortex even at a relatively high Deborah number. This is shown by the work of Viriyayuthakorn and Casewell [66] which has used an integral type of the upper convected Maxwell model and have reported a little vortex growth. However the effect of fluid elasticity was manifested very strongly by the stress and the pressure fields (intensive overshoots have been observed at the entry corner when compared to Newtonian fluid calculations). These stress and pressure overshoots were very sensitive to small changes of the velocity field, although velocity itself has shown a small overshoot. It was also claimed that intensification of stress and pressure singularities has demanded severe mesh refinement at the corner. Extra entry pressure loss has been measured by computing the Couette correction value for the first time in their work, and they have shown a linear decrease with respect to the Deborah number. All these results are to be expected because the upper convected Maxwell model has a constant shear viscosity (i.e., Newtonian viscosity—thus, no shear
thinning effect) and no secondary normal stress difference in the shear flow, and shows an infinite elongational viscosity at finite values of elongation rate.

However, difficult results for the couette correction value when compared to the upper convected Maxwell model have been reported by Keunings and Crochet [39], who have employed the Phan-Thien and Tanner model modified to include the retardation term. They have indicated that the couette correction value has initially decreased a little and then increased linearly with the Deborah number. The presence of the secondary normal stress difference in shear flows and the shear viscosity thinning effect in the Phan-Thien and Tanner model both seem to be responsible for this behavior. Another pronounced effect of their work is an enormous growth of the secondary flow vortex at relatively small Deborah numbers. A remarkable velocity overshoot has been observed using this model, also. However, they did not present the stress and the pressure fields, which would be expected to differ significantly from the Maxwell model behavior. It is generally believed that inclusion of the retardation term reduces the stiff stress gradient and consequently allows one to get a higher Deborah number convergence limit. However it has been criticized that this term may also essentially change the constitutive model itself.

Mendelson et al. [50] have attempted to find a connection between bifurcation points and the failure of the computation schemes using the upper convected Maxwell model. They have drawn the conclusion that no evidence for bifurcation points has been found for two-dimensional die-entry flow. Severe oscillations in stress and pressure fields before
numerical breakdown have been observed, which might be due to the existence of the stiff stress and pressure singularity at the corner.

Finally, Yeh et al. [70] have studied a possibility of limit points of the upper convected Maxwell model. They have concluded that the existence of limit points due to the structure of the model itself has been a major cause of the numerical breakdown, not the sharp edge singularity of the die-entry region.
III. MAXWELL-TYPE CONSTITUTIVE MODEL

3.1 Derivation

The most simple mechanical analog of the viscoelastic fluid is shown in Figure 1.

![Figure 1. A spring-dashpot mechanical model of a viscoelastic fluid.](image)

When a force $F$ is acting on the spring downward at $t = 0$, the deformation of the spring and the dashpot may be described as:

$$\tau = G\varepsilon_s$$  \hspace{1cm} (1) \\
and \\
$$\tau = \eta_0 \dot{\varepsilon}_d$$  \hspace{1cm} (2)

respectively, where $\tau$ is the stress (dynes/cm$^2$), $\varepsilon$ is the strain defined by $(L - L_0)/L_0$ (in which $L_0$ is the initial length of the spring at $t = 0$ and $l$ is its length at time $t$), $\dot{\varepsilon} = d\varepsilon/dt$ is the rate of strain (1/sec), $G$ is the elastic modulus (dynes/cm$^2$), and $\eta_0$ is the viscosity (poise). The spring exhibits purely an elastic effect (i.e., as a Hookean solid), while the dashpot exhibits purely a viscous effect (i.e., as a Newtonian
fluid). The total strain of the "spring and dashpot" at any time $t$ is the sum of that due to the dashpot (irreversible) and that due to the spring (reversible),

$$
\varepsilon = \varepsilon_s + \varepsilon_d.
$$

(3)

Combining Eqs. (1), (2) and (3) and formulating the resulting expression to a three dimensional form results in:

$$
\mathbf{I} + \lambda \frac{\partial \varepsilon}{\partial t} = 2\eta_0 \dot{D}
$$

(4)

where $\mathbf{I}$ is the stress tensor (dynes/cm$^2$), $\dot{D}$ is the rate of the deformation tensor (1/sec), and $\lambda = \eta_0 / G$ is a relaxation time (sec). Eq. (4) is called the classical Maxwell mechanical model, which is capable of qualitatively explaining many well known viscoelastic phenomena, such as stress relaxation after a sudden change in deformation and elastic recovery following a sudden release of imposed stress. It should be emphasized that Eq. (4) is formally valid only for infinitesimally small deformations.

The generalization of Eq. (4) to materials in general motion, in which the rate of deformation and peak strain are not necessarily small, must be subject to the following principles:

1. principle of material frame indifference--the equations must be independent of the frame of reference; this is satisfied by using invariant forms of tensors associated with the material elements in equations.
2. principle of determinism--the behavior of a material element which is described by equations depends only on its previous deformation history and not on the state of neighboring elements.

Based on these principles, the codeformational (or Oldroyd's convective) derivative,

\[ \frac{D}{Dt} - \mathbf{I} \cdot \mathbf{T} - \mathbf{T} \cdot \mathbf{I}^T \] (upper convective derivative) \hspace{1cm} (5)

\[ \frac{\Delta}{Dt} = \frac{D}{Dt} + \mathbf{I} \cdot \mathbf{I} + \mathbf{I}^T \cdot \mathbf{I} \] (lower convective derivative) \hspace{1cm} (6)

and the corotational derivative (or Jaumann derivative),

\[ \dot{\mathbf{I}} = \frac{D}{Dt} - \mathbf{w} \cdot \mathbf{I} - \mathbf{I} \cdot \mathbf{w}^T, \] \hspace{1cm} (7)

have been developed to replace the partial derivative term in Eq. (4) (refer to Bird et al. [5]). Here, D/Dt is a material (or substantial) derivative, \( \mathbf{I} \) a velocity gradient tensor (1/sec), \( \mathbf{w} \) a vorticity tensor (1/sec) and the superscript T represents a transpose.

We started above with a single "spring and dashpot" model. Unfortunately, polymeric materials can almost never be described by such a simple representation because of the complexity of the molecular structure. One way of avoiding this dilemma is to consider that a polymeric material consists of a very large number of sets of "spring and dashpots." If one assumes further that the stress \( \tau \) in the material
is the superposition of individual stresses $\mathbf{s}^i$ for each set of "spring and dashpot," Eq. (4) may be written as:

$$\mathbf{s} = \sum_{i=1}^{\infty} \mathbf{s}^i$$

$$\mathbf{s}^i + \lambda^i \frac{\mathbf{s}^i}{\partial t} = 2\eta^i_0 \mathbf{D}$$

(8)

where $\mathbf{s}^i$ is the stress tensor of the $ith$ mode, and $\lambda^i$ and $\eta^i_0$ are the relaxation time and the viscosity of the corresponding mode.

Substituting Eq. (5), (6) and (7) into Eq. (8) in place of the partial derivative term, we have the so-called upper convected and the lower convected Maxwell model, and the ZFD model [5]. These are the most simple implicit type of rheological equations of the state.

Our attention is paid particularly to the upper convected Maxwell and the ZFD model because these are building blocks of the most of the complicated, nonlinear and implicit-type of models. In addition, the bulk of the computational work in the past has been performed by employing one of these relatively simple models.

3.2 Definition of Material Functions in a Steady Simple Shear Flow.

Consider the flow of a fluid contained between two parallel plates, the upper one of which moves with constant velocity $v_0$. The velocity profile in the gap is given by

$$v_1 = \dot{\gamma} x_2, \quad v_2 = 0, \quad v_3 = 0$$

(9)
where $\dot{\gamma}$ is a constant shear rate (velocity gradient), with dimensions, 1/sec. This flow is known as steady simple shear flow and is the prototype viscometric flow. The values of differences of normal stress components are not altered by the addition of any isotropic pressure. It is believed that these differences depend on the rheological properties of the material. It follows that there are only three independent stress quantities which completely describe the rheological behavior of the steady simple shear flow: these are

\begin{align*}
\tau_{12} &= \eta(\dot{\gamma}) \dot{\gamma} \quad (10a) \\
\tau_{11} - \tau_{22} &= \psi_1(\dot{\gamma}) \dot{\gamma}^2 \quad (10b) \\
\tau_{22} - \tau_{33} &= \psi_2(\dot{\gamma}) \dot{\gamma}^2 \quad (10c)
\end{align*}

in which subscripts 1, 2, and 3 denote the direction of flow, the direction perpendicular to the flow, and the neutral direction, respectively. In Eq. (10), $\eta(\dot{\gamma})$ defines the shear dependent viscosity, $\psi_1(\dot{\gamma})$ and $\psi_2(\dot{\gamma})$ represents the primary and the secondary normal stress coefficients. $\eta(\dot{\gamma})$, $\psi_1(\dot{\gamma})$ and $\psi_2(\dot{\gamma})$ are called the material functions which depend only on the fluid, not on the particular flow (at given $\dot{\gamma}$).

It is further noted that the stress difference $\tau_{11} - \tau_{33}$ becomes redundant since we have
\[ \tau_{11} + \tau_{22} + \tau_{33} = 0 \]  \hspace{1cm} (11)

which follows from

\[ -P = \frac{1}{3} \text{tr} \ S \]  \hspace{1cm} (12)

and

\[ S = -P I + \tau \]  \hspace{1cm} (13)

where \( S \), \( \tau \), and \( P \) are called a stress tensor, an extra (or deviatoric) stress tensor and an isotropic pressure.

3.3 Definition of the Material Function in the Steady Simple Elongational Flow.

This type of flow is closely approximated in a thin filament of fluid that is being elongated by forces exerted on the two ends: it is sometimes called "uniaxial extensional" or "uniaxial elongational flow." This flow is defined to have only diagonal components of the rate of the deformational tensor and the extra stress tensor such as

\[
\mathbf{D} = \begin{pmatrix}
\varepsilon & 0 & 0 \\
0 & -\frac{\varepsilon}{2} & 0 \\
0 & 0 & -\frac{\varepsilon}{2}
\end{pmatrix}
\]  \hspace{1cm} and  \hspace{1cm}
\[
\tau = \begin{pmatrix}
\tau_{11} & 0 & 0 \\
0 & \tau_{22} & 0 \\
0 & 0 & \tau_{33}
\end{pmatrix}
\]  \hspace{1cm} (14)
In addition, the volume must remain constant,

\[ d_{11} + d_{22} + d_{33} = 0 \]  \hspace{1cm} (15)

and the symmetry condition requires

\[ \tau_{22} = \tau_{33} \]. \hspace{1cm} (16)

Thus, for a steady simple elongational flow, only one normal stress difference can be measured,

\[ \tau_{11} - \tau_{22} = \overline{n}(\dot{\varepsilon}) \dot{\varepsilon} \]. \hspace{1cm} (17)

Here, the quantities, \( \dot{\varepsilon} \) and \( \overline{n} \), are called the elongational rate and the elongational (or Trouton) viscosity. The zero-elongation-rate elongational viscosity \( \overline{n}_0 \) is approximately three times the zero-shear-rate viscosity \( \eta_0 \).

Now, we have defined material functions for steady simple shear and elongational flows. These material functions often provide an effective means of choosing successful constitutive equations because they can be measured experimentally as well as analytically predicted by particular rheological equations of the state. Because of their importance, we want to illustrate the material functions of the upper convected and corotational Maxwell models in the next section in order to observe some inherent characteristics of Maxwell fluids.
3.4 Material Functions of Maxwell Fluids.

Using the definitions given above, material functions of the upper convected Maxwell and of the ZFD fluids can be easily obtained, and are listed on Table 2.

Table 2. Material functions of Maxwell fluids in steady simple flows

<table>
<thead>
<tr>
<th>Constitutive model</th>
<th>Steady shear mat. functs.</th>
<th>Steady elongational viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper convected Maxwell</td>
<td>( n = \eta_0 )</td>
<td>( \bar{n} = \frac{3\eta_0}{(1-2\lambda \dot{\epsilon})(1+\lambda \dot{\epsilon})} )</td>
</tr>
<tr>
<td>( \dot{\gamma} + \lambda_{\dot{\gamma}}^0 = 2\dot{\gamma} )</td>
<td>( \psi_1 = 2\eta_0 \lambda )</td>
<td>( \psi_2 = 0 )</td>
</tr>
<tr>
<td></td>
<td>( \psi_2/\psi_1 = 0 )</td>
<td>( \psi_2/\psi_1 = 0 )</td>
</tr>
</tbody>
</table>

| ZFD                       | \( n = \eta_0/(1+\lambda^2 \dot{\gamma}^2) \) | \( \bar{n} = 3\eta_0 \) |
| \( \dot{\gamma} + \lambda_{\dot{\gamma}}^0 = 2\dot{\gamma} \) | \( \psi_1 = 2\eta_0 \lambda/(1+\lambda^2 \dot{\gamma}^2) \) | \( \psi_2 = -\eta_0 \lambda/(1+\lambda^2 \dot{\gamma}^2) \) |
|                           | \( \psi_2/\psi_1 = -0.5 \) | \( \psi_2/\psi_1 = -0.5 \) |

From Table 2, it is noted that the upper convected Maxwell model shows a constant shear viscosity (i.e., a Newtonian viscosity), shear independent first and zero second normal stress coefficients. It
clearly shows that this fluid cannot predict the shear behavior of most common polymer melts or solutions.

In contrast, the ZFD fluid demonstrates many observed characteristics of a shear flow such as a shear dependent viscosity, shear dependent primary and secondary normal stress coefficients and the negative value of the ratio of the normal stress coefficients although its absolute value is higher than the experimentally observed one. Thus, this fluid may qualitatively allow the prediction of shear behavior of polymer melts.

However, for elongational viscosity predictions for both fluids have defects. For instance, the upper convected Maxwell (UCM) fluid predicts an infinite viscosity at $\lambda = 1/2\dot{\gamma}$, while the ZFD fluid shows a constant elongational viscosity, independent of $\dot{\gamma}$.

Now, we would like to stress a critical view from the standpoint of numerical computation; that is, the material functions in the steady simple flows were derived in order to be compared to existing experimental data from simple flows, not for numerical analysts. Theoreticians who develop rheological constitutive equations of states have paid much attention to fitting their material functions to limited experimental data of polymer melts or solutions, but they have given little consideration to the computational aspects of their use. For example, to test the validity of any constitutive equation in a simple shear flow, the shear viscosity and normal stress differences have been plotted as a dependent variable with the shear rate as an independent variable, and these then compared to plotted curves of experimental data. However, in the computation the shear rate can not be assumed to
behave independently, but rather it is a quantity which has to be evaluated from the constitutive relations. Thus, even though some constitutive equations apparently work well in fitting simple shearing experimental data, it is still possible to say that they may fail to have computational success due to a shear-rate limitation present. As a matter of fact, we have found that several commonly used constitutive equations have serious defects in this regard.

To show this, our analysis begins with the steady viscometric flow of constitutive models in an axisymmetrical geometry. This is a very important subject because viscometric flow profiles are often used as boundary conditions for the die entry and exit problems. If limitations exist in the viscometric flow profiles, they may jeopardize the whole computational endeavor. For an investigation of the elongational flow limitation, please refer to later sections of this thesis, because a two-dimensional or a three-dimensional problem must be solved for a whole domain of the geometry given, particularly in the re-entrant corner region where these elongational flow effects can dominate.
IV. LIMITATION OF THE STEADY VISCOMETRIC FLOW IN DIFFERENTIAL MODELS

Consider an isothermal, isotropic, incompressible and low Reynolds number (pressure-driven) flow of a non-Newtonian fluid in a cylindrical axisymmetric channel. We will introduce the following dimensionless variables:

\[ r^* = \frac{r}{R}, \quad z^* = \frac{z}{R}, \quad \hat{V}^* = \frac{V}{<V_z>}, \]

\[ P^* = \frac{p}{\rho <V_z>^2}, \quad \hat{\tau}^* = \frac{\tau}{\rho R n_0 <V_z>}, \quad \hat{\gamma}^* = \frac{\gamma}{R <V_z>^2}, \quad (18) \]

\[ \text{De} = \frac{\lambda <V_z>}{R} \quad \text{and} \quad \text{Re} = \frac{\rho <V_z> R}{n_0}, \]

where the star sign indicates dimensionless variables, \( <V_z> \) the average axial velocity (cm/sec), \( r \) the radial distance from the center line (cm), \( z \) the axial distance from the inlet (cm), \( V \) the velocity vector (cm/sec), \( P \) the isotropic pressure (dynes/cm\(^2\)), \( \gamma \) the gravitational acceleration vector (cm/sec\(^2\)), \( \rho \) the density (g/cm\(^3\)), \( \tau \) the extra stress tensor (dynes/cm\(^2\)), \( n_0 \) the zero shear viscosity (g/cm·sec), and \( \lambda \) the relaxation time (sec).

