INFORMATION TO USERS

This was produced from a copy of a document sent to us for microfilming. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the material submitted.

The following explanation of techniques is provided to help you understand 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 you of complete continuity.

2. When an image on the film is obliterated with a round black mark it is an indication that the film inspector noticed either blurred copy because of movement during exposure, or duplicate copy. Unless we meant to delete copyrighted materials that should not have been filmed, you will find a good image of the page in the adjacent frame.

3. When a map, drawing or chart, etc., is part of the material being photographed the photographer has followed a definite method in “sectioning” the material. 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 any illustrations that cannot be reproduced satisfactorily by xerography, photographic prints can be purchased at additional cost and tipped into your xerographic copy. Requests can be made to our Dissertations Customer Services Department.

5. Some pages in any document may have indistinct print. In all cases we have filmed the best available copy.
LIN, YOW-THINK

A NUMERICAL STUDY OF NONLINEAR VISCOELASTIC FLOW AND NONISOTHERMAL POWER-LAW FLOW

Rice University

Ph.D. 1980

University Microfilms International
300 N. Zeeb Road, Ann Arbor, MI 48106
18 Bedford Row, London WC1R 4EJ, England
RICE UNIVERSITY

A NUMERICAL STUDY OF NON-LINEAR VISCOELASTIC FLOW
AND NON-ISOTHERMAL POWER-LAW FLOW

BY

YOW-THINK LIN

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

Doctor of Philosophy

APPROVED, THESIS COMMITTEE:

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

J. D. Hellums, Professor of Chemical Engineering

W. E. Walker, Professor of Mechanical Engineering

HOUSTON, TEXAS

APRIL, 1980
A NUMERICAL STUDY OF NON-LINEAR VISCOELASTIC FLOW
AND NON-ISOTHERMAL POWER-LAW FLOW

YOW-THINK LIN

ABSTRACT

Using the finite difference technique, the steady flow of a viscoelastic fluid through a contraction/expansion and a modified Graetz heat transfer problem for power-law fluids between parallel plates are numerically studied.

The constitutive model used for the viscoelastic fluid flow extends the Maxwell equation of linear viscoelasticity to the non-linear region by letting both relaxation time and elastic modulus depend upon the existing structure. Based on the calculations for a 3:1/1:3 contraction/expansion geometry with fully developed simple shearing flows at the entrance and exit, there exists a transition range for this fluid model, in terms of the Weissenberg number, beyond which elastic effects appear to become less dominant. The upstream vortex detachment length before the contraction is shown to grow with increasing Weissenberg number, and then reach a maximum value, until no converged solution can be obtained or possibly unsteady flow starts to develop.

Heat transfer to polymer melts or solutions flowing in a parallel plate system is of great importance in polymer processing, as for example in extrusion through a large aspect ratio slit die. The present work was undertaken to solve the energy equation for power-law fluids under various circumstances, including a temperature-dependent visco-
sity, viscous dissipation and heat convection across streamlines
induced by the abrupt change of boundary temperature and subsequent
velocity field rearrangement. In addition to the numerical solutions
given, an analytical approximation method for the Graetz-Nusselt problem
is also presented for comparison. This method divides the domain into
two sections for which two corresponding solutions, approximated by
polynomials, are solved by a thermal boundary layer theory and an in-
tegral method respectively. These two approximate solutions are then
matched at the intersection to give a continuous and consistent tempe-
rature profile. Although the analytical solutions application is limited
to the case with a temperature-independent viscosity, this simple ana-
lysis is believed to be better than the previous methods available in
the literature.
ACKNOWLEDGEMENTS

The author wishes to express his sincere appreciation to his advisor Professor Larry V. McIntire for his guidance and inspiration during the course of this investigation and his assistance in the preparation of this thesis.

Appreciation is also extended to Professors J. D. Hellums and W. F. Walker for their interest in this work and for serving on the oral examination committee.

Finally, the author wishes to thank his wife and parents for their constant encouragement and patient support.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>List of Tables</td>
<td>vii</td>
</tr>
<tr>
<td>List of Figures</td>
<td>viii</td>
</tr>
<tr>
<td><strong>Chapter</strong></td>
<td></td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Background</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Review of Previous Work</td>
<td>5</td>
</tr>
<tr>
<td>Contraction/Expansion Flow</td>
<td>5</td>
</tr>
<tr>
<td>Heat Transfer</td>
<td>8</td>
</tr>
<tr>
<td>II. MATHEMATICAL FORMULATION</td>
<td>11</td>
</tr>
<tr>
<td>2.1 Momentum Equation</td>
<td>11</td>
</tr>
<tr>
<td>2.2 Constitutive Equation of Viscoelastic Fluids</td>
<td>17</td>
</tr>
<tr>
<td>2.3 Energy Equation</td>
<td>20</td>
</tr>
<tr>
<td>III. NUMERICAL RESULTS AND DISCUSSIONS</td>
<td>34</td>
</tr>
<tr>
<td>3.1 Contraction/Expansion Flow of Viscoelastic Fluids</td>
<td>34</td>
</tr>
<tr>
<td>3.1-1 Flow Geometry</td>
<td>34</td>
</tr>
<tr>
<td>3.1-2 Constitutive Equation</td>
<td>34</td>
</tr>
<tr>
<td>3.1-3 Boundary Conditions</td>
<td>38</td>
</tr>
<tr>
<td>3.1-4 Numerical Formulation</td>
<td>41</td>
</tr>
<tr>
<td>3.1-5 Numerical Results</td>
<td>52</td>
</tr>
<tr>
<td>3.2 Heat Transfer Problem of Power-Law Fluids</td>
<td>72</td>
</tr>
<tr>
<td>3.2-1 Numerical Solutions</td>
<td>72</td>
</tr>
<tr>
<td>Chapter</td>
<td>Page</td>
</tr>
<tr>
<td>------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>3.2-2 Analytical Approximation Method for</td>
<td></td>
</tr>
<tr>
<td>Nusselt-Graetz Problem</td>
<td>86</td>
</tr>
<tr>
<td>IV. CONCLUDING REMARKS</td>
<td>96</td>
</tr>
<tr>
<td>BIBLIOGRAPHY</td>
<td>98</td>
</tr>
</tbody>
</table>
## LIST OF TABLES

<table>
<thead>
<tr>
<th>Table Number</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Number of Outer Iterations for the Converged Solutions obtained with various Weissenberg Numbers</td>
<td>53</td>
</tr>
<tr>
<td>2.</td>
<td>Comparison between Analytical and Numerical Solutions for the Nusselt-Graetz Problem of Newtonian Fluid</td>
<td>89</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Number</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Illustration for the Analytical Approximation Solution of Graetz-Nusselt Problem.</td>
<td>27</td>
</tr>
<tr>
<td>2.</td>
<td>Flow Domain for the Contraction/Expansion with ( h/a = 3 ).</td>
<td>35</td>
</tr>
<tr>
<td>3.</td>
<td>Iteration Scheme for determining Structure Variable.</td>
<td>39</td>
</tr>
<tr>
<td>4.</td>
<td>Typical Dimensionless Viscometric Material Functions</td>
<td>42</td>
</tr>
<tr>
<td></td>
<td>and values of the Structure Variable as a function of the Weissenberg Number for the model of Acierno et al.</td>
<td></td>
</tr>
<tr>
<td>5.</td>
<td>Flow Chart for Iteration Scheme of the Transport Equation</td>
<td>46</td>
</tr>
<tr>
<td>6.</td>
<td>Streamlines for the 3:1/1:3 Contraction/Expansion Flow with ( W_s = 0 ) and ( Re = 0.75 ).</td>
<td>55</td>
</tr>
<tr>
<td>7.</td>
<td>Streamlines for the 3:1/1:3 Contraction/Expansion Flow with ( W_s = 0.08 ) and ( Re = 0.75 ).</td>
<td>56</td>
</tr>
<tr>
<td>8.</td>
<td>Streamlines for the 3:1/1:3 Contraction/Expansion Flow with ( W_s = 0.20 ) and ( Re = 0.75 ).</td>
<td>57</td>
</tr>
<tr>
<td>9.</td>
<td>Streamlines for the 3:1/1:3 Contraction/Expansion Flow with ( W_s = 0.30 ) and ( Re = 0.75 ).</td>
<td>58</td>
</tr>
<tr>
<td>10.</td>
<td>Streamlines for the 3:1/1:3 Contraction/Expansion Flow with ( W_s = 0.45 ) and ( Re = 0.75 ).</td>
<td>59</td>
</tr>
<tr>
<td>11.</td>
<td>The Effect of Weissenberg Number on Vortex Intensity</td>
<td>61</td>
</tr>
<tr>
<td>12.</td>
<td>The Length of the Vortex Region in both Upstream and Downstream direction as a function of Weissenberg Number</td>
<td>62</td>
</tr>
<tr>
<td>13.</td>
<td>The Shear Stress along the Flow Direction on the Stationary Boundary ((y = 1)) as a function of Weissenberg Number.</td>
<td>65</td>
</tr>
<tr>
<td>Figure Number</td>
<td>The Structure Variable on the Moving Boundary $(y=0)$ as a function of Weissenberg Number</td>
<td>Page</td>
</tr>
<tr>
<td>---------------</td>
<td>--------------------------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>14</td>
<td>66</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>The Shear Stress $\tau_{xy}$ on the Moving Boundary $(y=0)$ as a function of Weissenberg Number</td>
<td>68</td>
</tr>
<tr>
<td>16</td>
<td>The Normal Stress Difference exerted on the Moving Boundary as a function of Weissenberg Number</td>
<td>69</td>
</tr>
<tr>
<td>17</td>
<td>The Velocity Profiles across the domain at various $x$ positions for $W_s = 0$ and 0.2</td>
<td>70</td>
</tr>
<tr>
<td>18</td>
<td>X-Component Velocity Profile at $j=6$ for Contraction /Expansion Flow of Viscoelastic Fluids</td>
<td>71</td>
</tr>
<tr>
<td>19</td>
<td>The Domain of Numerical Solution for Nusselt-Graetz Problem of Power-Law Fluids</td>
<td>73</td>
</tr>
<tr>
<td>20</td>
<td>Nusselt Number for various Power-Law Fluid Indices</td>
<td>77</td>
</tr>
<tr>
<td>21</td>
<td>Velocity Profile for various Power-Law Fluid Indices</td>
<td>78</td>
</tr>
<tr>
<td>22</td>
<td>The Effect of Power-Law Fluid Index on Temperature Distribution at $y=0$ and $y=0.9$</td>
<td>79</td>
</tr>
<tr>
<td>23</td>
<td>The Effect of Viscosity on Nusselt Number and Temperature for the flow with $n=0.25$</td>
<td>80</td>
</tr>
<tr>
<td>24</td>
<td>The Effect of Entry Condition and Viscous Dissipation for the flow with $n=0.5$ and $\mu \neq \mu(T)$</td>
<td>82</td>
</tr>
<tr>
<td>25</td>
<td>Nusselt Number Variation for different Entry Conditions of the flow with $n=0.5$, $Br^*=1.0$ and $\mu = \mu(T)$</td>
<td>83</td>
</tr>
<tr>
<td>26</td>
<td>Numerical Solution for a sample problem</td>
<td>85</td>
</tr>
<tr>
<td>27</td>
<td>Comparison of Analytical and Numerical Solutions with $Br^*=0$ and $n=1$</td>
<td>90</td>
</tr>
<tr>
<td>28</td>
<td>Comparison of Analytical and Numerical Solutions with $Br^*=1.0$ and $n=0.5$</td>
<td>94</td>
</tr>
</tbody>
</table>
I. INTRODUCTION

1.1 BACKGROUND:

Polymer processing can be described briefly as the controlled deformation of molten polymers by the application of heat and stress. To achieve an accurate design with the capability of good material quality control, it is necessary to understand the mechanical principles involved in these operations. These must be based on:

(1) relations between the deformation rate and applied stresses,
(2) relations between the generation and flow of heat and
(3) interaction between stress and temperature fields.

The first set of relations gives rise to the constitutive equation which determines the stress from the strain or strain rate. In Newtonian fluid mechanics, there are only viscous stresses, and the constitutive relationship is linear with a single material parameter, the viscosity. This may be a function of temperature and isotropic pressure. However, it has long been known that both viscous and elastic stress phenomena occur in the polymer flows. Except in very special cases, the constitutive relationship is very complex and cannot be described in a linear form. Over a century ago, Maxwell first speculated that the viscoelastic behavior might be synthesized by the series combination of a Hookean spring and a viscous dashpot. The contribution of viscous and elastic stresses in this linear viscoelastic model is weighted by a relaxation time, which is zero for Newtonian fluids. Although this simple mechanical analog still provides a convenient aid for thinking about the response of viscoelastic systems, it has been shown to be inadequate to represent quantitatively most observed phenomena. During
the last two decades, a considerable amount of research has been devoted to experimental rheological studies, and many suggestions have been made about how to modify the Maxwell model to describe better this experimental data. Most of these modifications have focused on letting the relaxation time, or the elastic modulus, or both, be variable. Different constitutive relations allow these material functions to depend on either the rate of strain, the deformation, or the stress. In addition the form of the non-linear dependence may vary. One of the most promising constitutive equation is the non-linear viscoelastic model proposed by Acierno et al. This model allows the relaxation time and elastic modulus depend on the existing network structure. The current structure depends on the whole past history of the motion, instead of just the instantaneous values of either the stress or the strain rate used by Carreau[7] and Kaye[26] for their modified network models. Because of this distinctive feature, we have adopted this constitutive model for analyzing the contraction/expansion flow in this work.

Relations (2) and (3) are concerned with the problem of heat transfer. For a steady polymer channel flow, the energy equation is usually dominated by (a) heat conduction across streamlines, (b) heat convection along streamlines and (c) heat generation due to viscous dissipation. It is also common in the case of polymer flow that the energy and momentum balance equations are strongly coupled through a shear viscosity, which is very strongly temperature-dependent. The situation can become more complicated when viscoelastic fluid flow is considered for which the relaxation time is also a function of temperature. In that case,
the time-temperature superposition should be employed, if the material is so-called "thermo-rheologically simple". The shift factor may be determined by an empirical correlation developed by Williams, Landel and Ferry[18], known as the WLF equation.

In industrial situations, polymer melts are often exposed to sudden changes in geometry and/or temperature. There is no doubt that an efficient numerical algorithm would be of interest in these cases for the use of theoretical calculation of velocity and stress fields. In view of the enormous difficulties associated with such a task in its full generality, it seems likely that a progressive tackling of the problem with simple constitutive models and simplified geometries may bring a better understanding of the important mechanisms involved.

