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<thead>
<tr>
<th>AUTHOR/FILING TITLE</th>
<th>KAKOULIS, A.P.</th>
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</thead>
<tbody>
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<td>28 JUN 1996</td>
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<td>6 UKC 1233</td>
<td></td>
</tr>
</tbody>
</table>

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DESIGN OF DIES WITH CONVERGENT AND NON-CIRCULAR SECTIONS

by

ANDREAS P KAKOURIS

A Doctoral Thesis submitted in partial fulfilment of the requirements for the award of the degree of Doctor of Philosophy of the Loughborough University of Technology

July 1986

Supervisor: P K Freakley
Institute of Polymer Technology

© by Andreas P Kakouris, 1986
Dedicated to my parents
Olga and Panos
DECLARATION

This thesis is a record of research work carried out by the author in the Institute of Polymer Technology of Loughborough University of Technology and represents the independent work of the author; the work of others has been referenced where appropriate.

The author also certifies that neither this thesis nor the original work contained herein has been submitted to any other institution for a degree.

........................................
A KAKOURIS
ACKNOWLEDGEMENTS

I would like to express my sincere thanks to Mr P K Freakley, my supervisor, for his help and encouragement given to me throughout this project. I am particularly grateful to Dr J Batchelor, Director of Research, for the fruitful discussions I had with him and his useful suggestions. My appreciation for assistance in his specialised subject goes to Dr M C Harrison of the Department of Engineering Mathematics.

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- Mr P Ramsey and Mr A J Davis for the IPT facilities made available whenever necessary
- Professor D J Evans for the beneficial discussions
- Mrs Janet Smith for offering her secretarial skills in preparing the thesis.
ABSTRACT

Quantitative design of extruder dies for rubber compounds and thermoplastics requires a knowledge of the pumping performance of the extruder; for an appropriate extruder-die interaction. The dies are generally formed from a succession of convergent, circular or non-circular ducts with axial varying geometrical dimensions. The design and operation of dies of these types is then a matter of sufficient importance to justify a detailed analysis of the factors involved.

In the light of the foregoing an investigation was set up with the following objectives:

a) provide a general theoretical treatment for conical and non-circular ducts of rectangular, square and triangular cross-sections, based on physical equations that link the velocity field with the pressure gradient and the rheological data of the medium; and for the solution of which the boundary conditions must, in each case, be fixed in accordance with the geometric data

b) simulate the flow in computer routines for each part of the die

c) provide experimental procedures to be used for the construction of accurate extrusion performance curves based on statistical experimental design methods.

The experimental work involved:

a) Extrusion trials in order to determine extrusion curves by selecting the main process variables i.e. set temperatures of the barrel and head, screw speed and back pressure, and examining their influence upon volumetric output and extrudate temperature. A special die fitted with an adjustable flow restrictor and a pressure transducer was designed and constructed, which incorporates a needle pyrometer for direct measurement of the melt at the end of the screw

b) Rheological trials to obtain the flow behaviour and viscosity-temperature dependence of the polymer used in this investigation, as well as some trials to evaluate the thermophysical properties of the medium
c) Extrusion-die trials based on pre-selected industrial channel cross-sections in order to obtain and consequently compare the experimental findings with the theoretically evaluated ones.
## NOMENCLATURE

Symbols appearing infrequently are generally not included.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Area</td>
</tr>
<tr>
<td>B</td>
<td>Extrudate swell</td>
</tr>
<tr>
<td>B_1</td>
<td>Biot number</td>
</tr>
<tr>
<td>b</td>
<td>Temperature coefficient of viscosity at constant shear rate</td>
</tr>
<tr>
<td>b*</td>
<td>Pressure coefficient of viscosity at constant shear rate</td>
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<tr>
<td>C, C_v</td>
<td>Specific heat at constant pressure and volume respectively</td>
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<tr>
<td>C_P, C_V</td>
<td>Specific heat</td>
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<tr>
<td>D</td>
<td>Circumference</td>
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<tr>
<td>D_h</td>
<td>Diameter</td>
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<tr>
<td>E</td>
<td>Activation energy</td>
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<tr>
<td>E'</td>
<td>Bagley correction</td>
</tr>
<tr>
<td>E_{A}</td>
<td>Integral defined by eqn. (6.83)</td>
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<tr>
<td>f</td>
<td>Friction factor</td>
</tr>
<tr>
<td>f(θ)</td>
<td>Quantity defined in eqn. (6.3a)</td>
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<tr>
<td>g</td>
<td>Gravitational acceleration constant</td>
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<tr>
<td>h</td>
<td>Height</td>
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<tr>
<td>K</td>
<td>Thermal conductivity</td>
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<tr>
<td>L, L'</td>
<td>Decay rate constant</td>
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<tr>
<td>M</td>
<td>Length</td>
</tr>
<tr>
<td>M_w</td>
<td>Coefficient of power-law equation for wall-slip</td>
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<tr>
<td>m</td>
<td>Weight-average molecular weight</td>
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<tr>
<td>m_w</td>
<td>Consistency index</td>
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<tr>
<td>N_1, N_2</td>
<td>Primary and secondary normal stress coefficients</td>
</tr>
<tr>
<td>n</td>
<td>Power-law index</td>
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<td>n*</td>
<td>Flow behaviour index</td>
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<tr>
<td>p</td>
<td>Pressure</td>
</tr>
<tr>
<td>Q</td>
<td>Volumetric flowrate</td>
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<tr>
<td>q</td>
<td>Heat flux vector</td>
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</tbody>
</table>
Greek symbols

\( \alpha \) - Thermal diffusivity
\( \gamma \) - Half angle of the cone
\( \dot{\gamma} \) - Shear rate
\( \dot{\gamma}_w \) - Shear rate at the wall
\( \Delta \) - Rate of strain tensor
\( \Delta P \) - Pressure drop
\( \eta \) - Viscosity
\( \eta_0 \) - Zero shear rate viscosity
\( I_1, I_2, I_3 \) - Scalar invariants of \( \dot{\gamma} \)
\( \kappa \) - Dilatational viscosity
\( \lambda \) - Time constant in Carreau model
\( \lambda(n) \) - Dimensionless flowrate or shape factor
\( \mu \) - Viscosity of Newtonian fluid
\( \rho \) - Density
\( \tau \) - Shear stress tensor
\( \tau \) - Shear stress
\( \tau_w \) - Shear stress at the wall
\( \tau_{11} - \tau_{22} \) - Primary normal stress difference
\( \tau_{22} - \tau_{33} \) - Secondary normal stress difference
\( \omega \) - Vorticity tensor
\( \omega \) - Relaxation factor
\( \omega_{opt} \) - Optimum relaxation factor
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page No</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acknowledgements</td>
<td>i</td>
</tr>
<tr>
<td>Abstract</td>
<td>ii</td>
</tr>
<tr>
<td>List of Symbols</td>
<td>iv</td>
</tr>
<tr>
<td>Table of Contents</td>
<td>vi</td>
</tr>
<tr>
<td><strong>CHAPTER 1:</strong> INTRODUCTION AND OBJECTIVES</td>
<td>1</td>
</tr>
<tr>
<td><strong>CHAPTER 2:</strong> RUBBER EXTRUSION AND DIE DESIGN: AN OVERVIEW</td>
<td>3</td>
</tr>
<tr>
<td>2.1 The Extrusion Process</td>
<td>3</td>
</tr>
<tr>
<td>2.2 Extrusion Developments</td>
<td>4</td>
</tr>
<tr>
<td>2.3 Die-Extruder Interactions</td>
<td>7</td>
</tr>
<tr>
<td>2.4 Theoretical Die Analysis in Relation to Practice</td>
<td>9</td>
</tr>
<tr>
<td>2.5 Elements of Die Design</td>
<td>12</td>
</tr>
<tr>
<td>2.6 Problems in Designing a Die</td>
<td>15</td>
</tr>
<tr>
<td>2.7 Comments on Available Literature</td>
<td>15</td>
</tr>
<tr>
<td>References</td>
<td>21</td>
</tr>
<tr>
<td><strong>CHAPTER 3:</strong> RHEOLOGICAL BEHAVIOUR OF MELTS</td>
<td>25</td>
</tr>
<tr>
<td>3.1 Flow Curve</td>
<td>25</td>
</tr>
<tr>
<td>3.1.1 The Stress Tensor</td>
<td>26</td>
</tr>
<tr>
<td>3.2 Rheological Measurements on Rubber</td>
<td>30</td>
</tr>
<tr>
<td>3.2.1 Rotational Rheometers and Viscometers</td>
<td>30</td>
</tr>
<tr>
<td>3.2.2 Capillary Rheometers</td>
<td>32</td>
</tr>
<tr>
<td>3.3 Hydrodynamic Entrance - Region Flow</td>
<td>35</td>
</tr>
<tr>
<td>3.4 Flow Phenomena</td>
<td>36</td>
</tr>
<tr>
<td>3.4.1 Extrudate Swell</td>
<td>36</td>
</tr>
<tr>
<td>3.4.2 Melt Fracture</td>
<td>40</td>
</tr>
<tr>
<td>3.4.3 Secondary Flows</td>
<td>41</td>
</tr>
<tr>
<td>References</td>
<td>43</td>
</tr>
</tbody>
</table>
### CHAPTER 4: NON-NEWTONIAN FLUID MECHANICS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page No</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1 General Considerations</td>
<td>47</td>
</tr>
<tr>
<td>4.2 Basic Equations of Non-Newtonian Fluids</td>
<td>47</td>
</tr>
<tr>
<td>4.3 Constitutive Equations</td>
<td>51</td>
</tr>
<tr>
<td>4.4 Equations of Energy</td>
<td>56</td>
</tr>
<tr>
<td>4.5 Boundary Conditions</td>
<td>57</td>
</tr>
<tr>
<td>4.5.1 Boundary Conditions in Heat Transfer</td>
<td>58</td>
</tr>
<tr>
<td>4.6 Effect of Temperature on Viscosity</td>
<td>60</td>
</tr>
<tr>
<td>4.7 Effect of Pressure on Viscosity</td>
<td>62</td>
</tr>
<tr>
<td>4.8 Selection and Discussion of Assumptions</td>
<td>63</td>
</tr>
<tr>
<td>References</td>
<td>68</td>
</tr>
</tbody>
</table>

### CHAPTER 5: AN OVERVIEW OF APPROXIMATE AND NUMERICAL SIMULATION AND OF EXPERIMENTAL DESIGN

<table>
<thead>
<tr>
<th>Section</th>
<th>Page No</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1 General Considerations</td>
<td>71</td>
</tr>
<tr>
<td>5.2 Finite Difference Method</td>
<td>72</td>
</tr>
<tr>
<td>5.3 Finite Element Method</td>
<td>74</td>
</tr>
<tr>
<td>5.4 Variational Principles</td>
<td>76</td>
</tr>
<tr>
<td>5.5 Experimental Design</td>
<td>76</td>
</tr>
<tr>
<td>References</td>
<td>80</td>
</tr>
</tbody>
</table>

### CHAPTER 6: MODELLING OF THE PROCESS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page No</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1 Converging Section</td>
<td>84</td>
</tr>
<tr>
<td>6.1.1 Transport Equations</td>
<td>84</td>
</tr>
<tr>
<td>6.1.2 Rheological Equation of State</td>
<td>85</td>
</tr>
<tr>
<td>6.1.3 Volumetric Flow Rate</td>
<td>86</td>
</tr>
<tr>
<td>6.1.4 Distribution of Pressure</td>
<td>86</td>
</tr>
<tr>
<td>6.1.5 Newtonian Fluids</td>
<td>89</td>
</tr>
<tr>
<td>6.1.6 Energy Equation</td>
<td>90</td>
</tr>
<tr>
<td>6.1.7 Comments</td>
<td>96</td>
</tr>
<tr>
<td>6.2 Estimation of Minimum Die Length in Non-Circular Ducts from Memory Effects</td>
<td>100</td>
</tr>
<tr>
<td>6.3 Rectangular and Square Ducts</td>
<td>105</td>
</tr>
<tr>
<td>6.3.1 Predicting Non-Newtonian Flow</td>
<td>105</td>
</tr>
<tr>
<td>Section</td>
<td>Page No</td>
</tr>
<tr>
<td>------------------------------------------------------------------------</td>
<td>---------</td>
</tr>
<tr>
<td>6.3.2 Prediction of Melt Elasticity from Viscosity Data</td>
<td>111</td>
</tr>
<tr>
<td>6.3.3 Correlation of Shear Stress with Pressure</td>
<td>116</td>
</tr>
<tr>
<td>6.4 Triangular Ducts</td>
<td>121</td>
</tr>
<tr>
<td>6.4.1 Variational Principle Method</td>
<td>121</td>
</tr>
<tr>
<td>6.4.2 Finite Difference Method</td>
<td>125</td>
</tr>
<tr>
<td>6.5 Comments</td>
<td>131</td>
</tr>
<tr>
<td>References</td>
<td>135</td>
</tr>
<tr>
<td>CHAPTER 7: EXPERIMENTAL</td>
<td>139</td>
</tr>
<tr>
<td>7.1 Material</td>
<td>139</td>
</tr>
<tr>
<td>7.2 Equipment</td>
<td>139</td>
</tr>
<tr>
<td>7.2.1 Mixing</td>
<td>139</td>
</tr>
<tr>
<td>7.2.2 Extrusion</td>
<td>139</td>
</tr>
<tr>
<td>7.2.3 Dies</td>
<td>139</td>
</tr>
<tr>
<td>7.2.4 Flow Properties</td>
<td>140</td>
</tr>
<tr>
<td>7.2.5 Thermophysical Properties</td>
<td>141</td>
</tr>
<tr>
<td>7.2.6 Miscellaneous</td>
<td>141</td>
</tr>
<tr>
<td>7.3 Procedure</td>
<td>141</td>
</tr>
<tr>
<td>7.3.1 Extrusion</td>
<td>141</td>
</tr>
<tr>
<td>7.3.2 Rheological Tests</td>
<td>143</td>
</tr>
<tr>
<td>CHAPTER 8: DISCUSSION</td>
<td>145</td>
</tr>
<tr>
<td>8.0 Analysis and Discussion of Results</td>
<td>145</td>
</tr>
<tr>
<td>8.0.1 Thermal Diffusivity</td>
<td>145</td>
</tr>
<tr>
<td>8.0.2 Specific Heat</td>
<td>146</td>
</tr>
<tr>
<td>8.0.3 Rheological Properties</td>
<td>146</td>
</tr>
<tr>
<td>8.1 Converging Section</td>
<td>148</td>
</tr>
<tr>
<td>8.1.1 Motion Equations</td>
<td>148</td>
</tr>
<tr>
<td>8.1.2 Energy Equations</td>
<td>151</td>
</tr>
<tr>
<td>8.2 Estimation of the Preform Section Based on Memory Effects</td>
<td>155</td>
</tr>
<tr>
<td>8.2.0 Extrusion</td>
<td>158</td>
</tr>
</tbody>
</table>
8.3 Square and Rectangular Sections .... 168
8.4 Triangular Section .... 173
8.5 Comments .... 178
  8.5.1 Feeding .... 178
  8.5.2 Limitations .... 179
  8.5.3 Summary of Equations for Each Section 181
8.5.4 Example .... 183
  References .... 186

CHAPTER 9: CONCLUSIONS AND RECOMMENDATIONS .... 188
  9.1 Conclusions .... 188
  9.2 Recommendations .... 190
  References .... 192

APPENDICES:

A: The Equation of Continuity in Two Coordinate Systems: Components of the Equation of Motion, the Function (|v|), the Rate-of-Strain Tensor in Two Co-ordinate Systems; Summary of Differential Operations Involving the \( \gamma \)-Operator. 193

B: Pressure Drop in Non-Newtonian Fluids due to an Entrance Region of Arbitrary Cross-Section 196

C1: Subroutine Used in Conjunction with NAG Library D02RAF to Evaluate the Volumetric Flow Rate in Converging Sections .... 208

C2: Logic Flowchart for Energy Calculations in Converging Sections .... 209

C3: Fletcher and Reeves Logic Diagram ... 210

C4: Logic Flowchart for the Correction of Capillary Data Using Bagley and Rabinowitsch Corrections .... 211

C5: Logic Flowchart for Non-Newtonian Flow in Non-Circular Ducts .... 212

D1: Evaluation of Thermal Diffusivity .... 213

D2: Treatment of Capillary Data Using:
   A. Bagley and Rabinowitsch Corrections (Figures D1 and D2)
   B. Two-point Method (Figures D3-D6)

D3: GLIM Output for the Extrusion Volumetric Flowrate Response .... 218
CHAPTER 1
INTRODUCTION AND OBJECTIVES

Die design in the polymer processing industry is a difficult and complicated area, even in designs for simple profiles such as tubes or slits. The situation becomes more complicated when non-circular ducts are involved; because apart from the strong non-Newtonian flow properties that characterise the materials, two- or three-dimensional analysis has to be included as well. This immediately leads to non-linear parallel differential equations where there is a tremendous degree of complexity when solving them, even (and sometimes especially) when one relies on numerical methods.

This is the reason why in the past, the industry has relied upon empirical approaches. Unfortunately, although such approaches are often satisfactory for known materials and applications, when one faces the vast range of compounds that exist in the rubber industry and the frequent introduction of new products, empirical trial and error methods of designing appear to be extremely time consuming and costly.

In order then to respond to the highly competitive demands of today's industry a quicker and more accurate approach is needed, which will involve rheological data easily obtainable in the laboratory and, on the other hand, mathematical principles to formulate such data into parameters necessary for the die-maker.

The aim of this investigation, which is solely based in conical and non-circular ducts of rectangular, square and triangular cross-sections, is to provide some design aids on the basis of approximate methods as well as some simple criteria which, in conjunction with the die-maker's experience, will lead to more efficient die design.

In view of the foregoing it is possible to frame a set of objectives for this work:

a) to provide a general theoretical treatment for evaluation of laminar flow and heat transfer to incompressible, non-Newtonian, viscous isothermal and non-isothermal fluids flowing in such ducts.
b) to obtain experimental results in preselected laboratory and industrial die cross-sections
c) to compare the obtained experimental results with the computed ones
d) to simulate the flow in computer routines for every part of the die.
The work reported in this thesis has been carried out wholly on rubber extrusion but the techniques developed also have some application in thermoplastics extrusion.
CHAPTER 2

RUBBER EXTRUSION AND DIE DESIGN: AN OVERVIEW

2.1 THE EXTRUSION PROCESS

Extruders are one of the most important items of processing equipment used in the rubber industry. They may be used in conjunction with mixing systems where, after accepting a batch from the mixing system, they either transform it to a suitable shape for further processing or a finished product. They can also act as mixing extruders converting particulate feedstock into homogeneous whole.

Depending on the temperature of the feedstock, extruders may be divided into hot- and cold-feed types. The former consists of taking slab rubber compound, passing it through a two-roll mill for prewarming, then feeding it to the extruder by rolling 'dollies' from the mill or in cut strips or by other automatic means. Cold feeding consists, as the name implies, of feeding the extruder with cold stock, which may be either in pellet, chunk or strip form. Hence, a hot feed extruder, generally speaking, is a simple transporting, compaction and pressurising device; while the cold feed extruder accomplishes these functions as well as warming up and mixing the stock as it moves along the barrel to the die. The merits of hot feeding versus the cold feeding of rubber have long been debated and indeed have not really been resolved.

Freakley et al [1a,2,3] discussed the merits of the various types of extruders and when discussing cold-feed machines summarised the factors governing their advantages over hot feed machines as follows:

a) Less capital cost - no mills etc.

b) Less labour involvement

c) Better temperature control of the compound

d) Better dimensional control of the extrudate

e) Capable of handling both low and high Mooney compounds.

However, when one examines closely each of the above claims several facts are revealed. When considering items (a) and (b), the capital cost of all the extra equipment and the labour involved in the preparation areas necessary to support a cold-feed extruder, introduces strong possibilities that the total set-up cost will be higher than that for hot feed.

Due to the long residence times associated with cold-feed extruder, the machines have been designed to offer better temperature control. This
in turn, does result in better dimensional control of the extrudate, since both extrudate swell and throughput are primarily affected by the material temperature and head pressure. Hot-feed extruders, on the other hand, have short residence time, thus relying largely on the two-roll mill for temperature control, but the chances for precise temperature control are limited because of the non-steady state conditions of the extruder feeding. The better dimensional control of the extrudate offered by cold-feed extruder arises from the elimination of the two-roll mills and the greater screw length in which the rubber compound can be conditioned. Although cold feed extruders are capable of handling both low and high Mooney compounds provided that special screw design is used, the range of materials which may be successfully extruded by a general purpose machine is narrower than for the equivalent hot-feed extruder.

The aspects addressed indicate that cold-feed extruders are preferable over hot-feed types when:

a) high precision extrusion is required
b) long runs are planned
c) limited range of mixes are to be extrudated.

2.2 EXTRUSION DEVELOPMENTS

The advances which have been made during recent years in the development of extruders and especially the advent of cold-feed extruders, put into perspective the general feeling of the industry at present. Independent work carried out in various companies has borne fruit in the form of new screw designs and marketable machines.

As it is obviously impossible to include all the marketable extruders, only some will be covered which appear to be making a significant contribution to advancement of cold-feed extrusion.

The more notable screw designs are those of 'Maillefer' [4] and 'Barr' [5] type. The former consists of two separate channels cut in the same shaft one of which connects with the feed point whilst the other channel supplies the melt to the die. This 'unorthodox' design increases the heat transfer from the screw and barrel wall, when compared to 'normal' designs; so that all elements of material reaching the output channel have been subjected to similar heating and shear effects. The makers also claim that better quality products at higher outputs per unit of energy are obtained in comparison with conventional screws.
A diagrammatic arrangement of the Maillefer screw is shown in Fig. 2.1a. Case (b) in Fig. 2.1 represents a closer view in the cross-section of channels showing the arrangement for the flights F and R.

The idea of using two channels has also been used in the 'Barr' screw, illustrated in Fig. 2.2, but instead of progressively varying the width of the channels to compress the material, as adopted by Maillefer, only the channel depths are changed. The design is said to give lower melt temperature compared with screws of 'orthodox' design.
The manufacture of the QSM pin extruder [6] by Troester, with its modified barrel/screw combination has attracted great interest, and a number of articles have been written on the advantages of the development. With this design, the homogenisation of the mix is carried out by pins, projecting through the barrel wall down to the root diameter of the screw. Up to ten rows of the radial pins, with eight pins in each row can be used. This arrangement of pins in the QSM barrel, Fig. 2.3, divides the material being transported in the rotary laminar flow along the screw flights, and it undergoes flow division and shifting with only a low shear rate, providing mixing and homogenisation without recourse to specialist screw design or thermal overstressing.

The development of vented extruders is synonymous with the development of the low-pressure continuous vulcanisation and fluid bed techniques for continuous vulcanisation of extrudates. It is designed to eliminate unwanted gases from compounds, so that the profiles produced from stocks could be vulcanised at, or near, atmospheric pressure, without problems of porosity occurring. The machine can be single-vented or multi-vented. The first stage of the screw is a cold feed section and the portion after the vent is a warm-feed screw matched to the throughput of the cold-feed section, to ensure maximum head pressure. It is usually necessary to have different screws for different types of application in order to ensure maximum efficiency and avoid extrusion from the vent.