Suppressing the star (*) sign, the dimensionless momentum balance equations lead us to,

\[ \frac{D\hat{V}}{Dt} = - \hat{\nabla} P + \frac{1}{\text{Re}} \hat{V} \cdot \hat{\tau} + \hat{\gamma} \]

(19)

where \( D/Dt \) is the material (substantial) derivative and \( \hat{\tau} \) the body force. The usual axisymmetric assumptions eliminate terms which
contain $\tau_{r\theta}$, $\tau_{\theta r}$, $\tau_{\theta z}$, $V_\theta$, and $\partial / \partial \theta$ in Eq. (19). For a pressure-driven
viscometric flow, it is assumed that profiles of velocities and stresses
are only the functions of the radial distance, and the axial pressure
gradient is constant (i.e., $-P_c$). In other words, we have

$$V_z = V_z(r), \quad V_r = 0, \quad \tau_{rr} = \tau_{rr}(r),$$

$$\tau_{rz} = \tau_{rz}(r), \quad \tau_{zz} = \tau_{zz}(r), \quad \tau_{\theta \theta} = \tau_{\theta \theta}(r),$$ (20)

and $\partial P / \partial z = -P_c$.

The above assumptions allow the momentum equation components to
be reduced to

$$\frac{\partial P}{\partial r} = \frac{1}{Re} \left( \frac{d \tau_{rr}}{dr} + \frac{\tau_{rr} - \tau_{\theta \theta}}{r} \right),$$ (21)

$$\frac{\partial P}{\partial z} = \frac{1}{Re} \left( \frac{1}{r} \frac{1}{dr} \frac{d}{dr} \left( r \tau_{rz} \right) \right).$$ (22)

The corresponding boundary conditions are given as

$$\tau_{rr} = \tau_{rz} = 0 \quad \text{at } r = 0$$ (23a)

$$P(0, z_0) = P_0 \quad \text{at } r = 0 \text{ and } z = z_0.$$ (23b)

Now, the assumed constant axial pressure gradient in Eq. (20) can
be expressed as

$$P(r, z) = -P_c z + P(r, z_0)$$

(24)

Thus, Eq. (22) can easily be integrated to obtain the shear stress,

$$\tau_{\theta z} = \frac{1}{2} \text{Re} \left( \frac{\partial P}{\partial z} \right) r = -\frac{1}{2} \text{Re} P_c r$$

(25)

At a given axial location $z_0$, the pressure distribution can be found from Eq. (21), (23) and (24):

$$P(r, z) = P_0 - P_c z + \frac{1}{\text{Re}} \left( \tau_{rr} + \int_0^r \frac{\tau_{rr} - \tau_{\theta \theta}}{r} \, \text{d}r \right)$$

(26)

Based on these results, we claim that some constitutive models are, indeed, shear-limited; that is, only impractically low ranges of shear rate give unique real solutions for velocity fields in spite of their ability to fit experimental simple shearing data quite well. These models include the ZFD, the Phan-Thien and Tanner [54], the Geiseukus [28] and the Leonov [44] constitutive equations. It could be possible that additional models also exhibit this shear limitation.

4.1 ZFD Fluid.

With a single relaxation time $\lambda$, the dimensionless ZFD model may be written in dimensionless form as:

$$\mathbf{I} + \text{De} \left( \frac{\mathbf{D}_T}{\text{Dt}} - \mathbf{\omega} \cdot \mathbf{I} - \mathbf{I} \cdot \mathbf{\omega} + \mathbf{T} \right) = 2 \mathbf{D}$$

(27)
where $\omega$ is the vorticity tensor (responsible for rotation) and $\mathbb{D}$ is the rate of the deformation tensor (responsible for stretching), defined as

\begin{align}
\omega &= (\nabla \cdot \mathbf{V} - (\nabla \cdot \mathbf{V})^T)/2, \quad (28a) \\
\mathbb{D} &= (\nabla \cdot \mathbf{V} + (\nabla \cdot \mathbf{V})^T)/2, \quad (28b) \\
\mathbb{L} &= \omega + \mathbb{D} = \nabla \cdot \mathbf{V}. \quad (28c)
\end{align}

Here, $\mathbb{L}$ is called the velocity gradient tensor.

For the axisymmetrically viscometric flow defined as in Eq. (20), equations (27) reduce to,

\begin{align}
\tau_{rr} + \text{De}V_z, r \tau_{rz} &= 0 \quad (29a) \\
\tau_{rz} + \text{De}(\tau_{zz} - \tau_{rr}) V_z, r/2 &= V_z, r \quad (29b) \\
\tau_{zz} - \text{De} V_z, r \tau_{rz} &= 0 \quad (29c) \\
\tau_{\theta\theta} &= 0 \quad (29d)
\end{align}

in which the comma indicates differentiation with respect to those variables which follows. Algebraic manipulation of Eq. (29) allows one to derive
\[ V_{z,r} = \frac{1 - \sqrt{1 - 4D\epsilon \tau_{rz}^2}}{2D\epsilon \tau_{rz}} \]  

\[ \tau_{rr} = -D\epsilon \mu V_{z,r} \tau_{rz} \]  

\[ \tau_{zz} = -\tau_{rr}; \quad \tau_{\theta \theta} = 0. \]  

Thus, complete viscometric flow profiles are determined from Eqs. (25), (26) and (30). These profiles can be used as boundary conditions for the axisymmetric die-entry and die-exit problems in numerical simulations. It is noted from Eq. (30) that there is a limitation in evaluating the axial velocity gradient; that is, 

\[ D\epsilon |\tau_{rz}| < 0.5 \]  

must be satisfied to allow for a real value in the square root term. Since \( D\epsilon \) and \( \tau_{rz} \) represent the elastic and shear forces, these forces are competing with each other and never allow both values to be large at the same time. For instance, a highly elastic flow (say, \( D\epsilon = 10 \)) reduces the maximum realizable value of the shear stress for real solutions to \( |\tau_{rz}| < 0.05 \). Unfortunately, this shear stress range is much too low for prediction of polymer melt or solution flows in the realistic situations.

Now, we will study the influence of a retardation term on the above limitation. If one adds a retardation term to the ZFD model, it turns out to generate the corotational Jeffreys model, i.e.,
\[ \mathbf{I} + \lambda_1 \mathbf{D} = 2\eta_0 (\mathbf{D} + \lambda_2 \mathbf{D}) \]  

(32)

where \( \mathbf{D} \) is the Jaumann derivative defined by Eq. (7). The dimensionless form for pressure driven viscometric pipe flow, we will have, similar to Eq. (29),

\[ \tau_{rr} + D_1 V_{z,r} \tau_{rz} = D_2 V_{z,r}^2 \]  

(33a)

\[ \tau_{rz} + D_1 (\tau_{zz} - \tau_{rr})V_{z,r}/2 = V_{z,r} \]  

(33b)

\[ \tau_{zz} - D_1 V_{z,r} \tau_{rz} = -D_2 V_{z,r}^2 \]  

(33c)

where \( D_1 = \lambda_1 \langle V_z \rangle/R \) and \( D_2 = \lambda_2 \langle V_z \rangle/R \). Rewriting the above equation gives us,

\[ - D_1 D_2 V_{z,r}^3 + D_1 D_1 V_{z,r}^2 V_{z,r} - V_{z,r} + \tau_{rz} = 0 \]  

(34a)

\[ \tau_{rr} = - (D_1 \tau_{rz} - D_2 V_{z,r})V_{z,r} \]  

(34b)

\[ \tau_{zz} = - \tau_{rr} \]  

(34c)

Here replace \( V_{z,r} \) in Eq. (34a) by \( x + \frac{D_1 \tau_{rz}}{2D_2} \), which results in an equation of the form

\[ x^3 + ax + b = 0 \]

where
\[ a = \frac{1}{D_1 D_2} - \frac{D_1^2 \tau_{rz}}{3D_2^2} \]

and

\[ b = -\frac{2D_1^3 \tau_{rz}}{27D_2^3} + \frac{\tau_{rz}}{3D_2^2} - \frac{\tau_{rz}}{D_1 D_2} \cdot \]

Three different root conditions for the above equations are found from the CRC standard math table. These are

\[ \frac{b^2}{4} + \frac{a^3}{27} > 0; \text{ for one real root and two conjugate imaginary roots} \]

\[ \frac{b^2}{4} + \frac{a^3}{27} = 0; \text{ for three real roots of which at least two are equal} \]

\[ \frac{b^2}{4} + \frac{a^3}{27} < 0; \text{ for three real and unequal roots.} \]

However, only one real root for \( x \) will provide a physically meaningful solution to the viscometric flow. Note that if the ratio of the retardation time to the relaxation time approaches a higher value, the flow becomes closer to Newtonian and the first condition is always satisfied. This indicates that the first criterion gives a stable root condition. Thus,

\[ \left[ -\left(\frac{D_1 \tau_{rz}}{3}\right)^3 + \frac{1}{6} (\frac{1}{2} - \frac{\gamma}{2}) D_2 \tau_{rz}\right]^2 + \left[ \frac{\gamma}{3} - \left(\frac{D_1 \tau_{rz}}{3}\right)^2 \right]^2 > 0 \]

where \( \gamma = \frac{D_2}{D_1} = \frac{\lambda_2}{\lambda_1} \).

The above inequality may be expressed in a simplified form for any finite values of \( D_1, D_2 \) and \( \tau_{rz} \) as;
\[ \gamma > \frac{1}{3} \text{ or } \text{De}_2 > \frac{1}{3} \text{De}_1. \]

This demonstrates that there exists a possibility of avoiding the shear limitation by adding a proper retardation time to the original constitutive model.

For computational purpose, another way of introducing the retardation term is to follow the work of Crochet and Keunings [22]. They have insisted that Eq. (32) is essentially the same as the following set of equations:

\[ \mathbb{I} = \mathbb{I}_1 + \mathbb{I}_2 \]  
(35a)

\[ \mathbb{I}_1 + \lambda_1 \frac{\partial}{\partial t} = 2 \eta_0 \mathbf{D} \]  
(35b)

\[ \mathbb{I}_2 = 2 \eta_0 \mathbf{D}. \]  
(35c)

A physical interpretation of the decomposition (35) holds for polymer solutions where \( \mathbb{I}_2 \) may be thought of as the Newtonian solvent contribution to the stress tensor while \( \mathbb{I}_1 \) is the polymer contribution. To show the identity of Eq. (32) and (35), they have started by calculating the Jaumann derivative of Eq. (35c) as

\[ \lambda_1 \frac{\partial}{\partial t} \mathbb{I}_2 = 2 \lambda_1 \eta_0 \frac{\partial}{\partial t} \mathbf{D}. \]  
(36)

By summing (35b), (35c) and (36), the original equation (32) is obtained:
\[ \mathfrak{I} + \lambda_0 \mathfrak{o}_0 = 2 \eta_0 (\mathfrak{D} + \lambda_2 \mathfrak{D}) \]

with

\[ \eta_0 = \eta_0^1 + \eta_0^2 \]

\[ \lambda_2 = \lambda_1 \eta_0^2 / \eta_0 \]

4.2 Phan-Thien and Tanner Network Model.

Macromolecules in polymeric liquids may interact with each other locally to break and reform the network junctions continually during the flow. The Cauchy stress tensor is assumed to depend on the history of the deformation of this network. Treating the rate of interaction of junctions on a manner similar to Boltzmann's kinetic theory of gases, Phan-Thien and Tanner [54] and Phan-Thien [55] have derived the following constitutive equations including the possibility of a nonaffine transformation of the entanglement point velocity with respect to the equivalent continuum velocity;

\[ \mathfrak{I} = \sum_i \mathfrak{I}_i \]

\[ K(\text{tr}\, \mathfrak{I}_i) \mathfrak{I}_i + \lambda_1 \left( \frac{D \mathfrak{I}_i}{Dt} - \mathfrak{C}_i \cdot \mathfrak{I}_i - \mathfrak{I}_i \cdot \mathfrak{C}_i^T \right) = 2 \eta_0 \mathfrak{D} \]

or using another expression,

\[ K(\text{tr}\, \mathfrak{I}_i) \mathfrak{I}_i + \lambda_1 [ (1 - \xi/2) \mathfrak{D} + (\xi/2) \mathfrak{D}^T ] = 2 \eta_0 \mathfrak{D} \]
where $\xi^i = \frac{1}{\lambda} - \xi^D$ is the effective velocity gradient and $\xi$ represents a measure of the deformation-induced slip between the network and the continuum (the recommended value is $0.1 \sim 0.2$). Phan-Thien and Tanner [54] have defined $K$ as,

$$K(\text{tr}^i) = 1 + \frac{\epsilon^i}{G^i} \text{tr}^i,$$  \hspace{2cm}(38)

while Phan-Thien [55] has used,

$$K(\text{tr}^i) = \exp\left(\frac{\epsilon^i}{G^i} \text{tr}^i\right),$$  \hspace{2cm}(39)

where $\epsilon^i$ is a parameter (the recommended value is $0.01 \sim 0.015$) which has the effects of controlling the infinite elongational viscosity and $G^i$ is a relaxation (rigidity) modulus. Equation (37) has several special cases which are shown in Table 3.

<table>
<thead>
<tr>
<th>Model</th>
<th>$\lambda$</th>
<th>$\xi$</th>
<th>$\epsilon^i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Johnson-Segalman [35]</td>
<td>$&gt;0$</td>
<td>$&gt;0$</td>
<td>0</td>
</tr>
<tr>
<td>Upper convected Maxwell</td>
<td>$&gt;0$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Newtonian</td>
<td>0</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

The material functions in a simple shear flow have been shown by Phan-Thien and Tanner [54] as
\[ n = \sum_{i} \frac{G_i \lambda^i}{1 + \xi(2-\xi)(\lambda_i^+)^2} + O(\varepsilon') \]  
(40a)

\[ N_1 = 2 \sum_{i} \frac{\xi^i (\lambda_i^+)^2}{1 + \xi(2-\xi)(\lambda_i^+)^2} + O(\varepsilon') \]  
(40b)

\[ N_2 = -\xi N_1/2 \]  
(40c)

where \( N_1 \) and \( N_2 \) are the normal stress differences. The elongational viscosity versus Deborah number (or \( \lambda^+ \)) has been derived by the work of Keunings and Crochet [39]. Phan-Thien and Tanner have claimed that these material functions fit available experimental data qualitatively as well as quantitatively. In spite of this limited agreement in simple shearing flows, we have found that this model also involves the same origin of the computational problem in pipe flows as in the ZFD model—low shear limitation.

For a single relaxation time, \( \lambda \), the usual steady viscometric assumption in the axisymmetric channel reduces Eq. (37) to

\[ K(\tau_{rz})\tau_{rr} + De\xi \tau_{rz} V_z, r = 0 \]  
(41a)

\[ K(\tau_{rz})\tau_{rz} - De(1 - \xi/2)\tau_{rr} V_z, r + De(\xi/2)\tau_{zz} V_z, r = V_z, r \]  
(41b)

\[ K(\tau_{rz})\tau_{zz} - De(2-\xi)\tau_{rz} V_z, r = 0 \]  
(41c)

\[ \tau_{\theta\theta} = 0 \]  
(41d)
Solve for $V_{zr}$, $\tau_{zz}$ and $\tau_{rr}$:

$$V_{zr} = \frac{K(t_{r^z})(1 - \sqrt{1 - 4\xi \varepsilon(2 - \xi)}\tau_{rz}^2}{2\xi \varepsilon(2 - \xi)\tau_{rz}}$$  \hspace{1cm} (42a)$$

$$\tau_{zz} = \frac{1 - \sqrt{1 - 4\xi \varepsilon(2 - \xi)}\tau_{rz}^2}{2\xi \varepsilon \xi}$$  \hspace{1cm} (42b)$$

$$\tau_{rr} = -\frac{\xi}{2 - \xi} \tau_{zz}$$  \hspace{1cm} (42c)$$

It is clear that this model inherently contains the shear limitation of

$$\sqrt{\xi(2 - \xi) \xi} \left| \tau_{rz} \right| < 0.5.$$  \hspace{1cm} (43)$$

Crochet and Bezy [19] have employed the Phan-Thien and Tanner fluid in simulating the 4:1 contraction die-entry problem. They have reported that numerical failure has occurred at $\text{De} = 1.15$ for unknown reasons. We believe that their numerical breakdown is due to the above shear limitation.