In that spirit, a 3:1/1:3 contraction/expansion geometry with a moving boundary is considered for the non-linear viscoelastic fluid model suggested by Acierno et al. These calculations are used to simulate the drag flow one might find inside an extruder. Using the SOR (Successive Over-Relaxation) iteration method with alternating direction to solve the governing equations, the observations deal primarily with the size of the vortices before and after the contraction. Similarly, the model of a power-law fluid is adopted for the case of non-isothermal flow between two parallel plates. The Crank-Nicholson implicit method of finite difference is employed to solve the energy equation, and the effects of viscous dissipation, temperature-dependent viscosity and heat convection across streamlines are discussed. Additionally, an analytical approximation method for the Graetz-Nusselt problem is also presented. It divides the domain into two sections for which two corresponding sol-
utions, approximated by polynomials, are solved by the thermal boundary layer theory and the integral method respectively. These two approximate solutions are then matched at the boundary of the two sections to give a continuous and consistent temperature profile. This simple analysis cannot be extended to the case with a temperature-dependent viscosity. Nevertheless, it certainly provides spot checks on the numerically computed values and is believed to be better than the previous analytical methods available.
1.2 REVIEW OF PREVIOUS WORK

CONTRACTION/EXPANSION FLOW

A limited number of investigations concerning steady contraction/expansion flows are available in the literature. Christiansen et al[9] used a finite difference method to study numerically the laminar tube flow of Newtonian fluids through an abrupt contraction. Solutions were obtained for the case where the large tube is either real, with no slip at the wall, or frictionless. Their results indicated that, for a given contraction ratio, the upstream vortex diminishes in size with increasing Reynolds number. Similarly, the entrance flow of a Powell-Eyring fluid was considered by Duda and Vrentas[16]. A prominent effect of shear thinning was shown by the increased size of recirculating eddies. It was also presumed that the more severe separation effects observed experimentally must be attributed to the elasticity of the fluids studied. In analyzing, both numerically and experimentally, the behavior of a power-law fluid flowing through a sudden expansion, Halmos et al [25] showed the effect of the Reynolds number on the reattachment length and the vortex. The reattachment length increases monotonically with increasing Reynolds number but the function becomes non-linear as inertia becomes increasingly important. This nonlinearity becomes more pronounced for power-law fluids as the index $n$ decreases from unity. In contrast to the contraction flow, not unexpectedly, it was found that the size of downstream vortex grows with increasing Reynolds number in this case. Deysarkar[15] also provided some interesting information for plane converging drag flow of Newtonian and inelastic power-law fluids. This flow is created by the drag forces brought about by a moving boundary with the other plate held stationary. A variational principle was
employed for the case with very small angles of convergence when an uni-
directional flow can be assumed, and a perturbation technique was used
when the two-dimensional flow should be considered. Their results con-
cluded that the unidirectional flow can be safely assumed for the con-
verging angles less than $8^\circ$. On the other hand, for any angle larger
than $17^\circ$, irrespective of the flow index or the gap ratio, a secondary
flow vortexing is always present.

As far as viscoelastic fluids are concerned, some results have been
recently presented for various constitutive models. Perera and Walters
[34,35] used a four-constant Maxwell/Oldroyd model to study numerically
the effect of high elasticity in flow situations involving L and T
shaped geometries as well as the contraction/expansion problem. Crochet
and Pilate[10] adopted the second-order approximation of Rivlin-Ericksen
constitutive equation to analyze plane flow through a contraction. Based
on their calculations, it was predicted that the upstream vortex grows
as elasticity increases for low values of the Reynolds number, while
the opposite is the case for the downstream vortex. Using a perturbation
scheme coupled with finite element technique, the creeping flow of a
second-order fluid through a tapered contraction was also studied by
Datta and Strauss[12]. However, they only indicated the existence of
circular motion in the contraction zone but failed to give any specific
prediction of its trend. Black and Denn[5] considered the extent to
which the sink flow approximation is valid for creeping converging flow
of viscoelastic liquids. The convected Maxwell model was used with con-
stant shear viscosity and elastic modulus, and a perturbation solution
was obtained for small values of Weissenberg number, $0 \leq \text{W}_{\text{s}} \leq 0.4$. It
was concluded that the sink flow may be used with confidence when the contraction ratios are of at least 5:1 and entry half-angles are of no more than 45°. Gatski[21] studied both Newtonian and three-constant Oldroyd B fluids in a contraction region, which is composed of rectangular hyperbolas, so that the strain rate will be constant along the centerline. Perera and Strauss[36] again used the four-constant Maxwell/Oldroyd model to analyze both contraction and expansion flow problems, and most of their results are the same as before except for the decreasing corner eddy of contraction due to elasticity. Nevertheless, this discrepancy stated in their paper does not seem to agree with the plots shown in the paper. Crochet and Bezy[11] considered the possibility of using the finite element method for non-Newtonian fluids in plane and axisymmetric contraction situations. They apparently did not show a convincing advantage of this method, compared with the finite difference technique, as the incompressibility of fluids leads to a very large number of variables and excessive constraints on the velocity field.

It must be mentioned, however, that the finite element method certainly will be easier to use when a situation of irregular geometry is considered, as demonstrated by Chang et al[8] for the die swell problem with a free surface.

Two papers, by Cable and Boger[6] and Davies et al[13] are closely related to this work and thus should be emphasized here. Cable and Boger have done a comprehensive experimental investigation of tubular entry flow for viscoelastic fluids. Although there is some evidence to suggest that there may not always be 1:1 correspondence between the flow behavior in the plane and the circular tube contraction/expansion problems,
we shall make no distinction between these two geometries as the general characteristics are believed to be equally applicable. Two flow regimes are identified for the entry flow in their observations: a vortex growth regime at low flow rates and a divergent flow regime at moderate flow rates. The vortex detachment length was found to be a linear function of the Weissenberg number in the vortex growth regime, and gradually reaches a maximum value before being reduced by the diverging effect. This is a very important illustration, and has never been shown by any of the numerical calculations based on the linear viscoelastic models before. It thus becomes the purpose of this work to confirm this observation by using a non-linear Maxwell model with structure-dependent relaxation time and elastic modulus. Davies et al gave further consideration to the use of four-constant Maxwell/Oldroyd model for the contraction flow with a moving boundary. This same geometry is adopted in our work because it was felt that the moving boundary can describe better the flow behavior inside the single-screw extruder of polymer processing [32]. In their calculations, it was reported that converged solutions were difficult to obtain for $\lambda_\perp$ above 0.2, and a comparably strong vortex after the contraction for $\lambda_\perp = 0.2$ was indicated.

HEAT TRANSFER

In view of its industrial importance, laminar heat transfer has been the subject of considerable study. The main contributions have been comprehensively reviewed by Porter[38], and only a brief summary of the various types of approach on the problem with constant wall temperature will be given here.
The first theoretical solution with some simplifying assumptions, which include temperature-independent viscosity and no viscous dissipation, was presented in 1885 by Graetz and again, in 1910 by Nusselt. Their results were extended to power-law fluids by Lyche and Bird[27] for tube flow, and Prins et al[39], Tien[45] and Suckow et al[43] for parallel plate system. Vlachopoulos and Keung[47] took viscous heating into account for a power-law fluid flowing between parallel plates, and the importance of variation in viscosity was considered by Gee and Lyon [24], Forrest and Wilkinson[20], Popovska and Wilkinson[37] and Winter [48] for various types of dependence on temperature. Since a high pressure drop is often encountered in polymer processing resulting from the very large shear stresses developed, the expansion effect caused by the compressibility of fluids was also included by Toor[46] and Gee and Lyon [24].

Theoretically, the discussion of these problems involves solving simultaneously the equations of motion and energy. When they are closely coupled through a temperature-dependent shear viscosity, a numerical solution is inevitable in most cases. However, some analytical solutions are still available under certain circumstances. Without considering the heat convection, Martin[28], and Gavis and Laurence[22,23] investigated plane and circular Couette flow as well as Poiseuille flow of both Newtonian and power-law fluids with an exponential dependence of viscosity on temperature. Their results showed that there is a maximum shear stress which can be applied and that two different temperature and velocity fields can exist at each applied stress below the maximum. This double-valued feature of simple shear flows was confirmed by the
experimental study of Sukanek and Laurence[44], and consequently a stability analysis of non-isothermal flow in channels was given by Shah and Pearson[42]. For the Graetz-Nusselt problem of both Newtonian and power-law fluids, the Sturm-Liouville type differential equation was solved by Lyche and Bird[27], using a power series expansion for tube flow, and Suckow et al[43], taking an iterative procedure for the parallel plate system. If viscous heating is not considered, an improved integral procedure was utilized by Young[49] to analytically study the laminar forced convection with a variable viscosity, which is restricted to have an inverse linear relation with temperature only. Meanwhile, combining orthogonal collocation with matrix diagonalization, a numerical method was introduced by Michelsen and Villadsen[31] to deal with this problem when the axial heat conduction should be considered for small Peclet numbers. An exact solution was also provided by Deavours[14] for the same case, but with viscous heating taken into account in a parallel plate system. The last two solutions suggested that the boundary condition at the entry cannot be relaxed to an uniform temperature, as it will lead to a mathematically inconsistent problem formulation.

In view of the complex behavior of viscoelastic fluids, very few quantitative studies have been made in the area of non-isothermal viscoelastic fluid flow. Typical results may be found in the work, both experimental and theoretical, by Matsui and Bogue[29]. However, there will be no intention in this thesis to add this complication of viscoelasticity into our analysis of heat transfer.
II. MATHEMATICAL FORMULATION

2.1 MOMENTUM EQUATION:

The fundamental equation for two dimensional, steady, incompressible flow, with no body forces, are the two component momentum equations (generalized Navier-Stokes) and the continuity equation. They can be written in a Cartesian coordinate system as[4]:

\[
\rho \left( \frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} \right) = - \frac{\partial \bar{P}}{\partial x} - \left( \frac{\partial \bar{\tau}_{xx}}{\partial x} + \frac{\partial \bar{\tau}_{yx}}{\partial y} \right) \quad (2.1.1)
\]

\[
\rho \left( \frac{\partial \bar{v}}{\partial x} + \frac{\partial \bar{v}}{\partial y} \right) = - \frac{\partial \bar{P}}{\partial y} - \left( \frac{\partial \bar{\tau}_{xy}}{\partial x} + \frac{\partial \bar{\tau}_{yy}}{\partial y} \right) \quad (2.1.2)
\]

\[
\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} = 0 \quad (2.1.3)
\]

where the overbars represent dimensional quantities. \( \bar{\tau}_{xx}, \bar{\tau}_{xy}, \bar{\tau}_{yx} \) and \( \bar{\tau}_{yy} \) are the components of the symmetric shear stress tensor, \( \bar{\tau} \), with \( \bar{\tau}_{xy} = \bar{\tau}_{yx} \); \( \rho \) is the density, \( \bar{P} \) is the isotropic pressure and \( \bar{v} = (\bar{u}, \bar{v}) \) is the velocity vector.

Defining dimensionless quantities by:

\[
\bar{u} = \bar{u}/u_0 \quad \bar{v} = \bar{v}/u_0 \]

\[
x = \bar{x}/L \quad y = \bar{y}/L
\]

\[
\bar{\tau} = \frac{L}{u_0 \nu_0} \quad \nu_0 \text{ is the reference viscosity}
\]

and with the introduction of stream and vorticity functions, \( \psi \) and \( \omega \) respectively:

\[
u = - \frac{\partial \psi}{\partial x}
\]

\[
u = - \frac{\partial \psi}{\partial x}
\]
\[
\omega = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} = \nabla^2 \psi
\]

The above equations (2.1.1-3) can be reduced to a dimensionless equation:

\[
\text{Re} \frac{\partial (\psi, \omega)}{\partial (x, y)} = \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) \tau_{xy} - \frac{\partial^2}{\partial x \partial y} (\tau_{xx} - \tau_{yy}) = \phi (\tau)
\]

(2.1.4)

where \( \phi \) is a tensor operator adopted for convenience, and \( \text{Re} \) is the Reynolds number defined by

\[
\text{Re} = \frac{\rho u_o L}{\nu_o}
\]

For a Newtonian flow with constant viscosity, which will be the reference viscosity in this case, the stress tensor can be expressed simply by

\[
\tau = 2D
\]

\[
D = \frac{1}{2} (\nabla v + \nabla v^T)
\]

is the rate of strain tensor

\[
\tau_{xx} = 2 \frac{\partial u}{\partial x} = 2 \frac{\partial^2 \psi}{\partial x \partial y}
\]

\[
\tau_{yy} = 2 \frac{\partial v}{\partial y} = -2 \frac{\partial^2 \psi}{\partial x \partial y}
\]

\[
\tau_{xy} = \tau_{yx} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = \frac{\partial^2 \psi}{\partial y^2} - \frac{\partial^2 \psi}{\partial x^2}
\]

By substituting these components of the Newtonian stress tensor, in terms of derivatives of stream function, into equation (2.1.4), it can be easily shown that the momentum equation can be expressed in an elliptic Poisson form.
\[ \nabla^2 \omega + \text{Re} \frac{\partial (\psi, \omega)}{\partial (x,y)} = 0 \]  \hspace{1cm} (2.1.5)

For Non-Newtonian flow, which can be either viscous (e.g. power-law fluids) or viscoelastic, or even with just Newtonian fluid flow with temperature-dependent viscosity, the operator \( \phi \) on the stress tensor cannot be reduced to a simple Laplacian form, and a different approach should be desirable.

If equation (2.1.4) is solved directly by finite difference method, as Gatski[21] mentioned in his thesis, the second-order central differencing of the advective terms of vorticity equation would yield a difference equation with no explicit dependence on the variable \( \omega_{ij} \), and the solution array would need to be determined implicitly by a matrix inversion. Hence he suggested the use of the unidirectional or upstream differencing for the advective terms. The major drawback of this scheme is the artificial viscosity errors[40] due to the first-order accuracy of the difference scheme. This can be very serious for highly viscous polymer melts, as their Reynolds numbers are usually very small. To prevent these numerical difficulties and also enhance the diagonal dominance in the numerical scheme at the same time, two alternatives can be used and both are suited for the second-order central differencing.

(a) For purely viscous fluids, if the viscosity is not directional, or may be called "isotropic", implying that it can only be a function of temperature or invariants of the rate of strain tensor, the vorticity equation can be rewritten by letting \( \phi \) operate on the stress tensor

\[ \tau = \mu(x,y) \phi \]
\[ \phi(\tau) = -\nabla^2 \mu_\omega + 2(\psi_{xx} \psi_{yy} - 2(\psi_{xy} \psi_{xy} + (\psi_{yy} \psi_{xx})) \]

\[ = -\nabla^2 \mu_\omega + 2(\mu_{xx} \psi_{yy} - 2\mu_{xy} \psi_{xy} + \mu_{yy} \psi_{xx}) \]

Such that

\[ \nabla^2 \mu_\omega + \text{Re} \frac{\partial (\psi, \omega)}{\partial (x, y)} = 2(\mu_{xx} \psi_{yy} - 2\mu_{xy} \psi_{xy} + \mu_{yy} \psi_{xx}) \quad (2.1.6) \]

where the subscripts represent partial differentiation, and \( \mu \) is the dimensionless viscosity based on a chosen reference.