The advent of powdered rubber [7] brought the problem of requiring the extruder to act as a mixer, converting a particulate feedstock into a homogeneous whole. Nevertheless, work in this area has resulted in a number of new machines. The EVK mixing extruder [8], designed by Werner and Pfleiderer, is a single screw continuous mixer/extruder, which differs from conventional extruders because of the barrier screw design, shown in Fig. 2.4.

![Fig. 2.4: Barrier screw design for the Werner and Pfleiderer EVK (Contimix) continuous mixer](image-url)
The machine offers the same maximum shear stress for each volume particle, despite the difference in distance travelled by each particle; and can operate when only partly filled because of the shearing barriers distributed along the whole of the length of the screw. The distributive mixing is influenced strongly by the length-to-diameter ratio of the screw and the dispersive mixing by the size of the narrow gap between barrier and barrel.

Single screw continuous mixers generally have a common disadvantage – they only operate efficiently with a limited range of compounds and extrudate cross-sections. However, the recent development of integrated mixing systems has overcome this drawback and a number of machines are now available capable of mixing and extruding in two separate functions. The Farrel-Bridge mix (mix-vent-extrude) [2] is the most highly developed of these machines. It has two separate variable-speed drive motors in order to achieve optimum conditions for both mixing extrusion. Independent adjustment of the motor speeds enables a wide range of compounds to be processed on the same machine, without needing to change the screw of mixing rotors. A vacuum unit removes air to ensure a porosity-free extrudate. Ellwood [9] claims a number of advantages offered by the MVX machine, which include:

a) energy savings
b) precise temperature control
c) better product uniformity
d) flexibility
e) reduction in capital cost and floor space.

Other companies have also developed similar machines for mixing and extrusion of powdered rubbers and the reader can refer to Evans [2] for a complete and detailed discussion of the currently available designs.

2.3 DIE-EXTRUDER INTERACTIONS

The interaction between extruder and die is usually represented by showing the dependence of the output on the pressure between screw and die head. Such a performance diagram is shown in Fig. 2.5 where the operating points A, B, C and D are identified at the intersection of the extruder and die operating curves.
To construct accurate extrusion curves, based on theoretical considerations, is a very difficult task, due to the complex non-linear interrelationship between extruder geometry and process variables. Alternatively, one has to rely on experimental procedures, by selecting the main process variables and examining experimentally their influence upon volumetric output and pressure. The set temperature for the barrel zones, screw, head, and die also influence strongly the extruder operation curve. Haul-off rate is an additional parameter but experimentation has shown this to have an insignificant effect on volumetric output [10]. Experimental procedures and analysis methods which will enable us to explore the influence on these process variables on the operation curve are discussed in Sections 6 and 7.

Once the experimental extruder curve has been determined, the next step is to match it with the theoretically determined characteristics of the die, which have been calculated from rheological data for a number of temperatures within the region of interest for high extruder productivity. Fig. 2.6 shows how such a procedure can be translated into an operating diagram, where the operating or 'working' points F, G, H and I are now defined by the intersection of volumetric output, pressure and temperature.
This procedure gives the die designer greater flexibility in that:

a) the operating points and the associated output performance can be estimated in advance of the die manufacture, so that alternative die forms can be examined without the necessity of time consuming and costly practical trials

b) minimises the assumptions and specifications necessary, if in addition to die equations, theoretical procedures were adopted for predicting the extruder operating curve.

2.4 THEORETICAL DIE ANALYSIS IN RELATION TO PRACTICE

Although the practice of polymer extrusion is well established, little information about the design of extrusion dies is available. Designers in the past have relied upon an empirical trial and error approach, mainly due to the complicated physical and mathematical nature of the subject. This empirical approach is often satisfactory for known materials and applications. With the introduction of new polymers and processes, however, and the trend towards higher outputs and better quality extrudate, such an approach often proves to be extremely costly, time-consuming, responding very slowly to customer's demands.
On the other hand theoretical methods of designing dies lag far behind practical advances. The reasons for this are:

a) the great mathematical complexity associated with transport equations describing flow motion and heat transfer

b) the linear (and non-linear) viscoelastic nature of the polymer melts, which leads to rheological models unexplored, even theoretically

c) the computational memory and time needed to solve such problems, where the use of large digital computers is essential; something the industry lacks at the present

d) the uncertainty and divergence in opinions when explaining phenomena associated with polymers as for example extrudate swell and second normal stress difference.

An adequate theoretical die design analysis should have the aim of determining a die-channel geometry which will achieve pressure drops compatible with the extruder and at the same time will give the required extrudate shape, free (as possible) from flow defects. While such an aim appears to be the ideal case from an engineering viewpoint, less detailed information can often be useful, for answering specific questions such as:

a) Is the pressure drop inside the die within the operating range for a given flowrate? This aspect is of primary importance, not only in the mechanical design of the die body and the bolts which hold the die assembly with the extruder but for the output rate which can be achieved as well.

b) What will be the restrictions on the flow if heat-sensitive compounds are to be extruded? This is of special importance for rubber compounds due to their high sensitivity to heat history.

c) How pressure drop is related to the flowrate inside the die for a certain die geometry?

d) What is the deviation in the extrudate shape caused by a deviation in the die channel geometry? i.e. what will be the deviation in extrudate swell, if, for example, a rectangular die is used, the length of which has been increased by 5%?

To provide sensible answers to the questions addressed one has to concentrate attention on, apart from the extruder operating variables, a number of interrelated factors such as the complexity of the flow (i.e. one-, two- or three-dimensional), viscoelasticity and memory effects.
Die design problems may be divided into two broad classes:

a) One-dimensional (1-D) flow dies where the velocity is changing in only one direction. Examples of this class include the capillary rheometer type and dies having circular, annular and thin split cross-sections.

b) Two- or three-dimensional (2-D or 3-D) flow which accounts for dies with geometries other than the ones above, e.g. profile dies.

With 1-D flow, the swelling of an extrudate, which results from the viscoelastic nature of rubber, is manifested as an increase in cross-section area, without a change of cross-section shape. With 2-D or 3-D flow, however, the situation becomes more complicated, because the amount of swelling is not uniform across the sides of the extrudate, thus producing a shape which can be different to that of the die orifice, Fig. 2.7.

Fig. 2.7: A possible difference that can occur between a die shape and the final extrudate

In this case the problem is to design an internal die geometry to give uniform exit velocities and hence to provide compensation for the effect of swelling, while working at defined and reasonable pressure drops, temperatures and flow rates. Fig. 2.8 gives an indication of the shape of die needed to produce a square profile.

Fig. 2.8: Shape of the die needed (dotted) to produce a square profile
A possible alternative is to run the extruder slowly enough, in order to give sufficient time to the stresses causing the shape distortion to relax. However, such an operation may limit the extrusion process to small volumetric outputs, uneconomical for the rubber industry.

2.5 ELEMENTS OF DIE DESIGN [11-15]

Strictly speaking, the die is an assembly of parts through which when attached to an extruder, rubber is forced in order to produce extrudates of chosen shape. The various components of a die body are shown in Fig. 2.9.

Fig. 2.9: Elements of a profile die body

A. Breaker Plate

This is a thick metal disk located at the discharge end of the screw. It is perforated with holes and serves the following functions:

a) breaks up the spiral flow pattern resulting from the screw
b) evens out temperature variations
c) supports metal mesh filter screens which filter out foreign matter or undispersed filler aggregates.

Fine mesh screens result in clean and smooth extrudates (in conjunction with adequate die design) but, on the other hand, reduce the extrudate output and may block quickly, which, in turn, means more time for screen changes. This can be overcome by the use of continuous screens.

If it is intended that a breaker plate and filter screens should be used, the pressure drop and temperature rise caused by their presence
must be added to that due to the die land and adaptor, in order to
determine the 'operating point' of the extruder. Theoretical expres­
sions in that respect can be found in Carley and Smith [16].

B. Die Adapter or Lead In

The internal shape of the die adapter (the part of the die body
which precedes the land) is designed to provide streamlined, unidirec­tional flow of the material from the extruder screw to the land section.
The reduction in area restricts the flow, so it is also utilised to
build up pressure at the end of the screw and thus the die cross-sec­
tion must be smaller than the extruder bore. The relationship between
these two depends on the material properties.

Two types of transition may be utilised in profile extrusion: the
fully streamlined transition and the abrupt transition. The former is
most desirable when extruding heat sensitive melts as, for example,
rubber compounds because it eliminates recirculatory flow areas so that
the rubber will not be exposed to long residence times at high tempera­
tures, which will cause scorch or onset of cross-linking. Abrupt trans­
itions to the die land are often utilised for either trial or short
run work since they are inexpensive die adapter constructions.

For profile cross-sections which have a relatively small area com­
pared to the adapter, a compromise is possible between the above two
types of transitions.

Fig. 2.10: Diagrammatic illustration of various internal angles $\theta$ to
the land length

A schematic diagram, illustrated in Fig. 2.10, shows some examples of
internal entrance angles to the die land. The shape of type I seems
to be the best transition, because although it may increase pressure
drop it minimises recirculatory flow regions and the small angle at the start of the land section permits material exit at high speed without melt fracture. Type II is probably easier to make it but the steep entrance angle may cause stagnation of the material and/or melt fracture.

C. **Land Section**

This section, also known as die land or land length, is the main extrudate forming part of the die and has a constant cross-section. Its functions are to:

i) reduce (or eliminate) 'memory effects'

ii) equalise any final velocity variations across the profile

iii) prepare and, finally, shape the extrudate.

The land section is commonly expressed as a ratio of the land length to the die opening. For the plastics industry, this ratio may vary from about 10:1 to 20:1 [11,17,18,19] depending on such factors as raw material, final wall thickness of section and extrusion rate. In rubber industry, where viscosities are generally an order of magnitude higher than in the plastics industry, such long lengths may give excessive pressure drops and temperatures; if short land lengths are used, then the die has to be shaped in such a way that will compensate for the distortion caused by the forces generated in the material during convergent flow.

Sometimes an extra die section has to be added between the lead-in and land to preform the melt [20]. The function of this preforming section is to set up a stress system which, in conjunction with that produced by the land section, brings about elastic recovery which imparts the desired geometry to the strand leaving the die.

The surface finish of the whole die and in particular the land is very important, since it imparts all its characteristics to the surface of the extrudate and usually it is highly polished.
2.6 PROBLEMS IN DESIGNING A DIE

A. Mechanical, Thermal and Construction Problems

They include areas such as [21]:

a) Attaching or adapting the die to the extruder
b) Minimising deformations of various flow and shape influencing parts of the die under pressure
c) Assembling the various components without interference
d) Building the die to facilitate clean-up, change-overs, adjustment of flow opening
e) Keeping temperature equal throughout the die
f) Dealing with all the above questions at a reasonable cost
g) Making the die body robust enough so that the deformation produced by the internal pressures to cause insignificant changes in the flow channel dimensions
h) Dimensioning the die overall.

B. Flow Problems

a) Internal dimensions needed to give the desired production rate at reasonable head pressure
b) Die shape required to give good surface finish and good extrudate properties
c) Internal dimensions needed to give the desired extrudate shape and dimensions
d) Flow channel design requirements needed to eliminate or at least minimise 'dead spots' i.e. regions of circulatory flow.

The combined solution of all problems addressed cannot be realised simultaneously with the same success and usually some sort of compromise is involved.

2.7 COMMENTS ON AVAILABLE LITERATURE

In contrast to the design of dies of circular, slit and annular shape, where a wealth of literature exists, there is a lack of information on the design of non-circular dies and converging sections; and only a small percentage of the available literature is devoted to the subject.
Also, the literature is full of terms, e.g. non-Newtonian fluids, non-circular ducts, polymer melts, which may be used in overlapping or conflicting senses. It is advisable at this stage to define clearly these terms as they are used in the present work, in order to be able to comment on the available literature of parallel known studies.

Polymeric melts by their nature are non-Newtonian fluids. The use then of Navier-Stokes equations to describe such fluids - although it gives an indication of some quantitative aspects - in reality oversimplifies the problem, especially when one deals with rubber materials whose power-law index is generally in the range 0.15-0.4 [1b]. Here a non-Newtonian fluid is regarded as a fluid whose behaviour cannot be predicted by the Navier-Stokes equations.

Sometimes the term 'non-circular ducts' is encountered for flow analysis in one dimension. Here this term is only used in relation to two-dimensional analysis while the use of the term slit (or parallel plates) will be kept for one-dimensional flow.

Many times, experimentation associated with die analysis has been carried out on dilute polymer solutions, where the effect of viscoelasticity and viscous heat generation are greatly reduced. The correlation between these studies and those involving melts is very poor.

Table 2.1 below attempts to place the work reported in this thesis in perspective with similar studies in a comparative form. However, it appears that while there have been extensive investigations for molten plastics, the situation for rubber extrusion through dies is completely different and only very few studies exist. Indeed the author is only aware of the work of Pearson et al [22-24]. This lack of information was also stressed by White and his co-workers [24] in a recent paper. Pearson and De Vine investigated power-law fluids with dies of crosshead type designed according to lubrication approximation theory for narrow-channel flow. The work also includes rheological investigation of rubber compounds with respect to shear stress vs shear rate at various temperatures, together with scorch time and extrudate swell and goes on to use theoretical methods to predict the flow of a variety of plastics and rubbers through selected die geometries. Vinogradov et al [23] considered the flow of a narrow-MWD polybutadiene through flat slits by the method of visualisation, showing that the development of elastic turbulence is associated with the transition of polymer systems to high elastic state. They
also observed that the transition gives rise to the 'stick-slip' process or to continuous slippage along the duct walls, depending on the velocity of polymer movement. Ma et al [24] carried out experimental studies of flow patterns in elastomers and their carbon black compounds in various extrusion geometries, reaching the conclusion that there is no evidence of vortices in converging dies, thus supporting the view of streamline flow into the entrance. Exception to these observations was a cold mastication degraded natural rubber which gave evidence of vortices in corners as well as in sharply diverging dies. Evidence indicating slippage in some of the rubber-carbon black compounds in the entrance region were also presented.

Although nearly all the literature listed in Table 2.1 involves polymeric flow in circular and slit dies, it was felt that its inclusion was necessary as contributing quite significantly towards improved die design. The table is by no means exhaustive.

### TABLE 2.1: COMMENTS ON THE AVAILABLE LITERATURE

<table>
<thead>
<tr>
<th>Reference</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abfel-Khalik et al [25]</td>
<td>Prediction of melt elasticity from viscosity data, Carreau model, combination of their theory with Tanner's theory on extrudate swell, experimental verification with melts</td>
</tr>
<tr>
<td>Arai and Toyoda [26]</td>
<td>Isothermal steady pressure flow of a power law fluid in non-circular ducts, successive over-relaxation technique, experimentation with an extruder using low pressure polyethylene</td>
</tr>
<tr>
<td>Bird et al [27]</td>
<td>Rather general treatment as far as die design is concerned, but a very valuable book on polymers</td>
</tr>
<tr>
<td>Boles et al [28]</td>
<td>Pressure drop and flow patterns in tapered and sharp-edged entrances, Newtonian and power-law fluids empirical formulations, quantitative studies using polymer solutions; experimentation with modified capillaries and Weissenberg rheogoniometer</td>
</tr>
<tr>
<td>Bond [29]</td>
<td>Newtonian fluid in converging section, analytical solution, paper more of historical interest</td>
</tr>
<tr>
<td>Briley [30]</td>
<td>3-D flow, Navier-Stokes eqns. rectangular ducts; Alternating-Direction Implicit (ADI) scheme, experimentation for Re&gt;1000</td>
</tr>
</tbody>
</table>
Table 2.1 (continued)

<table>
<thead>
<tr>
<th>Reference</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>Carley [31]</td>
<td>The first, rather simplified but useful approach to die design. It includes nearly all types of dies and discusses some practical aspects of design</td>
</tr>
<tr>
<td>Cogswell [32]</td>
<td>Converging flow analysis involves both shear and extensional flow, apparent viscosity</td>
</tr>
<tr>
<td>Cogswell [33]</td>
<td>Discussion of the rheological aspects of polymeric melts from the theoretical and practical viewpoint, good and practical discussion about elongational viscosity</td>
</tr>
<tr>
<td>Cogswell [34]</td>
<td>Review of the approaches and comparison of theories with experience for tapered channels</td>
</tr>
<tr>
<td>Fenner [35]</td>
<td>Newtonian and power law fluids in rectangular and converging sections, finite-difference vs finite-element, lubrication approximation in narrow channel flows</td>
</tr>
<tr>
<td>Fisher [36]</td>
<td>Practical aspects involved with extrusion dies</td>
</tr>
<tr>
<td>Forsyth [37]</td>
<td>Survey of convergent polymer flow until 1974</td>
</tr>
<tr>
<td>Han [38]</td>
<td>Correlation of exit pressure with swell</td>
</tr>
<tr>
<td>Han [39]</td>
<td>Isothermal, viscoelastic [3-constant Oldroyd] fluid, rectangular ducts, correlation of rheological properties of material with shear-rate and wall normal stress, experimentation with HDPE, correlation of swell with exit pressure</td>
</tr>
<tr>
<td>Han [40]</td>
<td>Rectangular and converging channels, range of constitutive eqns; some practical aspects are discussed</td>
</tr>
<tr>
<td>Han and Charles [41]</td>
<td>Measurement of the axial pressure distribution of melts flowing in rectangular ducts; some experimental verification</td>
</tr>
<tr>
<td>Hanks [42]</td>
<td>Additional work, in the same direction to that proposed by Miller [53]</td>
</tr>
<tr>
<td>Holmes &amp; Vermeulen [43]</td>
<td>Velocity profiles in rectangular ducts, experiments with Newtonian and power-law solutions visualisation technique based on phosphorescent tracers</td>
</tr>
<tr>
<td>Huang &amp; Shroff [44]</td>
<td>Converging channels, explicit relation between normal stress at the die wall and the experimentally measured pressure drop at the die entry, use of Weissenberg number</td>
</tr>
<tr>
<td>Ito et al [45]</td>
<td>Broken section method for analysing molten flow in extrusion die of plastic melts fluid, isothermal 2-D flow</td>
</tr>
<tr>
<td>Kaloni [46]</td>
<td>Incompressible viscoelastic fluid, Oldroyd's constitutive eqn. 2-D flow, conical and wedge shaped channels</td>
</tr>
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<td>Reference</td>
<td>Description</td>
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<tr>
<td>Kozicki et al [47]</td>
<td>Prediction of the flow rate and maximum velocity as function of pressure drop, use of geometric parameters for nearly all common shapes, comparison of analytical results with available experimental ones for Newtonian, power law, Bingham and Rabinowitsch fluids, effect of slip velocity</td>
</tr>
<tr>
<td>Lenk [48,49]</td>
<td>Simple straightforward approach to calculate pressure drop for wide-slit dies with and without taper, elliptical and regular polygonal channels, power-law fluid</td>
</tr>
<tr>
<td>Masberg &amp; Kleiner [50]</td>
<td>Navier-Stokes eqns., 3-D flow coupled with energy equation, finite-element</td>
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<tr>
<td>Menges et al [51]</td>
<td>Incompressible, inertialess, Newtonian, 3-D flow, finite element method</td>
</tr>
<tr>
<td>Middleman [52]</td>
<td>Flow of power law fluid in rectangular ducts, primarily concerned with screw extruders but equally applicable to rectangular dies, finite-difference using successive over-relaxation technique</td>
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<tr>
<td>Miller [53]</td>
<td>Non-Newtonian flow in ducts of unusual cross-sections based on geometrical shape factors and shear-stress vs rate data from circular tubes</td>
</tr>
<tr>
<td>Mitsoulis et al [54]</td>
<td>Newtonian, power-law and viscoelastic (CEF-model) fluids, slit dies, 2-D incompressible flow, finite element method</td>
</tr>
<tr>
<td>Oka et al [55-57]</td>
<td>Tapered tube, distribution of stresses, velocities and pressures, apparent viscosity, solution for Newtonian and power-law fluids, no experimentation</td>
</tr>
<tr>
<td>Okubo and Hori [58]</td>
<td>Simple model applicable to the converging flow of HDPE melt. Theoretical determination of swell and normal stress difference and comparison with the experimental results</td>
</tr>
<tr>
<td>Parnaby et al [59]</td>
<td>Die design using the lumped parameter method, non-isothermal flow, slit and circular dies experimentation with melts</td>
</tr>
<tr>
<td>Parnaby and Worth [60]</td>
<td>Blow moulding, power law model, experimentation with melts</td>
</tr>
<tr>
<td>Pearson [61]</td>
<td>Non-Newtonian flow, lubrication theory, cross-head and flat film dies</td>
</tr>
<tr>
<td>Pearson [62]</td>
<td>Theoretical treatment of die-design for plate, slot, annular, wire-coating and co-extrusion dies, lubrication method, Newtonian, power-law and Oldroyd models, instabilities and thermal effects</td>
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<td>Author(s)</td>
<td>Description</td>
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<td>---------------------------------</td>
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<tr>
<td>Philippoff [63]</td>
<td>Navier-Stokes equations, 2-D inertialess flow in converging channels, influence of Re number</td>
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<tr>
<td>Schechter [64]</td>
<td>Power-law fluid in rectangular ducts, variational principle, discussion of both theoretical and practical aspects involved in the design of dies</td>
</tr>
<tr>
<td>Schenkel [65]</td>
<td>Extrusion of plastics in rectangular ducts, use of correction factors (criteria), numerical examples</td>
</tr>
<tr>
<td>Sparrow [66]</td>
<td>Newtonian fluid flowing in isosceles triangular duct</td>
</tr>
<tr>
<td>Sutterby [67]</td>
<td>Newtonian fluid, converging flow in conical tubes, 2-D flow, finite-difference method</td>
</tr>
<tr>
<td>Tadmor &amp; Gogos [68]</td>
<td>Theoretical and practical aspects of nearly all kinds of dies; only Newtonian and power law fluid treatment for profile and rod dies</td>
</tr>
<tr>
<td>Tanner [69]</td>
<td>Conical flow, mainly discussion about the effect of the third invariant of rate-of-strain tensor</td>
</tr>
<tr>
<td>Tiu [70]</td>
<td>Simple way of predicting the extrusion pressure losses of a power law fluid through rectangular and trapezoidal dies based on the geometric parameter method proposed by Kozicki et al [47]</td>
</tr>
<tr>
<td>Weeks [71]</td>
<td>Prediction of flow and pressure drop in sheet and film dies, Newtonian and power law model, worked examples</td>
</tr>
<tr>
<td>Wheeler and Wissler [72]</td>
<td>Friction factor vs Re for power law fluid in rectangular sections, experimental verification</td>
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<tr>
<td>Wheeler and Wissler [73]</td>
<td>Steady flow of non-Newtonian fluids in square ducts</td>
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<tr>
<td>White and Huang [74]</td>
<td>Pressure flow rate relationship for power law fluids through rectangular and trapezoidal dies based on 1-D shear flow</td>
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<tr>
<td>Worth and Parnaby [75]</td>
<td>Blow moulding, calculation of die pressure drop and mandrel forces, relaxation effects, non-linear shear modulus, post-extrusion swell based on theories of strengths of materials</td>
</tr>
<tr>
<td>Yang and Price [76]</td>
<td>Laminar flow development and heat transfer of a Newtonian fluid in converging plane-walled channels, use of average Nusslet number</td>
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<td>Yoo and Han [77]</td>
<td>Stress distribution of polymers in extrusion through a converging die, use of Coleman-Noll second-order fluid; experimentation to measure wall normal stresses and stress birefringence using melts</td>
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3.1 FLOW CURVE

The generalised shear stress/shear rate curve of a polymer melt, known as the flow curve, may be subdivided into four regions as shown in Fig. 3.1.