Recently, Keunings and Crochet [39] have included the retardation in the Phan-Thien and Tanner fluid by under the consideration of the Oldroyd 8-constant model to increase the shear range of solution. This effort has also failed at a slightly higher Deborah number, $\text{De} = 1.76$,.
compared to the model without the retardation. The same conclusion can be drawn about the cause of this failure. They have used the following constitutive equations,

\[ k(\tau_{zz})_{z} + \lambda_{1} [(1-\xi/2)^{\frac{v}{2}} + (\xi/2)^{\frac{A}{2}}] = 2\eta_{0} [D + \lambda_{2}(1-\xi/2)^{\frac{V}{2}} + \lambda_{2}(\xi/2)^{\frac{A}{2}}] \]

with

\[ 9\lambda_{2}\xi(2-\xi) > \lambda_{1}\xi(2-\xi) > 0. \] (44b)

The axisymmetric and viscometric shear flow assumptions can reduce equations (44) to

\[ k\tau_{rr} + D_{e_{1}}\xi\tau_{rz} V_{z,r} = D_{e_{2}}\xi V_{z,r}^{2} \]

\[ k\tau_{rz} - D_{e_{1}}(1 - \xi/2)^{\frac{v}{2}} \tau_{rr} V_{z,r} + D_{e_{2}}\xi^{2} \tau_{zz} V_{z,r} = V_{z,r} \]

\[ k\tau_{zz} - D_{e_{1}}(2 - \xi)^{\frac{v}{2}} \tau_{rz} V_{z,r} = -D_{e_{2}}(2 - \xi) V_{z,r}^{2} \]

\[ \tau_{\theta\theta} = 0 \]

Here, \( k(\tau_{zz}) \) is assumed to be unity, which is not a bad assumption for viscometric shear flow. An explicit formulation for the variables gives rise to

\[ V_{z,r}^{3} - \frac{D_{e_{1}}\tau_{rz}}{D_{e_{2}}} V_{z,r}^{2} + \frac{V_{z,r}}{D_{e_{1}}D_{e_{2}}\xi(2-\xi)} - \frac{\tau_{rz}}{D_{e_{1}}D_{e_{2}}} = 0 \]
\[
\tau_{zz} = \text{De}_1 (2-\xi) \tau_{rz} V_{z,r} - \text{De}_2 (2-\xi) V_{z,r}^2 \\
\tau_{rr} = -\frac{\xi}{2-\xi} \tau_{zz}; \quad \tau_{\theta\theta} = 0.
\]

For a single real value of \( V_{z,r} \) in the above equation, the following inequality must be satisfied, as with the ZFD model;

\[
\left[ -\left( \frac{\text{De}_1 \tau_{rz}}{3} \right)^3 + \left( \frac{1}{6} - \frac{\gamma}{2} \right) \frac{\text{De}_2 \tau_{rz}}{\xi(2-\xi)} \right]^2 + \left[ -\left( \frac{\tau_{rz}}{3} \right)^2 + \frac{\gamma}{3\xi(2-\xi)} \right]^3 > 0
\]

It is obvious that this inequality may imply

\[
\gamma > \frac{1}{3} \quad \text{or} \quad \text{De}_2 > \frac{1}{3} \text{De}_1.
\]

Keunings and Crochet [39], have used \( \gamma = 1/8 \) in their simulation. As shown above, the one real root condition is likely not to be satisfied for relatively high values of \( \text{De}_1 \) or \( \text{De}_2 \) at this \( \gamma \) value. We do not know what is happening in the solution field when the multiple solutions are encountered due to the small \( \gamma \) value, \( \gamma < 1/3 \), but it is strongly suspected that this may cause the numerical failure.

Now, for an easier implementation, equations (44) may be decomposed as given below:

\[
\mathcal{I} = \mathcal{I}_1 + \mathcal{I}_2 \quad \text{(45a)}
\]

\[
K(\tau_{rz}) \mathcal{I}_1 + \lambda_1 \left[ (1-\xi/2) \mathcal{I}_1 + (\xi/2) \mathcal{I}_2 \right] = 2\tau_{10} \quad \text{(45b)}
\]
\[ I_2 = 2n_0^2 \tilde{\Omega} \]  \hspace{1cm} (45c)

with

\[ n_0^2 = n_0 \lambda_2 / \lambda_1, \quad n_0 = n_0^1 + n_0^2 \text{ and } 8n_0^2 > n_0^1. \]  \hspace{1cm} (45d)

It is noted that by putting \( \xi = 0 \) in Eq. (37) and (44), one can eliminate the problem of the low shear limit, but this leads to the upper convected Maxwell (UCM) and Oldroyd fluid-B type models.

4.3 Giesekus Model.

The dimensionless form of the Giesekus fluid [28] is written as

\[
(\tilde{\sigma} + \alpha D_{1}\tilde{\eta}) \cdot \tilde{\eta} + D_{1} \frac{\tilde{\nabla} \cdot \tilde{V}}{\tilde{\eta}} = 2(\tilde{D} + D_{2}\tilde{\nabla} \cdot \tilde{V}) \]  \hspace{1cm} (46)

where \( D_{1} \) is the dimensionless relaxation time, \( D_{2} \) the dimensionless retardation time, \( \tilde{\sigma} \) the unit tensor and \( \alpha \) is the dimensionless Giesekus mobility ratio (\( \alpha = \theta \eta_0 : \theta = \) the Giesekus mobility ratio, cm·sec/g).

The following special cases can be derived from this model, as shown in Table 4.
Table 4. Special cases of Gieseikus model.

<table>
<thead>
<tr>
<th>Constitutive equation</th>
<th>$D_{e1}$</th>
<th>$D_{e2}$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Newtonian (NEW)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Upper convected Maxwell (UCM)</td>
<td>$D_{e1}&gt;0$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Leonov-like (LEL)</td>
<td>$D_{e1}&gt;0$</td>
<td>0</td>
<td>$1/2$</td>
</tr>
<tr>
<td>Corotational Maxwell-like (CML)</td>
<td>$D_{e1}&gt;0$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Second-order fluid (SOF)</td>
<td>0</td>
<td>$D_{e2}&lt;0$</td>
<td>-</td>
</tr>
<tr>
<td>Oldroyd-B (OLD)</td>
<td>$D_{e1}&gt;0$</td>
<td>$D_{e2}&gt;0$</td>
<td>0</td>
</tr>
</tbody>
</table>

The viscometric material functions for each model plotted by Beris et al. [2] are shown in Fig. 2. The most interesting one as far as the material functions are concerned is the Leonov-like model in which a shear thinning of the viscosity and the first normal stress difference coefficient is predicted (in agreement with most experimental data), and also the elongational viscosity approaches to an asymptotic limit of $\bar{\eta} = 4\eta_0$ at high elongational rates starting from $\bar{\eta}_0 = 3\eta_0$ initially. It is recognized that the full Gieseikus model has one additional retardation term when compared to this Leonov-like model.

The steady shear pipe flow viscometric equations for the Leonov-like model are,

\[
\alpha D_1 \frac{\partial^2 \tau_{rr}}{\partial r^2} + \tau_{rr} + \alpha D_2 \frac{\partial^2 \tau_{rz}}{\partial r \partial z} = 0 \quad (47a)
\]

\[
\alpha D_1 \frac{\partial^2 \tau_{zz}}{\partial z^2} + \tau_{zz} + \alpha D_2 \frac{\partial^2 \tau_{rz}}{\partial r \partial z} - 2\alpha V_z \tau_{rz} = 0 \quad (47b)
\]
Figure 2. Material functions for six limits of the Giesekus model listed in Table 4. All quantities are dimensional.
\[ \tau_{rz} (1 + \alpha \text{De}(\tau_{rr} + \tau_{zz})) - (\text{De}\tau_{rr} + 1) V_{z,r} = 0 \]  \hspace{1cm} (47c)\\
\[ \alpha \text{De}\tau_{\theta\theta} + \tau_{\theta\theta} = 0 \]  \hspace{1cm} (47d)

Explicit equations for \( \tau_{rr}, \tau_{zz}, \) and \( V_{z,r} \) are given as,

\[ \tau_{rr} = \frac{-1 + \sqrt{1 - 4\alpha^2 \text{De}\tau_{rz}^2}}{2\alpha \text{De}} \]  \hspace{1cm} (48a)

\[ \tau_{zz} = \frac{-1 + \sqrt{(1 + \text{De}\tau_{rr} - 2\alpha \text{De}\tau_{rz}^2)\sqrt{(1 + \text{De}\tau_{rr} - 2\alpha \text{De}\tau_{rz}^2)^2 + 4\alpha \text{De}\tau_{rz}^2 (\text{De}\tau_{rr} + 1)(2 - \alpha + \alpha \text{De}\tau_{rr})}}}{2\alpha \text{De}(\text{De}\tau_{rr} + 1)} \]  \hspace{1cm} (48b)

\[ V_{z,r} = \frac{(1 + \alpha \text{De}(\tau_{rr} + \tau_{zz})) \tau_{rz}}{\text{De}\tau_{rr} + 1} \]  \hspace{1cm} (48c)

\[ \tau_{\theta\theta} = 0 \]  \hspace{1cm} (48d)

with \( \alpha = 1/2 \). Thus, this model also has the limitation in estimating \( \tau_{rr} \) in Eq. (48a); that is,

\[ \alpha \text{De}|\tau_{rz}| < 0.5. \]  \hspace{1cm} (49)

Adding the retardation term does not change this limit at all. It is not like other models which we have seen before, because Eq. (47a) and (48a) remain unchanged under the addition of the retardation term. So, we can conclude that this limitation is an inherent feature of the
Giesekus fluid itself.

Beris et al. [2] have used the Leonov-like model in computing the journal bearing problem in which no sharp geometrical singularities have been present. They have found that the upper convected Maxwell model has generated severe spurious oscillations before the numerical breakdown, but the Leonov-like model, unlike the UCM model, has not shown any sign of oscillations before the numeral instability. We conclude that this observation may be due to the above limitation of Eq. (49).

4.4 Leonov Model.

Leonov et al. [44, 45, 46] have proposed a differential constitutive equation based on heuristic thermodynamic arguments; that is, for a single mode,

\[ \dot{\mathbf{C}} + \frac{1}{2\lambda} (\mathbf{C} \cdot \mathbf{C} - \mathbf{I} + \frac{1}{3} (\text{tr} \mathbf{C}^{-1} - \text{tr} \mathbf{C}) \mathbf{I}) = 0 \]  

(50a)

\[ \mathbf{I} = \frac{n_0}{\lambda} (\mathbf{C} - \mathbf{I}), \]  

(50b)

where \( \mathbf{C}, \mathbf{C}^{-1} \) and \( \mathbf{I} \) are the Cauchy-Green deformation tensor, the Finger deformation tensor and the unit tensor, respectively.

Consider the steady viscometric shearing flow which has the velocity field of the form,

\[ v_r = 0, \quad v_z = f(r), \quad v_{\theta} = 0. \]  

(51)
The relative deformation function $x'(t')$ can be found by solving the differential equations

$$\frac{dr'}{dt'} = 0, \quad \frac{dz'}{dt'} = f(r), \quad \frac{d\theta'}{dt'} = 0 \quad (52)$$

with initial conditions

$$x'(t')|_{t' = t} = x(t) = [r, z, \theta]^T \quad (53)$$

which gives rise to

$$r'(t') = r, \quad z' = z + (t' - t) f(r), \quad \theta' = \theta \quad (54)$$

Since

$$\frac{dx'(t')}{dt'} = F_{xt}(t') \cdot dx(t), \quad (55)$$

the relative deformation gradient tensor $F_{xt}(t')$ may be obtained as

$$F_{xt}(t') = \begin{bmatrix}
-1 & 0 & 0 \\
(t' - t)f'(r) & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} \quad (56)$$

where $f'(r) = df(r)/dr$. By the definition, we evaluate the Cauchy-Green tensor,
\[
\mathbf{C}_\pm(t', \tau) = \mathbf{F}_\pm^T(t', \tau) \cdot \mathbf{F}_\pm(t', \tau) = \begin{bmatrix}
-1+(t'-t)^2f', 2 & (t'-t)f' & 0 \\
(t'-t)f' & 1 & 0 \\
0 & 0 & 1
\end{bmatrix},
\]

(57)

and the Finger tensor,

\[
\mathbf{C}_\pm^{-1}(t', \tau) = \begin{bmatrix}
1 & -(t'-t)f' & 0 \\
-(t'-t)f' & 1+(t'-t)^2f', 2 & 0 \\
0 & 0 & 1
\end{bmatrix}.
\]

(58)

Now, it is clear that from Eqs. (57) and (58),

\[
\text{tr} \mathbf{C}_\pm = \text{tr} \mathbf{C}_\pm^{-1}.
\]

(59)

Thus, Eq. (50a) can be simplified to

\[
\mathbf{\Gamma} + \frac{1}{2\lambda}[\mathbf{C}_+ \cdot \mathbf{C}_- - \mathbf{\delta}] = 0.
\]

(60)

Substituting Eq. (50b) into Eq. (60) and knowing that

\[
\mathbf{\Gamma}_\delta = -2\mathbf{D},
\]

(61)

we find, in the dimensionless form,

\[
(\mathbf{\delta} + \frac{\mathbf{D}e_1}{2}) \cdot \tau + \mathbf{D}_\tau = 2\mathbf{D}
\]

(62)
which is the exactly same form of the Leonov-like model of the Giesekus fluid in the previous section. Hence, the same restriction is imposed for the Leonov model, i.e.,

$$\text{De} \left| \tau_{rz} \right| < 1.0 \ .$$

(63)

In summary, Table 5 lists the limiting expressions in pipe flows for several models which we have investigated in this chapter.

Table 5. Limitation of differential models in the viscometric pipe flow.

| Model                  | \(^\hat{\alpha} \text{De} | \tau_{rz} | < 0.5 |
|------------------------|-----------------------------|
| Corrotational Maxwell (ZFD) | \(^\hat{\alpha} = 1\)       |
| Phan-Thien and Tanner [54] | \(^\hat{\alpha} = \sqrt{\xi(2-\xi)}\) |
| Giesekus [28]          | \(^\hat{\alpha} = \alpha\)  |
| Leonov [44, 45, 46]    | \(^\hat{\alpha} = 0.5\)     |

Two notable points demand our particular attention from the above table. First, the limiting parameter \(^\hat{\alpha}\) seems to be a relative indication of involvement of the corrotational derivative to any particular model. For instance, \(^\hat{\alpha} = 1\) or \(^\hat{\alpha} = 0\) indicates either full or no involvement. Note that when \(\hat{\alpha}\) equals zero (i.e., \(\xi = 0\) or \(\alpha = 0\)), the Phan-Thien & Tanner and Giesekus models become the upper convected Maxwell-like models. So, we conclude that the shear limitation shown
relates directly to the inherent nature of the corotational (Jaumann) derivative itself.

Second, the upper bound of Deborah number convergence in the numerical computation is totally dependent on specification of the value of the shear stress $\tau_{rz}$ which, in turn, is determined by the Reynolds number (Re) and the axial pressure gradient as can be seen from Eq. (25). Only extremely low shear stresses allow calculations with highly elastic melts. This is not a practical situation for industrially important contraction or expansion flows.
V. SIMULATION OF THE EXTRUSION DIE-ENTRY

In the extrusion die-entry region, one may observe three types of flow fields. One is the steady viscometric pipe shear-flow field of the upstream and the downstream which we have already explored in the previous chapter. Another is the nearly shear-free elongational flow field in the region of the center axis. The remainder is formed by the combination of the two, and depends on the contraction ratio and geometric location of the material point of interest. Investigation of the latter two flow fields involve solving the full equations over the whole domain of our interest. By computational results obtained in this simulation, we will show how the nature of the infinite elongational viscosity predicted by some differential models gives rise to another possible numerical difficulty. For this purpose, the mixed finite element method is employed as our computational tool.

5.1 Problem Definition.

Consider a non-Newtonian fluid flowing through the axisymmetric channel with a sudden contraction shown in Figure 3.

![Figure 3. Schematic diagram of the axisymmetric die-entry region.](image-url)
A typical problem of this kind is found near the die-entry region. An incompressible and homogeneous fluid is assumed with pressure driven flow. It is also assumed to be an isothermal flow which remains at its steady state (that is, we neglect viscous dissipation and assume all surfaces are at the melt temperature). To predict such flow behavior numerically over the geometrical domain \((\Omega)\), Phan-Thien fluid [55] is adopted as our non-Newtonian constitutive equation. This constitutive model, together with momentum and continuity equations compose the total set of equations to be solved. These are expressed in a dimensionless tensor notation as,

\[
\exp(c'Det\tau) = -c'D \left[ \frac{\partial \tau}{\partial t} - \frac{\xi}{2} (\tau : \tau + \frac{\tau^T \tau}{3}) \right] + \left( \frac{\xi}{2} \right) (\tau : \tau + \frac{\tau^T \tau}{3}) = 2\Omega,
\]

(64a)

\[
\frac{DV}{Dt} = -Vp + \frac{1}{Re} V\tau + q*,
\]

(64b)

\[
V\cdot V = 0.
\]

(64c)

Corresponding boundary conditions are given as,

\[
\tau = \tau(r,0), \quad V = V(r,0), \quad P = P(r,0) \quad \text{on} \quad (r,z) \in \partial\Omega_{r1}
\]

(65a)

\[
V = V(r,L) \quad \text{on} \quad (r,z) \in \partial\Omega_{r2}
\]

(65b)

\[
V = V(R,z) = 0 \quad \text{on} \quad (r,z) \in \partial\Omega_{r1}
\]

(65c)

\[
V_r = \tau_{rz} = 0 \quad \text{on} \quad (r,z) \in \partial\Omega_{r2}
\]

(65d)
Expressing these in component tensor notation, one has

\[
\exp(e' De \tau_{kk}) \tau_i = \text{De}[V_k \tau_{ij,k} + (1 - \frac{\xi}{2})(V_i,k \tau_{kj} + \tau_{ik} V_j,k)] + (\frac{\xi}{2})(\tau_{ik} V_k,j + V_{k,i} \tau_{kj}) - (V_i,j + V_{j,i}) = 0, \quad (66a)
\]

\[
V_k V_{i,k} + p_{i} - \frac{1}{\text{Re} \tau_{ik,k}} - g_i = 0, \quad (66b)
\]

\[
V_{k,k} = 0 \quad (66c)
\]

with boundary conditions of

\[
\tau_{ij} = \tau_{ij}(r,0), \quad V_i = V_i(r,0), \quad P = P(r,0) \quad \text{on} \quad (r,z) \in \partial \Omega_{z1} \quad (67a)
\]

\[
V_i = V_i(r,L) \quad \text{on} \quad (r,z) \in \partial \Omega_{z2} \quad (67b)
\]

\[
V_i = V_i(R,z) = 0 \quad \text{on} \quad (r,z) \in \partial \Omega_{z1} \quad (67c)
\]

\[
V_r = \tau_{rz} = 0 \quad \text{on} \quad (r,z) \in \partial \Omega_{z2} \quad (67d)
\]

The reason for choosing the above boundary conditions becomes clear later when we formulate the Galerkin weak solutions of the given equations.
5.2 Boundary Conditions.