The advantages of this approach are the "symmetric" feature between the derivatives of the viscosity and stream function of its forcing term as well as the fact that lower order derivatives of better accuracy are involved. Although there is no theoretical proof available, some test calculations showed that equation (2.1.6) would provide better possibilities to obtain converged solutions than the next approach to be introduced below, especially when the viscosity is temperature-dependent only.

(b) For general Non-Newtonian fluids, particularly the viscoelastic case when the stress cannot be explicitly evaluated in terms of velocity gradients, an "extra stress" defined by

\[ \tau^e = \tau - \tau^N \]

where \( \tau \) is the actual stress and \( \tau^N = 2\mu \)

is the Newtonian stress.

can be introduced such that the equation (2.1.5) will become

\[ \text{Re} \frac{\partial (\psi, \omega)}{\partial (x, y)} = \phi(\tau^e) + \phi(\tau^N) \]
Since \( \phi(\tau_e^N) = -\nabla^2 \omega \), the above equation is equivalent to

\[
\nabla^2 \omega + \text{Re} \left( \frac{\partial (\psi, \omega)}{\partial (x, y)} \right) = \phi(\tau_e^e)
\]

(2.1.7)

This modification will enable us to employ the same numerical scheme for both Newtonian and Non-Newtonian flow problems. It can be seen that equation (2.1.7) will reduce to equation (2.1.5) for Newtonian fluids. On the other hand, since the forcing term \( \phi(\tau_e^e) \) is associated here with the second-order derivatives of velocity gradients (rate of strain), which in turn are also second-order derivatives of stream function, the numerical accuracy certainly will be reduced to some extent by the approximation for this fourth-order derivative. Moreover, for power-law fluids, i.e.

\[
\bar{\mu} = m(T) \{ \text{II}_D \}^{(n-1)/2}
\]

the power index \( n \) has an amplification effect on this truncation error. Hence, this formulation will not be recommended for purely viscous flow problems. However, partly because the stress is usually evaluated implicitly for most of the viscoelastic fluids, it has been found that, with careful treatment, this method is acceptable and will give reasonably converged solutions for most cases of the practical importance.

There are several iterative numerical methods[41] which may be used to solve the vorticity transport equation with its appropriate boundary conditions. Among them, SOR (Successive Over-Relaxation) and ADI (Alternating Direction Implicit) are the most popular in computational fluid dynamics problems. For line-SOR, which uses advance values at three neighbor points instead of two by point-SOR, and ADI, the conver-
gence rate may be slightly improved because both methods are solved implicitly in one direction. However, each iteration takes longer for the tridiagonal matrix solution involved. Overall, there may be no gain in computing speed, and it was felt that line-SOR was not worth the added complexity. A test numerical experiment showed that it actually took longer for line-SOR to converge than point-SOR. To combine its simplicity with the effectiveness of alternating direction, point-SOR with changing sweep direction at each iteration (say, from \( i^+, j^+ \) to \( i^+, j^- \)) has been used for the vorticity equation. This is an explicit method requiring no tridiagonal solutions, and the idea behind changing sweep direction is to let interior points sense the changes or values of all boundaries at an earlier stage. In other words, if the sweep proceeds in the \( i^+ \) direction starting from \( i=1 \), the effect of boundary condition at \( i=1 \) will be carried over the whole region but the boundary condition at \( i=N \) can only be felt as \( i \) gets close to \( N \) (i.e. at \( i=N-1 \) during the first iteration if five-point central difference formula is used). Thus, by alternating the direction, both boundary conditions have the same opportunity to proceed inside and hopefully the convergence rate will be improved.

It has also been found that, with relaxation factor larger than one, the dynamic overshoot of SOR will sometimes never be recovered and will likely cause the iteration to diverge. Therefore, Liebman's method, also known as Gauss-Seidel[41] method, with the relaxation factor equal to unity is preferable here. SUR(Successive Under-Relaxation) may work as well but its convergence rate generally will be slower. Also, in proceeding from one iteration to the next for the vorticity equation,
it is found to be beneficial to smooth the current solution by taking a weighted average with the previous corresponding iterate. The value of this weighting ratio is empirical, but (0.8 : 0.2) was used in this work. Some additional strategies concerning the use of the above numerical scheme may also be referred to the paper by Davies et al[13].

2.2 CONSTITUTIVE EQUATION OF VISCOELASTIC FLUIDS

Before presenting the non-linear viscoelastic fluid model suggested by Acierno et al[1], it should be mentioned here that the main concern of this study is the numerical simulation itself, but not the comparison or derivation of various rheological models. Some concepts of linear viscoelasticity may be reviewed briefly when needed. However, this section does not intend to give any detail of these concepts, merely to state the salient points.

For small deformation, the linear viscoelastic behavior of polymer fluids can be described by the Maxwell equation in a general form:

$$\tau + \lambda \frac{\Delta t}{\Delta t} \tau = 2 \mu D$$  \hspace{1cm} (2.2.1)

where is the relaxation time and $\Delta \frac{abc}{\Delta t}$ is a symmetry-preserving associated time derivative for a symmetric tensor such as $\tau$,

$$\frac{\Delta abc}{\Delta t} \tau = \frac{d}{dt} \tau + a(\tau \cdot \dot{D} + \dot{D} \cdot \tau) + b(\tau : D) + cD tr \tau$$

$d/dt$ is the Jaumann or corotational derivative.

Through the discussions of viscometric flows[3], it is common to choose $b=c=0$, $a=-1$ in order to obtain realistic results for normal stress
difference predictions. In this case, $\frac{\Delta}{\Delta t}^{abc}$ becomes the so-called contra-
variant convected derivative defined as:

$$\frac{\delta}{\delta t} \mathbf{T} = \frac{d}{dt} \mathbf{T} - (\mathbf{T} \cdot \mathbf{D} + \mathbf{D} \cdot \mathbf{T})$$

For steady-state viscometric flow, equation (2.2.1) will reduce to:

$$\mathbf{T} = \lambda (\mathbf{T} \cdot \mathbf{D} + \mathbf{D} \cdot \mathbf{T}) + 2 \mu \mathbf{D}$$

(2.2.2)

It has been shown that the quantitative rheological response of a viscoelastic fluid can not be described well using a single relaxation
time. The basic Maxwell model may be generalized by superposing an infi-
nite number of Maxwell elements for a whole spectrum of relaxation times
and viscosities.

$$\mathbf{T} = \sum \mathbf{T}_i$$

(2.2.3)

$$\mathbf{T}_i = \lambda_i (\mathbf{T}_i \cdot \mathbf{D} + \mathbf{D} \cdot \mathbf{T}_i) + 2 \mu_i \mathbf{D}$$

(2.2.4)

If one uses network theories[4], which assume that the probabilities
for the macromolecular strands to leave and join the network are constant ,
relaxation times and elastic moduli, $G_i = \mu_i / \lambda_i$, are constant for these linear viscoelastic models. Unfortunately, data have shown this to be
inadequate to explain the apparent shift in relaxation times caused by
large shear stresses. Many suggestions have been made about how to let
the relaxation spectrum depend on the motion. For instance, Carreau[7]
proposed a dependence on the second invariant of the rate of strain, and
the local state of stress was chosen by Kaye[26]. In the non-linear vis-
coelastic model proposed by Acierno et al[1], $\lambda_i$ and $G_i$ are selected to
be dependent on a scalar dimensionless quantity $\xi_i (0 < \xi_i < 1)$ as:
\[ G_i = G_{o_i} \xi_i \quad (2.2.5) \]

\[ \lambda_i = \lambda_{o_i} \xi_i^{1.4} \quad (2.2.6) \]

where \( G_{o_i} \) and \( \lambda_{o_i} \) are the "equilibrium values" in the limit of linear viscoelasticity. \( \xi_i \) can be regarded as the structural variable which describes how the existing structure is far from equilibrium. The equation (2.2.5), expressing the fact that the elastic modulus is reduced proportionally to the concentration of junctions, is based on the classical result of the rubber elasticity theory. However equation (2.2.6) is essentially empirical. The power 1.4 is somewhat related to the experimental observation that the zero shear viscosity is proportional to the 3.4 power of the polymer concentration for concentrated solutions of high molecular weight polymers.

The structural variable \( \xi_i \) then is determined by the following kinetic equation:

\[ \frac{d}{dt} \xi_i = \frac{(1 - \xi_i)}{\lambda_i} - a \frac{\xi_i}{\lambda_i} \sqrt{\frac{E_i}{G_i}} \quad (2.2.7) \]

The rate of change of \( \xi_i \) is related to the rate of destruction of junctions due to the existing stress and the net rate of reformation due to the thermal motion. For the destruction term, the "associates" elastic energy \( E_i \) is evaluated by the trace of the stress tensor, although this is still open to question. The constant "a" is the only adjustable parameter in this model. It is reported that "a" should be of order unity and essentially the same for all polymers. In Meister's work[30] the "interacting sphere" model seems to predict values of "a" between
0.25 and 0.4.

To use this model to numerically simulate a non-linear viscoelastic steady-state flow, it is necessary to solve a whole system of equations, including equations (2.2.3) through (2.2.7) combined with the momentum balance equation, for a whole spectrum of relaxation times and elastic moduli. However, as the purpose of this work is to demonstrate the numerical algorithm, it is convenient to use only one single relaxation time and elastic modulus instead. For the kinetic equation (2.2.7) at steady state, a Newton-Raphson iteration method was found to be effective with a careful choice of its starting guesses.

2.3 ENERGY EQUATION:

According to the first law of thermodynamics, the energy equation for a steady-state, incompressible flow with no body forces can be written as:

$$\rho C_p \left( \nabla \cdot \text{grad} \bar{T} \right) = -\left( \nabla \cdot \mathbf{q} \right) - \left( \tau : \nabla \mathbf{v} \right)$$

(2.3.1)

where $C_p$ is the heat capacity, $\bar{T}$ is temperature and $\mathbf{q}$ is the energy flux defined by $\mathbf{q} = -k \text{grad} \bar{T}$, with a single thermal conductivity $k$ for isotropic materials. The term on the left side of the above energy equation is identified as the change caused by heat convection, and two terms on the right side are for heat conduction and viscous dissipation respectively.

In a two-dimensional Cartesian coordinate system, if all physical properties except viscosity are assumed to be constant, equation (2.3.1) can be expressed in terms of dimensional quantities as:
\[ \rho C_p \left( \frac{\bar{u}}{\partial x} \frac{\partial \bar{T}}{\partial x} + \frac{\bar{v}}{\partial y} \frac{\partial \bar{T}}{\partial y} \right) = k \left( \frac{\partial^2 \bar{T}}{\partial x^2} + \frac{\partial^2 \bar{T}}{\partial y^2} \right) - \left\{ \tau_{xx} \frac{\partial \bar{u}}{\partial x} + \tau_{yy} \frac{\partial \bar{v}}{\partial y} + \tau_{xy} \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right) \right\} \]  

(2.3.2)

By choosing a proper reference temperature \( T_0 \), with those dimensionless variables already defined for the momentum equation in section 2.1 and two dimensionless groups:

\[
\text{Peclet Number} \quad Pe = \frac{\rho C_p u_o L}{k}
\]

\[
\text{Brinkman Number} \quad Br = \frac{\mu u_o^2}{k T_0}
\]

Equation (2.3.2) can be written in a dimensionless form for viscous fluids:

\[
u \frac{\partial \bar{T}}{\partial x} + v \frac{\partial \bar{T}}{\partial y} = \frac{1}{Pe} \left\{ \left( \frac{\partial^2 \bar{T}}{\partial x^2} + \frac{\partial^2 \bar{T}}{\partial y^2} \right) + Br \mu \left[ \left( \frac{\partial \bar{u}}{\partial x} \right)^2 + \left( \frac{\partial \bar{v}}{\partial y} \right)^2 \right] + \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right)^2 \right\}
\]

(2.3.3)

It is common to assume that axial heat conduction (along streamlines) can be neglected when compared with radial heat conduction (across streamlines) and heat convection. This is always true for polymer melts of moderately high Peclet numbers in a thermal entry flow. If this is the case and an unidirectional flow is considered, i.e. \( u = u(y) \), equation (2.3.3) can be reduced to

\[
u \frac{\partial \bar{T}}{\partial x} = \frac{1}{Pe} \left\{ \frac{\partial^2 \bar{T}}{\partial y^2} + Br \mu \left( \frac{\partial u}{\partial y} \right)^2 \right\}
\]

(2.3.4)

Here the axial coordinate \( x \) may be further combined with the Peclet
number to form a new dimensionless coordinate:

\[ z = \frac{x}{Pe} \]

and equation (2.3.4) becomes

\[ u \frac{\partial T}{\partial z} = \frac{\partial^2 T}{\partial y^2} + Br \mu \left( \frac{\partial u}{\partial y} \right)^2 \]  

(2.3.5)

The use of \( z \) is to generalize the results. Additionally, \( z \) can be related to the inverse of Graetz number, the importance of which has been discussed by Pearson[33] and Winter[48]. For small Graetz numbers (or large \( z \)), the convection term is negligible compared with the conduction term and so fully-developed flow will occur. If its magnitude is of order unity, both convection and conduction will be equally comparable. In the case of large Graetz numbers, the convection usually dominates over the conduction terms, and this is the case of most interest in polymer processing, as \( Gz=100 \) is a common value for extruder dies.