Fig. 3.1: Generalised flow curve (logarithmic coordinates)

The first linear region, OA, represents the behaviour of a melt which is subjected to a shear-rate between zero and some finite value, in which region Newton's law of viscosity holds. The slope of this linear portion of the curve is known as the 'limiting viscosity', the (first or initial) 'Newtonian viscosity' or the 'zero-shear-rate viscosity', \( \eta_0 \), [1a]. It is sensitively connected with the molecular weight average, \( \bar{M}_w \), such that for linear molecules and a sufficiently high \( \bar{M}_w \) the relation [2]:

\[
\eta_0 = \bar{M}_w^{3.4}
\]  

(3.1)
holds. The second region, called the pseudoplastic region shows a convex curvature with respect to the shear axis (i.e. decreasing slope), which is characterised by the apparent viscosity, \( \eta_a = \tau/\dot{\gamma} \). Here, the material is shear-softening, a phenomenon which has its precise counterpart in the solid state where it is known as strain softening. The curve then is the second Newtonian viscosity, followed by a so-called dilatant region from C to F, where the flow, hitherto laminar, becomes turbulent. This point corresponds with the fracture point of highly stressed solids, thus it is referred to as melt fracture (see Section 3.3.2).

Polymer melt behaviour can be rationalized in terms of molecular structure [3]. The orientation process needs both force and time to change the structural state of the melt. At low shear, the randomising effect of the thermal motion of the chain segments overcomes any tendency toward molecular alignment in the shear field. The molecules are thus in their most random and highly entangled state and have their greatest resistance to slippage (flow). As the shear is increased, the flow behaviour index diminishes gradually to less than unity because the frictional resistance between aligned macromolecular shear planes is steadily decreasing. When all the flow units are aligned in laminar fashion along the shear planes so that the molecules have reached a state of minimum resistance to flow, then any further increase in shear rate cannot cause any more orientation (see Fig. 3.1). This state of flow, accompanied by higher pressure, intensifies the internal friction and results in an increase of both viscosity and flow behaviour index and explains the gradual change from pseudoplasticity to dilatancy at very high shear rates.

The main region of interest is the pseudoplastic region, since it covers nearly all the polymer processing range and especially of extrusion, where the shear rate spectrum lies between 100 s\(^{-1}\) and 1000 s\(^{-1}\).

### 3.1.1 The Stress Tensor

Nine quantities are necessary for specifying the state of stress at a point completely, and these are the components of the stress tensor which in a matrix form are:

\[
\tau = \begin{bmatrix}
\tau_{11} & \tau_{12} & \tau_{13} \\
\tau_{21} & \tau_{22} & \tau_{23} \\
\tau_{31} & \tau_{32} & \tau_{33}
\end{bmatrix}
\]  \quad (3.2)
The stress tensor is usually broken into an isotropic or hydrostatic pressure and a deviatoric stress tensor.

\[
\tau = \begin{pmatrix}
P & 0 & 0 \\
0 & P & 0 \\
0 & 0 & P
\end{pmatrix} + \begin{pmatrix}
S_{11} & \tau_{12} & \tau_{13} \\
\tau_{21} & S_{22} & \tau_{23} \\
\tau_{31} & \tau_{32} & S_{33}
\end{pmatrix}
\] (3.3)

where \( P \) is the hydrostatic pressure, arbitrarily defined as \(-\frac{t_{11} + t_{22} + t_{33}}{3}\) and \( S_{ii} = t_{ii} + P \) are the deviatoric normal stresses.

The negative signs arise from the historical convention of treating both hydrostatic pressure (an inward force on the element) and tensile stress (an outward force on the element) as positive. Shear stresses act parallel to the surface, while the normal stresses act normal to the surface as in Fig. 3.2.

Fig. 3.2: The nine Cartesian components of the stress tensor

Only shear stresses and differences between normal stresses in different directions have rheological significance, though individual normal stresses can have a mathematical significance. The differences \( \tau_{11} - \tau_{22} \) and \( \tau_{22} - \tau_{33} \) are called first- or primary- and secondary-normal stresses difference respectively. They are related to the shear rate as:
\[ \tau_{11} - \tau_{22} = -N_1(\dot{\gamma}) \dot{\gamma}_{21}^2 \]
\[ \tau_{22} - \tau_{33} = -N_2(\dot{\gamma}) \dot{\gamma}_{21}^2 \]

where \( N_1 \) and \( N_2 \) are the primary and secondary normal stress coefficients respectively.

A very considerable amount of effort has been devoted to obtaining reliable values for the first normal stress function \( N_1 \). It is generally agreed that \( N_1 \) is positive and this corresponds to a tension along the flow streamlines. Some typical plots of \( N_1 \) are given in Figs. 3.3 and 3.4 for a polymer melt [4,5] and polymer solutions [6], respectively.

![Fig. 3.3: Dependence of non-Newtonian viscosity \( \eta \) on shear rate [4] and primary normal stress coefficient \( N_1 \) on shear rate for a low density polyethylene melt [5]](image)

![Fig. 3.4: Dependence of viscosity \( \eta \) and primary normal stress coefficient \( N_1 \) on shear rate for two polymer solutions (\( O, A \)) and an aluminium soap solution (\( O \)). (Reproduced from Huppler et al [6])](image)
It is seen that it has a large power law region in which it decreases by as much as a factor $10^6$. Most often, the rate of decline of $N_1$ with $\dot{\gamma}$ is greater than that of $\eta$ with $\dot{\gamma}$. Also at low shear rates a linear proportionality appears to exist between $N_1$ and $\dot{\gamma}$ so that $N_1 \rightarrow N_{1,0}$ as $\dot{\gamma} \rightarrow 0$. However for high shear rates values, a limiting $N_1$ value corresponding to $n_\infty$ does not seem to exist. A number of phenomena are attributed to the existence of the primary normal stress, some of which are:

a) The well-known Weissenber effect [7]

b) The torsional flow between a flat disk and cone (cone and plate viscometer)

c) The torsional flow between two parallel disks where a pressure is generated that increases with decreasing radius. Actually this geometrical arrangement has been utilised to develop the normal stress extruder [8a]

d) Extrudate swell (see Section 3.4.1).

The behaviour of the second normal stress difference is not nearly as well understood and characterised experimentally as $\eta$ and $N_1$. A large divergence in opinions [9] has arisen as to its existence and magnitude. Some investigators [7,10] regarding it as being zero, some [11,12] as being negative (this is the most widely accepted proposition) and some [13] suggest that its value may even change sign and become positive at large shear rates. However, our knowledge about $N_2$ is still incomplete and the available facts are based on data for moderately concentrated solutions of relatively few different kinds of polymers. The most important point to note that $N_2$ is that it is much smaller than $N_1$, probably an order of magnitude smaller [8b] and routine determination is still not practicable. The effect of $N_2$ in hydrodynamic calculations is considered as not very important. One possible exception is wire coating [14] where, if the wire is eccentric to the die, there exist forces (attributed to $N_2$) that tend to diminish this eccentricity. A final point concerning $N_1$ and $N_2$ is that both are zero for Newtonian fluids.
3.2 RHEOLOGICAL MEASUREMENTS ON RUBBER

While in the plastics industry, materials change little in properties from the raw material to the final product and often only one processing step is employed, in the rubber industry production materials are compounds, usually containing two or more different raw polymers and large quantities of other materials such as fillers and processing oils. As a result, the demands made on rubber rheologists are difficult. The fact that rubber compounds are highly trixotropic, non-Newtonian, elastic and undergo molecular changes during processing makes the situation more difficult. A large number of rheological tests have been developed for routine testing and process control purposes, but the majority only provide arbitrary variables for comparative measurements (e.g. plasticity); there are very few ways of characterising rheologically a rubber or rubber compound [15].

3.2.1 Rotational Rheometers and Viscometers

Rotational instruments are suitable for testing rubber mixes because of the control which can be exercised over the total shear strain input to the test sample. This is necessary to overcome the problems caused by the marked thixotropy of elastomers. More precisely, thixotropy which results from the breakdown of weak rubber-filler linkages, gives an initial viscosity when the deformation begins, which may be ten times greater than the later, steady-state viscosity [16]. Such thixotropic behaviour makes it impossible to interpret reliably any test in which the deformation is limited. The state of true thixotropic equilibrium causes problems in that, in addition to rapid breakdown of recoverable thixotropic structure, there is usually a slow, permanent softening of the elastomer. Consequently a strictly steady-state of viscosity may not be attainable; and if a single figure is to be reported as the 'viscosity' an arbitrary criterion must be adopted as to when the viscosity is changing slowly enough to be considered essentially steady.

The most widely used rotational instrument is the Mooney viscometer, where the delta-Mooney [17] measurement assesses the initial thixotropic contribution to torque, while the Mooney ML(1+4) test [17], involving 1 min preheat time and 4 min running time prior to a measurement being made, is designed to give the steady-state torque value. Both of these times are rather short due to the speed of test requirements for quality control.
Perhaps the major criticism of rotational rheometers is that the range of shear rates available to the instruments is considerably lower than that experienced in processing machinery (see Fig. 3.5). The reason for using low shear rates with rotational instruments is to avoid any significant temperature rise in the test sample caused by viscous dissipation during the deformation period.

![Graph showing viscosity vs shear rate for various processes and testing equipment](image)

**Fig. 3.5: Viscosity vs shear rate for various processes and testing equipment**

An interesting development in rotational rheometers during recent years is the prototype Sondes Place TMS rheometer [18,19], shown in Fig. 3.6. This is a variable speed rotary rheometer having a biconical rotor, which gives an approximately uniform shear rate through the test sample. Some more of its virtues are that:

a) it measures wall slip velocities and stress relaxation 
b) the influence of thixotropy or time-dependence on the flow properties of rubber mix can be overcome by taking measurements after an approximately constant torque level has been achieved (i.e. in the same way as with Mooney viscometer) 
c) the pressure in the cavity is controlled by the force applied to the injection ram 
d) the cavity is always closed during filling
e) due to (c) and (d) the clearances between cavity and rotor remain constant from test to test.

f) it gives a flow curve between 0.1 and 100 s\(^{-1}\).

Fig. 3.6: Schematic diagram of (a) TMS rheometer and (b) its biconical rotor.

3.2.2 Capillary Rheometers

These are popular devices due to their capability to operate over a wide shear-rate range, something that rotational-rheometers and viscometers cannot achieve, and the similarities between their flow and that of extrusion dies. The theoretical assumptions derived for capillaries include a number of assumptions [20a]; and although these expressions have mainly been developed for plastic melts, they are usually applicable to raw elastomers provided that the critical shear-stress for melt fracture is not exceeded. However, rubber mixes behave in a much more complicated manner and often the validity of these expressions is seriously questionable, especially when one faces the assumption of zero slippage, time-independence and isothermal conditions [21]. To isolate the relative
magnitude of the contributions from these effects is rather difficult, due to the lack of control of shear history or total shear; which is a function both of capillary length and radial position within the capillary.

In order to measure the viscosity function as well as its functional relationships, Newtonian flow behaviour is assumed initially, and the apparent quantities (apparent shear rate and apparent viscosity) are obtained for the pseudoplastic materials investigated by means of equations:

\[
\tau_w = \frac{\Delta P \cdot R}{2L} \tag{3.6}
\]

\[
u = \frac{R \cdot \Delta P}{2L} / \gamma_w \tag{3.7}
\]

\[
\gamma_w = \frac{4Q}{\pi R^3} \tag{3.8}
\]

where \( R \) = radius of the capillary
\( L \) = length of the capillary
\( \Delta P \) = pressure drop
\( Q \) = volumetric flow rate

These quantities are then translated to the true quantities using a technique ascribed to Rabinowitsch [22a] by means of equations:

\[
\dot{\gamma}_{\text{corr}} = \frac{\gamma_w}{4} \left[ 3 + \frac{1}{n^*} \right] \tag{3.9}
\]

\[
n^* = \frac{d(\log \tau_w)}{d(\log \dot{\gamma}_w)} \tag{3.10}
\]

where \( \dot{\gamma}_{\text{corr}} \) = wall shear rate corrected by the use of Rabinowitsch theory
\( n^* \) = fluid behaviour index

The transition of the polymer melt from a large reservoir into the capillary forms a region of convergent flow with a portion of applied pressure being lost. This loss arises from increase in kinetic energy of the melt, storage of elastic energy, structural alignment of macromolecules and viscous losses upstream of capillary. Two methods are available for making end corrections: the 'two-point Couette-Hagenbach method [20a] and the Bagley correction [23]. The former method, which is a special case of the Bagley method, and involves the use of two dies of similar radius but different length under similar conditions of flow-rate and temperature, enabling the shear stress at the wall to be determined from
The pressure \( P \) obtained with the die \( L/R = 0 \) is assumed to embrace both entrance and exit corrections and its value has been found to be slightly higher than that predicted by a conventional Bagley plot. This is due to the assumption that the flow is fully developed, thus ignoring entrance length errors. Therefore, the method, though simple, cannot be used for scale-up work. In addition, the method fails to give any indication of the compliance of the material to the general assumption for capillary flow.

The Bagley correction overcomes the shortcomings of the 'two point' method by using a number of dies of similar radius but different lengths. A plot of \( P \) vs \( L/R \) gives a straight line with a negative intercept \( E \) on the \( L/R \) axis provided that the general assumptions for capillary flow are satisfied. This negative intercept is referred to as Bagley or end correction and can be incorporated in the following equation to calculate the true wall shear stress:

\[
\tau_w = \frac{\Delta P}{2(L/R + E)}
\]  

(3.12)

For a long time now Bagley correction procedure has been the ground of interesting scientific arguments and developments: some investigators [24] argued, after experimentation, that the positive exit pressure, \( P_{\text{exit}} \), should be subtracted from the pressure term of eqn. (3.12), while others [25] considered such a case as unnecessary pointing out also that if such a case exists then an exit correction term \( X \) should be introduced into the denominator:

\[
\tau_w = \frac{P-P_{\text{exit}}}{2[L/R + E-X]}
\]  

(3.13)

Others [26] consider the end correction to be the sum of: (1) the viscous dissipation caused by the convergence of flow prior to entering the capillary entrance, and (2) the storage of elastic energy caused by the chain uncoiling.

The theory behind these corrections can be found in any standard textbook [1b,8c,20b,c,22a,b]. However, two important points for the evaluation of the capillary data used in this work will be outlined and reasoned below:
a) Often the Q vs ΔP data obtained from capillaries, when plotted on logarithmic scales, do not fall on a straight line as it is usually assumed [22c]. This indicates that the power-law model is not applicable i.e. \( ΔP \neq KQ^n \). As an alternative then, the dependence of pressure on flow rate is fitted through other expressions such as

\[ \log ΔP = a + b \log Q + c(\log Q)^2 \]  

(3.14)

b) Similarly to (a), where the normal power-law rheological model, expressed in terms of shear-stress and shear-rate, fails to express the situation adequately, a logarithmic parabola form of equation (3.15) is recommended:

\[ \log τ_w = A + B \log \dot{γ}_w + C(\log \dot{γ}_w)^2 \]  

(3.15)

The need for such expressions can be appreciated if one examines the shape of Fig. 3.1.

3.3 HYDRODYNAMIC ENTRANCE-REGION FLOW

When a viscous fluid enters a duct from a large upstream reservoir, the velocity profile of the flow changes continuously because of the retarding action of the wall. This is called 'developing flow'. After some distance downstream, however, the flow profile changes no more and the flow is said to be 'fully developed'. The flow in the intermediate region is the so called 'hydrodynamic entrance-region flow'.

The study of the entrance-region flow is of considerable interest and is of practical application in polymer processing industries. Knowledge of the pressure losses in the entrance region will help the engineer in specifying appropriate pumping requirements. It is, therefore, important to know the exact distance from the entrance after which the conditions of fully developed pressure distribution are established, so that meaningful measurements for the adequate length of a die (or a capillary) can be obtained. Knowledge of the velocity distribution in the entrance region is also important from the viewpoint of estimating heat and mass transfer rates especially when one deals with non-Newtonian fluids.

While the problem is of engineering significance and of academic interest, it is somewhat difficult and of a sensitive nature, due to the problem of solving exactly the equation of motion which represents the flow development in the duct and, more precisely, its non-linear inertia
terms. Different techniques have been used by different investigators; and a very brief account will be given here, categorising the surveys of all the investigations into the following six approaches:

a) involves the linearisation of momentum equations to obtain an approximate solution [27], which originates basically from the work of Langhaar [28]

b) treats the entrance-region flow as a boundary-layer flow problem by using perturbation techniques [29]

c) describes the entrance flow problem as a boundary-layer flow problem and the solution is obtained through the well known Von Karman-Pohlhausen momentum integral technique [30,31]

d) involves the use of the variational technique and relatively little computational effort is needed [32]

e) numerical solutions of the relevant equation of continuity and motion are obtained by using finite difference techniques [33,34]

f) the integral approach by Campbell and Stattery [35] is combined with the differential momentum equation in such a way that by eliminating the pressure gradient term, it will lead to a solution capable of closed-form expression [36].

Mention must be made at this point of the fact that most of the studies involve circular pipes, Newtonian fluids and high Reynolds numbers. A review of nearly all the methods adopted for solving the entrance flow of both Newtonian and non-Newtonian fluids, until 1978, is given by Shah and London [37] who evaluate critically the procedures used and also discuss the range of applicability of the results.

Although in this work fully developed flow was assumed throughout all regions thus neglecting entrance region-flow, for academic interest a theoretical analysis was carried out for non-Newtonian fluids through non-circular cross-sections, based on the work of Lundgren et al [27] for Newtonian fluids, a detailed procedure of which can be found in Appendix B.

3.4 FLOW PHENOMENA

3.4.1 Extrudate Swell [38]

One of the most important and elusive properties of polymers is extrudate swell [39,40]. For a circular cross-section area, extrudate swell \( B \) is defined as the ratio of the diameter of the extrudate \( D \) divided by that of the circular die (or capillary) \( D_0 \), i.e.
This dimensional change (swelling) of the melt which takes place at the exit of the die occurs even in Newtonian fluids at low Reynolds number [41,42], while it is more pronounced in viscoelastic materials (e.g. 100-200% increase is possible [43a]).

In the rubber industry, changes in the shape and size of the extrudate can be very troublesome to both processor and die manufacturer. This can be appreciated by considering the extrusion process of tyre tread compounds. Upon extrusion it is common for such materials to swell sometimes to twice the area of the die, depending of course on the extrusion temperature and volumetric flowrate. A major problem in controlling the process is that both the viscosity and the elastic memory of the compound will vary from batch to batch due to variations in the raw materials properties and the conditions under which the batches were mixed. Such variations cause changes in extrusion rate, extrudate shape and size. It is, then, obvious how detrimental these changes can be to the tyre process and to efforts to improve the uniformity of the final product.

A considerable number of studies have been devoted to swell from capillary dies; this can be attributed to:

a) relative simplicity of the experimental techniques
b) ease of carrying out quantitative analyses.

in contrast to swell in non-circular ducts, where the research is sparse.

With the ground work now available, one may review and discuss extrudate swell as follows:

**CORRELATION WITH INFLUENTIAL FACTORS** - There are a considerable number of factors [44] which have been proven to affect extrudate swell. They include viscosity, shear-rate, molecular weight distribution, geometric die parameters and extruder operating conditions. The first step then is to identify clearly all the factors and then to correlate them quantitatively with the extrudate swell. This can be done by means of, say, a factorial design (see Section 5.4). However, there are two main disadvantages with this way:

a) the possibility of not identifying all the influential factors
b) some difficulty in producing a quantitative relation including all these factors.
METHODS OF MEASURING EXTRUDATE SWELL - Several techniques have been proposed to measure swell, the most important of which are:

a) ASTM [D-2230, Method B] technique originated by Dannenberg and Stokes [45]

b) Monsato Automatic Die Swell Detector based on the use of a sweeping laser to measure the extrudate profile [46]

c) Die swell test introduced by Pliskin [47]

d) Volumetric methods

The disadvantage with these methods is that they follow rather than predict i.e. they estimate extrudate swell once the die has been made, instead of predicting it in advance.

ORIGINS OF EXTRUDATE SWELL - A number of qualitative explanations have been given of the source of extrudate swell which according to Bagley et al [48], may be summarised as follows:

First, swelling arises as the approximately parabolic velocity distribution in the die transforms to a constant velocity distribution subsequent to extrusion, as discussed by Middleman and Gavis [49].

Second, swelling may be due partly to randomization of polymer molecules oriented during transit into the die [50,51]. The simple analysis by Spencer and Dillon [52] seemed to lead to reasonable results but, as pointed out by Mooney [16], the type of shearing deformation assumed by Spencer and Dillon should 'lead to a telescopic elastic deformation not to a longitudinal contraction and diameter swell'. There are thus theoretical troubles here, but it is certainly conceivable that molecular randomisation may well contribute to the swelling of the extrudate, particularly in the higher shear rate region. Again, as in the first case, the swelling should vary with the capillary length-to-radius ratio if the molecular deformation and orientation are determined only by the shear stress and shear modulus, which appear to be independent of die length [53].

A third explanation of post-extrusion swelling, termed the 'memory effect' [50,51] is needed to account for the variation of swelling with capillary length. This decay of swelling with capillary length might be expected to be a typical relaxation process, showing an exponential dependence on the time of transit through the die, i.e. if B, is the swell ratio and t is an average time of transit through the die, then an equation of the following form might be expected to hold:
\[ (B - B_\infty) = (B_0 - B_\infty) \exp(-kt) \]  
(3.17)

where \( B_0 \) and \( B_\infty \) are values of \( B \) at zero and infinite transit times, respectively, and \( k \) is a decay rate constant.

On the basis of this third explanation, a procedure is proposed in Section 6.2, where the minimum land length or preform section of a non-circular die is estimated by using capillary data.

**QUANTITATIVE ANALYSIS BASED ON TRANSPORT AND BOUNDARY CONDITIONS EQUATIONS:** The first theoretical treatments of the phenomenon for circular capillaries were introduced by Nakajima and Shida [54], Bagley and Duffey [55], Graessley, Glascock and Crawley [56] and Tanner [57]. However, Tanner's analysis seems to be the most satisfactory formulation and is based on ideas set by Lodge [58] using the theory of Bernstein et al [59] in order to relate (balance) the elastic recovery with the shear-stresses developed in the die. He found that:

\[ B = \left[ 1 + \frac{1}{2} S_r^2 \right]^{1/6} \]  
(3.18)
\[ S_r = \frac{1}{2} \frac{N_1}{\eta} \frac{\gamma}{w} \]  
(3.18a)

where \( S_r \) = recoverable shear strain
\( N_1 \) = first normal stress difference coefficient.