We have derived the viscometric flow profiles of the Phan-Thien fluid for a cylindrical axisymmetric channel as shown in Eqs. (25), (26) and (42). Detailed analytical expressions are given in Table 6.

Table 6. Viscometric flow profiles of the Phan-Thien model for a cylindrical axisymmetric channel.

<table>
<thead>
<tr>
<th>Model</th>
<th>Profiles of velocities, extra-stresses and a pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phan-Thien</td>
<td>( \frac{\partial P}{\partial z} = -P_c; \tau_{\theta \theta} = V_{r} = 0 )</td>
</tr>
</tbody>
</table>

\[
P(r,z) = P_0 - P_c z + [-1 + f(r) + \frac{1}{2} \ln(\frac{2}{1+f(r)})]/[(2-\xi)\text{DeRe}]
\]

\[
\tau_{rz}(r) = \frac{1}{2} \text{Re} \left( \frac{\partial P}{\partial z} \right) \frac{1}{2} \quad \tau_{zz}(r) = \frac{1-[1-f(r)]}{(2\xi \text{De})}
\]

\[
\tau_{rr}(r) = -\xi \tau_{zz}(r)/(2-\xi)
\]

\[
V_z(r) = e^a \left[ (e^{-f(r)} - e^{-f(R)})/a + e^a \left[ \ln \left( \frac{1+f(r)}{1-f(R)} \right) \right] \right.
\]

\[
- \frac{a[(1+f(r))-1+f(R)]}{1+1!} + \frac{a^2[(1+f(r))^2 - (1+f(R))^2]}{2+2!} - \frac{a^3[(1+f(r))^3 - (1+f(R))^3]}{3+3!} + \ldots \right) / (\xi(2-\xi)\text{ReDe}(\frac{\partial P}{\partial z})}
\]

where \( a = \epsilon'(1-\xi)/\xi(2-\xi) \) and \( f(r) = [1-4\xi(2-\xi)\text{De} \tau_{rz}]^{1/2} \).
Note that above viscometric flow profiles will be valid in both boundaries of the reservoir \( (\partial \Omega_{z1}) \) and the capillary section \( (\partial \Omega_{z2}) \) as long as the correct shear stress (or, the correct axial pressure gradient at a fixed Reynolds number) in each location is used. Of course, different values of pressure gradients (thus, shear stresses) depending on the upstream and the downstream locations will be used due to the difference in cross-sectional areas. One way of finding consistent pressure gradients is to impose a mass balance between the two locations. Assuming a constant density, the mass balance relates the average velocity of the reservoir (indicated by the subscript \( r \)) to that of the capillary (denoted by the subscript \( c \)) on the boundaries as follows:

\[
<V_z>^c = <V_z>^r \cdot \left( \frac{R_r}{R_c} \right)^2
\]

\[
= <V_z>^r \cdot \text{(contraction ratio)}^2
\]

where \( <V_z> \) represents the average axial velocity defined by

\[
<V_z> = \frac{\int_0^R v_z \cdot rdr}{\int_0^R rdr}.
\]

For a given axial pressure gradient in the reservoir section, one can compute the axial velocity from the Table 6. Then, the average velocity, \( <V_z>^r \), can be evaluated from Eq. (69). So does \( <V_z>^c \) from Eq. (68), provided that the contraction ratio is known for the given
geometry. Now, one can guess the axial pressure gradient of the capillary tube arbitrarily to estimate a corresponding \( \langle V_Z \rangle_C^* \) by the same procedure and check how closely the guessed \( \langle V_Z \rangle_C^* \) approaches to the exact \( \langle V_Z \rangle_C \) estimated. If an error criterion

\[
|\langle V_Z \rangle_C - \langle V_Z \rangle_C^*| < \varepsilon
\]

(70)

is met for a small prescribed \( \varepsilon \), then corresponding velocities, extra-stresses, and the pressure can be found in the downstream section by the help of the assumed pressure gradient and Table 5. If the error criterion is not satisfied, another pressure gradient is chosen and the iteration continues until a satisfactory convergence criterion is attained.

To accelerate this process, an efficient secant method is going to be introduced. That is, for a given equation \( f(x) = 0 \), the Newton-Raphson method in solving a nonlinear equation is given by

\[
X_i = X_{i-1} - \frac{f(X_{i-1})}{f'(X_{i-1})}.
\]

(71)

Since \( f'(X_{i-1}) \) is not known in our problem, \( f'(X_{i-1}) \) is approximated as

\[
f'(X_{i-1}) = \frac{f(X_{i-1}) - f(X_{i-2})}{X_{i-1} - X_{i-2}},
\]

(72)

which is known as the secant method. Combining Eqs. (71) and (72), one obtains the following form:
\[ x_i = x_{i-1} - \frac{f(x_{i-1}) * (x_{i-1} - x_{i-2})}{f(x_{i-1}) - f(x_{i-2})} \]  

(73)

For most cases, 4 or 5 iterations are sufficient to give a converged solution with the error tolerance \( \epsilon = 10^{-12} \), if two initial starting guesses for \( X_0 \) and \( X_1 \) are selected as \((0.85)(\partial P/\partial z)_{r}(\text{cont. ratio})^{4} \) and \((0.95)(\partial P/\partial z)_{r}(\text{cont. ratio})^{4} \). In this case \( \chi \) corresponds to the pressure gradient at the capillary section and \( f(x) \) is equal to \( \langle V^2 \rangle_c - \langle V^2 \rangle_{c}^{*} \), where the superscript * indicates the iteration value. Thus, one obtains the values of the variables at the upstream and downstream boundaries which are required in Eq. (65a) and (65b). By knowing that velocities vanish at the wall boundary, all boundary values can be specified for Eq. (65). Now, let us briefly review the mathematical background of the Galerkin finite element method.

5.3 Galerkin Weak Solution Formulation -- Mathematical Approach.

Consider the following boundary value problem,

\[ \nabla^2 u - u = f(x,y) \quad \text{on} \quad (x,y) \in \Omega, \]  

(74a)

\[ u(x,y) = 0 \quad \text{on} \quad (x,y) \in \partial \Omega \]  

(74b)

where \( \nabla \) denotes the gradient operator, and \( \Omega \) is a bounded domain in the plane with the boundary \( \partial \Omega \), and it is assumed \( f \in L^2(\Omega) \). If \( u \) is a solution of Eq. (74), then clearly
\[ \nabla^2 u \cdot v - u \cdot \nabla v = f \cdot v \]  \hspace{1cm} (75)

for any \( v \in H^1_0(\Omega) \). Integrating Eq. (75) over \( \Omega \) gives

\[ -(\nabla u, \nabla v)_\Omega + \langle \nabla u \cdot n, v \rangle_{\partial \Omega} - (u, v)_\Omega = (f, v)_\Omega \]  \hspace{1cm} (76)

where \((, , \rangle\) denotes the usual \(L^2\) inner product on \((x, y) \in \Omega\). In the above, we used Green's first Identity which, for \( w \in H^2(\Omega) \) and \( v \in H^1(\Omega) \), takes the form

\[ (\nabla^2 w, v) = -(\nabla w, \nabla v) + \langle \nabla w \cdot n, v \rangle \]  \hspace{1cm} (77)

in which \( \nabla w \cdot n = \partial w / \partial n \) indicates differentiation in the direction of the outward normal to \( \partial \Omega \). Since \( v(x, y) = 0 \) for \((x, y) \in \partial \Omega\),

\[ (\nabla u, \nabla v) + (u, v) + (f, v) = 0 \quad \text{for all} \ v \in H^1_0(\Omega). \]  \hspace{1cm} (78)

Thus, any solution of \( u \) of Eq. (74) is also a solution of Eq. (78). We say that \( u \) is a weak solution of Eq. (74) if \( u \in H^2_0(\Omega) \) and satisfies Eq. (78), and also \( u \) is a classical solution of Eq. (74) if \( u \in C^2(\Omega) \) and satisfies Eq. (74) pointwise.

Now, one chooses a suitable finite dimensional space \( M \), the trial space, of \( H^1_0(\Omega) \), and a basis \( \{ \psi_1, \psi_2, \ldots, \psi_N \} \) of \( M \). The Galerkin method then consists in finding an approximation to \( u \) of the form
\[ u_h(x,y) = \sum_{j=1}^{N} \psi_j(x,y)u_j \] (79)

where \( u_j \) are scalars. The Galerkin weak solution of Eq. (74) is defined to be the element \( u_h \in M \) satisfying

\[ (\nabla u_h, \nabla V_h) + (u_h, V_h) + (f, V_h) = 0 \] (80)

for all \( V_h \in M \).

Substitution of Eq. (79) into Eq. (80) leads to a system of linear algebraic equations

\[ \bar{A} \cdot \bar{u} = \bar{k} \] (81)

where \( \bar{u} = (u_1, u_2, \ldots, u_N)^T \), \( \bar{A} = (\nabla \psi_i, \nabla \psi_j) \) and \( \bar{k} = (f, \psi_i) \).

Suppose that a smooth function \( u \) in Eq. (74) has a partial derivative of order \( m \). We wish to interpolate \( u \) by a finite element representation \( u_h \), as in Eq. (80), which contains complete polynomials of degree \( r \). The \( H^1 \)-norm in two dimensions is defined, as usual,

\[ \|u\|_{1,1}^2 = \int_{\Omega} [u^2 + (\frac{\partial u}{\partial x})^2 + (\frac{\partial u}{\partial y})^2] \, dx, dy. \] (82)

Then, the following theorem has been proved by Fairweather [26].
Theorem:

Choose \( M \) from a family of spaces of class \( S_{1,r}^0, r > 2 \).

If \( u \in H^m(\Omega) \quad H^1_0(\Omega), 1 \leq m \leq r \), then there exists a constant \( C \) independent of \( u \) and \( h \), such that

\[
\|u-u_h\|_2 + h\|\nabla(u-u_h)\|_2 \leq Ch^m\|u\|_m
\]  

(83)

where \( h \) is the maximum diameter of all elements in the mesh.

Starting from this brief review, we want to elaborate further the actual implementation aspects of the Galerkin finite element method to our systems which were in the section 5.1.

5.4 Construction of System Residual Vector by the Mixed Finite Element Method.

5.4.1 General Considerations.

The finite element procedure begins with the division of the continuum region into a number of simply shaped domains, called finite elements, as shown in Figure 4. Since the Eulerian description of the fluid motion is going to be used in the field equation (64), these elements are assumed to be fixed in space. Within each element, the variables, \( \tau_{ij}, V_1 \) and \( P \), are interpolated by continuous functions of compatible order, in terms of values to be determined at a set of nodal points. In other words, the space of admissible functions is defined for each variable for error consistency reasons as,

\[
\tau_{ij} \text{ and } V_1 \in H^2(\Omega); \quad (84)
\]

\[
P \in H^1(\Omega).
\]
Figure 4. Formation of finite element meshes near the contraction region.
With these spaces, the stress, velocity and pressure fields are approximated for each element by

\[ \tau_{ij}(r,z) = \psi_{\alpha}(r,z)\tau_{ij\alpha} \]  
(85a)

\[ V_i(r,z) = \psi_{\alpha}(r,z)V_{i\alpha} \]  
(85b)

\[ P(r,z) = \theta_\beta(r,z)P_\beta \]  
(85c)

where repeated indices denote summation, \( \alpha \) and \( \beta \) are nodal point indices, \( \tau_{ij\alpha}, V_{i\alpha} \) and \( P_\beta \) are unknown scalar quantities of given nodal points, and \( \psi_{\alpha} \) and \( \psi_\beta \) are admissible basis functions, respectively.

Substitution of Eq. (85) into the field equations (64) yields the following sets of equations:

**constitutive equations:**

\[ f_1 (\psi_{\alpha}, \psi_{\alpha j}, \tau_{ij}, V_i, \varepsilon', \xi, \text{De}) = R_1 \]  
(86a)

**incompressibility equation:**

\[ f_2 (\psi_{\alpha k}, V_i) = R_2 \]  
(86b)

**momentum equations:**

\[ f_3 (\psi_{\alpha}, \psi_{\alpha k}, \theta_{\beta k}, \tau_{ij}, V_i, P, g_i, \text{Re}) = R_3 \]  
(86c)

where \( R_i \) are the residuals resulting from the use of approximation in Eq. (85). The Galerkin form of the method of weighted residuals seeks
to reduce these errors to zero, in a weighted sense, by making the residuals orthogonal to the basis functions over each element. These orthogonality conditions are expressed by,

\[ \langle f_1, \psi \rangle = \langle R_1, \psi \rangle = 0 \]  
\[ \langle f_2, \theta \rangle = \langle R_2, \theta \rangle = 0 \]  
\[ \langle f_3, \psi \rangle = \langle R_3, \psi \rangle = 0 \]

where \( \langle \cdot, \cdot \rangle \) denotes the inner product, defined by, in the axisymmetric cylindrical case as,

\[ \langle a, b \rangle = \iiint_V ab \, rdr \, dz \, d\theta \]

\[ = 2\pi \iint_{\Omega} ab \, rdr \, dz \]

with \( V \) and \( \Omega \) being the volume and the domain of the element.

It is mentioned that the Galerkin weak solution formulation is performed on the momentum equation (87c) only by using Green's first identity given in Eq. (77), while the constitutive and continuity equations are just weighted with basis functions, such as in Eqs. (87a) and (87b). This is a consistent way of introducing Galerkin weighted residuals to our non-Newtonian flow. It is known in the literature as the mixed method, the direct method, or the primitive variable method.

Writing out Eq. (87) in detail, one obtains the following
equations:

\[ R_{1a}^e = 2\pi \int_{\Omega} \phi_a \{ \exp(\epsilon' \text{De}(\tau_{rr} + \tau_{zz} + \tau_{r\theta})) \tau_{rr} + \text{De}[V_r \tau_{rr}, r + V_z \tau_{rr}, r] - (2 - \xi)(V_r, r \tau_{rr} + V_r, z \tau_{rz}) \]

\[ + \xi(V_r, r \tau_{rr} + V_z, r \tau_{rz}) - 2V_r, r \} \text{ rdrdz} = 0 \]

\[ R_{2a}^e = 2\pi \int_{\Omega} \phi_a \{ \exp(\epsilon' \text{De}(\tau_{rr} + \tau_{zz} + \tau_{r\theta})) \tau_{rz} + \text{De}[V_r \tau_{rz}, r + V_z \tau_{rz}, r] - (1 - \xi)(V_r, z \tau_{rz} + V_z, r \tau_{rr}) \]

\[ + \frac{\xi}{2} (V_r, z \tau_{rr} + V_z, r \tau_{zz}) - (1 - \xi)(V_r, r + V_z, z) \tau_{rz} \} - (V_r, z + V_z, r) \} \text{ rdrdz} = 0 \]

\[ R_{3a}^e = 2\pi \int_{\Omega} \phi_a \{ \exp(\epsilon' \text{De}(\tau_{rr} + \tau_{zz} + \tau_{r\theta})) \tau_{zz} + \text{De}[V_r \tau_{zz}, r + V_z \tau_{zz}, r] - (2 - \xi)(V_z, r \tau_{rz} + V_z, z \tau_{zz}) \]

\[ + \xi(V_r, z \tau_{rz} + V_z, z \tau_{zz}) \} - 2V_z, z \} \text{ rdrdz} = 0 \]

\[ R_{4a}^e = 2\pi \int_{\Omega} \phi_a \{ \exp(\epsilon' \text{De}(\tau_{rr} + \tau_{zz} + \tau_{r\theta})) \tau_{r\theta} + \text{De}[V_r \tau_{r\theta}, r + V_z \tau_{r\theta}, r] - 2(1 - \xi)V_r \tau_{r\theta} / r \]

\[ - 2V_r / r \} \text{ rdrdz} = 0 \]

\[ R_{5a}^e = 2\pi \int_{\Omega} \phi_a \{ V_r / r + V_r, r + V_z, z \} \text{ rdrdz} = 0 \]
\[ R_{6\alpha}^e = 2\pi \int_{\Omega} \phi_\alpha (V_r V_r, r + V_z V_r, z) - (\phi_\alpha/r + \phi_\alpha, r)^p + (\phi_\alpha, r \tau_{rr} + \phi_\alpha, z \tau_{rz} + \phi_\alpha \tau_{\theta \theta}/r)/Re \]

\[ - \phi_\alpha g_r \} r d\Omega + 2\pi R \int_{\partial \Omega} \phi_\alpha (P - \tau_{rr}/Re) n_r d\Omega = 2\pi L \int_{\partial \Omega} \phi_\alpha \tau_{rz} n_z r dr/Re = 0 \]

\[ R_{7\alpha}^e = 2\pi \int_{\Omega} \{ \phi_\alpha (V_r V_z, r + V_z V_z, z) - \phi_\alpha, z^p + (\phi_\alpha, r \tau_{rz} + \phi_\alpha, z \tau_{zz})/Re - \phi_\alpha g_z \} r d\Omega \]

\[ + 2\pi R \int_{\partial \Omega} \phi_\alpha \tau_{rz} n_r dz/Re + 2\pi L \int_{\partial \Omega} \phi_\alpha (P - \tau_{zz}/Re) n_z r dr = 0. \]

In the above, the residual expressions of \( R_{6\alpha}^e \) and \( R_{7\alpha}^e \) contain the boundary integrals. Setting up boundary conditions such as in Eq. (65) can avoid evaluation of these integrals. This makes the finite element method be favored over the finite difference method, especially when complex geometries are involved. Writing the residuals in the vector form one has

\[ R^e(\phi^e(De), De) = 0 \] (88)

where \( \phi^e = [\tau_{rr}^e, \tau_{rz}^e, \tau_{zz}^e, D_{\theta \theta}^e, \rho^e, \bar{V}_r^e, \bar{V}_z^e]^T \) is a solution vector and the superscript \( e \) represents equations for a single element.