For pseudo-unidirectional flow problems of power-law fluids, the velocity \( u \) may change along the streamlines. The radial (or \( y \)) component of velocity \( v \), however, is neglected against \( u \). This means that the local continuity equation of incompressibility is not satisfied, but an overall continuity equation is in the form of integral balance across the flow field at each \( x \). If a dimensionless temperature-dependent viscosity is defined as:

\[ \mu(T) = m(T) \left| \frac{\partial u}{\partial y} \right|^{n-1} \]  

(2.3.6)

the energy equation, (2.3.4) or (2.3.5), has to be solved simultaneously
with the one-dimensional momentum equation

\[
\frac{dP}{dx} = -\frac{\partial}{\partial y} \left[ \frac{\partial}{\partial y} \left\{ m(T) \left| \frac{\partial u}{\partial y} \right|^n \left| \frac{\partial u}{\partial y} \right|^{n-1} \right\} \right]
\]  \hspace{1cm} \text{(2.3.7)}

If the centerline of a parallel-plate system is taken to be at \(y=0\), the symmetry of velocity profile will give us the boundary condition:

\[
\frac{\partial u}{\partial y} = 0 \quad \text{at} \ y=0
\]

Thus the normalized velocity, based on the average velocity, can be obtained directly by integrating equation (2.3.7) and assuming no pressure drop across streamlines.

\[
u(y) = \int_y^1 \left( \frac{y'}{m(T)} \right)^{1/n} dy', \quad \int_0^1 \left( \frac{y'}{m(T)} \right)^{1/n} y'dy'
\]  \hspace{1cm} \text{(2.3.8)}

If the viscosity is independent of temperature, the velocity of power-law fluids flowing between two parallel plates can be shown to be:

\[
u(y) = \frac{2n+1}{n+1} \left( 1 - y^{(n+1)/n} \right)
\]  \hspace{1cm} \text{(2.3.9)}

Without considering axial heat conduction, the energy equation is a self-starting problem for the finite difference method. Providing the velocity field is given, the temperature profile at position \(i+1\) of \(x\) can be obtained directly from the calculated or boundary values at \(i\). If the pseudo-unidirectional flow is assumed for the case of temperature-dependent viscosity, the velocity should be explicitly determined through equation (2.3.8) by an iterative procedure. The iteration proceeds by assuming the same velocity profile at \(i\) exists at \(i+1\), to give
a first estimate of temperature there. Based on this new $T_{i+1}$, the corrected velocity at $i+1$ from equation (2.3.8) is then used to improve the next estimate of temperature. The procedure is repeated until two consecutive iterates of temperature (and velocity) are consistent within a given convergence criterion. These same iterating steps then start again at the next increment. However, for two-dimensional flow problems, which can be either due to a change of geometry or induced by the abrupt change of boundary temperature for incompressible fluids with a temperature-dependent viscosity, it is necessary to solve the elliptic momentum equation for each iterated temperature field. In this case, a boundary condition of velocity is needed at the end of our domain of interest and thus the region must be extended to where either the velocity profile is known or can be reasonably approximated by equation (2.3.8).

For the traditional Graetz-Nusselt problem, which is usually defined by a step-change boundary temperature at the entry with a fully-developed velocity field, no viscous dissipation and temperature-independent viscosity, there are several analytical results available in the literature. The governing heat transfer equation of power-law fluids in a parallel-plate system has a simple form in this case:

$$u \frac{\partial T}{\partial z} = u_{\text{max}} \left( 1 - y^{(n+1)/n} \right) \frac{\partial T}{\partial z} = \frac{\partial^2 T}{\partial y^2}$$  \hspace{1cm} (2.3.10)

with boundary conditions:

(1) at $z=0$, $T(0,y) = 1$

(2) at $y=1$, $T(z,1) = 0$

(3) at $y=0$, $\frac{\partial}{\partial y} T(z,0) = 0$

Theoretically there should be no problem to solve this linear par-
tial differential equation. The standard technique is to apply the method of separation of variables, and the problem will be reduced to the determination of the eigenvalues and eigenfunctions for an ordinary differential equation of Sturm-Liouville type. However, to determine these eigenvalues and eigenfunctions with reliable accuracy can be a very tedious task. The classical procedure, as shown by Lyche and Bird [27] for tube flow problems, is to use a power series expansion, for which the coefficients are expressed in terms of the eigenvalues. Then the boundary conditions (2) and (3) are used to obtain these eigenvalues. It can be easily seen that, in addition to the complexity of the calculations involved, this method is not applicable if $(n+1)/n$ is not an integer, and its practical use is thus very limited.

A different approach, which partly utilizes thermal boundary layer theory[17] has been found to be useful in obtaining an analytical solution for the Graetz-Nusselt problem. It divides the region into two sections, as shown in Fig. 1. Thermal boundary layer theory is applied to the first section, called thermal entry region, starting from the entry to the point where the thermal boundary layers just merge together at the centerline. The integral form of the energy equation is then used for the second section, called the developing region, to obtain the eigenvalues as well as the coefficients of the approximating polynomials. Finally, these two solutions are matched at the intersection to give a continuous temperature profile at the centerline. The results turn out to be quite satisfactory when compared with the numerical solutions. The range of application can also be extended to cases with viscous dissipation, as long as the viscosity is not temperature-dependent and the entry
boundary condition of fully-developed temperature is also properly defined.

For example, consider the case with no viscous heating. (Note the centerline in Fig. 1 is located at y=1)

**Thermal Entry Region (0 \leq z < z_f)**

It is assumed that the actual temperature profile within the thermal boundary layer can be approximated by one which merges into the uniform temperature, T=1, of the bulk fluid at y=\(\delta_T\), the thickness of thermal boundary layer. Since the velocity profile is fully-developed and not affected by temperature, the so-called flow or momentum boundary layer thickness \(\delta\) is always treated as constant, i.e. \(\delta=1\) and \(\delta \geq \delta_T\) in this case.

With following boundary conditions:

1. \(T=0, \text{ at } y=0\)
2. \(T=1, \text{ for } 1 \geq y \geq \delta_T\)
3. \(\frac{\partial^2 T}{\partial y^2} = 0, \text{ at } y=0; \text{ for } u=0 \text{ of no slip at wall.}\)
4. \(\frac{\partial^i T}{\partial y^i} = 0, \text{ at } y=\delta_T; \ i=1,2,\ldots\text{to } n.\)

The temperature is approximated by a polynomial:

\[
T = \sum_{j=0}^{n+2} a_j \eta^j \quad \eta = y/\delta_T(z)
\]

where the number of terms for this solution is determined by how many boundary conditions are applied, as the coefficient \(a_j\) must be determined by them.

Next, consider the integral form of equation (2.3.10) by integrating it across the flow direction:
Fig. 1 Illustration for the Analytical Approximation Solution of Graetz-Nusselt Problem (the scale is not in proportion).
\[
\int_0^1 u \frac{\partial T}{\partial z} \, dy = \frac{\partial T}{\partial y} \bigg|_{y=1} - \frac{\partial T}{\partial y} \bigg|_{y=0}
\]

Since the temperature profile is symmetric with respect to the centerline, and velocity \( u \) is only \( y \)-dependent, the above equation thus becomes:

\[
\frac{3}{\partial z} \int_0^1 uTdy + \frac{\partial T}{\partial y} \bigg|_{y=0} = 0 \quad (2.3.11)
\]

This does not show any dependence on the thermal boundary layer thickness, however, because of boundary condition (2), equation (2.3.11) can be written as:

\[
\frac{3}{\partial z} \int_0^{\delta_T(z)} u(1-T)dy = \frac{\partial T}{\partial y} \bigg|_{y=0} \quad (2.3.12)
\]

Substituting the polynomial form of temperature obtained earlier into equation (2.3.12), the thermal boundary layer thickness \( \delta_T(z) \) can be determined for any chosen axial distance between \( \delta_T=0 \) at \( z=0 \) and \( \delta_T=1 \) at \( z=z_f \). The latter will be used as the intersection to match with the second solution obtained from the developing region.

**Developing Region** ( \( z > z_f \) )

In the thermal entry region, \( \delta_T(z) \) is used to transform temperature profiles within the thermal boundary layer into one similar form which can be approximately described by a polynomial with its applicable boundary conditions. Similarly, the centerline temperature, \( T_0(z) = T(z,y=1) \), is chosen in this region for the same purpose, but some of the boundary conditions will be different.

Let \( \theta = T/T_0(z) \) and start with four basic boundary conditions first:

1. \( \theta=0 \), at \( y=0 \)
(2) $\Theta = 1$, at $y = 1$

(3) $\frac{3\Theta}{\partial y} = 0$, at $y = 1$

(4) $\frac{2\Theta}{\partial y^2} = 0$, at $y = 0$

$\Theta$ is then approximated by a third-order polynomial,

$$\Theta = \sum_{j=0}^{3} b_j y^j$$

with $b_0 = b_2 = 0$, $b_1 = 1.5$ and $b_3 = -0.5$

Substitute $\Theta$ into equation (2.3.11), it can be shown that

$$\{ \int_0^1 u \Theta dy \} \frac{dT_o}{dz} = -b_1 T_o$$

Therefore, $T_o = \exp(-\beta(z-z_f))$

$$\beta = b_1 / \int_0^1 u \Theta dy$$

This form of exponential dependence is identical with the solution derived from the method of separation of variables. It indicates that $T_o$ should be constructed from a combination of "eigenfunctions". In addition, using only "one eigenfunction" for $T_o$, as in the case of third order polynomial approximation, will inevitably lead to a constant Nusselt number for this whole region. Hence, it is necessary to have more boundary conditions than the basic four outlined above so that higher order approximations can be used and more than one eigenvalue can be obtained.

If the temperature distribution in this region is expressed by a summation:
\[ T(z, y) = \sum_{i=1}^{n} a_i \exp(-\beta_i z) \Theta_i(y) \]

(It should be noted that this is an exact solution with \( n \to \infty \), as shown by the method of separation of variables. \( \beta_i \) and \( \Theta_i \) are then the eigenvalue and eigenfunction respectively.)

At the centerline, \( y=1 \), from the energy equation (2.3.10) with new \( \zeta = x/Pe' \) (Pe' is based on the centerline velocity), the first additional boundary condition will be:

\[ (5) \text{ at } y=1, \quad \frac{\partial^2 \Theta_i}{\partial y^2} = -\beta_i \]

If equation (2.3.10) is differentiated once with respect to \( y \):

\[ \frac{\partial u}{\partial y} \frac{\partial T}{\partial \zeta} + u \frac{\partial^2 T}{\partial y \partial \zeta} = \frac{\partial^3 T}{\partial y^3} \]

Since

\[ \frac{\partial u}{\partial y} = 0 \text{ and } \frac{\partial^2 T}{\partial y \partial \zeta} = \frac{\partial}{\partial \zeta} \left( \frac{\partial T}{\partial y} \right) = 0 \text{ at } y=1, \]

Thus

\[ (6) \text{ at } y=1, \quad \frac{\partial^3 \Theta_i}{\partial y^3} = 0 \]

As this procedure goes on, more boundary conditions at \( y=1 \) can be drawn. Such as:

\[ (7) \frac{\partial^4 \Theta_i}{\partial y^4} = \beta_i^2 + 2\beta_i \]

\[ (8) \frac{\partial^5 \Theta_i}{\partial y^5} = 0 \text{ etc.} \]

With six boundary conditions, a fifth-order polynomial can be used
to approximate \( \Theta_i \) and two eigenvalues \( \beta_i \)'s will be obtained through equation (2.3.11). Although it is possible to determine \( \beta_i \)'s solely by applying more boundary conditions, the results will not be as good as these from the integral method. This can be explained by the characteristics of the method of weighted residuals[19], as the former will be equivalent to the collocation method with one point only at \( y=1 \), while in contrast, the integral method attempts to satisfy the original differential equation on an average basis for the whole domain from \( y=0 \) to \( y=1 \). On the other hand, the Galerkin method or the method of moments may be used to determine these coefficients for the assumed polynomials instead of employing the extra boundary conditions. However, the problem will then become more complicated and beyond reach for analytical solutions.

Finally, solutions from these two regions have to be matched at the intersection \( z=z_f \) to determine \( \alpha_i \)'s. It is obvious that the centerline temperature must be continuous, i.e.

\[
\sum_{i=1}^{n} \alpha_i \exp(-\beta_i z_f) = 1
\]

For \( n>2 \), the derivatives of \( T_o \) may also be required to be continuous,

\[
\frac{d^{n-1}}{dz^{n-1}} T_o = 0, \text{ at } z = z_f \tag{2.3.13}
\]

which implies that

\[
\sum_{i=1}^{2} \alpha_i \beta_i \exp(-\beta_i z_f) = 0
\]

is needed for \( n=2 \). Meanwhile, it should be noted here that the polynomials used must be of the same order on both sides. Otherwise, it is not possible to have a correct matching condition at the intersection because
equation (2.3.13) will not be true, and may also result in an inconsistent temperature profile.

If the problem with viscous dissipation is considered, it is known that as long as the entry condition of uniform temperature at \( z=0 \) is replaced by a fully-developed profile,

\[
T = 1 \quad \text{for } z \to -\infty \quad \text{and} \quad \frac{\partial T}{\partial z} = 0 \quad \text{at } z=0
\]

the solution can be simply obtained by superposing an asymptotic particular solution \( T_\infty \) on the solutions previously derived for the case without viscous dissipation. i.e.

\[
\frac{d^2 T_\infty}{dy^2} + Br \left| \frac{\partial u}{\partial y} \right|^{n+1} = 0 \quad \text{for power-law fluids}
\]

with boundary conditions:

(1) at \( y=0 \), \( T_\infty = 0 \)

(2) at \( y=1 \), \( \frac{dT_\infty}{dy} = 0 \)

By integrating, \( T_\infty \) can be obtained as:

\[
T_\infty = Br^* \frac{n^2}{(2n+1)(3n+1)} \{1 - (1-y)^n\}^{1/3} \]

(2.3.14)

\[
Br^* = Br \left(\frac{2n+1}{n}\right)^{n+1} \quad \text{the modified Brinkman number.}
\]

It is important to realize that the thermal boundary layer theory in this case can only be applied when the entry condition includes a fully-developed temperature profile. If an uniform temperature is assumed there, a small temperature peak due to the viscous heating may occur locally in the entry region and the existence of thermal boundary layer
will thus be impossible to define. In fact, as also indicated by Michelson and Villadsen[31], the use of uniform temperature may possibly lead to a mathematically inconsistent problem formulation due to the indirect negation of some physical terms, such as the viscous effect in this problem.
III. NUMERICAL RESULTS AND DISCUSSIONS

3.1 CONTRACTION/EXPANSION FLOW OF VISCOELASTIC FLUIDS

3.1-1 FLOW GEOMETRY:

One of the most important flow geometries found in the polymer processing industry is the contraction/expansion flow. Such a flow field is encountered in fiber spinning, extrusion molding and also in the capillary viscometer, an instrument widely used for fundamental fluid property measurements. The flow geometry investigated in this study for non-linear viscoelastic fluids is identical with the one used by Davies et al[13], as shown in Fig. 2. The boundary AH moves with a constant velocity $u = u_o$, generating a drag flow in the direction indicated. A contraction ratio of $h/a = 3$ is chosen with $a/b = 5/6$. The entrance AB and exit GH are taken to be sufficiently far from the obstruction CDEF so that fully-developed Couette flow may be assumed at AB and GH. It has been found that $BC = FG = 3b$ is long enough to justify this assumption for Newtonian fluids. However, a length of $3.5b$ was used to further assure the fully-developed flow for the case of viscoelastic fluids. The dimensionless variables chosen for this geometry are:

$$x = \frac{x}{h} \hspace{1cm} y = \frac{y}{h}$$

$$u = \frac{u}{u_o} \hspace{1cm} v = \frac{v}{u_o}$$

3.1-2 CONSTITUTIVE EQUATION:

Most of the recent numerical analyses of viscoelastic fluids involving abrupt changes in geometry are based on linear rheological models, for which the rheological material parameters are constant. The
Fig. 2 Flow Domain for the Contraction/Expansion with $h/a = 3$
adoption of a nonlinear model suggested by Acierno et al[1] here corrects this inadequacy. As described in the preceding chapter, the most distinctive feature of this nonlinear constitutive equation is the dependence of its relaxation time and elastic modulus on a structure variable, which takes the whole past history of the motion into account instead of just the instantaneous values of either stress or deformation. In a two-dimensional Cartesian coordinate system, the steady-state dimensionless stress components will be determined by:

\[
\begin{align*}
\tau_{xx} &= 2Ws \, \xi^{1.4} \left( u_x \tau_{xx} + u_y \tau_{xy} \right) + 2u_x \, \xi^{2.4} \\
\tau_{xy} &= Ws \, \xi^{1.4} \left( v_x \tau_{xx} + u_y \tau_{yy} \right) + (u_y + v_x) \, \xi^{2.4} \quad (3.1.1) \\
\tau_{yy} &= 2Ws \, \xi^{1.4} \left( v_x \tau_{xy} + v_y \tau_{yy} \right) + 2v_y \, \xi^{2.4}
\end{align*}
\]

where \( u_x, u_y, v_x \) and \( v_y \) are the components of velocity gradient, and \( Ws \) is the Weissenberg number defined by:

\[
Ws = \frac{\dot{u}_o}{\dot{\gamma}_o} = \frac{\mu \dot{u}_o}{\gamma_o h}
\]

with the structure variable \( \xi \) obtained from the steady-state kinetic equation:

\[
\begin{align*}
a(WsE)^k + \xi &= 1 \quad (0 < \xi \leq 1) \\
E &= \frac{1}{2} \text{tr} \tau = \frac{1}{2} (\tau_{xx} + \tau_{yy})
\end{align*}
\]

By solving equaiton (3.1.1), \( \tau_{xx}, \tau_{yy} \) and \( \tau_{xy} \) can be expressed in terms of the velocity gradients and the structure variable:

\[
\tau_{xx} = \frac{2Ws \, \xi^{3.8} \left( 2u_x^2 + u_y v_x + u_y^2 \right) + 2u_x \, \xi^{2.4}}{1 + 4Ws \, \xi^{2.8} \left( u_x v_y - u_y v_x \right)}
\]
\[
\tau_{xy} = \frac{2W_\xi \xi^{3.8} (v_x - u_y)u_x + \xi^{2.4} (u_y + v_x)}{1 + 4W_\xi \xi^{2.8} (u_y v_x - u_x v_y)} \tag{3.1.3}
\]

\[
\tau_{yy} = \frac{2W_\xi \xi^{3.8} (2v_y^2 + u_y v_x + v_x^2) + 2v_y \xi^{2.4}}{1 + 4W_\xi \xi^{2.8} (u_y v_x - u_x v_y)}
\]

As the structure variable \(\xi\) has to be determined indirectly by the trace of stress tensor, it is necessary to evaluate these components implicitly by an iterative method. The Newton-Raphson method was found to be effective, with some precautions, for this use.

Consider the associated elastic energy \(E\), which is related to the first invariant of the stress through the generalization of the shear rate\([1]\). It is clear that a positive value of \(E\) is required so that the square root in equation (3.1.2) can be taken and thus the numerical iteration will not be interrupted. If the third invariant(determinant) of the velocity gradient is positive, i.e.

\[
\det(\nabla v) = u_x v_y - u_y v_x > 0 \tag{3.1.4}
\]

the condition of positive \(E\) can be fulfilled and any initial value of the structure variable between zero and unity may be used to start the iterative procedure, as indicated by the denominator of equation (3.1.3). However, if \(\det(\nabla v) < 0\), there may exist a critical structure value \(\xi_c\) at which the linear models predict an infinite stress or, rather, no steady state is possible. This critical state can be determined by:

\[
\xi_c^{2.8} = (4W_\xi^2 | \det(\nabla v) | )^{-1} \tag{3.1.5}
\]

If \(\xi_c > 1\), since it is beyond the range of the structure variable,
the implied "instability" will never occur and there will be no problem to obtain an equilibrium value. If $\xi_c \leq 1$ is the case, it is necessary to let the initial guess of $\xi$ be less than $\xi_c$ and also make sure to keep $0 < \xi < \xi_c$ during the iterative procedure. A flow chart is shown in Fig. 3 with equation (3.1.2) being rewritten as:

$$F(\xi) = a(W_se\xi)^{\frac{1}{2}} + \xi - 1 = 0$$

For the only adjustable parameter "a" in this method, a=0.4 is taken by fitting the viscosity and the first normal stress difference with the experimental results for steady shear flow, as shown by Acierno et al[2].

3.1-3 BOUNDARY CONDITIONS

To solve the vorticity transport equation, it is necessary to specify either the value of stream function (Dirichlet condition) or its normal derivative (Neumann condition) along the boundaries of the flow domain so that the equation for the stream function, $\nabla^2 \psi = \omega$, can be numerically iterated with equation (2.1.7). The Dirichlet condition is preferred because of its simplicity and accuracy, but the Neumann condition will be also included in the evaluation of the boundary vorticities.

Since the boundary AH(y=0) is moving with a constant velocity $u_o$ (u=1) of fully-developed Couette flow, the no-slip condition gives us a linear velocity profile at both the entrance AB and exit GH:

$$u = 1 - y \quad (3.1.6)$$

Integrating equation (3.1.6), the stream function at AB and GH can be written as:
Fig. 3 Iteration Scheme for determining Structure Variable
\[ \psi = y - 0.5y^2 \] \hspace{1cm} (3.1.7)

Therefore, \( \psi = 0 \) is taken at \( y=0 \) for the moving boundary, and \( \psi = 0.5 \) along the fixed boundary BCDEFG.

Although the forcing values \( \Phi(\xi^2) \) for equation (2.1.7) are only needed at the interior points, it is necessary to have boundary values of the stress components so that \( \Phi(\xi^2) \) can be evaluated by central differencing. On AH and BCDEFG the stress components must be determined from equations (3.1.2) and (3.1.3) with appropriate values of the velocity gradients. They will, in general, be different each time after the equation of stream function has been iterated upon. Therefore, it is worthwhile to summarize all the velocity gradients on boundaries.

On AH, BC, DE and FG

\[ u_x = v_x = v_y = 0, \quad u_y = \omega \] (to be determined)

On AB and GH

\[ u_x = v_x = v_y = 0, \quad u_y = -1 \]

On CD and EF

\[ u_x = u_y = v_y = 0, \quad v_x = -\omega \] (to be determined)

It thus can be seen that, at points C and F, all the velocity gradients and stress components vanish, and their structure variables should be unity as expected. On AB and GH, the fully-developed stress components will be constant and can be easily determined by:

\[ \tau_{xy} = -\xi^{2.4} \]

\[ \tau_{xx} = 2W\xi^{3.8} \quad \tau_{yy} = 0 \] \hspace{1cm} (3.1.8)
with the structure variable obtained from

\[ 0.4 \, Ws^2 \xi^{2.4} + \xi = 1 \]

Fig. 4 shows the viscosity, normal stress difference and structure variable of this constant shear flow for various Weissenberg numbers, ranged from \( Ws = 0.02 \) to 5. It should be noted that stable flow usually only exists (at least from the numerical standpoint) for the Weissenberg numbers less than unity. On the other hand, the normal stress difference in this case will start to decrease after reaching its maximum at \( Ws = 3.798 \) with \( \xi = 7/12 \). It clearly indicates that the elastic effects will be of less importance after that point due to the decrease in effective crosslinks caused by the flow.

Finally, except that the fully-developed flow gives us \( \omega = -1 \) on AB and GH, the vorticity on the boundary must be obtained numerically and will be described in the next section on numerical formulation. It is through this important evaluation, which connects the equations of vorticity and stream function, that the overall numerical iteration is actually driven. Therefore, we should not be surprised to learn that the computational boundary conditions, besides affecting numerical stability, greatly affect the accuracy of the finite difference solution.

3.1-4 NUMERICAL FORMULATION

In order to obtain a numerical solution using finite difference method for this problem, the domain shown in Fig. 2 is covered with a rectangular mesh of 80x30 grids (10x20 grids of region CDEF are not used) for which \( \Delta x = 1/25 \) and \( \Delta y = 1/30 \). This mesh size was chosen after con-
Fig. 4. Typical Dimensionless Viscosimetric Material Functions and values of the Structure Variable as a function of the Weissenberg Number for the Model of Acierno et al. [1]
sidering the computing cost and the numerical accuracy involved. By com-
comparison, there are 10 grid length across the confined region instead of
only five used by Davies et al[13]. It is expected that using a mesh
with half of the grid size should give us better results.

The governing equations, both for the stream function and for vort-
icty, basically are of the same Poisson type with the exception of
their forcing terms. They may be represented by a single form

\[ \nabla^2 p(x,y) = q(x,y) \]

\[ p(x,y) = \psi(x,y) \] and \[ q(x,y) = \omega(x,y) \] for stream function,

\[ p(x,y) = \omega(x,y) \] and \[ q(x,y) = \psi(x,y) - \Re \frac{3(\psi,\omega)}{3(x,y)} \] for vorticity.

Using the five-point formula, equation can be differenced to second-
order accuracy as:

\[ \nabla^2 p_{i,j} = \frac{\delta_x^2 p_{i,j}}{\delta x^2} + \frac{\delta_y^2 p_{i,j}}{\delta y^2} = q_{i,j} \]

\[ = (p_{i+1,j} - 2p_{i,j} + p_{i-1,j})/(\Delta x)^2 \]

\[ + (p_{i,j+1} - 2p_{i,j} + p_{i,j-1})/(\Delta y)^2 \]

\((i,j)\) refers to \(x\) and \(y\) indices of the grid point with \(i\) from
1 to 81 and \(j\) from 1 to 31, and symbol \(\delta^n\) represents the \(n\)-th
order central differencing.

Since \(\Delta x \neq \Delta y\), it is convenient to define a mesh aspect ratio
\(r = \Delta x/\Delta y\) and the above differencing equation can be rewritten in a two-level
equation for the iteration:

\[ p^{(k+1)}_{i,j} = \frac{1}{2(1+r^2)} \left[ p^{(k+1)}_{i+1,j} + p^{(k+1)}_{i-1,j} + r^2 p^{(k+1)}_{i,j+1} \right] \]
\[ + p_{i,j+1}^{(k)} - (\alpha x)^2 q_{i,j} \]  

(3.1.10)

where the superscripts in parentheses indicate iteration level, and equation (3.1.10) is called Richardson's method requiring storage \( p^{(k+1)} \) and \( p^{(k)} \).

If the sweep direction is in \( i \) (small to large) and \( j \) (and new values of function \( p \) are used wherever available in equation (3.1.10), we obtain:

\[ p_{i,j}^{(k+1)} = \frac{1}{2(1+r^2)} \{ p_{i+1,j}^{(k)} + p_{i-1,j}^{(k)} + r^2 (p_{i,j+1}^{(k)}) 
+ p_{i,j-1}^{(k+1)} - (\alpha x)^2 q_{i,j} \} \]  

(3.1.11)

which is Liebman's method, also known as Gauss-Seidel method. This method can be programmed with only one storage level due to the nature of successive replacements.

To improve convergence rate, the SOR (Successive Over-Relaxation) method is commonly used, which increases the iterating increment by introducing a relaxation factor \( s (1 \leq s < 2) \)

\[ p_{i,j}^{(k+1)} = p_{i,j}^{(k)} + \frac{s}{2(1+r^2)} \{ p_{i+1,j}^{(k)} + p_{i-1,j}^{(k)} + r^2 (p_{i,j+1}^{(k)}) 
+ p_{i,j-1}^{(k+1)} - (\alpha x)^2 q_{i,j} - 2(1+r^2)p_{i,j}^{(k)} \} \]  

(3.1.12)

There exists an optimum value for this relaxation factor, which depends on the size of mesh, the shape of the domain and the type of boundary conditions. However, \( s \) must be determined empirically. If \( k \)-th iteration level values of \( p_{i,j} \) and \( p_{i,j+1} \) on the right side of equation (3.1.12) are replaced by \((k+1)\)th level, one obtains the so-called line-
SOR and must be solved implicitly for the \( p^{(k+1)} \). The number of iterations is thus reduced by the use of these advanced values. However, due to the tridiagonal solution involved, there may be no gain in overall computing speed as already discussed in section 2.1.

To select an appropriate numerical iteration method, we have to consider the whole iteration procedure, which will be described in the following, and the degree of non-linearity involved. The main difference between the Newtonian case and non-Newtonian is that the forcing term is constant (zero) for the former, whereas for the non-Newtonian case this term is a very sensitive variable through the high-order derivatives of stream function. Failure to realize this will possibly cause the iteration to diverge no matter which numerical method is used.

The basic approach is to solve the two elliptic equations for the stream and vorticity together, subject to their appropriate boundary conditions. To do this, we proceed iteratively from an initial guess for all the unknown function values until all the required criterions are satisfied. There are three iteration loops involved; two inner loops for iterating stream function and vorticity separately, and one outer loop to connect them. The whole procedure is summarized by the steps listed below with some detailed discussion, and also shown by a flow chart in Fig. 5.

1. Prescribe all the known or constant boundary conditions, as described in the preceding section 3.1-3.

2. Have a fair initial guess for the stream values at interior points.

3. Obtain the initial guess for vorticity. This includes
Fig. 5 Flow Chart for Iteration Scheme of the Transport Equation.

INPUT
\( \psi^0_{ij}, \omega^0_{ij} \)

Specify Boundary Condition

Velocity and its Gradients

Using New \( \psi^{k+1}_{ij} \) to Correct \( \omega \) at Boundaries

Constitutive Equation + \( \phi(T_e) \)

Iteration of Vorticity Equation by Lieberman Method with Alternating Direction

Converged? _Y_ or _N_?

Three Iterations for Stream Function

Converged OR 3 Iterations Exceeded?

Are Both \( \psi^k_{ij}, \omega^k_{ij} \) Converged?

OUTPUT
both the interior and the undetermined boundary values. However, except for Newtonian flow, all the initial guessing values of stream function and vorticity will be read in from the results of the previous case with a smaller Weissenberg number.