The simplicity of eqn. (3.18) and its success in describing data on extrudate swell recommends its use for estimation purposes. The method does not include the rearrangement of the velocity and stress field at the die exit, thus the factor 0.1 had to be empirically added.

Metzner et al [60] succeeded in relating swell with the first normal stress difference, at the die wall in the region of fully developed flow of high Reynolds number, \( Re \), but failed on low \( Re \), underestimating the value of \( N_1 \) as was proven by Graessley et al [56].

McIntosh and MacKelvey[22d] considered that an average recoverable elastic shear strain is imparted to the fluid during its passage through the tube, which recovers in the exit region thus causing swell. Their concept was simplified by assuming that the behaviour of a viscoelastic fluid can be described by a single Voigt element.
Huseby et al [61] related swell to a recoverable shear strain, the strain was obtained by applying Pao's theory [62] for viscoelastic fluids.

Some attempts [63] have been made to obtain extrudate swell using the "thrust-jet" method, a technique for measuring axial normal stresses (by measuring the thrust of the emerging horizontal jet on the tube) and relating these stresses to swell. Pearson and Trottnow [43b] demonstrated the use of the "jet swell" method according to which the change in the diameter of the emerging jet from the die can be combined with the abrupt change in stress boundary conditions as the liquid moves from a confined flow pattern into a stress-free-boundary flow. However, all these analyses have assumed that there is a fully developed velocity profile up to the exit plane and there is no "exit region" in the last section of the tube. The failure of all these theories to predict the amount of swell for low Reynolds number flows (which are the flows encountered in industrial processing units and thus the ones of practical interest) gave rise to speculations regarding the validity of this assumption. Bird et al [64] showed that because of a possible velocity rearrangement in the exit region, any formula for jet swell derived from the macroscopic balances will depend strongly on the details of the flow field in the exit region.

Abdel-Khalik et al [65] presented a simple method for estimating the primary normal stress function $N_1$ from viscosity data and then related $N_1$ with extrudate swell, as has been formulated by Tanner [57]. The present author extended Abdel-Khalik et al theory to non-circular dies, a detailed account of which can be found in Section 6.3.

Tanner [44] gives a full account, including a number of interesting references, of the methods available to tackle extrudate swell. However, the main problem when one uses transport equations to predict swell is with boundary conditions. This is because the boundary conditions involved are mixed i.e. wall boundaries inside the duct (usually no-slip conditions) and free boundaries at the surface of the extrudate emerging from the die. The difficulty is, then, to locate the exact position of the free boundaries. Further, thermal boundary conditions may also be present.

3.4.2 Melt Fracture

During the extrusion of melts through dies a puzzling phenomenon takes place known as melt fracture [66] or elastic turbulence [67], which
manifests itself by a rough and periodically deformed surface. Theoretical explanations and experimental evidence have been rather contradictory [20d,68a], possible causes of melt fracture are considered to be: a critical value of shear stress [86], slippage at the die wall [69,70], a critical value of high elasticity modulus [71], a die entry-or die exit-effect [72], Reynolds turbulence [73]. Therefore, as Brydson [20d] states "like the phenomenon itself, the present state of theory is one of instability".

Pearson and Petrie [74] investigated, theoretically, melt fracture based on linearised stability theory for breakdown of flow within the channel, and regarded both entry and exit effects as playing a secondary role. Vlachopoulos and Chan [75] report that the melt fracture sets in at a constant wall shear stress value, which for polymer melts is of the 0.1 MPa order. The corresponding critical recoverable shear strain has been found to vary between about 1 and 60 units. Further, Petrie and Denn [76] discuss the whole subject of polymer instabilities, among which melt fracture is included.

With die design calculations, melt fracture is dealt with through the shear stresses and shear rates which must remain inside certain operating limits and never exceed the critical values beyond which the instability occurs.

3.4.3 Secondary Flows

In the entrance region of the die the flow may become unsteady, and disturbed due to the elastic stresses which develop and decay; and circulating flow patterns may occur. Schematic representation of such flows are shown in Fig. 3.7.

![Diagram of Secondary Flows](image)

Fig. 3.7: (a) Entry flow field for Newtonian and elastic fluids, (b) Schematic of secondary flow patterns of viscoelastic fluids in a conical die.
Ericksen [77] was the first to show that flow in capillaries and
dies cannot be rectilinear unless the duct is of circular cross-section
or the apparent viscosity is related to the normal stress coefficient in
a certain manner. He used the constitutive equations of a Reiner-Rivlin
fluid for his analysis.

Green and Rivlin [78] approximated the velocity field of the circu­
latory motion found to exit in elliptical cross-sections. Of particular
interest is the analysis of Laglois and Rivlin [79] who, using the general
constitutive equation advanced by Rivlin and Ericksen, found that it took
a fourth-order fluid to yield secondary flows, with the second-order fluid
only affecting the pressure field and the third-order fluid only distor­
ting the normal Newtonian velocity profile. Oldroyd [80] investigated
fluid flow in an annulus between two cones with common axis of rotation
and vertex but different generating angles while Gieseikus [81] obtained
analytical solutions for secondary flows as well as flow instabilities in
2-D flows of non-Newtonian fluids between plane walls including the effect
of inertia. In fact, he predicted two types of secondary flow depending
on the predominance of elastic or shear thinning fluid properties.

Han [68b] speculates that the effect is a weak one, at least for
polymer melts, and that it may be necessary to use high axial velocities
before the secondary flow becomes apparent. This view was also shared
by Mashelkar [82], that although secondary flows do exist for elastic
solutions, it is quite weak with a negligible influence on flow rate.
Recently Ma et al [83] investigated flow patterns in elastomerics during
extrusion through dies. The general observations showed no vortices in
converging dies, thus verifying earlier studies by Vinogradov et al [84].
However, sharply diverging dies produced large dead regions.

For flow through non-circular tubes, a necessary but not entirely
sufficient condition for secondary flow to exit, is that the secondary
normal stress coefficient has to be non-zero. When secondary flow is
included in a theoretical treatment, it comes into consideration through
the velocity field relationships and, consequently the transport equa­
tions. For example, when Cartesian and spherical coordinates are used
the velocity fields are given, respectively, by:

\[
\begin{align*}
    v_x &= v_x(x,y) \\
    v_y &= v_y(x,y) \\
    v_z &= v_z(x,y) \\
    v_r &= v_r(r,\theta) \\
    v_\theta &= v_\theta(r,\theta) \\
    v_\phi &= v_\phi(r,\theta)
\end{align*}
\]
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4.1 GENERAL CONSIDERATIONS

Polymer melts are non-Newtonian fluids possessing a memory of past deformation, due to which they are termed viscoelastic materials. Contrary to the behaviour of polymers, most of the analysis to date has been carried out for Newtonian fluids, presumably due to the ease of quantitative analysis. Although such simplified analysis may be useful as:

a) to gain an 'insight' of the process
b) to provide some quantitative aspects
c) an initial decision-design method

it must be used only as a first approximation method since the constant viscosity assumption may lead to enormous errors in many cases.

Space limitations will not allow an exhaustive treatment on the subject of non-newtonian fluid mechanics to be presented here. The reader is referred to a number of excellent textbooks [1-5]. However, an attempt will be made to 'shape' the basic equations of transport phenomena i.e. continuity, momentum and energy equations, and also the relevant rheological equations of state with respect to non-Newtonian fluids, so that they will be in a convenient form for immediate use when the case arises. Also some practical aspects of these equations will be discussed, to help justify their application later on.

4.2 BASIC EQUATIONS OF NON-NEWTONIAN FLUIDS

A: Flow Fields

There are two forms for representing flow fields in fluid mechanics: Euler's and Lagrange's form. The difference between them lies in the way that the position in the field is identified. More specific, in the Lagrangian approach, the coordinates \((x,y,z)\) are the coordinates of the element of fluid and represented as function of time. So if at some arbitrary time, usually \(t_0 = 0\), the coordinates of a particle \((x_0,y_0,z_0)\) are identified, then that particle can be followed through fluid flow; hence the position of the particle at any other instance is given by a set of equations of the form:
\[ u = f_1(x_o, y_o, z_o, t) \]
\[ v = f_2(x_o, y_o, z_o, t) \]
\[ w = f_3(x_o, y_o, z_o, t) \]

or in a functional form as:
\[ V = V(x_o, y_o, z_o, t) \]

where \( u, v, \) and \( w \) are the components of velocity in \( x, y \) and \( z \) directions respectively. The Lagrangian approach then gives information about a fluid variable experienced by an element of fluid along its trajectory, rather than giving the value of a particular fluid variable at a fixed point in the flow. This description may be seen to be a natural way to set up fluid dynamics problems, but, in practice, it is not very convenient. For instance, a steady flow receives no special treatment and shows no simplification whatsoever in this description. Also, the expression for mass conservation turns out to be rather unwieldy.

The Eulerian form approaches the problem differently by giving the value of a fluid variable in a given point at a given time i.e.
\[ u = f_1(x, y, z, t) \]
\[ v = f_2(x, y, z, t) \]
\[ w = f_3(x, y, z, t) \]
or
\[ V = V(x, y, z, t) \]

The Eulerian approach then provides information of the type, for example, where the deformation on a stationary body in a flow field is required, by giving information about the pressure and shear stress at every point in the body. This more powerful and convenient method that the Eulerian description adopts, makes it the main tool in fluid dynamics.

However many times when clarification of certain aspects of fluid flow or physical interpretations are required, the Lagrangian description appears to be the best of the two forms. As an example of its usefulness in polymer processing, one may refer to Pearson [6a], where comparison of extension and blow moulding have been treated by using a Lagrangian frame of reference rather than Eulerian one, thus relating the situation to material particles rather than to fixed points in space.
B: The Equation of Continuity

The continuity equation arises from the principle of conservation of mass and it is expressed in the following form [2a]:

\[
\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0
\]  \hspace{1cm} (4.1)

where \( \rho \) = density
\( \mathbf{u} \) = velocity
\( t \) = time

\( D/ Dt \) is the material time derivative or "substantial derivative" defined, in Eulerian coordinates by:

\[
\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla
\]  \hspace{1cm} (4.2)

where \( \nabla \) is the gradient operator in a coordinate system \( \mathbf{x} \) (with dimensions of reciprocal length).

In almost all applications encountered in non-Newtonian fluid mechanics, \( \rho \) is taken to be constant and so the incompressibility condition is imposed, which implies that

\[
\frac{D\rho}{Dt} = 0
\]  \hspace{1cm} (4.3)

so eqn. (4.1) takes the form

\[
\nabla \cdot \mathbf{u} = 0
\]  \hspace{1cm} (4.4)

Table A1 in Appendix A, expresses eqn. (4.4) in the rectangular and spherical coordinates which will be used in this work.

C: The Equation of Motion

The stress equations of motion are mathematical expressions of Newton's second law of motion applied to a moving continuum, or the principle of balance of linear momentum, as well as the local expression of the principle of balance of the angular momentum. The momentum conservation equation is conveniently written in the following single vector form [3a]:

\[
\rho \frac{D\mathbf{u}}{Dt} = - \nabla P - [\nabla \tau] + \rho g
\]  \hspace{1cm} (4.5)

where \( \nabla P \) = gradient of \( P \), sometimes written as \( \text{grad} \ P \)
\( \tau \) = stress tensor (see Section 3.1.1)
\( g \) = gravitational acceleration, assumed to be the only body force acting, if significant.
Neglecting acceleration and body forces, then eqn. (4.5) reduces to:

\[ 0 = -\nabla \rho - [\nabla \tau] \quad (4.6) \]

Table A2, in Appendix A, lists the components of the momentum conservation equation in the two coordinate systems used in this work.

D. Navier-Stokes Equations

The rheological equation for a Newtonian fluid in an arbitrary flow has been generalised according to the following form [2b]:

\[ \tau = - \mu [\nabla u + (\nabla u)^T] + \left( \frac{2}{3} \mu - \kappa \right) (\nabla \cdot u) \delta \quad (4.7) \]

where
- \( \mu = \) viscosity of Newtonian fluid
- \([\nabla u]^T = \) transpose of the dyadic
- \( \kappa = \) dilatational viscosity
- \( \delta = \) unit tensor

For incompressible fluids, eqn. (4.7) is simplified by means of the continuity eqn. (4.4) to give:

\[ \tau = - \mu [\nabla u + (\nabla u)^T] \quad (4.8) \]

Combine eqn. (4.4), (4.5) and (4.8) to obtain the Navier-Stokes equation (4.9) which holds for incompressible and Newtonian fluids:

\[ \rho \frac{D\mathbf{u}}{Dt} = -\nabla \rho + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} \quad (4.9) \]

where \( \nabla^2 = \) Laplacian operator, given in Table A5 in Appendix A.

Note that the brackets product in eqn. (4.8) is identified to be the rate-of-strain tensor, \( \Delta \), i.e.

\[ \Delta = [\nabla u + (\nabla u)^T] \quad (4.10) \]

in which case eqn. (4.8) becomes

\[ \tau = -\mu \Delta \quad (4.11) \]
4.3 CONSTITUTIVE EQUATIONS [7]

The constitutive equations or rheological equations of state relate the stresses to the motion of the continuum and generally vary from one non-Newtonian fluid to another, in contrast to the field equations which are the same for all fluids. Actually, this variation is the distinct point of departure of the non-Newtonian fluids from the classical ones, whose behaviour may be predicted on the basis of the Navier-Stokes equations.

A: What Rheological Equation of State?

To construct suitable constitutive equations, which then will allow computational tractability is a very difficult task. It is even more difficult to draw boundaries and establish criteria upon which the choice (or formulation) of the rheological equations will be based. However, some general points are worthy of mention, since they constitute the criteria upon which the rheological models for this work were chosen.

a) There is no one complete satisfactory model which, by using simple rheometric experimental data, will describe complicated flow problems in simple form without concessions; consequently, the more complicated the problem, the more compromise is required.

b) In many cases, the engineer has to combine analytical, numerical and empirical methods. The use then of a complex rheological model may worsen the situation in the respect that the engineer may not have the needed mathematical background, many times equivalent to that of an applied mathematician, to solve such complicated problems. It is interesting to notice at this point the reference made by Middleman [8], to the work carried out by Schechter [9] on the steady flow of a non-Newtonian fluid in rectangular ducts, emphasising Schechter's intention of using polymers to illustrate an application of a variational principle, and not to discuss the physical problem used for the illustration. Further to appreciate the complexity of the rheological models involved with polymers and at the same time to show the failure of classical Newtonian equations to describe melt flows and phenomena arising due to the viscoelastic nature of the melts, consider eqn. (4.12) below [2c]:

\[
(4.12) 
\]
\[
\tau = - (\eta_s + \frac{2}{5} \frac{n k T \lambda}{t}) \dot{\gamma} - \frac{3}{5} n k T \int_0^t e^{-(t-t')/\lambda} \dot{\gamma}' dt' \\
- \frac{6}{35} n k T \int_0^t \int_0^t e^{-(t-t')/\lambda} \{\dot{\gamma}', \dot{\gamma}' + \dot{\gamma}', \dot{\gamma}'\} dt'' \\
- \frac{3}{10} n k T \int_0^t \int_0^t \int_0^t e^{-(t-t'')/\lambda} \left[ \frac{3}{7} \{\dot{\gamma}'', \dot{\gamma}'' + \dot{\gamma}''', \dot{\gamma}'''\} \right] dt'' dt'' + \ldots
\]

+ isotropic terms containing integrals of \( \dot{\gamma} \) \hspace{1cm} (4.12)

This rigid dumbbell model, is one of the few models for which stress-tensor expressions have been found and as Bird et al [2c] emphasise, they were able to obtain only the first few terms of a 'memory integral expansion'. Eqn. (4.12) is far from simple since the expansion continues with triple, quadruple etc. integrals and triple, quadruple etc. products of velocity gradients. A comparison with the simple stress tensor expression for Newtonian fluids, proves that the classical (Newtonian) hydrodynamics will be of little value for describing the flow of polymeric fluids and that a large number of new physical phenomena (e.g. stress difference) can be expected; phenomena that can be described only by stress-tensor expressions that are highly non-linear and strongly time-dependent.

c) Additional constraints may arise, over and above those deriving from the basic formulation principles of the rheological equation of state. As an example consider the so-called stress-overshoot phenomenon. When a simple shear flow is started from rest in elastic liquids, the shear and normal stresses are often found to overshoot their equilibrium values before reaching a steady state. The constitutive equation employed should be expected to predict such behaviour when it occurs. Another example which has been suggested as providing a severe constraint on constitutive equations is the case associated with non-linear effects in oscillatory shear flow; and the question posed is the following. Is the departure from linear viscoelastic behaviour strain dependent or strain-rate dependent? Astarita and Marrucci [1a] for example, suggest a strain dependent departure from linear behaviour, deprecating the use of strain-rate dependent integral models. Having recognised these problems, it is then impractical to seek for a complicated rheological model rather than seeking for a model involving a minimum of parameters which will adequately describe the range of flow behaviour in a specific problem. However care must be taken
not to lose the essentiality of the problem by trying to employ too a simple rheological model.

Throughout this work, the generalised power-law model was the basis upon which equations for the flow of generalised incompressible non-Newtonian fluids was related to the degree of pseudoplasticity. In one case, the Carreau model was also used.

B: The Power Law Model

The most commonly used rheological equation portraying pseudoplasticity, which has enjoyed a wide degree of acceptance between scientists and engineers despite its pure empirical form, is the 'power-law' equation proposed by Ostwald-de Waele [10a]. It relates shear stress, \( \tau \), and shear rate \( \dot{\gamma} \), through two experimentally determined constants, \( n \) and \( m \) and can be expressed as:

\[
\eta = m \left| \frac{\dot{\gamma}}{\dot{\gamma}_0} \right|^{n-1} = m \left( \frac{\tau}{\tau_0} \right)^{\frac{n-1}{n}} \tag{4.13a}
\]

\[
\tau = m \left| \frac{\dot{\gamma}}{\dot{\gamma}_0} \right|^{n-1} \dot{\gamma} \tag{4.13b}
\]

where \( \tau_0 \) and \( \dot{\gamma}_0 \) represent values of shear stress and shear rate respectively in arbitrarily chosen standard state, \( m \) commonly called consistency index, represents the non-Newtonian viscosity in arbitrarily chosen standard state, usually at \( \dot{\gamma}_0 = 1 \text{ s}^{-1} \). \( n \) is the power-law index, dimensionless and for \( n<1 \) the fluid is 'pseudoplastic' while for \( n>1 \) is 'dilatant'.

Note that when the flow index \( n \) is unity, the power law reduces the fluid into a Newtonian one, where:

\[
\tau = \mu \dot{\gamma} \tag{4.14}
\]

where \( \mu \) is the Newtonian viscosity, constant for a given temperature, pressure and composition.

There is some criticism concerning the use of the power-law model in designing extrusion dies. Rautenbach [11] argues that the errors which occur in computation are too great. Vaughn et al [12] goes further, by rejecting the Fredrickson et al theory [13] concerning non-Newtonian annular flow on the grounds that the power-law model is invalid. Parnaby et al [14], on the other hand, defend and recommends its use, in spite of its deficiencies.
The following two comments are characteristic of the power-law model with respect to extrusion dies:

a) Polymer melts are viscoelastic fluids. The power-law equation can only describe the viscous part of the fluid behaviour and it is unable to describe the elastic part (i.e. normal stresses), in which case other means may be used. For example, extrudate-swell measurements can give an estimate of the elastic effects, since the latter are responsible for the swelling of the material.

b) For a given value of the power-law index, \( n \), the model holds exactly only for limited ranges of shear rate. This can be appreciated by examining the rheogram of Fig. 3.3. At low shear rate the viscosity is constant, which implies more or less Newtonian behaviour of the melt. At higher shear rates, the log-log plot of \( \eta \) vs \( \dot{\gamma} \) approaches a straight line indicating a power law behaviour in this range. The flow through dies creates a shear rate gradient ranging from \( \dot{\gamma} = 0 \) in the die-centre to \( \dot{\gamma} = \dot{\gamma}_\text{max} \) at the die wall, and this could presumably lead to great errors. Surprisingly enough, this may not be the case because as Knappe et al [15] proved in a study of volumetric throughput, the computation is influenced little more than one power of ten of \( \dot{\gamma} \), see Fig. 4.1. Lower levels of \( \dot{\gamma} \), towards the die centre, have only insignificant influence on throughput.

![Graph showing relative error, \( F \), occurring in throughput computations when power-law model or Prandtl-Eyring law are used (applicable to polystyrene 165H). (Reproduced from Knappe et al [15])]
C. The Carreau Model

A four parameter model that has the useful properties of the power law model has been proposed by Carreau [2d] and is described by:

\[
\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = \left[ 1 + (\lambda \dot{\gamma})^2 \right]^{\frac{n-1}{2}}
\]  
\hspace{2cm} (4.15)

where \( \eta_0 \) = zero shear rate viscosity
\( \eta_\infty \) = infinite shear rate viscosity
\( \lambda \) = time constant for the material

The model has the advantage that it asymptotes to \( \eta_0 \) as \( \dot{\gamma} \to 0 \) and to \( \eta_\infty \) as \( \dot{\gamma} \to \infty \) thus avoiding the singularities of the power-law equation. Having four parameters, the model can be usefully fitted to much melt data over a rather wider range than eqn. (4.13), and is suitable for numerical work.

D. Generalisation of Incompressible Non-Newtonian Fluids

The general rheological equation for incompressible non-Newtonian fluids has been postulated by analogy to eqn. (4.11), in terms of the invariants \( \Delta \) and \( \tau \) as follows [10b]:

\[
\tau = n\Delta
\]  
\hspace{2cm} (4.16)

\( \eta \) is a scalar quantity and in order to be a scalar function of the tensor \( \Delta \), it must depend only on the 'invariants' of \( \Delta \). The scalar invariant of the rate of strain tensor is

\[
I_1 = \Sigma_i \Delta_{ii} = 2(\nabla \cdot u)
\]
\[
I_2 = \Sigma_i \Sigma_j (\Delta_{ij})^2 = (\Delta \cdot \Delta)
\]
\[
I_3 = \text{det} \Delta = \Sigma_i \Sigma_j \Sigma_k \varepsilon_{ijk} \Delta_{li} \Delta_{lj} \Delta_{lj}
\]  
\hspace{2cm} (4.17)

For incompressible fluids, the first invariant, \( I_1 \), vanishes since \( \Delta_{xx} + \Delta_{yy} + \Delta_{zz} = 0 \). In rectilinear flow and in 2-D flow, the third invariant is zero and is also considered as not important in other types of flow. Hence viscosity can be expressed as a function of the second invariant only.