Finally, total system residual vector can be constructed through an assemblage of individual element residual vectors such that interelement continuity of the approximating stress, velocity and pressure must be enforced. This continuity requirement is satisfied through the appropriate summation of equations for nodes common to adjacent elements. Further detailed procedures are given in subsequent sections.
5.4.2 The Master Element and Shape Functions.

Let our attention be focused on a partitioned physical element \( \Omega^e_h \) of length \( h \), and consider possible choices of shape functions \( \psi^e_h \). We begin this by taking tensor products of sets of polynomials (degree \( r \)) in \( x \)-coordinate with sets of polynomials (degree \( r \)) in \( y \)-coordinate. Combinations of all resulting terms constitute a complete polynomial basis of degree \( r \) that is continuous throughout \( \Omega^e_h \). For example, a bilinear basis function which is continuous on the 4-node quadrilateral element has

\[
\psi^e_h(x,y) = a_1 + a_2 x + a_3 y + a_4 xy
\]

(89)

since

\[
\begin{bmatrix} 1 \\ x \end{bmatrix} \cdot [1, y] = \begin{bmatrix} 1 \\ y \\ x \end{bmatrix} = \begin{bmatrix} 1 & y \\ x & xy \end{bmatrix}.
\]

Likewise, a biquadratic basis function which is smooth on the 9-node quadrilateral element,

\[
\psi^e_h(x,y) = a_1 + a_2 x + a_3 y + a_4 x^2 + a_5 xy + a_6 y^2
\]

\[
+ a_7 x^2 y + a_8 xy^2 + a_9 x^2 y^2,
\]

(90)

contains the following terms,
\[
\begin{bmatrix}
1 & \cdot \\
x & [1, y, y^2] = \\
x^2 & x
\end{bmatrix} \begin{bmatrix}
y \\
xy \\
x^2y
\end{bmatrix}.
\]

Now, we want to evaluate coefficients of polynomials. For example, taking coordinates of a 4-node quadrilateral physical element, which have \((x_1, y_1), (x_2, y_2), (x_3, y_3)\) and \((x_4, y_4)\), then Eq. (89) can be written for each coordinate as,

\[
V_1 = \psi_h^{e}(x_1, y_1) = a_1 + a_2x_1 + a_3y_1 + a_4x_1y_1
\]

\[
V_2 = \psi_h^{e}(x_2, y_2) = a_1 + a_2x_2 + a_3y_2 + a_4x_2y_2
\tag{91}
\]

\[
V_3 = \psi_h^{e}(x_3, y_3) = a_1 + a_2x_3 + a_3y_3 + a_4x_3y_3
\]

\[
V_4 = \psi_h^{e}(x_4, y_4) = a_1 + a_2x_4 + a_3y_4 + a_4x_4y_4
\]

Solving for \(a_1, a_2, a_3,\) and \(a_4\) from Eq. (91), and substituting them into Eq. (89) results in

\[
\psi_h^{e}(x, y) = V_1\psi_1^{e}(x, y) + V_2\psi_2^{e}(x, y) + V_3\psi_3^{e}(x, y) + V_4\psi_4^{e}(x, y)
\]

\[
= \sum_{i=1}^{4} \psi_i^{e}(x, y) V_i
\tag{92}
\]

where \(\psi_i^{e}\) is called a Lagrangian family of shape functions which have following properties;
\[
\sum_{i} \psi_i^e = 1 \tag{93a}
\]

\[
\psi_i^e(x_j, y_j) = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j
\end{cases} \tag{93b}
\]

The same procedure can be applied to an arbitrary 9-node quadrilateral physical element to give

\[
\psi_h^e(x, y) = \sum_{i=1}^{9} \psi_i^e(x, y) V_i. \tag{94}
\]

Computation of variables in the physical domain is possible by using interpolation functions of Eq. (92) or (94), but actual calculation is not performed this way. Instead, to avoid evaluation of the individual physical element differently, the concept of the Master element (\(\hat{\Omega}\)) and its transformation to the physical element is usually employed.

The master element (\(\hat{\Omega}\)) for quadrilateral elements is the square which has Cartesian coordinates of \(\xi\) and \(\eta\) with the origin \((0, 0)\) located at the center of \(\hat{\Omega}\). With this element, necessary conditions for the shape function in Eq. (93) allow the construction of master element shape functions. Details can be found in Becker, Carey and Oden [1]. Four node and nine node quadrilateral master elements and their shape functions are shown in Figure 5.
Figure 5. Master element, node numbering and shape functions for 4-, 9- and 8-node quadrilateral finite elements.
5.4.3 Element Transformations.

The whole idea of this section is to introduce an invertible transformation between a master element (\( \hat{\Omega} \)) and an arbitrary physical element (\( \Omega^e_h \)). Then we can perform the calculations conveniently on the master element instead of on the physical element. This transformation is accomplished by a simple coordinate transformation or mapping of points from \( \hat{\Omega} \) into points in each element, such as:

\[
x = x(\xi, \eta) = \sum_{i=1}^{N} x_i \hat{\varphi}_i(\xi, \eta)
\]

\[
y = y(\xi, \eta) = \sum_{i=1}^{N} y_i \hat{\varphi}_i(\xi, \eta)
\]

Thus, partitioning the physical domain into NE elements is viewed as a sequence of transformation \( \{T_1, T_2, ..., T_{NE}\} \) of the above equation in which each element \( \Omega^e_h \) is the image of the fixed master element \( \hat{\Omega} \) under a coordinate map, \( T_e \). These transformations generally must satisfy the following conditions:

1. Within each element, the function \( \xi = \xi(x, y) \) and \( \eta = \eta(x, y) \) must be invertible and continuously differentiable;

2. The sequence of mappings \( \{T_e\} \) must generate a mesh with no spurious gaps between elements and with no element overlapping another.

Assuming that the above conditions are satisfied, then

\[
dx = \frac{\partial x}{\partial \xi} \, d\xi + \frac{\partial x}{\partial \eta} \, d\eta
\]

and
\[
\begin{align*}
\text{d}y &= \frac{\partial y}{\partial \xi} \text{d}\xi + \frac{\partial y}{\partial \eta} \text{d}\eta \\
\text{ which can be rewritten as; } \\
\begin{pmatrix}
\text{d}x \\
\text{d}y
\end{pmatrix} &= \begin{pmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{pmatrix} \cdot \begin{pmatrix}
\text{d}\xi \\
\text{d}\eta
\end{pmatrix}.
\end{align*}
\]  

(96)

The above matrix is called the Jacobian matrix of the transformation of Eq. (95) and is denoted \( J \).

A necessary and sufficient condition for the system of Eq. (96) to be invertible is that the determinant \(|J|\) of the Jacobian matrix is nonzero at \((\xi, \eta) \in \hat{\Omega}\). Here, \(|J|\) is defined as,

\[
|J| = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi}
\]

\[
= \left\{ \sum_{i=1}^{N} \frac{\partial x}{\partial \xi} x_i \right\} \left\{ \sum_{i=1}^{N} \frac{\partial y}{\partial \eta} y_i \right\} - \left\{ \sum_{i=1}^{N} \frac{\partial x}{\partial \eta} x_i \right\} \left\{ \sum_{i=1}^{N} \frac{\partial y}{\partial \xi} y_i \right\}. \tag{97}
\]

For \(|J| \neq 0\), the inverse map of Eq. (96) is given by:

\[
\begin{pmatrix}
\text{d}\xi \\
\text{d}\eta
\end{pmatrix} = \frac{1}{|J|} \begin{pmatrix}
\frac{\partial y}{\partial \eta} & -\frac{\partial y}{\partial \xi} \\
-\frac{\partial y}{\partial \xi} & \frac{\partial x}{\partial \eta}
\end{pmatrix} \cdot \begin{pmatrix}
\text{d}x \\
\text{d}y
\end{pmatrix}. \tag{98}
\]

An infinitesimal vector in \(\hat{\Omega}\) can be written as in Eq. (96),
\[
\begin{bmatrix}
\frac{\partial \xi}{\partial x} \\
\frac{\partial \eta}{\partial x}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y}
\end{bmatrix} \begin{bmatrix}
\int_0^1 \\
\int_0^1
\end{bmatrix}.
\]

Equating terms in Eqs. (98) and (99), we get

\begin{align*}
\frac{\partial \xi}{\partial x} &= \frac{1}{\frac{1}{\xi}} \frac{\partial y}{\partial \eta} = \frac{1}{\frac{1}{\xi}} \left( \sum_{i=1}^{N} \frac{\partial \xi}{\partial \eta} y_i \right) & (100a) \\
\frac{\partial \xi}{\partial y} &= \frac{-1}{\frac{1}{\xi}} \frac{\partial x}{\partial \eta} = \frac{-1}{\frac{1}{\xi}} \left( \sum_{i=1}^{N} \frac{\partial \xi}{\partial \eta} x_i \right) & (100b) \\
\frac{\partial \eta}{\partial x} &= \frac{-1}{\frac{1}{\eta}} \frac{\partial y}{\partial \xi} = \frac{-1}{\frac{1}{\eta}} \left( \sum_{i=1}^{N} \frac{\partial \eta}{\partial \xi} y_i \right) & (100c) \\
\frac{\partial \eta}{\partial y} &= \frac{1}{\frac{1}{\eta}} \frac{\partial x}{\partial \xi} = \frac{1}{\frac{1}{\eta}} \left( \sum_{i=1}^{N} \frac{\partial \eta}{\partial \xi} x_i \right) & (100d)
\end{align*}

Field variables and their derivatives in the discretized set of equations are defined on \( \hat{\psi}_i^e \), where the element shape function \( \psi_i^e(x, y) \) can be obtained from the master element shape function \( \hat{\psi}_i(\xi, \eta) \) by

\[
\psi_i^e(x, y) = \hat{\psi}_i(\xi(x, y), \eta(x, y)), \quad i = 1, 2, \ldots, N.
\]

The derivatives of \( \psi_i^e(x, y) \) are obtained using the chain rule from Eq. (101):

\[
\frac{\partial \psi_i^e}{\partial x} = \frac{\partial \hat{\psi}_i}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial \hat{\psi}_i}{\partial \eta} \frac{\partial \eta}{\partial x} \quad (102a)
\]
\[ \frac{\partial \psi_i^e}{\partial y} = n \frac{\partial \psi_i}{\partial y} + \frac{\partial \psi_i}{\partial n} \frac{\partial n}{\partial y} \quad (102b) \]

We use Eqs. (100) and (102) to get:

\[ \frac{\partial \psi_i^e}{\partial x} = \frac{1}{|\Omega|} \left\{ \frac{\partial \psi_i}{\partial x} \sum_{k=1}^{N} \frac{\partial \psi_k}{\partial n} y_k - \frac{\partial \psi_i}{\partial n} \sum_{k=1}^{N} \frac{\partial \psi_k}{\partial x} y_k \right\} \quad (103a) \]

\[ \frac{\partial \psi_i^e}{\partial y} = \frac{1}{|\Omega|} \left\{ - \frac{\partial \psi_i}{\partial x} \sum_{k=1}^{N} \frac{\partial \psi_k}{\partial n} x_k + \frac{\partial \psi_i}{\partial n} \sum_{k=1}^{N} \frac{\partial \psi_k}{\partial x} x_k \right\} \quad (103b) \]

Note that the partial derivatives of \( \psi_j^e \) with respect to \( x \) and \( y \) are completely determined by calculations defined only on the master element \( \hat{\Omega} \).

5.4.4 Integration by Gaussian Quadrature.

Formulation of the element residual vector in Eq. (88) involves integrations of variables and their derivatives over the physical domain. We will study this aspect in this section.

Let \( u \) be a scalar-valued function of \( x \) and \( y \) defined on an element \( \Omega_h^e \). Then, we can convert \( u \) to a function \( \hat{u} \) of \( \xi \) and \( \eta \) defined on \( \hat{\Omega} \) by setting

\[ u(x, y) = u(x(\xi, \eta), y(\xi, \eta)) = \hat{u}(\xi, \eta) \quad (104) \]

where \( x(\xi, \eta) \) and \( y(\xi, \eta) \) are given by Eq. (95). By knowing that the determinant \( |\Omega| \) of the Jacobian matrix is the ratio of the area in the physical domain to that in the master element domain, it is clear that
\[ \int_{\Omega} u(x, y) \, dx \, dy = \int_{\Omega} \hat{u}(\xi, \eta) \, |y| \, d\xi \, d\eta. \] (105)

Thus, integrals of functions over elements \( \Omega_h \) can be evaluated using calculations on \( \hat{\Omega} \). In actual computations, numerical quadrature rules are generally employed to estimate all integrals. Quadrature rules are typically defined for standard regions of integration, such as our master element, by specifying the quadrature points \((\xi_i, \eta_i)\) as well as quadrature weights \((W_i)\) for \(i = 1, 2, \ldots, N_1\). In most finite element calculations, Gaussian quadrature points and weights are used (refer to Zienkiewicz [71]).

Quadrature rules for quadrilateral elements are usually derived from one dimensional quadrature formulas by treating the integration over the master element as a double integral,

\[ \int_{\Omega} \hat{u}(\xi, \eta) \, |y| \, d\xi \, d\eta = \int_{-1}^{1} \left[ \int_{-1}^{1} \hat{u}(\xi, \eta) \, d\xi \right] \, d\eta \]

\[ = \sum_{m=1}^{N} \left[ \sum_{n=1}^{N} \hat{u}(\xi_n, \eta_m) \cdot |y| \hat{u}(\xi_n, \eta_m) \right] \cdot W_n \cdot W_m. \] (106)

For computational convenience, the double summation can be reduced to a single summation over the entire set of integration points by relabeling the point \((m,n)\) with the single index \(l\) with \(N_1 = N^2\),

\[ \sum_{m=1}^{N} \left[ \sum_{n=1}^{N} \hat{u}(\xi_n, \eta_m) \cdot |y(\xi_n, \eta_m)| \cdot W_n \right] W_m = \sum_{l=1}^{N^2} \hat{u}(\xi_l, \eta_l) \cdot |y(\xi_l, \eta_l)| \cdot W_l. \] (107)

5.4.5 Summary.

We now summarize the essential steps in the element matrix
calculation.

1. Choose a master element \(\hat{\Omega}\) and shape functions
   \(
   (\hat{\psi}_j, j = 1, 2, ..., N_e)\). Specify the \(x, y\)-coordinates \((x_1, y_1),
   (x_2, y_2), ..., (x_{N_e}, y_{N_e})\) of nodal points of each physical element.

2. Determine a set of \(N_1\) Gaussian quadrature points
   \((\xi_1, \eta_1), l = 1, 2, ..., N_1\), and weights \(W_l\) for a given master
   element.

3. Evaluate values of \(\hat{\psi}_j, \partial \hat{\psi}_j/\partial \xi, \partial \hat{\psi}_j/\partial \eta\) at the integration points
   \((\xi_1, \eta_1)\).

4. Compute values of \(x = x(\xi, \eta), y = y(\xi, \eta)\) of Equation (95).

5. Calculate values of the Jacobian determinant \(|\mathcal{J}(\xi, \eta)|\) as in Eq.
   (97), and functions \(\partial x/\partial \xi, \partial x/\partial \eta, \partial y/\partial \xi\) and \(\partial y/\partial \eta\) at the integration
   points \((\xi_1, \eta_1)\), as in Eq. (100).

6. Estimate \(\partial \hat{\psi}_j/\partial x\) and \(\partial \hat{\psi}_j/\partial y\) at each integration point \((\xi_1, \eta_1)\) as
   shown in Eq. (103).

7. Using the above information, compute integral functions at the
   integration point \((\xi_1, \eta_1)\) and multiply each by \(W_l |\mathcal{J}(\xi_1, \eta_1)|\).

8. Sum the values evaluated in step 7 in accordance with Eq. (107) to
   obtain the element residual vector of Eq. (88).

After the element residual equations have been established, the
contribution of each of the element equations at the same node is added
to form the system equations. This process is called an assembly.