4. Calculate the velocity, velocity gradients and extra stress components (only for non-Newtonian flow), so that the advective and forcing terms can be obtained. For viscoelastic flow, the stress components have to be determined through a subroutine as described in Fig. 3.

5. Iterate the vorticity equation:

\[ \nabla^2 \omega = \phi (\underline{e}) - \text{Re} \frac{\partial (\psi, \omega)}{\partial (x, y)} \]

6. Iterate the stream function equation:

\[ \nabla^2 \psi = \omega \]

7. Correct the boundary conditions of vorticity.

8. Go to step 4, and repeat the procedure until both inner loops in steps 5 and 6 are converged within the same outer loop.

In step 2, since the iteration is based on the idea of trial-and-error, it is therefore not surprising that for Newtonian flow the quality of these initial guesses affect quite markedly the computing time taken to reach convergence. For viscoelastic fluids, this quality may dictate whether the algorithm even converges at all. A natural approach is to take the corresponding Newtonian results as the initial guess for
the viscoelastic flow with a small Weissenberg number (say, \( W_s = 0.01 \) for example). Then the converged solution of the latter is used in turn for the next case with a larger Weissenberg number and so on. Therefore, only the initial guess for the Newtonian case needs to be determined and it will be shown here. It should be noted that the following simple estimate is far from perfect and must not be mistaken as an unique solution. However, it is certainly better than any arbitrary guess.

A symmetric flow based on the centerline of the contraction region \((i=41, x=1.6)\) is assumed in this case as indicated by the low Reynolds number, \( Re = 0.75 \). Hence only half of the domain needs to be considered, which is divided into four sections: two fully-developed regions at the entrance and the confined part, a \( 45^o \) plane sink flow between them and a stagnant corner.

The detachment length is thus the same as the height of CD, \( h-a \), and the sink flow will start approximately from \( i=19(x=0.72) \) to \( i=36 \) \((x=1.4)\). To determine the locus of this detachment plane, a linear function is used which gives us:

\[
y^* = \frac{26}{15} - x^* \quad (0.72 \leq x^* \leq 1.4)
\]

The starting values of stream function for Newtonian flow can thus be obtained as:

A fully-developed flow in the entry region \((1 \leq i \leq 19)\)

\[
\psi = y - 0.5y^2 \quad \text{as given by the boundary condition.}
\]

A fully-developed flow in the contraction region \((36 \leq i \leq 41)\)

\[
\psi = y + 7.5y^2 - 18y^3 \quad \text{derived from no-slip at wall.}
\]
A stagnant region under the detachment plane (\(19 < i \leq 36\) and \(y^* < y < 1\)) \(\psi = 0.5\)

A sink flow in the converging region (\(19 < i \leq 36\) and \(0 \leq y < y^*\))

\[
\psi = y + cy^2 + dy^3 \quad \text{with} \quad c = (3-4y^*)/2y^{*2} \quad \text{and} \quad d = (y^*-1)/y^{*3}
\]

From steps 5 and 6, it can be seen that the forcing terms are still far from correct at earlier stages for two governing equations. Trying to satisfy either of them before advancing to the next step will be a very inefficient effort, and may even possibly never converges at all. It was found that no more than three iterations should be sufficient enough to be considered effective. In addition, due to the fact that the boundary values of vorticity change after each iteration of stream function, it will be beneficial to employ the alternating direction feature so that all the "corrected" boundary conditions can have the same opportunity to proceed inside, as mentioned in section 2.1. Therefore, it was chosen to iterate vorticity equation only twice in step 5; once for \(i^+, j^+\), followed by \(i^+, j^+\). For the stream function in step 6, because all the boundary values are constant it is thus not necessary to change the sweep direction and three iterations are allowed in this loop.

Basically, the solution of (steady) elliptic equations by iteration is analogous to solving a time-dependent problem to an asymptotic steady state. Each iterated value corresponds to the solution at certain time. The over-relaxation technique described earlier attempts to reach the steady state faster by increasing the time step, and this is meaningful only if the time-dependence is known to be bounded. In other words, if either the boundary condition or the forcing term is fixed, the extra
increment added by the relaxation factor will accelerate the convergence eventually. (In the first few iterations, the over-relaxation may bring the solution further away from the converged value resulting from this extrapolation effect.) On the other hand, without these independent restraints to stabilize the overall iteration, a small overshoot by the over-relaxation will never be recovered and consequently may cause the whole iteration to diverge. This is the reason why SOR is particularly not recommended for the vorticity equation and Liebman's method, equation (3.1.11) is thus preferred here. Meanwhile, since the forcing term $\Phi(e)$ is quite sensitive to changes of the stream function values, it was decided to sacrifice some small gain in speed (if any) by not using SOR for the stream function in step 6 so that the stability of step 5 can be more assured.

Because the boundary values of vorticity corrected in step 7 dictate the iteration in step 5, it was felt that their accuracy should be at least consistent with those of interior points, for which central-differencing of second-order accuracy is used.

Consider the vorticity on the moving boundary AH for example. We expand the stream values $\psi_{1,1}$ and $\psi_{1,2}$ by Taylor series based on the boundary values as:

$$\psi_{1,1} = \psi_{1,0} + \frac{\partial \psi}{\partial y}_{i,0} \Delta y + \frac{1}{2} \frac{\partial^2 \psi}{\partial y^2}_{i,0} (\Delta y)^2 + \frac{1}{6} \frac{\partial^3 \psi}{\partial y^3}_{i,0} (\Delta y)^3 + O(\Delta y)^4$$

$$\psi_{1,2} = \psi_{1,0} + 2 \frac{\partial \psi}{\partial y}_{i,0} \Delta y + 2 \frac{\partial^2 \psi}{\partial y^2}_{i,0} (\Delta y)^2 + \frac{4}{3} \frac{\partial^3 \psi}{\partial y^3}_{i,0} (\Delta y)^3 + O(\Delta y)^4$$

Since the no-slip boundary condition is defined by a constant stream function value, the second-order derivative in above equations is iden-
tified as the vorticity to be sought, \( \omega_{i,0} \). By eliminating the third-order derivative term and rearranging the resulting equation, a second-order from can be obtained:

\[
\omega_{i,0} = \frac{-7\psi_{i,0} + 8\psi_{i,1} - \psi_{i,2}}{2(\Delta y)^2} - \frac{3}{\Delta y} \frac{\partial \psi_{i,1}}{\partial y} \bigg|_{i,0} + O(\Delta y)^2 \tag{3.1.13}
\]

Here, the Neumann condition is applied. For stationary boundaries, the normal derivative of stream function should vanish, which is the case for boundary BCDEF in this problem. On AH, the constant moving velocity gives:

\[
\omega_{i,0} = \frac{-7\psi_{i,0} + 8\psi_{i,1} - \psi_{i,2}}{2(\Delta y)^2} - 90 + O(\Delta y)^2 \quad \text{for } \Delta y = 1/30
\]

The total number of iterations required depends on the convergence criterion. With all calculations performed in double precision, it was felt that each convergence criterion chosen for the stream function and vorticity respectively should be consistent with the discretization errors of the formulae used to approximate the governing equations. Since all the values of velocity and velocity gradients are based on the stream function, which is usually confined between 0 and 0.5 in this case except in the vortex region, an absolute tolerance is taken for the stream function in step 6, i.e.

\[ |\psi_{i,j}^{(k+1)} - \psi_{i,j}^{(k)}| < 10^{-6} \]

Considering the magnitude of vorticity, which can range from -40 to 20 in the contraction region, and also the way step 5 is being iterated, a relative tolerance is considered adequate for vorticity as:

\[ |\omega_{i,j}^{(k+1)} - \omega_{i,j}^{(k)}| < 10^{-2} |\omega_{i,j}^{(k)}| \]
Finally, in proceeding from one iteration to the next, the current solution was smoothed by taking its weighted average with previous corresponding iterate. This is equivalent to the SUR method with an under-relaxation factor less than unity.

\[
\frac{p_{i,j}^{(k+1)}}{p_{i,j}^{(k)}} = \alpha p_{i,j}^{(k+1)} + (1-\alpha) p_{i,j}^{(k)} \quad (0 < \alpha < 1)
\]

\[
= \frac{\alpha}{2(1+r^2)} \{ p_{i+1,j}^{(k)} + p_{i-1,j}^{(k+1)} + r^2 p_{i,j+1}^{(k)} + p_{i,j-1}^{(k+1)} - \Delta x^2 q_{i,j} \} + (1-\alpha) p_{i,j}^{(k)}
\]

\[
= \frac{\alpha}{2(1+r^2)} \{ p_{i+1,j}^{(k)} + p_{i-1,j}^{(k+1)} + r^2 p_{i,j+1}^{(k)}

+ r^2 p_{i,j-1}^{(k+1)} - \Delta x^2 q_{i,j} - 2(1+r^2) p_{i,j}^{(k)} \} + p_{i,j}^{(k)}
\]

Again this technique is only applied to step 5 to assure the numerical stability for the vorticity equation, and should be mutually exclusive with the use of SOR. However, it is interesting to note that Davies et al also applied it to the stream function with which the SOR method was used by them. The same effect can be achieved simply by reducing the over-relaxation factor as shown above.

3.1-5 NUMERICAL RESULTS

Employing the numerical scheme outlined above, converged solutions have been obtained for the following cases with the same Reynolds number of 0.75, as shown in Table 1.

For the 3:1 contraction geometry considered here, Davies et al reported that it was difficult to obtain converged solutions for the
<table>
<thead>
<tr>
<th>Weissenberg Number</th>
<th>Number of Outer Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>case studied/initial guess used</td>
<td></td>
</tr>
<tr>
<td>0 (i.e. Newtonian)</td>
<td>52</td>
</tr>
<tr>
<td>0.01/0</td>
<td>25</td>
</tr>
<tr>
<td>0.05/0</td>
<td>83</td>
</tr>
<tr>
<td>0.08/0.05</td>
<td>71</td>
</tr>
<tr>
<td>0.10/0.08</td>
<td>60</td>
</tr>
<tr>
<td>0.125/0.10</td>
<td>66</td>
</tr>
<tr>
<td>0.15/0.125</td>
<td>63</td>
</tr>
<tr>
<td>0.20/0.10</td>
<td>109</td>
</tr>
<tr>
<td>0.25/0.20</td>
<td>70</td>
</tr>
<tr>
<td>0.30/0.25</td>
<td>52</td>
</tr>
<tr>
<td>0.35/0.30</td>
<td>29</td>
</tr>
<tr>
<td>0.40/0.35</td>
<td>25</td>
</tr>
<tr>
<td>0.45/0.40</td>
<td>30</td>
</tr>
<tr>
<td>0.50/0.40</td>
<td>not converged</td>
</tr>
<tr>
<td>0.50/0.45</td>
<td>not converged</td>
</tr>
</tbody>
</table>
Maxwell/Oldroyd model with the relaxation time above 0.2 (equivalent to Weissenberg number 0.267 here). However, there was no difficulty for this nonlinear model until the Weissenberg number was over 0.45. Although this may have been partly associated with the numerical algorithms involved, such as the mesh size or the iteration procedure, it may also be due to the characteristics of different viscoelastic models themselves. The difficulty in obtaining converged solutions for the model with constant relaxation time and elastic modulus is usually caused by the very high values of stress components generated in the confined region. In contrast, the nonlinear model used here always gives finite stress values. Nevertheless, when the Weissenberg number reaches to a certain limit, the rapid changes in structure will make the stress become very sensitive to the strain rate. Thus, no steady-state solution can be obtained within the chosen tolerance although the numerical iteration did not actually diverge for Weissenberg number larger than 0.45. This result is supported by the experimental investigation of Cable and Boger[6], in which two distinct flow regimes are identified for the tubular entry flow of viscoelastic fluids. At moderate flow rates, a divergent flow will develop as the vortex detachment plane is approached, and this may result in the numerical instability encountered above.

Figures 6 to 10 show the relevant streamlines for cases with Weissenberg numbers \( Ws = 0 \) (Newtonian), 0.08, 0.2, 0.3 and 0.45. \( Ws=0.08 \) was chosen because it is equivalent to the result of Davies et al for \( \lambda = 0.06 \). Basically, for Weissenberg number less than 0.25, the fluid elasticity was found to accentuate the size and the intensity of the upstream (before the contraction) vortex, and this prediction is consis-
Fig. 6 Streamlines for the 3:1:1:3 contraction/expansion flow with $M_b = 0$ (Newtonian) and $Re = 0.75$
Fig. 7 Streamlines for the 3:1/1:3 Contraction/Expansion Flow with $We = 0.08$ and $Re = 0.75$
Fig. 8 Streamlines for the 3:1:1:3 Contraction/Expansion Flow with $M_s = 0.20$ and $Re = 0.75$
Fig. 9 Streamlines for the 3:1/1:3 Contraction/Expansion Flow with \( W_s = 0.30 \) and \( Re = 0.75 \)
Fig. 10 Streamlines for the 3:1/1:3 Contraction/Expansion Flow with $W_s = 0.45$ and $Re = 0.75$
tent with most of the previous results. On the other hand, the downstream corner eddy was shown to decrease, but in not as pronounced a manner as the upstream eddy after the Weissenberg number is larger than 0.1. However, due to the nature of this nonlinear model, there exists a transition range ($Ws=0.2\pm0.25$) beyond which the intensity of the upstream vortex starts to decrease and the downstream vortex begins to increase again. This has never been found in the earlier numerical calculations, and has to be related to the fact that the elastic effect will gradually become less dominant for this nonlinear model when the number of "cross-linkings" in the structure is reduced by a relatively high strain rate. Since the linear model could not predict such a continuous transition, most of the results for the linear model, except $Ws=0.267$ used by Davies et al[13], have been within this limit to avoid the instability caused by the extremely high stress. When the Weissenberg number is beyond this transition range, it is believed that the linear model will incorrectly predict a high intensity of vortices downstream because of the possible elastic turbulence developed after the contraction, as shown by the result of Davies et al.