With the foregoing in mind, the power-law model, as expressed by eqn. (4.13), can now be rewritten in a more general form, allowing for estimation of flow in complex geometries.
Replacing $\gamma_0$ and $\dot{\gamma}$ in eqn. (4.13) by 1 s$^{-1}$ and $[(\Delta:\Delta)/2]^{1/2}$, respectively:

$$\eta = m \left| \frac{(\Delta:\Delta)}{2} \right|^{n-1}$$

(4.18a)

$$\tau = m \left| \frac{(\Delta:\Delta)}{2} \right|^{n-1} \Delta$$

(4.18b)

In this way, then, the viscosity depends on the magnitude of the entire tensor $\Delta$, through $(\Delta:\Delta)$, i.e. it is a function of all the velocity gradients. On the negative side, it is inadequate for describing normal stress differences and viscoelastic responses e.g. stress relaxation. Criticism must also be made of the neglect - mainly due to the lack of experimental information - of the $I_3$ effect [16].

To utilise eqns. (4.18), the scalar quantity $(\Delta:\Delta)$ and the components of the rate of deformation tensor, $\Delta$, have to be expressed in the appropriate coordinates. These are tabulated in Tables A3 and A4 in Appendix A.

4.4 EQUATIONS OF ENERGY

Isothermal and adiabatic flows are two distinct cases describing the heat transfer operation: isothermal operation is the case in which the fluid temperature is the same at all points in the die channel and is easily subjected to mathematical analysis. Adiabatic operation is the case in which there is no heat transfer through the walls of the die but all the heat energy comes from viscous dissipation.

However, actual flow lies between these two extremes, so no real fluid could ever be pumped isothermally, since heat generation due to viscous shear is inevitable in melt flows at moderate and high shear rates; thus setting up temperature gradients for any fluid having a finite conductivity. These considerations are very important and must be taken into account, especially for temperature sensitive materials such as rubber compounds which are subjected to chemical cross linking and thermal degradation; and also when extrudate surface quality (and properties) are of critical importance.

The equation of energy in terms of the fluid temperature is given by [3b]:

$$\rho \ C_v \frac{DT}{Dt} = - (V \ q) - T \left( \frac{\partial P}{\partial T} \right)_v (V.u) - (\tau:Vu)$$

(4.19)

where $C_v$ = specific heat at constant volume
q = heat flux vector
$DT/Dt$ = substantial time derivative.
Expressing heat flux in terms of the temperature gradient using the generalised form of Fourier equation (4.20) [2e] and assuming that the thermal conductivity, $K$, is constant, then

$$q = -K \nabla T$$

(4.20)

$$-(\nabla q) = (V \cdot K \nabla T) = K \nabla^2 T$$

(4.21)

The last term of eqn. (4.19) accounts for the viscous heat generated during the flow of the fluid, and it can be expressed in a different form as [5a]:

$$(\tau: Vu) = \frac{1}{2} (\tau: \Delta + \tau: \omega)$$

(4.22)

Assuming that the fluid is incompressible, and $C = C_V = C_p$ ($C_p$ = specific heat at constant pressure) the middle term in the RHS of eqn. (4.19) disappears. Also by assuming that there is no rotary motion, the last term of eqn. (4.22) is eliminated, thus eqn. (4.19) transforms to:

$$\rho C \frac{DT}{Dt} = KV^2 T - \frac{1}{2} (\tau: \Delta)$$

(4.23)

Eqns. (4.2) and (4.23), assuming steady-state conditions, yield

$$\rho C u \cdot V T = KV^2 T - \frac{1}{2} (\tau: \Delta)$$

(4.24)

Combine eqns. (4.18) and (4.24) to obtain:

$$\rho C u \cdot V T = KV^2 T - m \left[ \frac{\Delta: \Delta}{2} \right]^{n+1}$$

(4.25)

### 4.5 BOUNDARY CONDITIONS

In order to solve the constitutive equation in conjunction with the transport equations the appropriate boundary conditions have to be specified. Usually the 'no slip at the wall' condition is sufficient to provide a complete solution. However, certain complications may arise if one takes into account fluid memory, in which case the complete history of deformation prior to entry must be known. Also, if the boundary of the domain contains an entry region then the strain history of the fluid entering the domain - i.e. stress field on entry - must also be known; this can be best appreciated if one studies 'the hydrodynamic entrance region' section as it has been derived in Appendix B.

In studying extrudate swell using transport equations, one of the problems encountered is the involvement of mixed boundary conditions on the fluid, where part of the fluid surface has velocity boundary conditions
called rigid boundaries, while another part has stress (or truncation) boundary conditions, called free boundaries. In addition, there may be thermal boundary conditions.

4.5.1 Boundary Conditions in Heat Transfer

The differential equation of heat transfer will not have a unique solution unless a set of boundary conditions and initial conditions are specified. A general classification of thermal boundary conditions is as follows:

a) **Boundary Conditions of the First Kind:**

Temperature $T$ is prescribed along the boundary surface $S_i$, i.e.

$$T_i = f_i(r) \text{ on } S_i$$

(4.26)

where $r$ describes the position of a point in the three space variables $x$, $y$ and $z$ (for Cartesian coordinate systems). Special case includes temperature as being constant.

b) **Boundary Condition of the Second Kind:**

The normal derivative of temperature prescribed at the boundary surface, $S_i$, may be a function of position i.e.

$$\frac{\partial T}{\partial n_i} = f_i(r) \text{ on } S_i$$

(4.27a)

where $\partial T/\partial n_i$ denotes differentiation along the outward drawn normal at the $S_i$. Multiplying both sides of eqn. (4.27a) by the thermal conductivity, $K_i$, then gives:

$$\frac{\partial T}{\partial n_i} \cdot K_i = f_i(r) \cdot K_i$$

(4.27b)

The LHS of eqn. (4.27b) is the heat flux $q(r)$, thus

$$q(r) = K_i f_i(r)$$

(4.27c)

c) **Boundary Condition of the Third Kind:**

Temperature and its normal derivative, linearly combined, are prescribed at the boundary surface, $S_i$, i.e.

$$K_i \frac{\partial T_i}{\partial n_i} + h_i T = f_i(r)$$

(4.28)

To demonstrate the physical significance of eqn. (4.28) we can apply an energy balance for the boundary surface $S_i$ of the die, which in fact is the contact layer between melt and (inside) die wall.
\[
 q_{\text{wall}} = -K \left( \frac{\partial T}{\partial n} \right)_S = h (T - T_c) \quad (4.29)
\]

where \( K \) is the thermal conductivity of the melt; \( h \) is the heat transfer coefficient of the die wall between the inside surface of the die which comes in contact with the melt and the outside surface of the die (at distance 1), where the temperature is \( T_c \) (i.e. controller-temperature) \( T \) and its outward normal derivative in the melt are evaluated at the boundary. The negative sign indicates that heat is assumed to flow in the opposite direction to that in which melt-temperature increases algebraically.

Eqn. (4.29) describes convection boundary conditions and states that the rate of flow of energy conducted to the surface is equal to the energy leaving the surface or vice-versa.

Combine eqn. (4.29) with the dimensionless Biot number, \( B_i \) [17], given by eqn. (4.30), to obtain:

\[
 B_i = h 1/K \quad (4.30)
\]

\[
 \left( \frac{\partial T}{\partial n} \right)_S = B_i \frac{T - T_c}{l} \quad (4.31)
\]

A note on Biot number which indicates whether the process of heating is dominated by internal conduction or external convection, is that only heat flux vertical to the contact layer melt/die is described, thus neglecting heat conduction in the \( r \)-direction, for spherical co-ordinates.

Since, then \( \theta \) is the polar coordinate perpendicular to the inner wall, eqn. (4.29) can be written as:

\[
 - \left( \frac{\partial T}{\partial \theta} \right) = \frac{r h}{K} (T - T_c) \quad (4.32)
\]

In the majority of problems associated with heat transfer calculations a boundary condition of this kind is used as being more realistic condition. Recently this has been criticised by Dorfman [18] as failing to represent the real situation because it neglects the fact that the heat transfer coefficient is a function of the boundary conditions, thus leading to both quantitative and qualitative errors.

The foregoing three kinds of boundary conditions cover nearly all the cases of practical importance in polymer heat transfer and they are linear boundary conditions. Non-linear boundary conditions usually involve thermal variation boundary conditions which obey the fourth-power temperature law, boundary conditions associated with changes of phase (e.g. melting,
solidification). For an extensive discussion on thermal boundary conditions, the reader can refer to an extensive article by Shah and London [19].

4.6 EFFECT OF TEMPERATURE ON VISCOSITY

The form of the dependence of Newtonian viscosity on temperature, known as Arrhenius [10c], has been known for a long time. It is a simple exponential viscosity-temperature dependence:

\[ \mu = A \exp\left(\frac{E}{R_g T}\right) \]  \hspace{1cm} (4.33)

where \( A \) is a coefficient depending upon the nature of the fluid.
\( E \) is the energy of activation for flow.
\( R_g \) is the gas constant (8.314 J/K gr mole).
\( T \) is the absolute temperature.

A plot of \( \log \mu \) vs \( (1/T) \) gives, for most fluids, a reasonably good straight line over a temperature range of 40°C. Beyond this, curvature usually becomes more pronounced, indicating that variation in the quantities \( A \) and \( E \) is becoming significant.

Since polymers are rarely in the lower Newtonian range in commercial processing operations, the viscosity in eqn. (4.33) can be replaced by the apparent viscosity \( \eta_a \) in which case two equations result because the activation energy \( E \) assumes different values if temperature is varied at constant shear rate \( E'_y \) or constant shear stress \( E_T \):

\[ \eta_a = f(\gamma, T) = A \exp\left(\frac{E'_y}{R_g T}\right) \] \hspace{1cm} (4.34a)
\[ \eta_a = f(\tau, T) = A \exp\left(\frac{E_T}{R_T T}\right) \] \hspace{1cm} (4.34b)

Over a similar temperature range, the ratio of activation energies becomes:

\[ \frac{E_T}{E'_y} = 1 - \gamma \left(\frac{\partial \eta_a / \partial \tau}{\partial \eta_a / \partial T}\right) T \] \hspace{1cm} (4.35)

which shows that \( E'_y = E_T \) as \( \gamma \to 0 \). For Newtonian fluids \( E'_y = E_T \) under all conditions because \( (\partial \eta_a / \partial \tau)_T = 0 \). For pseudoplastic fluids \( (\partial \eta_a / \partial \tau)_T < 0 \) and therefore \( E_T > E'_y \).

The fact that activation energy of a non-Newtonian fluid varies with temperature in addition to shear stress or shear rate means that an
increasing temperature causes a decrease in the activation energy and also tends to suppress non-Newtonian effects. Therefore, if wide temperature ranges are encountered, the activation energy and fluid models parameters have to be repeatedly re-evaluated under local conditions in relatively narrow temperature ranges.

When the temperature dependence of \( \eta_a \) shown in eqns. (4.34), is incorporated in flow equations, it often leads to mathematical difficulties. A more convenient empirical form is, therefore, frequently used:

\[
\eta_a = ae^{-bT} \tag{4.36}
\]

where \( a \) and \( b \) are constants.

A more useful form of eqn. (4.36) relates apparent viscosity at one temperature to that at a different temperature

\[
\eta_{aT} = \eta_{a_o} \exp\{-b(T-T_o)\} \tag{4.37}
\]

where \( \eta_{aT} \) and \( \eta_{a_o} \) are the apparent viscosities at temperature \( T_o \) (reference temperature) and \( T \) (any temperature) respectively. The constant \( b \) assumes different values at constant \( \tau \) and \( \gamma \). McKelvey [10c] calculated some representative values from data collected by Westover [20a].

For polymers following the power-law model, eqn. (4.37) in conjunction with eqns. (4.13) can be written as

\[
\eta(T) = e^{-b(T-T_o)} \bigg| \frac{Y}{Y_o} \bigg|^{n-l} \tag{4.38a}
\]

\[
\tau = m'e^{-b(T-T_o)} \bigg| \frac{Y}{Y_o} \bigg|^{n-l} \tag{4.38b}
\]

where \( \eta(T) \) and \( m' \) are, respectively, viscosities at temperature \( T \) and \( T_o \) reference temperature. Investigation with rubber [21], showed that two values of \( b \) may be needed to define this dependence because a change of slope may occur in the region of 100°C.

Many other theoretically and empirically based expressions have been proposed by various investigators; however the choice is often dictated by the mathematical formulation of the problem and the required accuracy when representing data.
4.7 EFFECT OF PRESSURE ON VISCOSITY

The viscosity of fluids depends on intermolecular forces, which in turn are dependent on intermolecular distances. It is not surprising, therefore, to find that the compression of fluids tends to increase the viscosity. Moreover, the compressibility of polymer melts at processing temperatures is higher than that of ordinary liquids [20b]. Hence a greater effect of pressure on viscosity can be expected.

The dependence of melt viscosity on pressure is normally approximated by

\[ \eta(P) = m^* e^{\frac{b^*}{n} (P-P_o)} \]

(4.39)

where \( \eta(P) \) and \( m^* \) are, respectively, the viscosities at pressure \( P \), and reference pressure \( P_o^* \), \( b^* \) is the pressure coefficient of viscosity and \( m^* \) is a function of temperature and shear rate (or shear stress). Therefore the power-law equation would become

\[ \tau = m \left( \frac{\dot{\gamma}}{\dot{\gamma}_o} \right)^{n-1} \dot{\gamma} \exp\{b^* (P-P_o)\} \]

(4.40)

Coupling together the effects of both temperature and pressure on viscosity, the power law equation (4.13) becomes:

\[ \tau = m \left( \frac{\dot{\gamma}}{\dot{\gamma}_o} \right)^{n-1} \dot{\gamma} \exp\{-b^* (T-T_o) + b^* (P-P_o)\} \]

(4.41)

where \( m^* \) is the viscosity at \( T_o^* \) and \( P_o \) (the reference temperature and pressure respectively) and \( b^* \) is defined at constant shear rate.

The experimental determination of \( b^* \) is difficult, and consequently rarely attempted. Maxwell and Jung [22] obtain a few results for polyethylene and polystyrene using a capillary rheometer in which a high pressure was maintained on both sides of the capillary. Westover [23] and Senjonow [24] developed a special rheometer and obtained values of \( b^* \) (at constant shear rate) of 3.2-6.1 m²/GN for various polyethylenes and 7.4-15 m²/KN for polypropylene, all under very limited conditions of temperature and shear rate.

Similarly, Hellwege et al [25] obtained values of 42-91 m²/KN for various polyesters. Duvdevani and Klein [26] also developed a method for obtaining the pressure coefficient from ordinary capillary viscometric pressure data, by a method which involves differentiation of the reservoir versus die length. They quote \( b^* \) in the vicinity of 48 m²/KN for polyethylene.
This would imply that a 70 MN/m² increase in pressure will cause the viscosity to increase by about 35% which is, of course, a significant effect. However Fenner [27a] criticises these findings as extremely unreliable, due to the fact that the experimental method involved is unacceptable. Carley [28] has critically reviewed work on polymer melts and concludes that pressure effects are of minor significance in most processing situations, provided that the temperature is not too close to a transition. High pressures raise both glass transition temperature \( T_g \) and crystalline melting temperature \( T_m \) slightly, and the viscosity shoots up tremendously as either is reached. Cogswell [29], on the other hand, considers the influence of pressure on viscosity as playing a major role, outlining that 1000 atmospheres (\( \approx 10^8 \text{ N/m}^2 \)) increase in pressure has as much effect on viscosity as a reduction of 50°C in temperature, while causing a 10% increase in density. He also reports that a decrease in pressure during extrusion, for a pressure gradient of 0.1 GN/m² could lead to isentropic reduction in the average melt temperature of the order of 15°C and introduce an error of the order 10 to 50% in viscosity.

### 4.8 SELECTION AND DISCUSSION OF ASSUMPTIONS

To solve the field and constitutive equations, once the boundary conditions have been specified, a number of simplifications and assumptions must be made if solutions are to be obtained with a reasonable amount of effort. The simplifications and the assumptions which will be examined in this section are valid for all cases throughout this work, except where stated otherwise.

1. The die can be supplied with melt at any pre-requested pressure and temperature.
2. Die-entrance pressure must not exceed that available from the extruder.
3. Output of the extruder must be known as a function of head pressure, screw speed and temperature.
4. Polymer melts are non-Newtonian fluids at processing conditions.
5. Body forces (e.g. gravity) are negligible in comparison with viscous and pressure forces.
6. The third invariant of the rate-of-deformation tensor is small - see Section 4.3D.
7. Fully developed flow - see Section 3.3.
8. No recirculatory flow at the entrance - see Section 3.4.3.
9. The fluid is incompressible - see Section 4.7.
10. Steady-state flow. This assumption implies that the flow characteristics are independent of time, \( \frac{d}{dt}=0 \). In reality, few processes are truly steady, from the simple fact that factors such as boundary conditions, systems resistance etc. introduce small fluctuations which in turn introduce process changes. However in such cases the pseudo-steady-state approximation, described briefly by Tadmor and Gogos [5b], may be used.
11. Inertia forces are negligible [5c,6b,14,27b,30]. When inertia forces are either zero or negligibly small, the flow is called "creeping". In such flows, the viscous forces predominate over inertia forces, and in terms of Reynolds number this means that it has to be less than about 0.1 [3c]. Polymer processing flows are generally viewed as creeping flows. This view is best explored in studies related with "thrust" measurements. For example Pearson [31] commenting on the "direct-thrust" technique adopted by Shertzer and Metzner [32] for the measurement of normal stresses in viscoelastic fluids, rejects the method as being irrelevant to polymer melts because the Re used was greater than 100, while for molten polymer extrusion Re<1. Bird et al [33] in a detailed study of extrudate swell analysis by macroscopic balances distinguishes between two regimes: a high Re regime and a low Re regime stressing that only the latter is relevant to polymers.
Classical examples of creeping flows include those treated by the hydrodynamic theory of lubrication, Hele-Shaw flows and the flow of very viscous fluids past immersed bodies, a detailed account of which can be found in Happel and Brenner [34] and Langlois [35].
12. No slip at the wall. This is one of the most common assumptions made during any polymer processing analysis. However its validity has been seriously questioned by some investigators during recent years when it is applied to rubber mixes, UPVC and high molecular weight polyethylenes. From the plastics viewpoint, most research in this area is attributed to Den Otter et al [36], Uhland [37] and Worth [38]. With rubber mixes, on the other hand, experimental work [39] in a TMS binonical rotor rheometer using polished and grooved rotors has shown the existence of slip between rubber and polished metal surfaces. Also it was suggested that wall slip velocities, \( V_s \),
can be measured from the results on the grooved and smooth rotors at a given shear stress, according to:

\[ V_s = R(w_s - w_g) \]

where \( R = \) rotor radius

\( w_s, w_g = \) angular velocity of smooth and grooved rotors, respectively (radians/sec).

This suggestion was based on the fact that wall slip manifests itself by the difference in rotational rate between the smooth and grooved rotors, and in that smooth rotors allow slip to occur, probably due to formation of a lubricating layer, while grooved rotors inhibit slip by breaking the continuity of this layer.

A method of characterising wall slip is to use the power-law eqn. (4.43) [40] below

\[ V_s = M_s \tau^s \]  

(4.43)

where \( M_s, s = \) coefficients of power-law equation for wall slip, determined experimentally.

Using the assumption of zero wall slip on a Newtonian fluid, one may expect a flow pattern like the one shown in Fig. 4.2a where a globular mass of material is forced at the die exit due to equalisation of flow velocities. With a power law material and zero wall slip, a 'plug-like' profile is expected thus ending up with a more conventionally shaped extrudate. If, on the other hand, slip was present, case b, shown in Fig. 4.2b, would be the probable result.

**Fig. 4.2:** (a) Flow pattern of a Newtonian fluid in the absence of wall slip, (b) Flow pattern of a power-law fluid in the presence of wall slip.

Wall slip is related, indirectly, to extrudate swell in that increase in slip velocity will reduce strain rates. This is due to the dependence between strain-rates and swelling (see Section 3.4.1), where
swell is the result of the elastic recovery of strains set-up during the melt passage through the die, hence any increase in slip will reduce swell. The overall contribution of slip to volumetric flow rate is additive and for a circular die the formula expressing it may be written as

\[ Q = \frac{n}{3n+1} \left( \frac{\Delta P}{2mL} \right)^{1/n} \pi R \frac{3n+1}{2} \tau R^2 + \pi R^2 V_s \]  

(4.44)

13. Constant thermophysical properties \((\rho, K, C)\). The thermophysical properties of polymers which are required for the present heat transfer calculations include: density \(\rho\) (or its reciprocal specific volume), specific heat \(C\), thermal conductivity \(K\) (or thermal diffusivity which is a function of specific heat, conductivity and density) and melt viscosity (discussed in Sections 4.6 and 4.7). These are mainly dependent, to a greater or lesser extent, on polymer type, molecular weight (and its distribution), orientation, previous history of temperature or shear (memory effects), temperature, pressure and flow conditions.

Although we are concerned primarily with the effects of pressure and temperature on these parameters, it must be pointed out that the effects resulting from polymer type and molecular weight are considerably different for rubber materials (as compared to plastics). The reason is that the rubber compounds may contain two or more different raw polymers and quantities of other materials such as fillers and processing oils.

The pressures involved in dies are relatively low, not more than about 20 MPa. This, in turn, means that both thermal conductivity- and density-pressure dependence can be neglected on the grounds that for every 10³ psi (≈7 MN/m²) there is a 1% increase in conductivity [5] and a 10² MN/m² pressure causes a 10% increase in density [29]. Pressure independence can also be assumed for the specific heat of melts, based on the work reported by Anderson and Sundqvist [41] who in extensive work investigated the effect of pressure on thermal properties.

As far as the temperature is concerned, experimental evidence provided by Tadmor and Gogos [5], and Anderson and Sundqvist [41] do seem to indicate that thermal conductivity, density and specific heat can be treated as temperature-independent. However, some serious reservations must be kept about the influence of temperature on these
thermal properties when glass- and melting-temperature are involved: a review can be found in Tadmor and Gogos [5e]. From the foregoing it is evident that whether a property can be assumed as temperature-dependent or independent, depends on whether the temperature range of the system under consideration passes through a temperature transition state; but since for extrusion dies only the melt state is encountered it seems reasonable enough to assume these thermophysical properties are temperature-independent.

14. The heat transfer coefficient is infinitely large. This assumption implies that the thermal contact between the metal surfaces and the polymer melt is excellent. Experimental evidence [42], though limited, exists for the barrel-melt-screw combination. However, Tadmor and Klein [43] expressed some reservations about this evidence, since the experiments were carried out under near isothermal conditions and therefore do not answer questions about temperature fluctuations.
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33. BIRD, R.B., R.K. PRUDHOMME and M. GOTTLIEB, The University of Wisconsin, Rheology Research Centre Report, RRC-35, 1975, (Adapted from Tadmor et al [5d]).


CHAPTER 5
AN OVERVIEW OF APPROXIMATE AND NUMERICAL SIMULATION AND OF EXPERIMENTAL DESIGN

5.1 GENERAL CONSIDERATIONS

For complicated engineering design analyses, especially those involving the interaction of transport and constitutive equations, it is often necessary to seek engineering approximations to make the solution of difficult problems more tractable and the computation more economical. This is a motivation for using approximate methods for the numerical simulation of the non-Newtonian polymer flow equations in this work.

The numerical analysis involved is shown diagrammatically in Fig. 5.1. A simplified view is taken here as the subject is discussed excellently elsewhere [1-7]; also some basic ideas and principles are introduced which will be adopted later on during the modelling of the process.