Thus, we obtain the final form, which is a system of nonlinear equations
such as,

\[
R(\phi(De), De) = 0
\]  \hspace{1cm} (108a)
where
\[ \phi = [\tau_{rr}, \tau_{rz}, \tau_{zz}, \tau_{\theta\theta}, P, V_r, V_z]^T. \]  

(108b)

5.5 Nonlinear Iteration Method.

In literature of non-Newtonian fluid simulations, three types of nonlinear iteration methods, have most often appeared. These are the successive substitution with SOR (refer to Coleman [15], Crochet and Keunings [20] and Davies and Walters [24]), the Newton-Raphson (refer to Finlayson [36], Crochet et al. [39] and Viriyayuthakorn et al. [66]), and the Newton-Raphson with the continuation method (refer to Mendelson et al. [50], Beris et al. [2] and Yeh et al. [70]). After briefly reviewing them, our numerical scheme, which may be thought of as an initial value approach, will be discussed in greater detail.

5.5.1 Successive Substitution Method with SOR.

Rewriting Eq. (108) in the form of,
\[ \mathbf{R}(\phi, \text{De}) = \mathbf{A}(\phi, \text{De}) \cdot \phi - \mathbf{R}(\text{De}) = 0, \]  

(109)

one can easily devise the successive substitution scheme with SOR;

\[ \mathbf{A}(\phi_k^n, \text{De}_k) \cdot \phi_k^{n+1} = \mathbf{R}(\text{De}_k) \]  

(110a)

and
\[ \phi_k^{n+1} = \omega \phi_k^n + (1 - \omega) \phi_k^n \]  

(110b)

with \( \text{De}_k = \text{De}_{k-1} + \Delta \text{De} \) and \( \phi_k^n = \phi^n(\text{De}_k) \) where the indices \( n \) and \( k \) indicate the iteration number and the De number increment-level,
and \( \omega \) is the relaxation parameter, the value of which usually ranges from 0.4 to 0.6.

It is well known that this method converges linearly but has greater stability when compared to the Newton-Raphson method.

5.5.2 Newton-Raphson Method.

This method exhibits a quadratic rate of convergence but with generally a poor stability range. Thus, a good starting vector must be provided. It can be written as,

\[
\begin{align*}
\mathbf{J}(\phi_k^n, \text{De}_k) \cdot \Delta \phi_k^{n+1} &= - R(\phi_k^n, \text{De}_k) \quad (111a) \\
\phi_{k+1}^n &= \phi_k^n + \Delta \phi_k^{n+1} \quad (111b)
\end{align*}
\]

where \( \mathbf{J} = (\partial R / \partial \phi) \), or in tensor component notation \( J_{ij} = (\partial R_i / \partial \phi_j) \).

5.5.3 Newton-Raphson with the Continuation Method.

This method is essentially the same as the Newton-Raphson, but it creates a better starting vector for each De number increment. As long as the De number stepsize, \( \Delta \text{De} \), remains at a small value, this could be by far the most efficient method. It also possesses the ability to sometimes skip singular or bifurcation points caused by incrementing the De number. Thus, it is called a continuation method. However, the small \( \Delta \text{De} \) requirement could result in an excessive amount of computational time. This method is illustrated in two phases, that is, the initial step,
\[ J(\phi_{k-1}, D\epsilon_{k-1}) \cdot \frac{d\phi}{d\epsilon} = - \frac{\partial R}{\partial \epsilon} \quad (112a) \]

\[ \phi_0 = \phi_{k-1} + \left( \frac{d\phi}{d\epsilon} \right)_{k-1} \Delta \epsilon, \quad (112b) \]

and the iteration step,

\[ J(\phi^n, D\epsilon_k) \cdot \Delta \phi^n = - R(\phi^n, D\epsilon_k) \]

\[ \phi^{n+1} = \phi^n + \Delta \phi^{n+1}. \]

5.5.4 Initial Value Approach.

It is recognized that the nature of approximating errors in our problem involves two processes; one is to deal with errors generated from Deborah number increment procedures. The second one is the discretization error of finite element procedures at a specified Deborah number as shown in Eq. (83). From this point of the view, the role of the Deborah number corresponds to that of time in a transient problem. For the latter error, the Newton-Raphson iteration scheme may still be applied if an efficient and reliable Deborah number increment method is devised to reduce the former error. Thus, much of our attention is directed to the development of an effective Deborah number marching scheme.

(1) Deborah Number Marching Scheme--General Aspects.

Differentiation of Eq. (108) with respect to the incremental
parameter $De$ gives rise to

$$\frac{dR}{dDe} = \left( \frac{\partial R}{\partial \phi} \right) \left( \frac{d\phi}{dDe} \right) + \left( \frac{\partial R}{\partial De} \right) = 0.$$ 

Thus,

$$\left( \frac{\partial R}{\partial \phi} \right) \left( \frac{d\phi}{dDe} \right) = -\left( \frac{\partial R}{\partial De} \right)$$ \hspace{1cm} (113)

or,

$$\left( \frac{d\phi}{dDe} \right) = -\left( \frac{\partial R}{\partial \phi} \right)^{-1} \cdot \left( \frac{\partial R}{\partial De} \right) = - \frac{1}{y} \left( \phi, De \right) \cdot \left( \frac{\partial R}{\partial De} \right)$$ \hspace{1cm} (114)

with the starting vector,

$$\phi(De_0) = \phi_0.$$ 

Comparing Eq. (114) to an initial value problem of the form,

$$\frac{dy}{dt} = f(t, y)$$ \hspace{1cm} (115)

subject to the initial condition,

$$y(a) = x,$$

we see they are the same problem with the derivative function defined as,

$$f(t, y) = - \frac{1}{y} \left( \phi, De \right) \cdot \left( \frac{\partial R}{\partial De} \right).$$ \hspace{1cm} (116)

The continuation method introduced in the section 5.5.3 is nothing but the most simple, one-step and explicit Euler approximation, because Eq. (112b) can be rewritten as
\[
\frac{d\phi}{(d\Delta e)^{k-1}} = \frac{\phi_k - \phi_{k-1}}{\Delta e}.
\]

This consideration allows one to expand the limited numerical schemes used at present in the non-Newtonian simulation field to the numerous methods of solving the initial value problem of the ordinary differential equation field. Depending on how one can reduce the truncation error in solving Eq. (113) or (114) various numerical strategies can be implemented. For example, since the evaluation of the derivative function in Eq. (116) of our problem is the most time consuming and difficult process, the method which requires the least function evaluations is more favorable. In other words, a higher order method may be favored over a lower order one in our situation of advancing the Deborah number. Also, for the same reason, the multistep method is considered to be advantageous when compared to the single step method of the Runge-kutta type for nonstiff systems.

Presently, several general purpose codes of the initial value problem of the O.D.E. are in our disposal, like DIFFSUB of Gear [27], STEP of Shampine [59] and EPISODE of Hindmarsh [30], etc. Because these codes have been developed with relatively simple derivative functions \(f(t, y)\) in mind, they may not be suitable for our purpose, in which the dimension of the function is huge and the evaluation of the function itself involves solving a large system of equations. In this respect, we have constructed our own code from the Adams-type of predictor-corrector methods.
(2) Adams-Type Predictor-Corrector Multistep Method.

Multistep methods are known to utilize previous solutions computed at $t_0, t_1, \ldots, t_i$ in order to calculate the next step solution at $t_{i+1}$. The definition of the multistep method is given below (refer to Ralston et al. [56]).

**Definition:** A multistep method for solving the initial value problem $y' = f(t, y)$, $a < t < b$, $y(a) = \alpha$ is one whose difference equation for finding the approximation $y_{i+1}$ at the mesh point $t_{i+1}$ can be represented by the following equation, where $m$ is an integer greater than 1:

$$
\begin{align*}
    y_{i+1} &= a_{m-1} y_i + a_{m-2} y_{i-1} + \ldots + a_0 y_{i+1-m} \\
    &+ h \left[ b_m f(t_{i+1}, y_{i+1}) + b_{m-1} f(t_i, y_i) \\
    &+ \ldots + b_0 f(t_{i+1-m}, y_{i+1-m}) \right]
\end{align*}
$$

(118)

for $i = m - 1, m, \ldots, N - 1$, where the starting values $y_0 = \alpha_0$, $y_1 = \alpha_1$, $y_2 = \alpha_2$, $\ldots$, $y_{m-1} = \alpha_{m-1}$ are specified and $h = (b-a)/N$. And the local truncation error for the step $i+1$ is defined as

$$
\begin{align*}
    E_{i+1} &= (y_{i+1} - a_{m-1} y_i - \ldots - a_0 y_{i+1-m})/h \\
    &+ b_m f(t_{i+1}, y_{i+1}) \\
    &+ \ldots + b_0 f(t_{i+1-m}, y_{i+1-m})].
\end{align*}
$$

(119)

When $b_m = 0$, Eq. (118) becomes an explicit method in which $y_{i+1}$ is expressed explicitly in terms of previously determined values.

When $b_m \neq 0$, this is called an implicit method, since $y_{i+1}$ occurs on both sides of Eq. (118) and is determined only in an implicit manner.

For example, let $m = 4$, $a_3 = 1$, $a_2 = a_1 = a_0 = 0$, $b_4 = 0$, $b_3 = 55/24$, $b_2 = -59/24$, $b_1 = 37/24$ and $b_0 = -9/24$ in Eq. (118). Then,
\[ y_{i+1} = y_i + h[55f_{i} - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}] \]  

(120)

for each \( i = 3, 4, \ldots, N-1 \), defines an explicit four-step method, which is known as the fourth-order Adams-Bashforth technique, provided that \( y_0 = a_0, \ y_1 = a_1, \ y_2 = a_2, \) and \( y_3 = a_3 \). It has a local truncation error of

\[ E_{i+1} = \frac{251}{720} y^{(5)}(\mu_i) h^4, \]  

(121)

where \( t_{i-3} < \mu_i < t_{i+1} \). For another example, let \( m = 4 \) with \( a_3 = 1, a_2 = a_1 = a_0 = 0, b_4 = 251/750, b_3 = 646/750, b_2 = -264/750, b_1 = 106/750 \) and \( b_0 = -19/750 \) in Eq. (118). This turns out to be an implicit four-step method, namely the fifth-order Adams-Moulton technique:

\[ y_{i+1} = y_i + h[251 f_{i+1} + 646 f_{i} - 264 f_{i-1} + 106 f_{i-2} - 19 f_{i-3}] / 720 \]  

(122)

where \( i = 3, 4, \ldots, N-1 \) and starting values must be supplied like \( y_0 = a_0, \ y_1 = a_1, \ y_2 = a_2, \ y_3 = a_3 \). The local truncation error of this method is estimated as

\[ E_{i+1} = -\frac{3}{160} y^{(6)}(\mu_i) h^5. \]  

(123)

In general, the implicit method has greater stability and fewer rounding errors than the explicit method, but is hard to implement. Thus, in actual practice, implicit multistep methods are not used directly; rather, they are used to improve upon an approximation.
obtained by explicit methods. The usual procedure, involving the combination of an explicit and an implicit technique, is called a predictor-corrector method. Here, we use the fourth order Adams-Bashforth method as a predictor and the fifth order Adams-Moulton method as a corrector. This predictor-corrector method requires the initial four starting values such as $y_0$, $y_1$, $y_2$, and $y_3$. To generate these values, we choose the fourth order Runge-Kutta method. The most common Runge-Kutta method of order four is given as:

$$
\begin{align*}
    y_0 &= a \\
    k_1 &= hf(t_i, y_i) \\
    k_2 &= hf(t_i + \frac{h}{2}, y_i + \frac{1}{2} k_1) \\
    k_3 &= hf(t_i + \frac{h}{2}, y_i + \frac{1}{2} k_2) \\
    k_4 &= hf(t_{i+1}, y_i + k_3) \\
    y_{i+1} &= y_i + (k_1 + 2k_2 + 2k_3 + k_4)
\end{align*}
$$

for each $i = 0, 1, 2$. This one-step method is known to have the local truncation error $O(h^4)$, provided that the solution $y(t)$ has five continuous derivatives. As far as stability of the predictor-corrector and the Runge-Kutta methods are concerned, both are called conditionally stable methods, such that a large stepsize may produce instability due to accumulating errors. To control error propagation, we must devise a stepsize control scheme, unless excessively small steps are taken. The following subsection is devoted to this subject (refer to Burden et al. [6]).
(3) Local Error Control.

Since the global error of a difference method cannot be determined, we may work instead with a concept known as the local error. The local error is defined as

$$e_{i+1}(h) = \max_k | Z^k(t_{i+1}) - W_{i+1}^k|$$  \hspace{1cm} (125)

where $Z(t)$ is the exact solution to the initial-value problem

$$\frac{dZ}{dt} = f(t, Z), \quad t_i < t < b, \quad Z(t_i) = W_i$$  \hspace{1cm} (126)

and $W_i$ is the approximation of the difference method.

We will now determine how the estimation of the local error of a difference method can be used to control the global error. The Adams-Bashforth four-step method has the following local truncation error,

$$Z_{i+1} = W_{i+1} + \frac{251}{720} y^{(5)}(u_i) \cdot h^4$$  \hspace{1cm} (127)

for $t_{i-3} < u_i < t_{i+1}$, while the Adams-Moulton four-step method gives

$$Z_{i+1} = ^\wedge{W}_{i+1} - \frac{3}{160} y^{(6)}(\hat{u}_i) \cdot h^5$$  \hspace{1cm} (128)

for $t_{i-3} < \hat{u}_i < t_{i+1}$. Suppose that solutions of the above two methods agree at $(t_i, W_i)$ and let $h$ denote the initial choice for the stepsize at $t_i$. Then,
\[ Z_{i+1} - W_{i+1} = Z_{i+1} - W_{i+1} + \tilde{W}_{i+1} - W_{i+1} = 0(h^5) + \tilde{W}_{i+1} - W_{i+1} \]

(129)

and

\[ e_{i+1}(h) = \max_k |Z^k_{i+1} - W^k_{i+1}| = \max_k |\tilde{W}^k_{i+1} - W^k_{i+1}| + O(h^5). \]

(130)

Moreover, \(e_{i+1}(h)\) is of order \(O(h^4)\) from Eq. (127). Therefore, a constant \(C > 0\), independent of \(h\), exists with

\[ e_{i+1}(h) < Ch^4 + O(h^5). \]

(131)

Equations (130) and (131) imply that a valid estimate for the smallest \(C\) could be given by

\[ Ch^4 = \max_k |\tilde{W}^k_{i+1} - W^k_{i+1}| \]

or

\[ C = \frac{\max_k |\tilde{W}^k_{i+1} - W^k_{i+1}|}{h^4}. \]

(132)

Since the purpose of above argument is to allow a variable step size, we want \(h\) replaced by the variable stepsize \(Sh\), where \(S\) is positive but bounded from above and is also bounded away from zero. Then,
\[ e_{i+1}(Sh) < C(Sh)^4 + O((Sh)^5) \]  

(133)

and the boundedness of \( S \) implies that

\[ e_{i+1}(Sh) < CS^4h^4 + O(h^5). \]

Using Eq. (132) results in

\[ e_{i+1}(Sh) < S^4 \cdot \max_k |\tilde{W}_{i+1}^k - W_{i+1}^k| + O(h^5) \]  

(134)

The most significant portion of the local error \( e_{i+1}(Sh) \), that is, the portion that is order \( O(h^4) \), is consequently bounded by

\( S^4 \cdot \max_k |\tilde{W}_{i+1}^k - W_{i+1}^k| \). Thus, we can ensure that the local error is bounded by \( \epsilon \) times the stepsize provided that

\[ S^4 \cdot \max_k |\tilde{W}_{i+1}^k - W_{i+1}^k| < \epsilon Sh, \]

which implies that

\[ S < \left( \frac{\epsilon h \max_k |\tilde{W}_{i+1}^k - W_{i+1}^k|}{10} \right)^{1/3}. \]  

(135)

Usually, \( S \) tends to be chosen rather conservatively in practice, such as:

\[ S = \left( \frac{\epsilon h \max_k |\tilde{W}_{i+1}^k - W_{i+1}^k|}{10} \right)^{1/3}. \]  

(136)
It should be noted that since the multistep methods require an equal stepsize for the starting values, any change in the stepsize necessitates recalculating new starting values at that point. Thus, whenever the stepsize changes its value, the Runge-Kutta method must be called again to generate new starting values.

We have seen that depending on the specified $\epsilon$ value, the corresponding stepsize may be determined, i.e., for a small $\epsilon$, the incrementing error has to remain less so that a very small stepsize may be necessary. If one wants to allow as large a stepsize as possible, he has to pay the penalty of crude solutions due to the large stepsize. However, combining the Newton-Raphson nonlinear iteration scheme with the multistep marching technique at each given incremental level, may allow both relatively larger step-increment and still acceptably accurate solutions. This combination scheme has proven to be very effective for our problem.

(4) Stiff Problem.

A stiff system of ordinary differential equations (whose exact solutions contain a function of the form $e^{\lambda t}$) may be defined as one in which the maximum eigenvalue $\lambda_{\text{max}}$ is sufficiently large so that either stability or an error bound of numerical solutions can be obtained only by unreasonable restrictions on the numerical integration stepsize. In other words, it requires an excessively small stepsize which results in an enormous amount of computing time necessary to solve the system equations. Usually stiffness is measured by its stiffness ratio, the ratio of the largest to the smallest eigenvalue of the system. By this
definition, one may hypothesize that a system may be called a nonstiff system if stiffness ratio is less than $10^2$, and a stiff system if stiffness ratio is greater than $10^2$.