The exact effect of the Weissenberg number on the vortex intensity (as characterized by the maximum value of the stream function) is shown in Fig. 11. Except at $Ws=0.01$, the intensity of upstream vortex grows with the increasing Weissenberg number and reaches its maximum at $Ws=0.24$. After that, the intensity begins to diminish gradually. The opposite is the case for the downstream vortex with a minimum at $Ws=0.21$. Similarly, by determining the separation points on the fixed boundaries BC and FG, the size of two vortex regions is shown in Fig. 12. It can
Fig. 11 The Effect of Weissenberg Number on Vortex Intensity
Fig. 12 The Length of the Vortex Region in both Upstream and Downstream direction as function of Weissenberg Number.
be seen that the detachment length increases with the Weissenberg number. However, the decreasing slope after $W_s=0.2$ seems to indicate that the value at $W_s=0.45$ is the maximum. Whereas at the downstream section, the reattachment length drops dramatically at small Weissenberg numbers and then remains nearly constant from $W_s=0.1$ to $W_s=0.3$ before increasing again. The prediction of the upstream detachment length here is in accordance with the experimental results of Cable and Boger. They reported that the detachment length increases almost linearly with the Weissenberg number in the so-called vortex growth regime of low flow rates. At higher flow rates, the vortex size will be reduced as the flow diverges upstream of the detachment plane. Incidentally, they also indicated that the maximum detachment length occurred at $W_s=0.45$ for the fluid F9 used by them in a 4:1 contraction, but the exact comparison with the experimental data is not possible as real elastic fluids are known to have a spectrum of rheological parameters instead of the single value considered here. Nevertheless, the good agreement of the qualitative trend clearly shows the excellence of this numerical solution and the nonlinear viscoelastic model proposed by Acierno et al.

To explain the deviation of both the size and the intensity of the upstream vortex which occurred at $W_s=0.01$, it is necessary to reconsider the definition of Reynolds number. The same Reynolds number, $Re=0.75$ based on the equilibrium value of viscosity (i.e. in the limit of linear viscoelasticity), was used for all the cases studied here. However, the local Reynolds number could have been very different. Recall that the Reynolds number is an index for the ratio between the inertia and the viscous forces as:
\[
Re = \frac{\rho u^2}{\tau_{xy}}
\]

For a very small Weissenberg number, such as \(Ws=0.01\), the velocity field is not too different from the Newtonian case, but the shear force will be reduced significantly due to the "drag reduction" effect of the elasticity. Fig. 13 shows the shear stress at boundary BC from \(i=6\) to \(i=31\) for \(Ws=0, 0.01, 0.2, 0.45\). In other words, the flow with a very small Weissenberg number is actually similar to the corresponding Newtonian case with a larger Reynolds number. Since the upstream corner eddy will decrease with the increasing Reynolds number for the Newtonian flow, as shown by Crochet and Pilate[11], it is therefore not surprising that a slight reduction of the upstream vortex should be expected. When the Weissenberg number becomes larger, the elastic effects become totally dominant over the inertia ones and the upstream vortex starts to grow both in size and intensity. It can thus be concluded that the flow behavior is determined by the "competition" between these two factors, and this relationship is quite nonlinear, to the extent that neither of them can be discussed separately. As it has been described previously, the inertia may again show its influence when the Weissenberg number reaches a certain limit, because of dramatic structural alterations caused by flow for those cases.

A typical profile of the structure variable \(\xi\) along the flow direction, taking the moving boundary \((j=1, y=0)\) for example, is shown in Fig. 14. It should be unity everywhere when the fluid is inelastic, i.e. \(Ws=0\). As the Weissenberg number increases, the profile becomes less symmetric with respect to the center of the contraction region.
Fig. 13 The Shear Stress along the Flow Direction on the Stationary Boundary (y = 1) as a function of the Weissenberg Number.
Fig. 14 The Structure Variable on the Moving Boundary \((y = 0)\) as a function of Weissenberg Number.
and the structure is further away from its equilibrium state in the contraction region. Due to the acceleration and deceleration caused by the geometry change, there will be two points on the moving boundary where all the velocity gradients are zero. The cross-sectional area available for the flow in the upstream section is reduced by the vortex corner, where the acceleration starts. Thus the location of this strain-rate-free point will be closely related to the detachment length. From Fig. 14, it can be seen that the upstream point with \( \xi = 1 \) is farther away from the confined region when the Weissenberg number increases. Meanwhile, the downstream one seems to occur at the same spot and this may be due to the fact that the reattachment length is almost constant for \( W_s = 0.1 \sim 0.3 \).

Figures 15 and 16 contain the corresponding shear stress and normal stress difference at the moving boundary. The shear stress is reduced quite considerably as the elasticity is increased. For \( W_s = 0.05 \), the shear stress at the center of the contraction is 25% less than the Newtonian case, whereas for \( W_s = 0.45 \) the value is only less than one third of that. On the other hand, the normal stress difference increases dramatically with a slight elasticity. This is related to the well known Weissenberg effect. The velocity profile is shown in Fig. 17 for \( W_s = 0.2 \), and compared with the Newtonian flow profile. Partly due to the shear-thinning viscosity, the upper portion of the fluid (adjacent to the moving boundary) is accelerated faster than in the Newtonian case and then starts to relax in the confined region. Finally, if we plot the velocity profile at \( j = 6 \) (i.e. \( y = 1/6 \), however, the maximum velocity will occur at \( y = 5/36 \) for fully-developed flow.) across the domain, as shown in Fig. 18,
Fig. 15 The Shear Stress $\tau_{xy}$ on the Moving Boundary ($y = 0$) as a function of Weissenberg Number.
Fig. 16 The Normal Stress Difference exerted on the Moving Boundary\((y = 0)\) as a function of Weissenberg Number.
Fig. 17 The Velocity Profiles Across the Domain at various x positions for $W_s = 0$ and 0.2
Fig. 18 X-Component Velocity Profile at $j = 6$ for Contraction/Expansion Flow of Viscoelastic Fluids
the same effect can be seen. The maximum velocity in the contraction region is reduced by the elasticity and the whole velocity profile becomes flatter for the incompressible fluid assumed.

3.2 HEAT TRANSFER PROBLEM OF POWER-LAW FLUIDS

3.2-1 NUMERICAL SOLUTIONS

The geometry is shown in Fig. 19 for a parallel plate system. Since the temperature profile is expected to be symmetric with respect to the centerline at \( y=0 \), only half of the domain needs to be considered. The half-width of the slit is taken as the characteristic length for the dimensionless coordinates, so that \( y=1 \) is at the upper plate. The boundary conditions at \( x=0 \) and \( y=1 \) will vary, depending on the situation involved and the reference temperature chosen. Basically, there are two types of problems:

At \( x=0 \),

1. A uniform temperature, if viscous dissipation is not considered.

2. Otherwise, a fully-developed temperature profile.  
   i.e. \( \frac{\partial T}{\partial x} = 0 \)

At \( y=1 \),

1. Isothermal.

2. Linearly decreasing temperature.

As mentioned in section 2.3, the energy equation, neglecting the axial heat conduction, is numerically a self-starting problem providing the velocity field is known. In this case, the Crank-Nicholson
Fig. 19 The Domain of Numerical Solution for Graetz-Nusselt Problem of Power-Law Fluids
method was found to be effective. If the equation (2.3.3) is rewritten as:

\[ u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{1}{Pe} \left( \frac{\partial^2 T}{\partial y^2} + \Omega \right) \quad (3.2.1) \]

where \( \Omega \) is the viscous dissipation.

For power-law fluids, \( \Omega = Br \mu \left\{ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right\} \)

with a dimensionless viscosity \( \mu \) based on the Newtonian viscosity.

Employing a central difference formula, the above equation can be differenced at \((i+\frac{1}{2}, j)\) to have a tridiagonal form as:

\[-a_j T_{i+1,j-1} + b_j T_{i+1,j} - c_j T_{i+1,j+1} = d_j\]

where \( a_j = \frac{\Delta x}{2u_{i+1,j}} \left( \frac{1}{Pe(\Delta y)^2} + \frac{\nu_{i+1,j}}{2y} \right) \)

\( b_j = 1 + \frac{\Delta x}{Pe(\Delta y)^2 u_{i+1,j}} \)

\( c_j = \frac{\Delta x}{2u_{i+1,j}} \left( \frac{1}{Pe(\Delta y)^2} - \frac{\nu_{i+1,j}}{2\Delta y} \right) \)

\( d_j = \left\{ \frac{\Delta x}{2u_{i,j}} \left( \frac{1}{Pe(\Delta y)^2} + \frac{\nu_{i,j}}{2\Delta y} \right) \right\} T_{i,j-1} + \right\} T_{i,j+1} + \right\} T_{i,j} + \left\{ 1 - \frac{\Delta x}{Pe(\Delta y)^2 u_{i,j}} \right\} T_{i,j} = \frac{\Delta x}{2Pe} \left\{ \frac{\Omega_{i+1,j}}{u_{i+1,j}} + \frac{\Omega_{i,j}}{u_{i,j}} \right\} \]

This can be solved simply by backward substitution without the use of matrix inversion, and is of second-order accuracy. For the Graetz-Nusselt problem, due to the step-change boundary condition at the entry, it is necessary to have a very fine grid in the flow direction near the entry so that a continuous and consistent temperature field can be
obtained. After several attempts, an optimum variable-spacing mesh was chosen as shown also at the bottom of Fig. 19. Meanwhile, 20 grids in y-direction will be enough to give a satisfactory result.

Four categories of heat transfer problem were studied for power-law fluids in this work; i.e.

(a) temperature-independent viscosity without viscous heating,
(b) temperature-independent viscosity with viscous heating,
(c) temperature-dependent viscosity without viscous heating,
(d) temperature-dependent viscosity with viscous heating.

The first two are used primarily to compare with the previously published results. Only the last one will be applied to the case in which two-dimensional flow is taken into consideration. Most of their results are represented by the local Nusselt number defined as:

\[ \text{Nu} = \frac{2}{T_{\text{ave}}} \left| \frac{\partial T}{\partial y} \right|_{y=1} \]

where \( T_{\text{ave}} \) is the flow-average(bulk) temperature.

\[ T_{\text{ave}} = \frac{\int_0^1 (uT)dy}{\int_0^1 udy} \]

The integration will be carried out by the Simpson's method, and the temperature gradient at boundary is approximated by the backward difference formula of second-order accuracy as:

\[ -\left( \frac{\partial T}{\partial y} \right)_{i,j=n+1} = \frac{1}{6\Delta y} \left( -11T_{i,n+1} + 18T_{i,n} - 9T_{i,n-1} + 2T_{i,n-2} \right) \]

which is suggested by Vlachopoulos and Keung[47].
For the last two cases, the Arrhenius equation is assumed for the temperature dependence of viscosity with an activation energy $\Delta E/R$ of $2920^\circ K$. The velocity has to be calculated from equation (2.3.8) also by the Simpson's integration method, if only a unidirectional flow is considered.

For the simplest case (a), Fig. 20 shows the Nusselt numbers along the flow direction for power-law fluids with power-law index $n = 0.25$, $0.5$, $1.0$ and $2.0$ respectively. The higher Nusselt number for the fluids with smaller index seems to indicate that they are more difficult to be cooled. This is due to the fact that the velocity profile becomes flatter as $n$ decreases, shown in Fig. 21, and the temperature near the wall will thus be higher, as the faster velocity there provides shorter contact time for the heat conduction. In Fig. 22, the centerline temperature and the one near the wall ($y=0.9$) are compared for two extreme cases, $n = 0.25$ and $2.0$, and clearly confirm the above expectation.

Similarly, if the viscosity is temperature-dependent, the temperature near the wall will be lower, compared with the temperature-independent case for the same power-law index fluid, due to the slower velocity caused by the cooler temperature (higher viscosity) there before this effect can be compensated for by the heat conduction from the central core of fluid. The Nusselt number and the temperature at $y = 0.9$ for $n = 0.25$ are shown in Fig. 23 to illustrate this influence. Because the relatively high temperature at the center is weighted more by the velocity readjustment, there will be a minimum of Nusselt number occurring around $z = 0.2$ before reaching its equilibrium value.

The effect of viscous dissipation on the Nusselt number is shown
Fig. 20 Nusselt Number of the Flow with Various Power-Law Indices
Fig. 21 Velocity Profile for various Power-Law Fluid Indices
Fig. 22 The Effect of Power-Law Fluid Index on Temperature Distribution at $y = 0$ and $y = 0.9$
Fig. 23 The Effect of Viscosity on Nusselt Number and Temperature for the Flow with $n = 0.25$
in Fig. 24 for the power-law fluid with \( n = 0.5 \). For the modified Brinkman number \( Br^* = 1.0 \), there is a minimum in the curve and the Nusselt number increases further downstream because of the viscous heating until it is balanced by the heat being conducted outwards. If the viscosity is not temperature-dependent, the entry conditions (i.e. uniform temperature, \( T = 1 \), or a developed temperature profile such as equation (2.3.14)) do not seem to make much difference except in the entry region. This is obviously due to the slightly different temperature field used at the entrance. However, the discrepancy is certainly not negligible if the viscosity is temperature-dependent as a very different velocity field, including radial convection, will be involved. In Fig. 25, this difference is clearly indicated. On the other hand, also shown in Fig. 25 is the result of solving the two-dimensional momentum equation (2.1.6) coupled with the energy equation (3.2.1) for the case of \( Pe = 5000 \). The heat transfer will be enhanced by the radial (across streamlines) heat convection, and thus the Nusselt number is reduced in the entry region to some extent. Although the effect can only be felt for \( z < 0.01 \), it is expected to be more important for the case with smaller Peclet number. Unfortunately, no reasonably converged solutions have been obtained for \( Pe < 5000 \). This is believed to be because of the singularity of the step-change boundary condition at the entry and the neglect of axial heat conduction.

Finally, to demonstrate the actual application in polymer processing, a sample problem was calculated for the situation of a molten plastic entering a horizontal slit die of length \( L = 1.28 \) cm and width \( 2h = 0.0788 \) cm. All the following physical properties were taken from the example
Fig. 24 The Effect of Entry Condition and Viscous Dissipation for the Flow with $n = 0.5$ and Temperature-Independent Viscosity
Fig. 25 Nusselt Number Variation for Different Entry Conditions of the Flow with $n=0.5$, $\text{Br}^*=1.0$, and Temperature-Dependent Viscosity.
problem (5.4-5) in reference[4], in which the entry temperature is assumed to be uniform so that the importance of viscous heating can be illustrated.

\[ \rho C_p = 1.8 \times 10^6 \text{ J/m}^3\text{K} \]
\[ k = 4.184 \times 10^{-2} \text{ W/m}^0\text{K} \]
\[ n = 0.5 \]
\[ m(T) = 6.9 \times 10^3 \text{ Ns}^{\frac{1}{2}}/\text{m}^2 \text{ at } 463^0\text{K} \]

A linearly decreasing temperature, from \( T_o = 463^0\text{K} \) to \( T_e = 413^0\text{K} \), was assumed at the die wall, with the same activation energy \( \Delta E = 2920^0\text{K} \) used for the temperature dependence of the viscosity. The corresponding dimensionless groups are:

\[ \text{Re} = 4.9 \times 10^{-5} \]
\[ \text{Pe} = 1.122 \times 10^3 \]
\[ \text{Br}^* = 2.348 \]

Fig. 26 shows the average temperature and the Nusselt number of this solution for both the unidirectional and two-dimensional flow cases. A small rise of temperature is clearly indicated as the result of viscous dissipation, and then both the temperature decreases and Nusselt number increases almost linearly due to the linearly decreasing boundary temperature. Since the singularity of step-change boundary condition is removed in this case, a converged solution for the two-dimensional flow has been obtained. However, the difference is still not very significant as the Peclect number is relatively high and the temperature difference
Fig. 26 Numerical Solution for a sample problem
is only moderate. Qualitatively, the unidirectional flow calculation seems to under-estimate the cooling effect and thus should be sufficient for practical conservative design use if the viscous heating is the problem.