![Diagram](Fig. 5.1: Simplified logical diagram for numerical simulation)
5.2 **FINITE DIFFERENCE METHOD**

It is one of the oldest and most widely used methods because the mathematical concept of discretisation is relatively simple. A continuous domain is replaced with a network or mesh of discrete spatial grid-points (nodes) and the field unknowns to be calculated are precisely the unknown values of the variables at these points. The approximations used in this work are listed in Table 5.1; they were obtained from the Taylor's series expansion.

**TABLE 5.1:** Finite difference approximation of first and second derivatives

<table>
<thead>
<tr>
<th>Derivative</th>
<th>Operator</th>
<th>Difference Approximation</th>
<th>Order of Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{du}{dx} )</td>
<td>Forward (( \Delta f_, P ))</td>
<td>( \frac{f_{P+1} - f_P}{h} )</td>
<td>0(h)</td>
</tr>
<tr>
<td></td>
<td>Backward (( \nabla f_, P ))</td>
<td>( \frac{f_P - f_{P-1}}{h} )</td>
<td>0(h)</td>
</tr>
<tr>
<td></td>
<td>Central (( \delta f_, P ))</td>
<td>( \frac{f_{P+1} - f_{P-1}}{2h} )</td>
<td>0(h²)</td>
</tr>
<tr>
<td></td>
<td>Average (( \mu f_, P ))</td>
<td>( \frac{f_{P+1} + f_{P-1}}{2h} )</td>
<td>0(h²)</td>
</tr>
</tbody>
</table>

In its simplest form, the basic steps for a finite different method are:

a) choose a mesh on the interval of interest i.e. for \([a,b]\)

\[ a = x_0 < x_1 < ... < x_n < x_{n-1} = b \]

such that the approximate solution will be sought at these mesh points.

b) form the equations required to satisfy the differential equations (either ordinary- or partial-differential equations) and the boundary conditions by replacing derivatives with difference approximations involving only the mesh points.

c) Consider how good the approximation to the solution of the corresponding equation is by checking for stability and convergence, (see Fig. 5.2).
A variety of solution methods, ranging from the common explicit- and implicit-forms, to a number of special purpose methods, exist. The choice of methods depends on a number of criteria namely: consistency, convergence, stability, computation time, accuracy; all of which are inter-related. Care must be given to the selection because their negligence or misapplication can lead to severe solution problems or wrong answers.

A brief and simplified error analysis will be encountered next, as more detailed treatments can be found in the literature. The error refers to the difference between the approximate calculation solution of the finite difference equations and the exact solutions of the governing partial differential equation, although one may not know and there may be no formal expression for this exact solution. There are two types of errors. The first is called truncation error, due to computing with derivatives replaced by finite differences and this depends on the choice of finite difference scheme (see Table 5.1), the choice of the step used in
the computation, the initial temperature (or velocity) distribution and the boundary conditions. If the boundary conditions are not of the Dirichlet type, they must also be approximated by finite differences thereby introducing an additional or boundary truncation error. Strictly speaking the error $O(h)$ and $O(h^2)$ shown in Table 5.1 is the truncation error of the finite difference equation and not of the solution. The error in the solution, due to replacement of the continuous problem by the discrete model, is called discretisation error. The second type of errors are numerical: round off errors which are caused by the finite significant figure restriction used in any calculation. Their contribution is difficult to ascertain because of its random nature; and probability studies may be used, in which case an assumption concerning the probability density function of the error is required. Thus we cannot guarantee that an error is less than, say $\varepsilon_0$, but can only estimate the probability that this is the case.

In most problems, where the truncation errors do not vanish, the mesh is refined to reduce these errors but this affects (increases) the round off errors. For this reason, one cannot generally assert that decreasing the mesh size always increases the accuracy. In large computational problems, it is not usually the rounding errors which dictate the limit on mesh-size, but the storage capacity of the computers.

5.3 **FINITE ELEMENT METHOD** [7]

An alternative method to finite difference is the finite element formulation, in which the variables are approximated over finite regions (or finite elements) with a grid pattern. The coefficients of the variables in this functional representation are then calculated. The number, sizes, shapes and arrangements of these elements are carefully chosen by subjective decision making.

The finite element method has been developed in a number of areas such as aerodynamics, civil engineering and metallurgy. In recent years, the first signs of its application in polymer fields have been seen but it still has not penetrated this industry adequately. Briefly, the finite element analysis offers the following advantages:

a) It is not limited to 'nice' shapes with easily defined boundaries, but irregular shaped boundaries can also be handled.
b) The size of the elements can be varied, thus allowing for the element grid to be expanded or refined as the case requires.
c) Any type of boundary conditions, e.g. mixed, can be approximated.
d) It can be applied to bodies composed of different materials, because the materials in adjacent elements do not have to be the same.
e) A general computer program, developed for a number of cases, can incorporate the particular subject area.

It is this last advantage which, in the end, turns out to be a disadvantage due to the need of digital computers with large core memory. Obviously, the use of desk calculations or hand computations is ruled out. Another disadvantage of the method is its failure to estimate error, in which case one has to rely on comparison with calculations on a simple problem for which an analytical solution exists.

At present it seems that although the finite element method offers certain advantages over the finite difference method, its application to polymer processing will be delayed by the fact that the computer programs available are very complicated and they can be used only by experienced users. It seems that only if user-friendly packages made will the finite element method be adopted in this industry.

As far as accuracy is concerned, this is an inappropriate criterion for the choice, since both finite difference- and finite element-methods offer the same degree of accuracy. Shih [5a] attempts, in a way, to identify the similarities and differences between the two methods in several aspects which include among others smoothness, numerical instability, accuracy, irregular geometries, non-linear problems and discretisation schemes of higher than second order accuracy of the approximated solutions.

In general, the choice between the two methods is a matter of subjective judgement. In this work, the finite-difference method was chosen, as both the background and the required mathematics were available.

Pittman et al [3,8,9] have discussed both methods as they are applied to polymer processing, giving also an account of nearly all the existing literature.
5.4 VARIATIONAL PRINCIPLES

A convenient approximate analysis of polymer melts flowing through complex geometries is the variational method. It is similar to that of weight residuals in that the assumed solution is expressed in terms of a linear combination of basic functions with coefficients to be determined. However with the variational method, which is based on variational calculus, the variational integrals are minimised while with the weighted residuals, the residuals are those which are minimised. The method, when applied, covers the whole region of the problem under consideration, and it offers the advantage over the finite difference techniques that one obtains analytical expressions rather than tabulations of numerical results.

It is undesirable to discuss the method here, as it may be found in the relevant literature [10-11]; instead its application will be demonstrated in Section 6.3.3 by means of studying the melt flow through triangular ducts.

5.5 EXPERIMENTAL DESIGN

Factorial experimental design and multi-variable regression methods have been widely used in the Chemical Engineering industries to optimise multivariable processes. They have also been introduced to the rubber industry under the name 'computer compounding' where they are used to determine the optimum levels of ingredients in the rubber compounds [12].

Here factorial experimental design is used to characterise extruder performance, thus providing an 'operating window' for die design.

With the factorial experimental design, it is possible to examine the influence of changing a number of process variables simultaneously. Thus overcoming the limitations of conventional experimental design, which usually involves changing one variable while holding others constant. The fact that these methods can deal with interactions between variables is particularly suitable for processes such as extrusion where a number of process variables may interact together to influence performance.

A variety of experimental designs exist, such as full factorial, fractional replicate of full factorials and special purpose designs [13, 14]. The Rotatable Centre Composite Factorial Design was selected due to
its successful performance in previous work [15,16]. The term rotatable refers to the variance of the predicted response, e.g. an extrusion property, being a function only of the distance from the centre of the design at which it is measured. A rotatable centre composite design is built up from a complete two level factorial design \(2^n\) by adding further experimental points known as "star" points \((2^n)\) and "centre" points (see Table 5.2). The \((2^n)\) supplementary points are added in pairs along the coordinate axes at \(\pm a_1, \pm a_2, \ldots \pm a_n\) respectively, as shown in Fig. 5.3. Addition of some replicate runs at the centre point will provide an estimation of the experimental error and hence the adequacy of the model. Linear and interaction relationships are determined by the two-level factorial, while the star points allow any curvature of the relationship between a response and the experimental variables to be modelled.

**TABLE 5.2: Central Composite Design for a \(2^4\) Factorial**

<table>
<thead>
<tr>
<th>Experiment No</th>
<th>Screw Speed S</th>
<th>Die Temperature DT</th>
<th>Head/Barrel Temperature HBT</th>
<th>Pressure P</th>
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</table>

Two-levels full factorial design in 4-variables

\((2^n=2^4=16)\)

\((2n=2^4=8)\)

Star or axial points

Centre points replicates
The value of $a$ is determined from the equation below [17]

$$a = \pm 2 \frac{P}{4}$$

where $p$ represents the total number of variables included in the design: thus for $p=4$ (as in the present work - see Section 7.3) then

$$a = \pm 2$$

A point of caution about the empirical models is that, in contrast to the mechanistic models, their usefulness is limited to inside the range of experimental data only, but the latter are less flexible and mathematically quite difficult to be handled.

Once the results are obtained they can be treated by multivariable regression analysis using the statistical package designated GLIM (Generalised Linear Interactive Modelling) [18]. Using this program, the coefficients of a second order polynomial equation, relating a selected response to the four independent variables: screw speed $S$, die temperature $DT$, head temperature/barrel temperature $HBT$ and pressure $P$, may be estimated. The polynomial approximation selected takes the general form:

$$Y = b_0 + b_1 S + b_2 DT + b_3 HBT + b_4 P - \text{linear or first order terms}$$

$$+ b_{11} S^2 + b_{22} (DT)^2 + b_{33} (HBT)^2 + b_{44} P^2 - \text{quadratic terms}$$

$$+ b_{12} S DT + b_{13} S HBT + b_{14} S P \quad \{ - \text{interaction terms}$$

$$+ b_{23} DT HBT + b_{24} DT P + b_{34} HBT P$$

where $Y =$ response or dependent variable

$b_0 =$ grand mean or zero order constant

$b_{ij} =$ coefficients.

In addition to listing the estimates of the coefficients of the polynomial equation, the GLIM program provides the associated standard error thus permitting the significance of each effect, either individual or interactive to be assessed. By selecting only those independent variables associated with coefficients which are statistically significant and which give rise to practically important variation in the rheological parameters, is it possible to reduce substantially the amount of information which requires detailed consideration.
Fig. 5.3: The central composite factorial experimental design in three variables
REFERENCES


CHAPTER 6
MODELS FOR DIE FLOW

In Chapters 2 and 3, we introduce some background information and the many kinds of flow phenomena that are encountered in the study of flow through extrusion dies. In Chapter 4 we concentrate our attention on the fluid mechanics equations governing the non-Newtonian flow of polymer melts in the dies. The equations were expressed in a form convenient for immediate use when the case arises, as well as in a vector form in order to accommodate any of the standard orthogonal coordinate systems, since in our case both Cartesian and spherical coordinates were used.

This chapter serves as a link between the above three chapters by means of the numerical and approximate analysis which occupied our attention in Chapter 5. The flow geometries of interest include: converging flow in conical channels and flow in non-circular ducts of rectangular, square and equilateral triangle shape.

The first part of this chapter is devoted to converging flow in conical channels, where both pressure and temperature distribution are calculated. Also a short discussion is given, presenting the most important points involved during the analysis and their consequences in the derived equations. Next in Section 6.2, a method is proposed as how to calculate the minimum die land length, or the length of the preform section, for each of the above three non-circular ducts, by using the theory of extrudate dwell based on 'memory effects' and capillary data. This leads naturally to the presentation of each of the non-circular ducts, which are discussed in Sections 6.3 and 6.4. Due to the complicated nature of the procedure proposed for the prediction of pressure drop and extrudate swell in Section 6.3, the section has been divided into three parts (Sections 6.3.1-6.3.3) as Figure 6.1 explains. Section 6.4 which follows, treats non-Newtonian flow in triangular ducts, incorporating both variational principle (Section 6.4.1) and finite difference (Section 6.4.2) methods. Finally, Section 6.5 presents a short discussion, highlighting the pros and cons of the methods proposed in Sections 6.2-6.4 indicating some aspects of the derivation and solution of the appropriate equations.
Fig. 6.1: Layout of Chapter 6
6.1 CONVERGING SECTION

6.1.1 Transport Equations

A. Velocity field

Using the spherical co-ordinates \((r, \theta, \phi)\) as shown in Fig. 6.2, with symmetry at the centre of the cone, where \(\theta = 0\), the velocity field is given by

\[
\begin{align*}
v_r &= v_r(r, \theta) \\
v_\theta &= v_\phi = 0
\end{align*}
\]

(6.1a) \hspace{1cm} (6.1b)

Eqns. (6.1) assume that there is no circulating flow within the converging flow field (see Section 3.4.3).

Fig. 6.2 Representation of the spherical co-ordinate system used for analysis of converging flow

B. Continuity equation

The continuity eqn. (4.4) for spherical co-ordinates, see eqn. (A1-B) of Appendix A, becomes:

\[
\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v_r) = 0
\]

(6.2)
which yields

\[ f(\theta) = v_r r^2 \]  \hspace{1cm} (6.3a)

\( f(\theta) \) is a yet undetermined function depending on \( \theta \) only, and holds for \( r_2 \gg r \gg r_1 \). From eqn. (6.3a) one may write:

\[ \frac{3v_r}{r} = -2 \frac{f(\theta)}{r} \]  \hspace{1cm} (6.3b)

\[ \frac{1}{r} \frac{3v_r}{\theta} = \frac{f'(\theta)}{r^2} \]  \hspace{1cm} (6.3c)

C. **Equation of motion**

The components of the momentum eqn. (4.6) in spherical coordinates \((r, \theta, \phi)\), see eqns. (A2-D) and (A2-E) of Appendix A, may be expressed as

**r-component:**

\[ -\frac{\partial p}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \tau_{rr} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \tau_{r\theta} \sin \theta \right) - \frac{\tau_{\theta \phi} + \tau_{\phi \theta}}{r} \]  \hspace{1cm} (6.4a)

**\( \theta \)-component:**

\[ -\frac{1}{r} \frac{\partial p}{\partial \theta} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \tau_{r\theta} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \tau_{\theta \theta} \sin \theta \right) + \frac{\tau_{r \theta}}{r} - \cot \theta \frac{\tau_{\phi \theta}}{r} \]  \hspace{1cm} (6.4b)

6.1.2 **Rheological Equation of State**

Combine eqn. (4.18b) with the components of the scalar quantity \((\Delta : \Delta)\) and the rate of deformation tensor \(\Delta\), as they are given in tables A3 and A4 of Appendix A, by also taking into account eqns. (6.1)

\[ \tau_{rr} = -m \left[ \frac{3v_r}{r} \right]^2 + \left( \frac{v_r}{r} \right)^2 + \left( \frac{1}{r^2} \right)^2 \right] \]  \hspace{1cm} (6.5a)

\[ \tau_{\theta \theta} = \tau_{\phi \phi} = -m \left[ \frac{3v_r}{r} \right]^2 + \left( \frac{v_r}{r} \right)^2 + \left( \frac{1}{r^2} \right)^2 \right] \]  \hspace{1cm} (6.5b)

\[ \tau_{r \theta} = \tau_{\theta r} = -m \left[ \frac{3v_r}{r} \right]^2 + \left( \frac{v_r}{r} \right)^2 + \left( \frac{1}{r^2} \right)^2 \right] \]  \hspace{1cm} (6.5c)

\[ \tau_{r \phi} = \tau_{\phi r} = \tau_{\theta \phi} = \tau_{\phi \theta} = 0 \]  \hspace{1cm} (6.5d)
6.1.3 Volumetric Flow Rate

The volumetric flow rate \( Q \) of a fluid, passing a spherical surface of radius \( r \) is given by:

\[
Q = \int_{r}^{2T} \int_{0}^{\pi} v_r \cdot r^2 \sin \theta \, dr \, d\phi d\theta
\]

or

\[
Q = 2\pi \int_{0}^{\pi} v_r \cdot r^2 \sin \theta d\theta
\]  \hspace{1cm} (6.6a)

Substitution of eqn. (6.3a) into the above eqn. yields

\[
Q = 2\pi \int_{0}^{\pi} f(0) \sin \theta d\theta
\]  \hspace{1cm} (6.6b)

6.1.4 Distribution of Pressure

Combine eqns. (6.5) with (6.3), differentiate \( \tau_{rr} \) and \( \tau_{\theta\theta} \) with respect to \( r \) and \( \theta \) respectively, and \( \tau_{r\theta} \) with respect to \( r \) and \( \theta \); and substitute them back to eqns. (6.4) to produce:

\[
- \frac{\partial P}{\partial r} = \frac{m}{r^{3n+1}} \left\{ 12f^2(\theta) + f'^2(\theta) \right\}^{\frac{n-1}{2}} \left[ 12(1-n)f(\theta)f'(\theta) \cot \theta - f''(\theta) \right]
\]

\[
- (n-1)(f'(\theta))^2 \left[ 12f(\theta) + f''(\theta) \right] \left[ 12f^2(\theta) + f'^2(\theta) \right]^{\frac{n-3}{2}} \]  \hspace{1cm} (6.7a)

\[
- \frac{\partial P}{\partial \theta} = \frac{m}{r^{3n}} \left\{ 3nf'(\theta) \left[ 12f^2(\theta) + f'^2(\theta) \right]^{\frac{n-1}{2}} - 5f'(\theta) \left[ 12f^2(\theta) + f'^2(\theta) \right]^{\frac{n-1}{2}} \right\}
\]

\[
- 2(n-1)f(\theta) f'(\theta) \left[ 12f^2(\theta) + f'^2(\theta) \right]^{\frac{n-3}{2}} \]  \hspace{1cm} (6.7b)

The pressure terms from eqns. (6.7) can now be eliminated by differentiating eqns. (6.7a) and (6.7b) with respect to \( \theta \) and \( r \) respectively.

\[
- \frac{\partial^2 P}{\partial \theta^2} = \frac{m}{r^{3n+1}} \left\{ 12f^2(\theta) + f'^2(\theta) \right\}^{\frac{n-1}{2}} \left[ 12(1-n)f'(\theta) + f'(\theta) \cot^2 \theta - f''(\theta) \cot \theta \right]
\]

\[
- f'''(\theta) \]  \hspace{1cm} (n-1)(n-3) f'^3(\theta) (12f(\theta) + f''(\theta))^{2} (12f^2(\theta) + f'^2(\theta))^{\frac{n-5}{2}}
\[ f'(\theta) + \left( \frac{12f^2(\theta)+f'^2(\theta)}{2} \right) \left[ (12(1-n)f(\theta)-f'(\theta)\cot\theta-f''(\theta)) \right] \]

\[ f''(\theta) - \frac{3f'f''}{2} = -\frac{m}{z^{3n+1}} \left\{ 6n(n-1)f(\theta)f'(\theta) (12f(\theta)+f''(\theta)) (12f^2(\theta)+f'^2(\theta))^2 \right\} \]

By eliminating the pressure terms in eqns. (6.7), the following differential eqn. is obtained

\[ f'''(\theta) \left[ 12f^2(\theta)+f'^2(\theta) \right] = (12f^2(\theta)+f'^2(\theta)) \left\{ 12(1-n) + \csc^2(\theta) + 3n(3n-5) \right\} \]

Eqn. (6.8) is subjected to the following boundary conditions

i) at the wall, where \( \theta = \alpha \), there is no-slip i.e. \( f(\theta) = f(\alpha) = 0 \) (6.10a)

ii) at the centre, where \( \theta = \pi \), \( f'(\theta) = f'(0) = 0 \) (6.10b)

Equation (6.9) is a highly non-linear differential equation and it is not possible to solve it analytically. Numerical methods must then be used in conjunction with a high speed computer. The solution is computed using a finite-difference technique [1,2] with deferred correction allied to a Newton iteration, i.e. "iterated deferred correction" [3]. Each step of deferred correction is used to produce an approximation with a smaller global error, so in the first approximation the usual \( O(h^2) \) error expansion is used, in the next the error \( O(h^4) \), then the \( O(h^6) \) and so on, thus producing the equivalent of the method of "deferred approach to the limit" on the same mesh and without obtaining \( O(h^2) \) solutions at successively smaller intervals.
Due to the complication of the equation, it was found that an initial mesh had to be supplied for the finite difference equations as well as an initial approximate solution. As initial approximation, the Newtonian fluids solution was used. Further, due to the difficulty of the Newton iteration to converge a continuation facility, $\epsilon$, was adopted, where the solution for each step was evaluated by using the solution of its predecessor as a starting approximation. $\epsilon$ ranges from 0 to 1 and is related to the power-law index, $n$, by the equation:

$$f(n) = 1 - (1-n)\epsilon$$

At the centre of the cone (i.e. $\theta=0$) the trigonometric functions $\cot \theta$ and $\csc^2 \theta$ of eqn. (6.9) lead to indeterminacy of their corresponding terms. This was overcome by using L'Hopital's rule.

The volumetric flow rate $Q$ was evaluated from eqn. (6.6b) by numerically integrating [4,5] the computed $f(\theta)$ profile of eqn. (6.9). Since the two boundary conditions, provided by eqn. (6.10) are not sufficient a trial and error procedure has to be followed until a value of $f(0)$ can be found which will satisfy the required flow rate. The necessary subroutine is listed in Appendix C1. Alternatively a table of $f(0)$ vs $Q$ values can be made and the required $f(0)$ value for the desired flow rate can be interpolated [6,7].

A. At the centre, where $\theta=0$, and from eqn. (6.7a) the pressure across direction $r$ becomes, if one introduces the boundary condition (6.10b).
\[ \frac{3P}{\partial r} \bigg|_{\theta=0} = - \frac{m}{r^{3n+1}} \left\{ \frac{12 f^2(0)}{2} \left[ \frac{12 (1-n) f(0) - f''(0)}{\frac{n-1}{12}} \right] \right\} \]

or
\[ \frac{3P}{\partial r} \bigg|_{\theta=0} = - \frac{12}{2} \frac{m f^n(0)}{r^{3n+1}} \left[ 12 (1-n) \frac{f''(0)}{f'(0)} \right] \]

(6.11a)

Integrate with respect to \( r \) to obtain
\[ \Delta P [r_2-r_1, 0] = - \frac{(\sqrt{12})^{n-1} m f^n(0)}{3 n} \left[ \frac{1}{r_1^{3n}} - \frac{1}{r_2^{3n}} \right] \]

(6.11b)

B. At the die wall, where \( \theta = \alpha \), by combining eqns. (6.7a) and (6.10a), the pressure drop becomes:
\[ \frac{3P}{\partial r} \bigg|_{\theta=\alpha} = + \frac{m f'^n(\alpha)}{r^{3n+1}} \left[ \cot \alpha + n \frac{f''(\alpha)}{f'(\alpha)} \right] \]

(6.12a)

Integration with respect to \( r \), yields
\[ \Delta P [r_2-r_1, \alpha] = - \frac{m f'^n(\alpha)}{3n} \left[ \cot \alpha + n \frac{f''(\alpha)}{f'(\alpha)} \right] \left[ \frac{1}{r_1^{3n}} - \frac{1}{r_2^{3n}} \right] \]

(6.12b)

6.1.5 Newtonian Fluids

For Newtonian fluids, where \( n = 1 \), eqn. (6.9) reduces to
\[ f''(\theta) + f''(\theta) \cot \theta + f'(\theta) (6 - \csc^2 \theta) = 0 \]

(6.13)

Eqn. (6.13) is the same with that derived by Bond et al [8].