Stability is one of the major factors in choosing a suitable numerical algorithm for solving stiff ordinary differential equations, with a reasonably large stepsize in mind. To study stability, we turn to the so-called test equation, which is the simplest type of a differential equation that has a solution of the form $e^{\lambda t}$;

$$\frac{dy}{dt} = \lambda y, \quad y(0) = \alpha. \quad (137)$$

Euler's approximation to the above equation gives us

$$y_0 = \alpha$$

$$y_{i+1} = y_i + \lambda h y_i = (1 + \lambda h)^i y_0. \quad (138)$$

Thus, for other one-step methods, one can generally write

$$y_{i+1} = u(\lambda h) y_i = u(\lambda h)^{i+1} y_0 \quad (139)$$

when that method is applied to the test equation. Note that an inaccurate approximation would be given by Eqs. (138) and (139)
unless $|\mu(\lambda h)| < 1$.

Stiffness is also observed most frequently in problems involving systems of differential equations. For example, a rapidly increasing elongational viscosity may indicate that the problem of a viscoelastic flow belongs to one of these systems. In these situations, it is more natural to consider the test equation with $\lambda$ a complex number with a negative real part. In this case, the domain in the complex plane which satisfies $|\mu(\lambda h)| < 1$, is called the region of absolute stability for the method. Given a value of $\lambda$, this region determines values of $h$ for which the method would be expected to give accurate approximations. The larger the area of absolute stability is, the more appropriate the method would be for handling problems involving stiff equations.

The following definition about stability is given by Lambert [40].

Definition: A numerical scheme is termed

A-Stable if for $-\infty < \text{Re}(\lambda h) < 0$, $|\mu(\lambda h)| < 1$

and Strongly-A-Stable if $|\mu(\lambda h)| \to 0$ as $\text{Re}(\lambda h) \to -\infty$.

For a system of equations, i.e., $dv/dt = Bv$, the eigenvalue $\lambda$ in the above definition is equivalent to the maximum eigenvalue of $B$, $\lambda_{\text{max}}$. On this basis, a good algorithm should first have the property of being A-Stable and then the further property of being Strongly-A-Stable. The explicit 4th order Runge-Kutta methods and the Adams-type predictor-corrector methods have neither property, and thus are completely unsuitable for stiff systems, even though they are computationally simple to use. For this reason, semi-implicit Runge-Kutta methods which can be A-Stable and Strongly-A-Stable, have been developed and are currently under further development by
mathematicians. Unfortunately, the derivative function of our problem is not given by such a simple form of those semi-implicit methods to allow differentiation with respect to the independent variable.

One possibility might be using the particular implicit method which Cash [8] has reported in terms of a general structure. Abstractions from a second-order and a third-order algorithm are shown below;

\[ y_{i+1} = y_i + k_2 \]

\[ k_1 = hf(t_{i+1}, y_{i+1}) \]

\[ k_2 = hf(t_{i+1} - \frac{1}{2}h, y_{i+1} - \frac{1}{2}k_1) \]

and

\[ y_{i+1} = y_i + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4) \]

\[ k_1 = hf(t_{i+1}, y_{i+1}) \]

\[ k_2 = hf(t_{i+1} - \frac{1}{2}h, y_{i+1} - \frac{1}{2}k_1) \]

\[ k_3 = hf(t_{i+1} - \frac{1}{2}h, y_{i+1} - \frac{1}{2}k_2) \]

\[ k_4 = hf(t, y_i). \]

The corresponding characteristic roots are, respectively

\[ \mu(\lambda h) = (1 - \lambda h + \frac{\lambda^2 h^2}{2})^{-1} \] (142)

and

\[ \mu(\lambda h) = \frac{1 + \frac{1}{6} \lambda h}{1 - \frac{5}{6} \lambda h + \frac{1}{3} \lambda^2 h^2 - \frac{1}{12} \lambda^3 h^3} \] (143)

which are both A-Stable and Strongly-A-Stable. Since a Strongly-A-
Stable second-order method is imbedded with a Strongly-A-Stable third-order method, we can control local errors without an additional function evaluation.

Application of the above algorithm to our problem requires calculation of the implicit term, \( f(t_{i+1}, y_{i+1}) \), which is given by the expression of Eq. (116). We estimate this term by a linear approximation using a Taylor series;

\[
f(t_{i+1}, y_{i+1}) = f(t_i, y_i) + \left( \frac{df}{dt} \right)_i h \tag{144a}
\]

\[
y_{i+1} = y_i + h \left( \frac{dy}{dt} \right)_i + \frac{1}{2} \frac{d^2y}{dt^2} i h^2 \tag{144b}
\]

\[
t_{i+1} = t_i + h \tag{144c}
\]

where

\[
f = \frac{dy}{dt} = - y^{-1} \cdot \frac{\partial R}{\partial t} \tag{145a}
\]

\[
\frac{df}{dt} = \frac{d^2y}{dt^2} = - y^{-1} \cdot \left[ \left( \frac{dy}{dt} \right)^T \left( \frac{\partial^2 R}{\partial y \partial y} \right) + 2 \left( \frac{\partial R}{\partial y} \right) \cdot \left( \frac{dy}{dt} \right) + \frac{\partial^2 R}{\partial t^2} \right] \tag{145b}
\]

It is mentioned that this algorithm has not been implemented in our present work, but, possibly, future work will be conducted to study its effectiveness.
VI. COMPUTATIONAL ASPECTS

6.1 Generation of the Starting Vector in the Initial Value Problem.

Implementation of the Deborah number marching scheme necessitates an initial solution vector to begin with. The solution to the Navier-Stokes equation is a natural choice for that vector because the Phan-Thien & Tanner constitutive equation reduces to a Newtonian fluid when the Deborah number is zero.

In the following, we would like to highlight some the steps taken in simulating a Navier-Stokes fluid in a cylindrical and axisymmetric contraction-channel, as shown in Fig. 3. An isothermal, incompressible and laminar flow is considered. The momentum and mass balances can be written as:

\[
V_r V_r, r + V_z V_r, z = -P, r + \frac{1}{Re} \left[ \left( \frac{1}{r} (r V_r), r \right), r + V_{r, zz} \right] + g_r \quad (146a)
\]

\[
V_r V_z, r + V_z V_z, z = -P, z + \frac{1}{Re} \left[ \frac{1}{r} (r V_z), r + V_{z, zz} \right] + g_z \quad (146b)
\]

\[
\frac{1}{r} (r V_r), r + V_{z, z} = 0 \quad (146c)
\]

To discretize the above equations over the domain of our geometry, a mixed finite element procedure which has been introduced in previous sections is employed. The usual Galerkin weak solution formulation yields,
\[ 2\pi \int_{\Omega} \left[ V_r^* (V_r + rV_z, V_z) r - (rV_r)^* \right] p + \frac{1}{\text{Re}} (rV_r^*), r \frac{1}{\text{Re}} rV_r^* \right] r \, dr \, dz \]

\[ = 2\pi \int_{\Omega} V_r^* g_r r \, dr \, dz - 2\pi \int_{\partial \Omega} V_r^* P_n r \, dr + 2\pi \int_{\partial \Omega} V_r^* r \, dr + 2\pi \int_{\partial \Omega} V_r^* r \, dr \]

\[ (147a) \]

\[ 2\pi \int_{\Omega} V_r^* (rV_r), r \, dr \, dz + 2\pi \int_{\Omega} V_{z,z}^* r \, dr \, dz = 0 \]

\[ (147b) \]

\[ 2\pi \int_{\Omega} V_z^* (V_r + rV_z, V_z) r - (rV_z)^* \right] p + \frac{1}{\text{Re}} V_z^* r \, dr \, dz + 2\pi \int_{\partial \Omega} V_r^* r \, dr \, dz + 2\pi \int_{\partial \Omega} V_r^* r \, dr \]

\[ (147c) \]

where the superscript * indicates the weighting function.

Choosing following boundary conditions to make all boundary integral terms in Eq. (147) vanish at once;

\[ V_r = 0, \quad V_z = V_z(r), \quad P = P_0 \quad \text{on} \quad (r, z) \in \partial \Omega_{z1} \]

\[ V_r = V_z = 0 \quad \text{on} \quad (r, z) \in \partial \Omega_{r1} \]

\[ V_r = V_z, r = 0 \quad \text{on} \quad (r, z) \in \partial \Omega_{r2} \]

\[ V_z = Z_z(r), \quad V_r, z = 0 \quad \text{on} \quad (r, z) \in \partial \Omega_{z2} \]

Substituting interpolation functions of the form,

\[ V_i^e = \sum_{\alpha=1}^{2} \phi_\alpha V_{i,a}, \quad V_i^* = \phi_\alpha^*; \]

\[ p^e = \sum_{\beta=1}^{4} \phi_\beta p_\beta, \quad p^* = \phi_\beta^*; \]

\[ (149a) \]

\[ (149b) \]
to Eq. (147) yields the following element residual equations:

\[ R_1^e = 2\pi\int_{\Omega^e} \left[ \phi^e_\alpha (V_r r, r + V_z z, r) - (\phi^e_\alpha + r_\phi^e_\alpha, r) \right] d\Omega + \frac{1}{Re} (\phi^e_\alpha + r_\phi^e_\alpha, r)(V_r + rV_r, r)/r \]

\[ + \frac{1}{Re} \phi^e_\alpha, z^r r, z r dr dz \]  \hspace{1cm} (150a)

\[ R_2^e = 2\pi\int_{\Omega^e} \theta^e_\alpha (V_r + rV_r, r + rV_z, z) d\Omega \]  \hspace{1cm} (150b)

\[ R_3^e = 2\pi\int_{\Omega^e} \left[ \phi^e_\alpha (V_r r, r + V_z z, z) - \phi^e_\alpha, z^p, \right] d\Omega \]

\[ + \frac{1}{Re} (\phi^e_\alpha, r z, z + r_\phi^e_\alpha, z z, z) dr dz \]  \hspace{1cm} (150c)

where \( \phi^e_\alpha \) and \( \theta^e_\beta \) represent a 9-node bi-quadratic and a 4-node bi-linear shape functions, respectively.

The contributions of each element residual vector are assembled together to form a system residual vector given by:

\[ R(\phi) = 0. \]  \hspace{1cm} (151)

A Newton-Raphson iteration scheme such as given in Eq. (111) requires the formulation of the Jacobian matrix in solving the above nonlinear residual equations. These are given below in an element block matrix form:

\[ \hat{y}_{11}^e = 2\pi\int_{\Omega^e} \left[ \phi^e_\alpha (V_r r, r + V_z z, z) - (\phi^e_\alpha + r_\phi^e_\alpha, r) \right] d\Omega + \frac{1}{Re} (\phi^e_\alpha + r_\phi^e_\alpha, r)(\phi^e_\beta + r_\phi^e_\beta, r)/r \]

\[ + \frac{1}{Re} \phi^e_\alpha, z^r r, z r dr dz \]  \hspace{1cm} (152a)
\[ \mathbf{u}^{e}_{12} = -2\pi \int_{\Omega} \left( \phi_{a} + r\phi_{a,r} \right) r d\theta \quad (152b) \]

\[ \mathbf{u}^{e}_{13} = 2\pi \int_{\Omega} \theta_{\alpha} \phi_{\beta} V_{r,z} r \, dr \, dz \quad (152c) \]

\[ \mathbf{u}^{e}_{21} = 2\pi \int_{\Omega} \theta_{\alpha} \left( \phi_{\beta} + r\phi_{\beta,r} \right) r \, dr \, dz \quad (152d) \]

\[ \mathbf{u}^{e}_{22} = 0 \quad (152e) \]

\[ \mathbf{u}^{e}_{23} = 2\pi \int_{\Omega} \theta_{\alpha} \phi_{\beta,z} r \, dr \, dz \quad (152f) \]

\[ \mathbf{u}^{e}_{31} = 2\pi \int_{\Omega} \theta_{\alpha} \phi_{\beta} V_{z} r \, dr \, dz \quad (152g) \]

\[ \mathbf{u}^{e}_{32} = -2\pi \int_{\Omega} \phi_{a,z} \theta_{\beta} r \, dr \, dz \quad (152h) \]

\[ \mathbf{u}^{e}_{33} = 2\pi \int_{\Omega} \left[ \phi_{\alpha} \left( V_{r,\phi_{\beta,z}} + r\phi_{\alpha,r} V_{z,\phi_{\beta,z}} + V_{z,\phi_{\beta,z}} \right) \right] r \, dr \, dz \quad (152i) \]

For a strong viscous creeping flow \( \text{Re} = 10^{-2} \sim 10^{-5} \), three to four Newton-Raphson iterations starting from a zero vector with specified boundary conditions have given very accurate solutions for velocities and pressure. Now, from the velocity field obtained, stress profiles must be established at each nodal point on the domain in order to include those as the starting vector for the non-Newtonian simulation; this is because a mixed finite element method requires stress
information as independent variables. This can be done by introducing the interpolation functions into the definition of a Newtonian extra stress, such as

\[ \tau_{ij}(r, z) = \sum_{\alpha=1}^{N} (V_{i\alpha} \phi_{\alpha,j} + V_{j\alpha} \phi_{\alpha,i}). \]  

(153)

6.2 Computational technique and parameter specification.

The physical domain (4:1 axisymmetric cylindrical contraction-channel) is divided into streamline-oriented, four-node quadrilateral element meshes. Meshes near the reentrant corner are refined to minimize the large discretization errors due to the sudden contraction. To reduce the singularity present at that corner, an insignificant amount of the sharp edge is smoothed out. This transitional portion of the channel is manually woven and its four-node element information is read in as input data, while those of the wide upstream and the narrow downstream channel are automatically generated. This procedure has relieved much of tedious and time-consuming effort of data generation. A detailed picture of four-node space discretization over the transitional region is shown in Figure 4. After completion of four-node data generation, the nine-node element information is created automatically from the known data. It is also noted that long upstream and downstream channels are adopted in our problem to ensure viscometric flow profiles, at both channel ends, which are the numerical boundary conditions.
The above system contained 2639 nodes, 606 elements and 16,548 unknowns (or equations) and has been simulated by AS-II machine of the National Semiconductor Company, which had a memory capacity of 8 megabytes. For a solver, the unsymmetric version of "Frontal Method" developed by Hood [31] has been employed in order to save on core memory. This solver has greatly reduced the large amount of central memory requirement of our system to only 1.29 megabytes.

A brief description of the unsymmetric Frontal Solver may be helpful. The frontal routine starts by assembling each of the element stiffness matrices in turn into the core, until the core area allocated to the solution routine by the programmer is filled. Then, from within this assembled part of the complete matrix, a pivotal search is made to determine the largest entry from among those rows and columns which are fully summed. The pivotal row is then used to eliminate all of the coefficients in the pivotal column, after which it is placed on a backup storage disc. When sufficient coefficients have been eliminated it is possible to assemble the next element stiffness matrix, after which further elimination may take place. When finally all coefficients have been eliminated, the solution is obtained by a back-substitution routine. In order to minimize core requirements, the element numbering may be chosen in such a way as to keep the "front width" as small as possible. It may also be important to note that the computational time and core requirements of this frontal routine are strongly controlled by the amount of pivotal choice permitted, and the mode of pivoting.

This original frontal method has been modified for the purpose of accommodating boundary conditions in solving the Newton-Raphson
iteration scheme of Eq. (111). The terminating criterion of this nonlinear iteration method takes the form of the standard deviation between two consecutive iterated solutions; that is,

$$
\delta = \left( \frac{\sum (\phi_i - \phi_{i-1})^2}{\sum \phi_i \cdot \phi_i} \right)^{1/2} < \varepsilon = 1.0 \times 10^{-12}.
$$

(154)

Usually, three or four iterations have been enough to satisfy the above criterion.

The following parameters of the Phan-Thien fluid have been specified in our problem to allow a practical shear stress range even doing a high elongation rate flow (refer to the section 4.2);

$$
\varepsilon' = 0.015 \quad \text{and} \quad \xi = 1.0 \times 10^{-6}.
$$

(155)

Under these conditions, the Phan-Thien fluid [55] may behave very similarly to an upper convected Maxwell fluid, which has an infinite elongational viscosity and a constant shear viscosity.

Using considerations of actual polymer melts (polyethylene) at 200°C, viscosities of which range between $10^4 \sim 10^6$ poises, the upstream flow conditions in our numerical simulation may be selected to agree with the real situations, such as,

$$
\text{Re} = 10^{-4} \quad \text{and} \quad \left( \frac{\partial P}{\partial z} \right)_{(0,Z_0)} = -4 \times 10^2.
$$

(156)

Two sets of numerical simulations have been performed and listed below.
Table 7 lists results of the one-step, 4th-order Runge-Kutta type of the initial value approach with the Newton-Raphson iteration scheme (RK-Newton; refer to the section 5.5.4).

Table 7. Comparison between the STEP-Newton and the RK-Newton.