3.2-2 ANALYTICAL APPROXIMATION METHOD FOR NUSSELT-GRAETZ PROBLEM

As described in section 2.3, this method is applicable only when the viscosity is not temperature-dependent. In spite of this limitation, it is important to have an analytical result when possible, if only to provide spot checks on the numerically computed values. Therefore, the results approximated by third and fifth order polynomials respectively for this analytical method will be shown here to compare with the numerical solution obtained in the preceding part. Their good agreement seems to indicate that this simple and handy solution is certainly better than previous analytical results available, the inadequacy of which is probably due to the use of one single form of solution for the whole domain. It should be expected that the nearly uniform temperature profile at the entry region cannot be fairly represented by only few eigenfunctions with limited terms. Failure to realize this problem will possibly result in a physically unrealistic solution, such as that of Suckow et al[43].

The geometry is shown in Fig. 1, with y = 0 taken at the lower plate surface. This is mainly for the convenience in evaluating the boundary condition T = 0 there. In this case, the velocity profile will be defined as:

\[
\frac{u(y)}{u_{\text{max}}(y=1)} = 1 - (1 - y)^{(n+1)/n}
\]
The solution is very straightforward, as described in section 2.3. The corresponding results will be listed below without derivation. Using a reduced coordinate defined as $\eta = y / \delta_T(z)$ for the entry region, consider Newtonian flow without viscous dissipation as an example:

**THIRD-ORDER APPROXIMATION**

Thermal Entry Region ($z_f \geq z \geq 0$)

\[
T(z,y) = 1.0 \quad \text{for} \quad 1 \geq y \geq \delta_T
\]

\[
T(\eta) = 1.5\eta - 0.5\eta^3 \quad \text{for} \quad \delta_T \geq y \geq 0
\]

\[
T_{ave} = 1 - 0.3\delta_T^2 + \frac{1}{16} \delta_T^3
\]

\[
Nu = 3/(\delta_T T_{ave})
\]

The thermal boundary layer thickness, $\delta_T$, is determined from:

\[
\frac{2}{15} \delta_T^3 - \frac{1}{32} \delta_T^4 = 1.5z
\]

with $\delta_T = 1$ at $z_f = 0.068$

Developing Region ($z \geq z_f$)

\[
T(z,y) = 1.2224\exp(-2.951z) \{1.5y - 0.5y^3\}
\]

\[
T_{ave} = 0.932\exp(-2.951z)
\]

\[
Nu = 3.934
\]

**FIFTH-ORDER APPROXIMATION**

Thermal Entry Region ($z_f \geq z \geq 0$)

\[
T(z,y) = 1.0 \quad \text{for} \quad 1 \geq y \geq \delta_T
\]

\[
T(\eta) = 2.5\eta - 5\eta^3 + 5\eta^4 - 1.5\eta^5 \quad \text{for} \quad \delta_T \geq y \geq 0
\]
\[ T_{\text{ave}} = 1 - \frac{1}{7} \delta_T^2 + \frac{5}{224} \delta_T^3 \]

\[ \text{Nu} = \frac{5}{(\delta_T, T_{\text{ave}})} \]

The thermal boundary layer thickness, \( \delta_T \), is determined from:

\[ \frac{4}{63} \delta_T^3 - \frac{5}{448} \delta_T^4 = 2.5z \]

with \( \delta_T = 1 \) at \( z_f = 0.021 \)

**Developing Region ( \( z \geq z_f \))**

\[ T(z,y) = \frac{2}{\Sigma a_i \exp(-\beta_i z) \Sigma a_{ij} y^j} \]

\[ T_{\text{ave}} = 0.886\exp(-\beta_1 z) + 0.0852\exp(-\beta_2 z) \]

\[ \text{Nu} = \frac{(3.354\exp(-\beta_1 z) + 3.518\exp(-\beta_2 z))}{T_{\text{ave}}} \]

\[ \alpha_1 = 1.168 \quad \alpha_2 = -0.193 \quad \beta_1 = 2.839 \quad \beta_2 = 30.983 \]

\[ a_{10} = a_{12} = a_{20} = a_{22} = 0 \]

\[ a_{11} = 1.435 \quad a_{13} = -0.032 \quad a_{14} = -0.678 \quad a_{15} = 0.274 \]

\[ a_{21} = -9.119 \quad a_{23} = 49.221 \quad a_{24} = -56.966 \quad a_{25} = 17.864 \]

The comparison between the analytical approximation and the numerical results is shown in Table 2 and Fig. 27. With four basic boundary conditions, the third-order polynomial approximation inevitably leads to only one "eigenfunction" which resulted in having a constant Nusselt number, i.e. \( \text{Nu} = 3.934 \), in the developing region. However, it is known that the temperature profile is not really fully-developed in this region. To improve this inadequacy, the use of higher than third-order polynomial is recommended. For the Nusselt number in the entry region, the increa-
Table 2

Newtonian Flow (n = 1)

<table>
<thead>
<tr>
<th>$z = x / Pe$</th>
<th>$\delta_T$</th>
<th>$T_{ave}$</th>
<th>Nu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3rd order</td>
<td>5th order</td>
<td>3rd order</td>
</tr>
<tr>
<td>0.001</td>
<td>0.2282</td>
<td>0.3474</td>
<td>0.9851</td>
</tr>
<tr>
<td>0.0025</td>
<td>0.3119</td>
<td>0.4754</td>
<td>0.9727</td>
</tr>
<tr>
<td>0.005</td>
<td>0.3958</td>
<td>0.6039</td>
<td>0.9569</td>
</tr>
<tr>
<td>0.0075</td>
<td>0.4554</td>
<td>0.6955</td>
<td>0.9437</td>
</tr>
<tr>
<td>0.01</td>
<td>0.5034</td>
<td>0.7693</td>
<td>0.9319</td>
</tr>
<tr>
<td>0.02</td>
<td>0.6422</td>
<td>0.9838</td>
<td>0.8928</td>
</tr>
<tr>
<td>0.04</td>
<td>0.8231</td>
<td>1.0</td>
<td>0.8316</td>
</tr>
<tr>
<td>0.06</td>
<td>0.9545</td>
<td>1.0</td>
<td>0.7811</td>
</tr>
<tr>
<td>0.08</td>
<td>1.0</td>
<td>1.0</td>
<td>0.7361</td>
</tr>
<tr>
<td>0.10</td>
<td>1.0</td>
<td>1.0</td>
<td>0.6939</td>
</tr>
<tr>
<td>0.25</td>
<td>1.0</td>
<td>1.0</td>
<td>0.4457</td>
</tr>
<tr>
<td>0.50</td>
<td>1.0</td>
<td>1.0</td>
<td>0.2132</td>
</tr>
<tr>
<td>0.75</td>
<td>1.0</td>
<td>1.0</td>
<td>0.1019</td>
</tr>
<tr>
<td>1.00</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0488</td>
</tr>
</tbody>
</table>
Fig. 27 Comparison of Analytical and Numerical Solutions, with $Br^* = 0$, $n = 1$
sing deviation of fifth-order approximation from the numerical solution may be due to the large mesh size in y-direction used for the finite difference grid. This is also believed to be a partial cause of the numerical problem in obtaining converged solutions for the two-dimensional flow case. In the developing region, the better accuracy of fifth-order is clearly seen as its asymptotic Nusselt number 3.785 is only different from the theoretical value 3.767 by less than 0.5%.

Also shown in Fig. 27 is the result by Suckow et al[43]. The difference of their solution from the numerical value may be due to the use of only first two eigenvalues, as postulated by Vlachopoulos and Keung[47]. However, the truth may be that their analytical solution is very seriously wrong and thus not acceptable. We have made calculations of the heat flux at wall and the Nusselt number by using their solution. Both of them went from a negative value in the entry region to a positive value at $z \sim 0.05$. Since this is contrary to what is possible physically, their whole formulation should be viewed with doubt.

For the case with viscous dissipation, a solution using fifth-order polynomial has been obtained for $n=0.5$ and the modified Brinkman number $Br^*=1.0$. It is constructed from an asymptotic solution, as expressed by equation (2.3.14), and the solution to the case without viscous dissipation.

**SOLUTION WITHOUT VISCOUS DISSIPATION**

Thermal Entry Region ($z _f \geq z \geq 0$)

$$T(z,y) = 1.0 \text{ for } 1 \geq y \geq \delta_T$$
\[ T(\eta) = 2.5\eta - 5\eta^3 + 5\eta^4 - 1.5\eta^5 \text{ for } \delta_T \geq y \geq 0 \]

This temperature function is basically the same as the Newtonian case, but with a different thermal boundary thickness determined from:

\[ \frac{2}{21} \delta_T^3 - \frac{15}{448} \delta_T^4 + \frac{1}{210} \delta_T^5 = 2.5z \]

with \( \delta_T = 1 \) at \( z_f = 0.0266 \)

\[ T_{ave} = 1 - \frac{4}{21} \delta_T^2 + \frac{5}{84} \delta_T^3 - \frac{1}{126} \delta_T^4 \]

\[ Nu = \frac{5}{(\delta_T T_{ave})} \]

**Developing Region (\( z_f \leq z \))**

\[ T(z,y) = \sum_{i=1}^{2} \alpha_i \exp(-\beta_i z) \sum_{j=1}^{5} a_{ij} y^j \]

\( \alpha_1 = 1.1899 \quad \alpha_2 = -0.2247 \quad \beta_1 = 2.687 \quad \beta_2 = 27.622 \)

\( a_{11} = 1.492 \quad a_{13} = -0.297 \quad a_{14} = -0.375 \quad a_{15} = 0.179 \)

\( a_{21} = -7.858 \quad a_{23} = 43.339 \quad a_{24} = -50.244 \quad a_{25} = 15.764 \)

\[ T_{ave} = 0.881\exp(-2.687z) + 0.0852\exp(-27.622z) \]

\[ Nu = (3.551\exp(-2.687z) + 3.532\exp(-27.622z)) / T_{ave} \]

**Asymptotic Solution with \( Br^* = 1.0 \)**

\[ T_\infty(y) = \frac{1}{20} \{ 1 - (1-y)^5 \} \]

\[ T_{\inftyave} = \frac{5}{108} \]

The overall temperature will be the sum of above two solutions, the overall Nusselt number can be obtained as:
\[ \text{Nu}_{\text{overall}} = \left( \text{Nu} \times T_{\text{ave}} \right) + 0.5 \right) \left( T_{\text{ave}} + T_{\text{ave}} \right) \]

The result is shown in Fig. 28, and the excellence of this solution is again clearly indicated. To summarize this analytical approximation approach, it is necessary to mention a similar method developed by Yang[49]. Its existence was not realized until this work has been done, but the comparison is still quite interesting. Basically, Yang improved the third-order approximation by substituting it back into the original energy equation and then integrated it as an ordinary differential equation. This improvement is emphasized in generating a more accurate dependence in \( y \)-direction and will certainly give a better formulation for the asymptotic solution. For example, in the developing region, the third-order approximation will give us:

\[ T(z,y) = \exp(-\beta z) \left\{ 1.5y - 0.5y^3 \right\} \]

For the Newtonian case, by substituting the above temperature profile into:

\[ (2y - y^2) \frac{\partial T}{\partial y} = \frac{\partial^2 T}{\partial y^2} \]

The energy equation becomes:

\[ -\beta \exp(-\beta z) \left\{ 3y^2 - 1.5y^3 - y^4 + 0.5y^5 \right\} = \frac{\partial^2 T}{\partial y^2} \]

Integrating it twice with respect to \( y \) with the appropriate boundary conditions, a seventh-order form can be obtained:

\[ T(z,y) = \beta \exp(-\beta z) \left\{ \frac{61}{120} y - \frac{1}{4} y^4 + \frac{3}{40} y^5 + \frac{1}{30} y^6 - \frac{1}{81} y^7 \right\} \]
Figure 2.8: Comparison of Analytical and Numerical Solutions with $B = 1.0$, $n = 0.5$.
which will have an asymptotic Nusselt number 3.778, compared with \( \text{Nu} = 3.785 \) obtained before by the fifth-order polynomial and the theoretical value \( \text{Nu} = 3.767 \). However, there will still be only one Nusselt number for the whole developing region and this is not entirely adequate as discussed earlier. The effort here was to remove this inadequacy by introducing one more eigenvalue. In other words, the improvement in our method was made on the dependence in \( x \)-direction.

The main advantage of Yang's improved integral method is that it can be applied to the case with temperature-dependent viscosity if such dependence is of an inverse linear form. Nevertheless, considering the complexity involved (as shown in his results, there is a nonlinear equation for the determination of thermal boundary layer thickness and at least a tenth-order polynomial for the developing region.), it will be easier to use the Crank-Nicholson implicit method to serve the same purpose.
IV. CONCLUDING REMARKS

For the viscoelastic flow problems, the main motivation here was to demonstrate that meaningful solutions can be obtained for the cases involving high elasticity and abrupt changes in geometry. The numerical scheme described in this thesis can be extended to the case with fully-developed Poiseuille flow at both the entrance and exit, or to different contraction ratios so that the non-linear viscoelastic effects under these circumstances can be examined.

To have better accuracy, nine-point central formula of fourth-order accuracy can be used in the numerical iteration for the momentum equation. This may also help to obtain a converged solution for the viscoelastic flow problem at a higher Weissenberg number. For practical use, however, the improvement is not very significant if the added complexity and the longer computation time are considered. In particular, Cable and Boger have shown that the divergent flow regime was in fact metastable experimentally.

For the non-isothermal case of power-law fluids, the purpose was to solve the energy equation in the situation of two-dimensional flow with temperature-dependent viscosity. Unfortunately, it was found that the Graetz-Nusselt problem is not a good case to test its applicability due to the singularity involved. Nevertheless, there should be no problem if the two-dimensional flow is caused by a geometry change instead of being induced by a step-change boundary temperature.

The ultimate problem of non-isothermal extrusion of viscoelastic fluids is certainly one of vast mathematical difficulty. With the aid of
rapid modern computer development, it should constitute a future research ambition.
BIBLIOGRAPHY


13. Davies, A.R., Walters, K. and Webster, M.F., "Long Range Memory


41. Roache, P.J., Computational Fluids Dynamics, Hermosa Publishers, (1972)