The solution of eqn. (6.13) subjected to boundary conditions (6.10) gives
\[ f(\theta) = C \left[ \cos 2\theta - \cos 2\alpha \right] \]

(6.14a)

where \( C \) is a constant.
Also \( f'(\theta) = -2C \sin 2\theta \) \hspace{1cm} (6.14b)

\( f''(\theta) = -4C [\cos^2 \theta - \sin^2 \theta] \) \hspace{1cm} (6.14c)

\( f'''(\theta) = 8C \sin 2\theta \) \hspace{1cm} (6.14d)

From eqns. (6.6b) and (6.14a)

\[
Q = 2\pi \int_0^\theta C [\cos 2\theta - \cos 2\alpha] \sin \theta \, d\theta
\]

or \[
C = \frac{3Q}{4\pi(2\cos^3 \alpha - 3\cos^2 \alpha + 1)} = \frac{3Q}{4\pi(1 - \cos \alpha)^2(1 + 2\cos \alpha)}
\] \hspace{1cm} (6.15)

Eliminate \( C \), by substituting eqn. (6.15) into (eqn. (6.14a) and then combine the resulting equation with eqn. (6.3a) to get:

\[
\frac{3Q}{4\pi r^2} \left[ \frac{\cos 2\theta - \cos 2\alpha}{2\cos^3 \alpha - 3\cos^2 \alpha + 1} \right]
\] \hspace{1cm} (6.16a)

If eqn. (6.3a) is adopted, eqn. (6.16a) gives

\[
Q = \frac{4}{3} \pi f(\theta) \left[ \frac{2\cos^3 \alpha - 3\cos^2 \alpha + 1}{1 - \cos 2\alpha} \right]
\] \hspace{1cm} (6.16b)

6.1.6 Energy Equation

The energy equation for spherical co-ordinates is obtained by combining eqns. (4.25), (6.1), (A3-B), (A3-E) and (A5-F) of Appendix A and by assuming that energy transfer by conduction in the \( \phi \) component may be neglected as contributing very little.

\[
\frac{\partial T}{\partial r} + \alpha \left[ \frac{1}{r^2} \left( 2r \frac{\partial T}{\partial r} + r^2 \frac{\partial^2 T}{\partial r^2} \right) + \frac{1}{r^2 \sin \theta} \left( \cos \theta \frac{\partial T}{\partial \theta} + \sin \theta \frac{\partial^2 T}{\partial \theta^2} \right) \right]
\]

\[
+ \frac{\eta(T)}{\rho C} \left[ 2 \left( \frac{\partial T}{\partial r} \right)^2 + \left( \frac{\partial T}{\partial \theta} \right)^2 \right]
\]

where \( \alpha = \text{thermal diffusivity} = \frac{K}{\rho C} \) \hspace{1cm} (6.17)

\( K = \text{thermal conductivity} \) \hspace{1cm} (6.18)
\[ \rho = \text{density} \]
\[ C = \text{specific heat} \]
\[ \frac{\partial v_r}{\partial r} \text{ and } \frac{\partial v_r}{\partial \theta} = \text{local shear rates} \]
\[ \eta(T) = \text{viscosity which is temperature dependent according to eqn (4.36)} \]

Eqn. (6.17) may be written as

\[ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial T}{\partial \theta} + \frac{\eta(T)}{\rho C} \left\{ 2 \left( \frac{\partial v_r}{\partial r} \right)^2 + \left( \frac{\partial^2 v_r}{\partial r^2} \right)^2 \right\} \]

Eliminating local shear rates and the \( v_r r^2 \) term from eqn. (6.19), by using the \( f(\theta) \) functions as they are given in eqns. (6.3) yields

\[ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial T}{\partial \theta} + \frac{r^2 \eta(T)}{\rho C f(\theta)} \left\{ \frac{12f_2^2(\theta) + f_1^2(\theta)}{r^5} \right\} \]

If one assumes that \( \frac{\partial T}{\partial \theta} = 0 \) on the grounds that except in unusual problems [9a] - mainly in liquid metals - the heat conduction in the \( r \)-direction is much smaller than the heat convection in the \( r \)-direction (the heat transport by fluid flow), and also takes into consideration the viscosity-temperature dependence expressed by eqn. (4.36), then the above eqn reduces to the following parabolic one:

\[ \left[ 2r - \frac{f(\theta)}{\alpha} \right] \frac{\partial^2 T}{\partial r^2} + \cot \theta \frac{\partial T}{\partial \theta} + \frac{2}{\alpha} \frac{\partial^2 T}{\partial \theta^2} + \frac{r^2 \eta(T)}{\rho C f(\theta)} \left\{ \frac{12f_2^2(\theta) + f_1^2(\theta)}{r^5} \right\} \]

Eqn. (6.20) is subjected to the following boundary conditions:

\[ i) \quad \text{at the centre of the cone, where } \theta = 0 \quad \frac{\partial T}{\partial \theta} = 0 \quad (6.21a) \]
\[ ii) \quad \text{at the wall, where } \theta = a \quad T(a) = \text{constant (known)} \quad (6.21b) \]

Also the temperature of the fluid at the entrance in the cone is known.

Eqn. (6.20) is a parabolic equation and can be solved by numerical means only. In order, then, to approximate its solution by finite difference method, a network of mesh points is established through the regions \( r_1 \leq r \leq r_2 \) and \( 0 \leq \theta \leq a \).
An implicit finite difference scheme was chosen. The derivatives of temperature were approximated by the Crank-Nicolson method. The choice of this scheme was due to the fact that the method is unconditionally stable and the convergence is independent of the $[\Delta R/(\Delta \theta)^2]$ value which restricts the convergence of the explicit schemes [10a,11a].

Approximation of derivatives by finite difference for mesh point $(i,j)$ as described in Table 5.1, gives the following equation:

$$
\begin{align*}
&\left[2r - \frac{f(\theta)}{a}\right] \frac{T_{i+1,j}-T_{i,j}}{\Delta r} + \cot \theta \left[\frac{T_{i+1,j+1}-T_{i+1,j-1}+T_{i,j+1}-T_{i,j-1}}{2(\Delta \theta)}\right] \\
&+ \frac{1}{2} \left[\frac{T_{i+1,j+1}-2T_{i+1,j}+T_{i+1,j-1}+T_{i+1,j}+T_{i,j+1}-2T_{i,j}+T_{i,j-1}}{(\Delta \theta)^2}\right] \\
&+ \frac{r^2a}{T} \exp(-bT_{i,j}) \left[\frac{12f^2(\theta)+f^2(\theta)}{r_i^6}\right] \frac{n+1}{2} = 0
\end{align*}
$$

which after rearrangement becomes

$$
C_j T_{i,j+1} + a_j T_{i,j} + b_j T_{i,j-1} = d_j \quad \text{for } 1 \leq j \leq N-1
$$
where \( RA = \Delta r/\Delta \theta \)^2

\[
\begin{align*}
a_j &= 2 \left[ 2r - \frac{f(\theta)}{\alpha} + RA \right] \\
b_j &= \cot \theta \Delta r - RA \\
c_j &= - \left[ RA + \cot \theta \Delta r \right] \\
d_j &= \left[ \cot \theta \Delta r + RA \right] T_{i+1,j+1} + 2 \left[ 2r - \frac{f(\theta)}{\alpha} - RA \right] T_{i+1,j} + \\
&+ \left[ RA - \cot \theta \Delta r \right] T_{i+1,j-1} + \frac{2 \Delta r^2 \exp(-bT_{i+1,j})}{K} \\
&+ \{ 12 \frac{f^2(\theta) + f'^2(\theta)}{r^6} \}^{\frac{n+1}{2}} 
\end{align*}
\]

The boundary condition eqn. (6.21a) implies that the problem is symmetrical with respect to the centre of the cone, but this leads to indeterminacy of the term \( \cot \theta \left( \frac{3T}{3\theta} \right) = 0/0 \). There are two ways to deal with this complication. One is to replace the polar co-ordinates with its Cartesian equivalent [11b] and the other is to apply L'Hopital's rule. The second method was followed in this work, thus eqn. (6.20) becomes

\[
\left[ 2r - \frac{f(\theta)}{\alpha} \right] \frac{3T}{3r} + 2 \frac{3^2T}{3\theta^2} + \frac{\Delta T}{\Delta \theta} \frac{\exp(-bT)}{K} \left[ \frac{12f^2(\theta) + f'^2(\theta)}{r^6} \right] \frac{n+1}{2} = 0
\]

(6.24)

If eqn. (6.24) is approximated by adopting the implicit scheme used for eqn. (6.20), then at \( j=0 \) the finite-difference approximation will include a fictitious temperature at point \( j=-1 \), i.e.

\[
\begin{align*}
&2 \left[ 2r - \frac{f(\theta)}{\alpha} \right] \left[ T_{i+1,j} - T_{i,j} \right] + 2 \frac{\Delta r}{\Delta \theta} \left[ T_{i+1,j+1} - 2T_{i+1,j} \right] + \\
&+ T_{i+1,j-1} + 2T_{i,j} + T_{i,j-1} + \frac{2 \Delta r^2 \Delta T \exp(-bT_{i,j})}{K} \\
&+ \left[ \frac{12f^2(\theta) + f'^2(\theta)}{r^6} \right] \frac{n+1}{2} = 0
\end{align*}
\]

(6.25)
This can be overcome by using the boundary condition $\partial T/\partial \theta = 0$ i.e.

$$\frac{\partial T}{\partial \theta} = \frac{1}{2} \left[ \frac{T_{i+1,j+1} - T_{i+1,j-1} + T_{i,j+1} - T_{i,j-1}}{2(\Delta \theta)} \right] = 0$$

\[ T_{i+1,j+1} + T_{i,j+1} = T_{i+1,j-1} + T_{i,j-1} \]

Substitute the above eqn into eqn (6.25) for $j=0$ (i.e. at $\theta=0$) and rearrange to produce

$$c_0 T_{i,1} + a_0 T_{i,0} = d_0$$

(6.26a)

where $a_0 = 2(r-RA) - \frac{f(0)}{a}$

$$c_0 = -2RA$$

$$d_0 = \left[ 2(r-RA) - \frac{f(0)}{a} \right] T_{i+1,0} + 2RA T_{i+1,1} + \frac{\Delta r \Delta x^2 a_T \exp(-b T_{i+1,0})}{K}$$

$$\left\{ \frac{12f^2(0) + f'^2(0)}{x^6} \right\}^n+1$$

The wall boundary conditions (at $j=N+1$) will supply one more equation, i.e.

$$a_N T_{i,N} + b_N T_{i,N-1} = d_N$$

(6.26b)

where

$$a_N = 2 \left[ 2r - \frac{f(\theta)}{a} + RA \right]$$

$$b_N = \left[ \cot \theta \frac{\Delta r}{2(\Delta \theta)} - RA \right]$$

$$d_N = \left[ \cot \theta \frac{\Delta r}{2(\Delta \theta)} + RA \right] \left[ T_{i+1,N+1} + T_{i,N+1} \right] + 2\left[ 2r - \frac{f(\theta)}{a} - RA \right] T_{i+1,N} +$$

$$\left[ RA - \cot \theta \frac{\Delta r}{2 \Delta \theta} \right] T_{i+1,N-1} +$$

$$\frac{2 \Delta r \Delta x^2 a_T \exp(-b T_{i+1,N})}{K} \left\{ \frac{12f^2(\theta) + f'^2(\theta)}{x^6} \right\}^n+1$$
Having established the finite difference equations for each grid point, a system of $N+1$ equations will result, which if it is expressed in matrix form becomes

$$
\begin{bmatrix}
    a_0 & c_0 & 0 & & & & \\
    b_2 & a_1 & c_1 & & & & \\
    & b_2 & a_2 & c_2 & & & \\
    & & b_j & a_j & c_j & & \\
    & & & & b_{N-1} & a_{N-1} & c_{N-1} \\
    & & & & b_N & a_N \\
\end{bmatrix} \begin{bmatrix}
    T_{i,0} \\
    T_{i,1} \\
    T_{i,2} \\
    T_{i,j} \\
    T_{i,N-1} \\
    T_{i,N} \\
\end{bmatrix} = \begin{bmatrix}
    d_0 \\
    d_1 \\
    d_2 \\
    d_j \\
    d_{N-1} \\
    d_N \\
\end{bmatrix}
$$

(6.27)

The matrix of coefficients $a$, $b$ and $c$ alone is called a tridiagonal matrix. The system of equations described in (6.27) can be readily solved by using the Thomas algorithm [10b,12a] which is simply a form of Gaussian elimination method without pivot points. If the matrix equation is generalised in the form ($AX=V$) then the equations for reduction to triangular form in this algorithm are

$$
\begin{align*}
    a_0 &= a_o, \quad \gamma_0 = \frac{c_0}{a_0}, \quad u_0 = \frac{v_0}{a_0} \\
    a_j &= a_j - b_j \gamma_{j-1}, \quad u_j = \frac{v_j - b_j u_{j-1}}{a_j} \quad \text{for } j = 1, 2, \ldots, N \\
    \gamma_j &= c_j/a_j \quad \text{for } j = 1, 2, \ldots, N-1
\end{align*}
$$

and the back-substitution solution is given by

$$
\begin{align*}
    x_N &= u_N \\
    x_j &= u_j - \gamma_j x_{j+1} \quad \text{for } j = N-1, N-2, \ldots, 0
\end{align*}
$$

Calculations were accomplished with the aid of a high speed computer. The program listing is shown in Appendix C2.
6.1.7 Comments

In paragraphs 6.1.1-5, we succeeded in reducing the set of partial differential equations to a single differential equation, obtaining at the end a solution for generalised power-law fluids, with some difficulties due to the equation being highly non-linear of third-order. On the other hand, the solution of Newtonian fluids was easily obtained analytically so it can be used, in order to explore some aspects of converging flows, otherwise known as Hamel flows, after Hamel who first investigated such problems [13].

Eqn (6.3) i.e. \( v_r = \frac{f(\theta)}{r^2} \) assumes that the flow is entirely radial i.e. the fluid particles move to the vertex along lines of constant \( \theta \) so that \( v_\theta = 0 \). Firstly, it will be examined to see if this assumption can possibly pass the boundary conditions. In that respect and for \( \theta = \pm a \), \( f(\alpha) = 0 \) which is proper, although some questions may arise about the validity of the boundary condition assumption itself, especially when one deals with rubber compounds (for a detailed discussion see Section 4.8). Furthermore as \( r \to \infty \), \( v_r \to 0 \) which is again physically correct. However, eqn.(6.3) does give an unbounded \( v_r \) as \( r \to 0 \) with \(-\alpha < \theta < \alpha \), but fortunately enough this was overcome by equipping the converging channel with an opening \( D_1 \) at \( r=r_1 \) (see Fig. 6.2) and considering only the region \( r>r_1 \) as the physical domain of the flow, in which case the singularity at \( r=0 \) will be harmlessly outside the region of physical interest.

Another frustration resulting from the rather peculiar nature of this problem is if one assumes Newtonian flow again, where the Navier-Stokes eqn (4.9), for purely radial flow patterns, for the \( \theta \)-component becomes [14a]

\[
\frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{v_r}{r^2} \right) = \frac{\partial P}{\partial \theta} \frac{3P}{\partial \theta} = \frac{2\mu}{r^2} \frac{\partial v_r}{\partial \theta}
\]

Introducing eqn. (6.3c) into the above eqn. and integrating with respect to \( \theta \), yields

\[
P = \frac{2\mu}{r^2} f(\theta) + g(r)
\]

Differentiate with respect to \( r \) to obtain

\[
\frac{3P}{\partial r} = - \frac{2\mu f(\theta)}{r^2} + g'(r)
\]
Substitution of the above equation into the r-component of the Navier-Stokes equation including also the \( \frac{\partial v_r}{\partial r} \) acceleration term \([14a]\) gives:

\[
\rho v_r \frac{\partial v_r}{\partial r} - \frac{6 \mu f'(\theta)}{r^4} + g'(r) = \mu \left( \frac{\partial^2 v_r}{\partial r^2} - \frac{2}{r} \frac{\partial v_r}{\partial r} \right)
\]

Replace the Laplacian operator by its equivalent as it is given in eqn.A5-E of Appendix A5 and then insert eqns. (6.3) to obtain

\[
- \frac{2 \rho f^2(\theta)}{r} - 6 \mu f(\theta) + r^4 g'(r) = \mu \left[ 6 f(\theta) - 4f(\theta) \cot \theta f'(\theta) + f''(\theta) - 2f \right]
\]

or

\[
r^4 g'(r) - \frac{2 \rho f^2(\theta)}{r} = \mu \left[ f''(\theta) + \cot \theta f'(\theta) + 6f(\theta) \right]
\]

Since the LHS is a function of \( r \) and the RHS is not, both sides must be equal to some constant, say \( c \). But consider further: setting the LHS equal to \( c \) the above eqn gives

\[
2 \rho f^2(\theta) = rc + r^5 g'(r)
\]  \( (6.28) \)

Again, both sides must be equal to some constant, so that \( f(\theta) \) itself must be a non-zero constant at all values of \( r \). But \( v_r \) is zero at the wall, when \( \theta = \pm \alpha \), so \( f(\theta) \) vanishes. Consequently, this means that even at low flow rates and small values of \( \alpha \) there must be a component of flow in the \( \theta \)-direction so that an eddy pattern results. However, this conclusion is questionable if one compares it with the experimental studies of White and his co-workers \([15]\), who found that for rubber materials the flow pattern through converging channels is a purely radial flow without hint of vortices, a situation which is completely different for the same compounds in diverging channels, as well as for molten plastics in both converging and diverging channels.

Perhaps this conclusion has something to do with the inherent mathematical structure of the problem itself and this can be further demonstrated by comparing wedge and conical flow dimensionally \([16]\). For wedge flow the relevant physical parameters are the fluid density, its viscosity, the wedge half-angle \( \alpha \) and the source output per unit length. The dimensions of these quantities are:
\[ [\rho] = M \text{ L}^{-3} \]
\[ [\mu] = M \text{ L}^{-1} \text{ T}^{-1} \]
\[ \alpha = \text{ dimensionless} \]
\[ [Q]_w = \text{L}^2 \text{ T}^{-1} \]

No combination of these parameters yields a length, so if sink flow were to produce a steady-state eddy pattern, the eddies would presumably be characterised by a length, expressible in terms of the parameters of the problem, but this did not happen. For flow in a cone, the dimensions of \( \rho \), \( \mu \) and \( \alpha \) are the same as for wedge flow, but

\[ [Q]_c = \text{L}^3 \text{ T}^{-1} \]

\[ \therefore \quad \frac{[Q]}{\mu} = \text{L} \]

which in a sense proves the mathematical validity of the conclusion drawn from eqn. (6.28).

Of course, such paradoxes arise in the solution of other creeping motion equations as well, see for example Stokes paradox [17].

Since 1916, when Hamel published his paper, people have tried to obtain an exact solution for the Navier-Stokes equations including the component in the \( \theta \)-direction but without much success. For an extensive investigation one may refer to Goldstein [18].

Turning now to energy eqn (6.27), one may realise that a kind of singularity has arisen at the corners where the vertical line corresponding to the initial conditions meets the horizontal line of the boundary conditions as it is shown schematically in Fig. 6.4.

This discontinuity exists because the common point \( T(r, \theta) = T(0, \alpha) \), has two different values, one from the \( r \)-axis and the other from the \( \theta \)-axis.

* If the origin is a sink \( f(\theta) \) has minus sign (our case) if it is source has plus sign.
Fig. 6.4: Corner singularity in polar coordinates

In contrast to the analytical solution where the effect of such discontinuities does not penetrate into the field of integration [19], with the finite-difference equations one would expect inaccurate and doubtful results, unless the discontinuity was removed. Suitable approaches to this direction include [19-21]:

a) A calculation of an analytical solution that is continuous near the discontinuity.

b) An adoption of a new set of independent variables by transforming both variables \((r, \theta)\) to a new set, such as \((R, \Theta)\), by means of the eqn:

\[
R = r \cdot \theta^\frac{1}{2}, \quad \Theta = \theta^\frac{1}{2}
\]

c) The use of the arithmetic average corresponding to \(r \to 0\) and \(\theta \to \alpha\). Lapidus [21] claims that by using this approach "the actual numerical value used at the corners is quickly 'washed out' in subsequent calculations and thus is not too important".

Albasiny [20] examined the practical use of (a) and (b) in a cylindrical heat conduction problem of the form

\[
\frac{\partial^2 \phi}{\partial t^2} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right)
\]

having an initial discontinuity in both function and derivative at a boundary point; He found that no special starting procedure was necessary to deal with the singularity since the effect of initial discrepancies in the solution appeared to die away with increase of the value of time. However, the author was also cautious about the appearance of similar behaviour of an equation not of the above form and also for non-linear cases.

In the present work, the approach (c) was used.
6.2 ESTIMATION OF MINIMUM DIE LENGTH IN NON-CIRCULAR DUCTS FROM MEMORY EFFECTS

Among the various qualitative explanations given about the origins of extrudate swell (see Section 3.4.1) the one termed 'memory effects' will be used here as a means to provide information about the minimum die length or the length of the preform section (see Section 2.5C).

The profile of the extrudate is affected by the geometrical configuration of the die entrance region as a result of the fact that the elastic component of the fluid responsible for elastic recovery effects is dependent on flow history. This means that the longer the land or transit time of the melt, the less the effect will be. However, the stresses which occurred at the entrance into the die channel relax while the melt is in the channel, but at the same time the melt is placed in a different stress field due to a new die geometry which, for the example of rectangular dies, is the parallel sections of the die. Minimisation of these effects may be achieved if the die land length L, is long enough so that the average transit of the melt through the die is at least equal to the mean relaxation time of the melt $t_R$ [22], i.e.

$$L \geq t_R \bar{v} \quad (6.29)$$

where $\bar{v}$ is the average velocity of the fluid.

![Fig. 6.5: Typical curves of extrudate swell B vs capillary L/R for fixed shear rates, $\dot{\gamma}$](image)

The curves in Fig. 6.5, which are fairly typical of extrudate swell B vs capillary L/R and the considerations given concerning factors affecting swell, makes it possible to describe the decay of swelling with length as an exponential dependence on the time of passage of the melt through the channel [23,24].
\[ B - B_\infty = (B_0 - B_\infty) e^{-K t} \]  \hspace{1cm} (3.17)

where \( B_0 \) and \( B_\infty \) are values of \( B \) at zero and infinite transit times, respectively; \( K \) is the decay rate constant (\( = \frac{1}{t_R} \)) and \( t \) is the transit time of the melt.