<table>
<thead>
<tr>
<th>Step No.</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Newton-Raphson</td>
<td>STEP-Newton</td>
<td>RK-Newton</td>
<td>RK-Newton</td>
<td>RK-Newton</td>
</tr>
<tr>
<td>Total De</td>
<td>De = 0</td>
<td>De = 0.001</td>
<td>De = 0.151</td>
<td>De = 0.251</td>
<td>De = 0.351</td>
</tr>
<tr>
<td>ΔDe</td>
<td>0</td>
<td>0.001</td>
<td>0.15</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Iter. #1</td>
<td>δ = 0.9708</td>
<td>δ = 0.8176 x 10^{-4}</td>
<td>δ = 0.1317 x 10^{-4}</td>
<td>δ = 0.5813 x 10^{-5}</td>
<td>δ = 0.3235 x 10^{-1}</td>
</tr>
<tr>
<td>Iter. #2</td>
<td>δ = 0.3724 x 10^{-6}</td>
<td>δ = 0.1018 x 10^{-6}</td>
<td>δ = 0.5364 x 10^{-7}</td>
<td>δ = 0.1343 x 10^{-7}</td>
<td>δ = 0.1283 x 10^{-1}</td>
</tr>
<tr>
<td>Iter. #3</td>
<td>δ = 0.3110 x 10^{-15}</td>
<td>δ = 0.2587 x 10^{-13}</td>
<td>δ = 0.4578 x 10^{-12}</td>
<td>δ = 0.4551 x 10^{-14}</td>
<td>δ = 0.1678</td>
</tr>
<tr>
<td>Iter. #4</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>Iter. #5</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
</tr>
</tbody>
</table>

It is noted that numerical breakdown has taken place at De = 0.351. The possible cause of this failure will be given in the next chapter. From the above table, we want to stress particularly the advantage of the RK-Newton over the step-change in De number with the Newton-Raphson method (STEP-Newton; refer to the section 5.5.2). Note that the STEP-Newton only allows a small Deborah number increment at each step (here, ΔDe = 0.001) such that the convergence of the Newton-Raphson scheme can be assured; three function evaluations are required for this method. In contrast, the RK-Newton method can advance a large step (ΔDe = 0.15) mainly due to the higher order approximation, but
seven total function evaluations are needed for each increment-step (four for the Runge-Kutta and three for the Newton-Raphson). It is obvious that the initial value approach (i.e., RK-Newton method) is far superior over the STEP-Newton with respect to saving computational time. We feel that many future numerical computations of viscoelastic fluids should be directed at using one of the stable and efficient initial value algorithms of the ordinary differential equations with the Newton-Raphson iteration scheme.

We have attempted to test the efficiency of the predictor-corrector method, but due to our mistake in coding the results cannot be demonstrated. We only tabulate four initial steps of this method on Table 8, which is the same as the RK-Newton.

All values of variables listed on the table are dimensionless quantities. Plots and explanations of the stress, the velocity and the pressure distributions which have been obtained by the numerical procedures summarized in Table 8, will be given in the next chapter. The infinite elongational viscosity predicted by the upper convected Maxwell model be the major cause of numerical failure in the die-entry flow.
Table 8. Numerical performance of the RK-Newton.

<table>
<thead>
<tr>
<th>Step No.</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method</td>
<td>Newton-Raphson</td>
<td>RK-Newton</td>
<td>RK-Newton</td>
<td>RK-Newton</td>
</tr>
<tr>
<td>Total De</td>
<td>De = 0</td>
<td>De = 0.05</td>
<td>De = 0.10</td>
<td>De = 0.15</td>
</tr>
<tr>
<td>Δ De</td>
<td>0.0</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
</tr>
</tbody>
</table>

|        | δ=0.9708 | δ=0.9456x10^{-4} | δ=0.134x10^{-5} | δ=0.1629x10^{-5} |
| Iter. #1 | δ=0.3724x10^{-6} | δ=0.6068x10^{-5} | δ=0.1518x10^{-9} | δ=0.7172x10^{-9} |
| Iter. #3 | δ=0.3110x10^{-15} | δ=0.1226x10^{-8} | δ=0.1964x10^{-15} | δ=0.4407x10^{-15} |
| Iter. #4 | ----- | δ=0.2944x10^{-15} | ----- | ----- |

\((\hat{\sigma}/\hat{Z})_{res.}\)  
-0.4x10^{3}  
-0.4x10^{3}  
-0.4x10^{3}  
-0.4x10^{3}  

\(<V_{z}\rangle_{res.}\)  
0.08  
0.08  
0.08  
0.08  

\((\hat{\sigma}/\hat{Z})_{cap.}\)  
-0.1024x10^{6}  
-0.10227x10^{6}  
-0.10187x10^{6}  
-0.10123x10^{6}  

\(<V_{z}\rangle_{cap.}\)  
1.28  
1.28  
1.28  
1.28  

VII. COMPUTATIONAL RESULTS OF THE CONTRACTION FLOW

7.1 Possible Cause of Numerical Failure of the Upper Convected Maxwell Model.

In spite of much devoted effort and time of many researchers in the field of non-Newtonian fluid mechanics, the problem of the numerical breakdown of the upper convected Maxwell model has remained one of the most mysterious and challenging problems. Some results have been published showing large oscillations in the stress, velocity and pressure fields generated near the reentrant corner of a contraction channel [50], pointing out the limit point behavior of Deborah number convergence [70], and demonstrating that fine mesh refinement over the region trouble does not significantly help in getting a higher range of convergence [25,39,70]. Here we show by a simple analysis and then prove using computational results that the infinite constitutive prediction of elongational viscosity at finite elongation rate and shear stress may be to a large degree responsible for all of the confusion.

Even though the Phan-Thien model has been employed in our numerical study, the extremely small value of the parameter $\xi = 10^{-6}$ has rendered our analysis that of essentially the upper convected Maxwell type fluid. Thus, for simplicity, we analyze this fluid in the rest of the section. The contraction channel of our problem has several features which are summarized below.

1. both far upstream and downstream of the contraction there exists a viscometric flow;

2. a shear-free elongation takes place along the center line when the flow converges into the small channel;
3. the sharp reentrant corner can be a source of very large shear stresses.

Based on these observations, we write down the dimensionless form of the center line equations;

\[ \text{De} V_z \tau_{rr,z} + (1 - 2 \text{De} V_{r,r}) \tau_{rr} = 2 V_{r,r} \tag{157a} \]

\[ \text{De} V_z \tau_{zz,z} + (1 - 2 \text{De} V_{z,z}) \tau_{zz} = 2 V_{z,z} \tag{157b} \]

These are the first order differential equations for \( \tau_{rr} \) and \( \tau_{zz} \), but it is still not easy to obtain the exact solutions because \( V_{r,r} \), \( V_{z,z} \) and \( V_z \) are not known and must be obtained from the two dimensional problem. Fortunately, however, more simplification can be made to Eq. (157), knowing that there exists a maximum or a minimum point on the center line such that \( \tau_{rr,z} \) and \( \tau_{zz,z} \) vanish, because both ends of the center line must satisfy the viscometric flow conditions (i.e., \( \tau_{rr} = \tau_{zz} = 0 \) in our case). Thus, a maximum or a minimum point has the expression of

\[ (\tau_{rr})_m = \frac{2 V_{r,r}}{1 - 2 \text{De} V_{r,r}} \tag{158a} \]

\[ (\tau_{zz})_m = \frac{2 V_{z,z}}{1 - 2 \text{De} V_{z,z}} \tag{158b} \]

Eq. (158b) represents the locus of maximum points in the axial stress field of the centerline until the Deborah number arrives at the singular value of \( \text{De} = 1/(2V_{z,z}) \). This is well demonstrated in Figure
7. After passing through the singular point, the same equation now becomes the locus of minimum points in the same axial stress field, which is a physically unrealistic situation. Josse and Finlayson [36] have actually displayed these minimum values of the axial stresses on the centerline, although they have not realized the implication of their results.

This behavior is exactly the same as the elongational viscosity of the upper convected Maxwell model which has been demonstrated in Section 3.4. In other words, it can be said that the locus of maximum axial and radial stresses on the center line as a function of an increasing Deborah number is simply a reflection of the infinite elongational viscosity at finite elongation rate predicted by the model. This can be clearly shown by applying the definition of the steady simple elongational flow, such as given by Eqs. (14) and (17), to the expressions of the maximum axial and radial stresses on the center line of Eq. (158). One obtains an identical expression for the infinite elongational viscosity of the upper convected Maxwell model in dimensionless form given earlier (refer to Table 2).

\[
(\tau_{zz})_m - (\tau_{rr})_m = \frac{3\dot{\varepsilon}}{(1-2\dot{\varepsilon})(1+\dot{\varepsilon})}
\]

or

\[
\bar{n}(\dot{\varepsilon})_m = \frac{3}{(1-2\dot{\varepsilon})(1+\dot{\varepsilon})}.
\]

Next we turn our attention to the subject of how the shear stress is coupled with the infinite elongational viscosity in bringing about numerical problems. The question naturally arises because the numerical
procedures, as is widely known, have never failed on the center line, but rather have had their largest problems at the point just after the sharp edge of the reentrant corner of the wall, that is, the place which is expected to have the maximum shear stress rise.

Thus, we write down equations for the non-moving wall at which velocities are assumed to vanish, i.e., \( V_r = V_z = 0 \), and rearrange them into the explicit forms of \( \tau_{rr} \), \( \tau_{zz} \) and \( \tau_{rz} \).

\[
\tau_{rr} = \frac{2V_r r + 2De V_r z \tau_{rz}}{1 - 2De V_r r} \quad (159a)
\]

\[
\tau_{zz} = \frac{2V_z z + 2De V_z r \tau_{rz}}{1 - 2De V_z z} \quad (159b)
\]

\[
\tau_{rz} = \frac{(V_r r + V_z z + V_r z \tau_{zz} + V_z r \tau_{rr})}{1 - De(V_r r + V_z z)} \quad (159c)
\]

Surprisingly enough, Eq. (159) for the wall include both the singular behavior of the elongation term of the center line as well as the term due to the shear. Now, we begin to understand what is really happening near the sharp corner. The shear term \( 2De V_z r \tau_{rz} \) is believed to contribute some magnification of the singular behavior at positions where the wall shear rate \( (V_z r)_w \) and the wall shear \( (\tau_{rz})_w \) are most significant. This point is confirmed by the numerical results, shown in Figure 9, to be just behind the reentrant corner of the contraction channel. The extremely large growth of the wall axial stress is also demonstrated at this very spot, as shown in Figure 10. Note that the same magnitude of growth for \( \tau_{rr} \) and \( \tau_{rz} \) should be expected from Eq. (159a) and (159c) and have been verified by Figures 8 and 9. This sharp
and critical rapid rise of the stress field near the corner can surely cause numerical oscillations and the subsequent failure when one attempts to solve the equations using the nonlinear iteration routine. Also note that since the shear rate and the shear stress show maximum values at the wall and diminish toward the center axis, the same trend is followed in the normal stress field, which is given in Eq. (158) and (159) and shown in Figures 8, 9 and 10. For instance, the center axial stress is approximately ten times smaller than that of the wall at De = 0.15 in our problem. This phenomenon will become even more impressive when the Deborah number approaches the singular value.

Please understand that the large wall shear stress generated due to the geometric singularity present at the sharp corner is not the only major factor of the numerical breakdown; that is why the mesh refinement over the region cannot overcome this difficulty. Instead, we have to say that the singular behavior of the stress field for this constitutive model (or the infinite elongational viscosity) is the principal problem. In other words, the role of the large shear stress at the corner hastens the onset of singular behavior like a catalyst in a chemical reaction. This couples the shear stress with the Deborah number convergence indicator. That is, the Deborah number convergence may heavily depend on the shear stress specification (i.e., the axial pressure gradient and the Reynolds number; refer to Eq. (25)) at the upstream boundary. For example, at higher shear stress one must provide a lower Deborah number in order that convergence can be obtained. From this point of view, shear thinning behavior of polymer melts may help to raise the convergence limit. Finally, it may be concluded that any
constitutive model which contains the prediction of infinite elongational viscosity in the purely extensional flow must be avoided in the numerical simulation of the viscoelastic flows with complex geometries.

7.2 Physics of the Maxwell Fluid in the Contraction Channel.

Consider the cylindrical contraction channel which is shown in Figure 6. The wall and the centerline constitute the exact streamlines, but the inner two lines are arbitrarily drawn, hypothetical streamlines in order to obtain a physical pictures of variables seen when a material point proceeds along those lines. All figures in the following are based on these four lines as pre-determined. The line number is named from the center (or the first line) and toward the wall (or the fourth line). Also, it is mentioned that the values of all variables which appear are dimensionless quantities which have been defined by Eq. (18).

Figure 8 shows radial normal stress changes on the four different passages mentioned above. The most strong radial stress is shown to be present at the wall, but the region susceptible to this stress becomes extremely narrow. In contrast, the magnitude of radial stress towards the center decreases dramatically and is spread out widely upstream.

The magnitude of shear stress shown in Figure 9 has generally the same trend as the radial stress mentioned above. The second and the third lines demonstrate elongational characteristics of the contraction flow; that is, a decrease of the shear stress after a gradual increase indicates this phenomenon. Just after the reentrance corner, the extraordinarily large values of wall shear stress are clearly observed.
Some interesting results of the axial normal stress field can be found using Figure 10. Stresses on the second line show a small contraction force before embarking on the large extensional one. Particularly, the Newtonian stresses on the third and the fourth line are contractile for both lines. The huge and sharp axial normal stress appears right after the reentrance corner, which has been explained in the previous section.

The angular stress which is plotted on Figure 11 increases toward the center, while the maximum points on each line shift downwards with larger Deborah number.

Figure 12 demonstrates the effect of the pressure loss due to the reentrance section of the channel. Close to the wall, the sharp pressure decrease is observed after a remarkable pressure rise. Meanwhile, a smooth and gradual pressure loss is presented on the centerline without any prior pressure gain. Also, decrease of the pressure loss is observed with the increase of the Deborah number, which is a well known result for the Maxwell model.

The radial and the axial velocity fields are shown in Figure 13 and 14. Differences of the velocity field between the Newtonian and the non-Newtonian fluids are very small. However, it is observed that the axial slope decreases slightly with the increase of the Deborah number.

In general our results are in agreement with those of Viriyayuthakorn et al., [66] which have simulated the integral type of the upper convected Maxwell model. However, ours are more extensive and very clear in presenting the pathological behavior of the Maxwell fluid in the defined region.
A comment can be made about the shift of the stress curve to the downstream from that of the Newtonian when the Deborah number increases. This shift, which may be conceived as the actual magnitude of the elongation, is more pronounced toward the center axis as shown in Figures 8, 9, 10 and 11. Thus, one may expect that the maximum elongation would be experienced along the center line. Also, the axial normal stress and the shear stress on the second line tell us that there are two different flow mechanisms near the corner; one is the strong shear-induced flow and the other is the flow due to the strong elongational forces. Finally the stress field on the third line clearly indicates the existence of a weak vortex at the L-shaped corner. The size of the vortex can be visualized by drawing the contour lines of the stream function. However, we have omitted this in the present study.
Figure 6. Contour lines for plotting variables in the given geometry.
Figure 7. Axial normal stress fields with changes of the Deborah number on the centerline.
Figure 8. Radial stress distribution along the contour lines near the die-entry region.
Figure 8. Radial stress distribution along the contour lines near the die-entry region.
Figure 9. Shear stress distribution along contour lines near the die-entry region.

- dimensionless shear stress
- dimensionless axial distance (Z/R)

Chart showing the distribution of shear stress with respect to axial distance.
Figure 9. Shear stress distribution along contour lines near the die-entry region.
Figure 10. Axial stress distribution along contour lines near the die-entry region.
Figure 10. Axial stress distribution along the contour lines near the die-entry region.
Figure 11. Angular stress distribution along contour lines near the die-entry region.
Figure 12: Pressure distribution along contour lines near the die-entry region.
Figure 12 (a): Pressure distribution along contour lines near the die-entry region.
Figure 12 (b): Pressure distribution along contour lines near the die-entry region.
Figure 13: Radial velocity distribution along contour lines near the die-entry region

Dimensionless radial velocity

Dimensionless axial distance (Z/R)
Figure 14: Axial velocity distribution along contour lines near the die-entry region
VIII. CONCLUDING REMARKS

We have shown that almost all of the commonly used differential models contain either viscometric shear limitations in tube flow or they have infinite elongational viscosity problems. This work may have as its principal value clearly disclosing the inherent problems of these models from a computational view point. We have also indicated that these defects are directly related to the co-rotational (Jaumann) derivative and the upper (or lower) convective (Oldroyd) derivative, derived from the very essence of the continuum mechanics. This puts forward another dilemma -- finding proper differential constitutive models for future numerical prediction work. Our hope is that clear exposure of the nature of the numerical breakdown would help some theorists to mold sound constitutive models not only from the viewpoint of the experimentalist, but also from that of the numerical analyst in the near future.

Another important contribution of this work may be the introduction of the initial value approach in reducing errors due to the Deborah number increments. Particularly in the case of highly elastic fluid flow, the stiff problem method may overcome the barrier of the excessive computer time utilized in evaluating the ever-increasing stress field.

By a simple material balance, velocity boundary conditions for the downstream have been obtained for the contraction channel for the first time in our thesis. We have confirmed the effectiveness of the method by the experience of this work.

Finally we thank numerous people for their sincere advice and criticism which have helped us in laying the foundation of this thesis.
BIBLIOGRAPHY