Introducing the concept of apparent shear rate at the wall \( \dot{\gamma}_w \) into eqn. (3.17), Bagley et al [24] have derived eqn. (6.30) below, which holds independently as to whether \( (L/R) \), the actual length-to-radius ratio, or \( [(L/R)+\delta] \), the effective capillary length-to-radius ratio, has been used

\[ B - B_\infty = (B_0 - B_\infty) \exp\left\{ -[(L/R) + \delta] [4K/\dot{\gamma}_w] \right\} \]  \hspace{1cm} (6.30)

The next step is to derive an expression for non-circular ducts, so that in conjunction with the preceding analysis, it will provide information about the length of the duct under consideration. Kozicki et al [25] have demonstrated that the fully established friction factor, \( f \), of a power-law fluid through ducts of arbitrary cross-sectional shape can be obtained by the circular cross-sections relation:

\[ f = \frac{16}{Re^*} \]  \hspace{1cm} (6.31)

where \( Re^* \) is the dimensionless 'generalised' Reynolds number defined by Kozicki and his co-authors as:

\[ Re^* = \frac{\rho \frac{v^2}{2n} D_h^n}{8^{n-1} a + b n \frac{m}{n}} \]  \hspace{1cm} (6.32)

where \( \rho \) is the density of the melt

\( m \) and \( n \) are the consistency and power-law index, respectively

\( a,b \) are constants which depend on the geometry of the channel

\( D_h \) is the hydraulic diameter

From the definition of Fanning friction factor \( f \) one may write for the case of fully developed flow through a duct [25,26] that

\[ f = \frac{2 \tau_w}{\rho \dot{\gamma}^2} = \frac{D_h (\Delta P/L)}{2 \rho \dot{\gamma}^2} \]  \hspace{1cm} (6.33)
where $\tau_w$ is the average wall shear stress and $\Delta P/L$ is the pressure drop gradient through the duct length $L$.

Combine eqns. (6.32) and (6.33) to obtain

$$Re^* = \frac{\rho v^{-2-n}}{\frac{8n-1}{a+bn}} \frac{D_n}{m} \frac{1}{\frac{1}{m}} \frac{D_h(\Delta P/L)}{2\rho v^2}$$

Substitute in the above equation the product $Re^*$ by its equivalent as it is given in eqn. (6.31) and solve for $\bar{v}$

$$\bar{v} = \left(\frac{n}{a+bn}\right) \frac{D_h}{8} \frac{1}{n} \frac{D_h}{4L} (\Delta P)^{1/n}$$

Let $A$ and $C$ be the cross-sectional area and the wetted perimeter (channel circumference) of the non-circular duct, respectively, then

$$D_h = \frac{4A}{C}$$

If $Q_{ncd}$ is the volumetric flow rate through a non-circular duct, then

$$\bar{v} = \frac{Q_{ncd}}{A}$$

Combine eqns. (6.34) and (6.35) to yield

$$\frac{Q_{ncd}}{A} = \left(\frac{n}{a+bn}\right) \frac{A}{2C} \left(\frac{1}{m}\right) \left[\frac{A.DP}{C.L}\right]$$

The volumetric flow rate $Q_{cd}$ of a power-law fluid through a circular duct of radius $R$ is given by [27]

$$\frac{Q_{cd}}{\pi R^3} = \left(\frac{n}{3n+1}\right) \frac{1}{m} \left[\frac{R.DP}{2L}\right]$$

Miller et al [28,29] demonstrated that

$$\tau_{cd,w}(\gamma_w) = \tau_{n cd,w}(\gamma_w)$$

where $\tau_{cd,w}(\gamma_w)$ and $\tau_{n cd,w}(\gamma_w)$ are, respectively, the average wall shear stresses for circular and non-circular ducts; but

$$\tau_{cd,w}(\gamma_w) = \frac{R \Delta P}{2L}$$
Combine eqns. (6.36)-(6.38) to obtain

\[
\frac{[Q_{ncd}/A]}{[(3n+1/n)(Q_{ncd}/R^3)]]} = \left(\frac{n}{a+bn}\right)\left(\frac{A}{2C}\right)
\]  

(6.39)

Substitute the denominator in the LHS of eqn. (6.39) by its equivalent \(\dot{\gamma}_w\) and rearrange to yield

\[
\dot{\gamma}_w = \left(\frac{a+bn}{n}\right)\left(\frac{2C}{A}\right) Q_{ncd}
\]  

(6.40)

The values of \(a\) and \(b\) for both rectangular and triangular geometries are given in Table 6.1 as a function of the aspect ratio \(E'\) (= minor side/major side) and half angle opening \(\alpha\) of the duct, respectively.

<p>| TABLE 6.1 Values of constants (a) and (b) for rectangular and triangular ducts [25] |
|---------------------------------|---------------------------------|
| <strong>RECTANGULAR DUCTS</strong>           | <strong>TRIANGULAR DUCTS</strong>            |</p>
<table>
<thead>
<tr>
<th>(E')</th>
<th>(a)</th>
<th>(b)</th>
<th>(\alpha)</th>
<th>(a)</th>
<th>(b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.50</td>
<td>1.00</td>
<td>5°</td>
<td>0.1547</td>
<td>0.6287</td>
</tr>
<tr>
<td>0.25</td>
<td>0.3212</td>
<td>0.8182</td>
<td>10°</td>
<td>0.1693</td>
<td>0.6332</td>
</tr>
<tr>
<td>0.50</td>
<td>0.2440</td>
<td>0.7276</td>
<td>20°</td>
<td>0.1840</td>
<td>0.6422</td>
</tr>
<tr>
<td>0.75</td>
<td>0.2178</td>
<td>0.6866</td>
<td>30°</td>
<td>0.1875</td>
<td>0.6462</td>
</tr>
<tr>
<td>1.00</td>
<td>0.2121</td>
<td>0.6766</td>
<td>40°</td>
<td>0.1849</td>
<td>0.6438</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>45°</td>
<td>0.1830</td>
<td>0.6395</td>
</tr>
</tbody>
</table>

**PROCEDURE**

1. Obtain extrudate swell data for different L/R ratio over a range of shear rates and plot them according to Fig. 6.5.

2. Use eqn. (6.30) to obtain the values of \(B_o\), \(B_w\) and \(K\) for each \(\dot{\gamma}_w\). This can be done by using an optimisation technique; for the present work the Fletcher-Reeves conjugate gradient optimisation method [30] was used, a logical diagram of which can be found in Appendix C3. The program implementing the algorithm finds the unconstrained minimum of the multi-variable non-linear function from extrudate swell, \(B\), vs L/R data directly.
3. Plot $K$ vs $\dot{\gamma}_w$.

4. For a given non-circular duct, since $a$, $b$, $n$ and $Q_{ncd}$ are known, use eqn. (6.40) to obtain $\dot{\gamma}_w$.

5. Use the $\dot{\gamma}_w$ value found in step 4 and the plot $K$ vs $\dot{\gamma}_w$ from step 3 to find the value of $K$.

6. In order to minimise the entrance effects, the die must have such a length so that the melt-mean relaxation time $t_R$ has to be equal to its average transit time $t_R$ through the die. Use eqns. (6.29 and (6.35a) and the value of $K$ obtained from step 5 to evaluate the necessary length.

7. Plot $B_0$ and $B_\infty$ vs $\dot{\gamma}_w$ from the values obtained in step 2.

8. From the required $\dot{\gamma}_w$ (found in step 4), evaluate $B_0$ and $B_\infty$.

9. Once $B_0$, $B_\infty$ and $K$ are known, plot $B$ vs $t$ according to eqn. (3.17) to see the variation of extrudate swell with respect to the melt-transit time.
6.3  RECTANGULAR AND SQUARE DUCTS

This section deals specifically with rectangular and square ducts. In Section 6.3.1 the combined flow-rate/pressure drop expression will be derived, assuming that the area and the length of the duct are known i.e. without making any allowances for extrudate swell. In Section 6.3.2, the necessary equations will be put forward for the prediction of normal stress difference (responsible for the swelling of the material) from the viscosity function. Also a brief discussion of the method of obtaining viscosity from capillary data will be included. The next step, which will be the subject of Section 6.3.3, is to correlate the wall average shear stress $\tau_{ncd,w}$ and the primary normal stresses difference $N_{i,j}$ occurring in these non-circular ducts, with the pressure $P$. The reasons for these correlations is (a) to correct the duct length due to entrance pressure drop based on the $\tau_{ncd,w}$ vs $P$ relation, and (b) to reduce (improve) extrudate swell based on the $N_{i,j}$ vs $P$ relation. Further, a technique is also proposed for reducing swell based on the velocity distribution expression (isovels) described in Section 6.3.1.

6.3.1  Predicting Non-Newtonian Flow

6.3.1.1  Transport equations

A.  Velocity field

Using the Cartesian coordinate system $(x,y,z)$ for the rectangular or square duct of cross-section area, $A$, as shown in Fig. 6.6 and by assuming that no secondary flow pattern occurs, the velocity field is given by

$$v = v_z = v_z(x,y) \quad (6.41a)$$

$$v_x = v_y = 0 \quad (6.41b)$$

* For convenience the subscript $z$ in the velocity has been dropped in the following sections.
B. Continuity equation

Apply continuity eqn. (4.4) to rectangular coordinates as they are given in Table A1 in Appendix A and by taking into account eqns (6.41), then

\[ \frac{\partial v}{\partial z} = 0 \]  

(6.42)

C. Momentum equation

Expand the equation of motion (4.6) for rectangular coordinates, see Table A2 in Appendix A to obtain

\[ \frac{\partial P}{\partial x} = \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{yx}}{\partial y} \]  

(6.43a)

\[ \frac{\partial P}{\partial y} = \frac{\partial T_{xy}}{\partial x} + \frac{\partial T_{yy}}{\partial y} \]  

(6.43b)

\[ \frac{\partial P}{\partial z} = \frac{\partial T_{xz}}{\partial x} + \frac{\partial T_{yz}}{\partial z} \]  

(6.43c)
D. **Boundary conditions**

By assuming that there is no slip at the wall

\[ v = 0 \text{ (on } \partial A \text{)} \]  
(6.44)

where \( \partial A \) is the boundary of \( A \).

6.3.1.2 **Rheological equation of state**

Combine eqn (4.18b) with the components of the scalar quantity \( \frac{\Delta}{2} \) and the rate of deformation \( \Delta \), as they are given in Tables A3 and A4 of Appendix A, by also taking into consideration eqns. (6.41), to yield

\[ \tau_{xz} = -m \left( \frac{\partial v}{\partial x} \right) \left\{ \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right\}^{\frac{n-1}{2}} \]  
(6.45a)

\[ \tau_{yz} = -m \left( \frac{\partial v}{\partial y} \right) \left\{ \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right\}^{\frac{n-1}{2}} \]  
(6.45b)

\[ \tau_{yy} = \tau_{xx} = \tau_{xy} = \tau_{yx} = \tau_{zz} = 0 \]  
(6.45c)

6.3.1.3 **Solution of Equations for Rectangular and Square Ducts**

Combine eqns. (6.43) and (6.45) to obtain

\[ (- \frac{\partial P}{\partial z}) = \frac{3}{\partial x} \left( \eta \frac{\partial v}{\partial x} \right) + \frac{3}{\partial y} \left( \eta \frac{\partial v}{\partial y} \right) \]  
(6.46a)

or its equivalent

\[ 2(- \frac{\partial P}{\partial z}) = \nabla^2 (nv) + \eta \nabla^2 v - \nabla^2 \eta \]  
(6.46b)

where \( \nabla^2 \) is the Laplacian operator given by eqn. A5-B of Appendix A

and \( \eta = m \left| \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right|^{\frac{n-1}{2}} \)  
(6.47a)

A dimensionless formulation of eqns (6.46) and (6.47) may be written as

\[ \frac{3}{\hat{x}} \left( \hat{\eta} \frac{\partial \hat{v}}{\partial \hat{x}} \right) + \frac{3}{\hat{y}} \left( \hat{\eta} \frac{\partial \hat{v}}{\partial \hat{y}} \right) = -1 \]  
(6.46c)

\[ \hat{\eta} = \left[ \left( \frac{\partial \hat{v}}{\partial \hat{x}} \right)^2 + \left( \frac{\partial \hat{v}}{\partial \hat{y}} \right)^2 \right]^{\frac{n-1}{2}} \]  
(6.47b)

where \( \hat{x} = \frac{x}{H}, \hat{y} = \frac{y}{H}, \hat{v} = \frac{v}{H}, \hat{w} = \frac{w}{H}^{1/n} (- \frac{\partial P}{\partial z})^{-1/n} \)  
(6.48)
Eqn. (6.46c) is an elliptic partial differential equation and can be solved by numerical means only in conjunction with a high speed computer. A finite difference approach was used, the main points of which are outlined below.

A network of grid points is firstly established through the region $0 \leq \hat{x} \leq w$ and $0 \leq \hat{y} \leq h$ as shown in Fig. 6.7 with grid spacing $(\delta \hat{x})$ and $(\delta \hat{y})$ respectively.

![Grid Network](https://via.placeholder.com/150)

**Fig. 6.7:** Grid network for a channel of arbitrary cross-section (blue lines are extrapolated points, green lines are boundary points)

Upon approximation of derivatives by finite differences for grid point $(i,j)$ - see Table 5.1 - eqn. (6.46c) gives:

$$
\frac{1}{(\delta y)^2} \left\{ \hat{n}_{i,j+1} + \hat{n}_{i,j} \right\} \left[ \hat{v}_{i,j+1} - \hat{v}_{i,j} \right] - \frac{1}{2} \left[ \hat{n}_{i,j-1} + \hat{n}_{i,j} \right] \left[ \hat{v}_{i,j} - \hat{v}_{i,j-1} \right] = -1
$$

$$
\frac{1}{(\delta x)^2} \left\{ \hat{n}_{i+1,j} + \hat{n}_{i,j} \right\} \left[ \hat{v}_{i+1,j} - \hat{v}_{i,j} \right] - \frac{1}{2} \left[ \hat{n}_{i-1,j} + \hat{n}_{i,j} \right] \left[ \hat{v}_{i,j} - \hat{v}_{i-1,j} \right] = -1
$$
which after some rearrangement yields
\[
\hat{v}_{i,j} = \frac{A_{i,j} \hat{v}_{i,j+1} + B_{i,j} \hat{v}_{i,j-1} + C_{i,j} \hat{v}_{i+1,j} + D_{i,j} \hat{v}_{i-1,j} + 1}{A_{i,j} + B_{i,j} + C_{i,j} + D_{i,j}}
\]  
(6.49)

where
\[
A_{i,j} = \frac{\hat{n}_{i,j+1} + \hat{n}_{i,j}}{2(\delta y)^2}
\]  
(6.50a)

\[
B_{i,j} = \frac{\hat{n}_{i,j-1} + \hat{n}_{i,j}}{2(\delta y)^2}
\]  
(6.50b)

\[
C_{i,j} = \frac{\hat{n}_{i+1,j} + \hat{n}_{i,j}}{2(\delta x)^2}
\]  
(6.50c)

\[
D_{i,j} = \frac{\hat{n}_{i-1,j} + \hat{n}_{i,j}}{2(\delta x)^2}
\]  
(6.50d)

Similarly eqn. (6.47b) results
\[
\hat{\eta}_{i,j} = m \left\{ \frac{(\hat{\nu}_{i+1,j} - \hat{\nu}_{i-1,j})^2}{(2 \delta x)^2} + \frac{(\hat{\nu}_{i,j+1} - \hat{\nu}_{i,j-1})^2}{(2 \delta y)^2} \right\}^{\frac{n-1}{2}}
\]  
(6.51)

To solve eqn. (6.49), the values of \(\hat{n}_{i,j+1}, \hat{n}_{i,j-1}, \hat{n}_{i+1,j}\) and \(\hat{n}_{i-1,j}\) at the points 2 to N in all the four sides of the rectangle must be evaluated. This means from eqn. (6.51), that the velocities at the points 3 to N-1 must be known (i.e. the blue velocities coloured at Fig. 6.7). From the definition of the forward-difference operator, \(\Delta\) see Table 5.1, and by extrapolation it may be obtained that [31]
\[
\hat{v}_{i,N+1} = 5\hat{v}_{i,N} - 10\hat{v}_{i,N-1} + 10\hat{v}_{i,N-2} - 5\hat{v}_{i,N-3} + \hat{\nu}_{i,N-4}
\]  
(6.52a)

\[
\hat{v}_{i,j} = 5\hat{v}_{i,j} - 10\hat{v}_{i,j-1} + 10\hat{v}_{i,j+1} - 5\hat{\nu}_{i,j} + \hat{\nu}_{i,j+1}
\]  
(6.52b)

\[
\hat{v}_{N+1,j} = 5\hat{v}_{N,j} - 10\hat{v}_{N-1,j} + 10\hat{v}_{N-2,j} - 5\hat{v}_{N-3,j} + \hat{\nu}_{N-4,j}
\]  
(6.52c)

\[
\hat{v}_{i,1} = 5\hat{v}_{i,2} - 10\hat{v}_{i,3} + 10\hat{v}_{i,4} - 5\hat{v}_{i,5} + \hat{\nu}_{i,6}
\]  
(6.52d)

Eqn. (6.49) was solved iteratively using the successive over-relaxation technique [12b, 32] and the grid point viscosities were updated during the iteration process in the light of the current estimates of velocities.
To accelerate the convergence of the iteration process, the following formula was used:

$$
\hat{v}_{\text{NEW}(I,J)} = \hat{v}_{\text{OLD}(I,J)} + \omega \left[v_C - \hat{v}_{\text{OLD}(I,J)}\right]
$$

(6.53)

where

- $\hat{v}_{\text{NEW}(I,J)} = \text{accelerated velocity value}$
- $\hat{v}_{\text{OLD}(I,J)} = \text{velocity value calculated at the k-1 iteration}$
- $v_C = \text{velocity value calculated at the k(current) iteration}$
- $\omega = \text{relaxation factor}$

The volumetric flowrate $Q$ in the duct can be estimated as

$$
Q = \iiint_A v(x,y) \, dx \, dy
$$

(6.54)

Introducing the dimensionless variables into eqn. (6.54) yields

$$
\lambda(n) \frac{3^{1/n} \left(- \frac{dp}{dz}\right)^{1/n}}{m^{1/n}}
$$

(6.55)

where the shape factor $\lambda(n)$ is given as

$$
\lambda(n) = \iiint_A \hat{v}(x,y) \, dx \, dy
$$

(6.56)

which depends on the duct geometry and the power-law index $n$.

To obtain $\lambda(n)$, the computed velocity profile, from eqn. (6.49) was integrated numerically by using Simpson's cubature formulae [33] which when applied over the grid network gives

$$
\lambda(n) = \frac{wh}{9} \sum_{i=0}^{m} \sum_{j=0}^{m} \left\{ \left[ \hat{v}_{2i,2j} + \hat{v}_{2i+1,2j} + \hat{v}_{2i+2,2j} + \hat{v}_{2i+2,2j+2} + \hat{v}_{2i,2j+2} \right] + 4[\hat{v}_{2i+1,2j} + \hat{v}_{2i+2,2j+1} + \hat{v}_{2i+2,2j+2} + \hat{v}_{2i+2,2j+2} + \hat{v}_{2i+1,2j+1}] + 16\hat{v}_{2i+1,2j+1} \right\}
$$

(6.57)

where

$$
w = \frac{\text{width}}{2n} ; \ h = \frac{\text{high}}{2m}
$$
6.3.1.4 Shear Rate Distribution

The shear rate \( \dot{\gamma} \) can be determined from the second invariant of shear rate, \( I_2 \), as it has been outlined in Section 4.3D, i.e.

\[
\dot{\gamma} = \frac{(\Delta \Omega)^2}{2}
\]

(6.58a)

Combination of eqns. (6.41), (6.58a) and A3-A of Appendix A yields

\[
\dot{\gamma} = \frac{\partial^2 \Omega}{\partial x^2} + \frac{\partial^2 \Omega}{\partial y^2}
\]

(6.58b)

Approximation of the derivatives of eqn. (6.58b) by finite difference for grid point \((i,j)\) using central difference - see Table 5.1 - gives

\[
\dot{\gamma}_{i,j} = \left[ \frac{\dot{v}_{i+1,j} - \dot{v}_{i-1,j}}{2(\delta x)} \right]^2 + \left[ \frac{\dot{v}_{i,j+1} - \dot{v}_{i,j-1}}{2(\delta y)} \right]^2 \dot{\gamma}
\]

(6.59)

A straightforward substitution of the velocities, obtained from the computer results of iteration described previously, will give the distribution of the shear rate in the duct.

Calculations were accomplished with the aid of the Honeywell-Multics computer at Loughborough University of Technology.

6.3.2 Prediction of Melt Elasticity from Viscosity Data

There are two ways to deal with the viscoelasticity of polymer melts. One way is to use constitutive equations which relate the stress tensor \( \tau \) with suitable kinematic variables expressing the motion of the continuum; but in that respect we are faced with two difficulties: (a) to find the "right" constitutive equation which will describe this relationship adequately and (b) because of the complexity of the equation, or the complexity which arises when it is combined with transport equations, it has been found that it is rather difficult to be amended to mathematical analysis. (For more details see Section 4.3). The alternative way is to split the viscoelastic melt behaviour into two parts: a viscous and an elastic part. The former part is associated with pressure drops and viscous dissipation while the latter is associated with phenomena
such as extrudate swell and the Weissenberg effect. Of course, strictly speaking such a distinction may not be justifiable on scientific grounds in the sense that one may consider it as a kind of superposition, something analogous to the superposition of pressure and drag flows for the evaluation of the flow rate in the extrudate. However, this distinction does provide some qualitative understanding of the process; and for this reason was chosen in the present work.

A quantitative measure of melt elasticity is the primary normal stress. In general, to obtain normal stresses from direct experimentation is very rare in process engineering in the polymer industry. One reason is that in order for normal stresses to be determined, rotational viscometers are needed, which have the disadvantage over capillaries of being more expensive in terms of capital cost, running cost and maintenance cost; thus they can only be found in large companies and research centres. Also, the shear rates at which they operate are small (<10 s⁻¹) compared to the shear rates encountered in industrial situations (e.g. extrusion operates at $10^2$ s⁻¹ - $10^3$ s⁻¹). Consequently there is a need for quick and inexpensive methods for estimating the normal stress functions. The viscosity function seems to fulfil these requirements, being a quantity widely used in the polymer industry, since it is relatively easy to measure in rather inexpensive equipment, such as capillary viscometers.

In the following the method of relating normal stress functions with viscosity will be put forward. In addition, the procedure used to convert capillary data into melt viscosity data will be discussed, especially from the programming point of view.

**PRIMARY NORMAL STRESS DIFFERENCE AS A FUNCTION OF VISCOSITY**

Bird et al [9b, 34] have proposed the following semi-empirical formula relating the primary normal stress difference function $N_1(\dot{\gamma})$ with the viscosity function $n(\dot{\gamma})$

$$ N_1(\dot{\gamma}) = \frac{4K}{\pi} \int_{0}^{\infty} \frac{n(\dot{\gamma}) - n(\dot{\gamma}')}{(\dot{\gamma}')^2 - \dot{\gamma}^2} d\dot{\gamma} $$

where $K$ is an empirical factor having the values of 2 for solutions and 3 for melts.
Equation (6.60) follows directly from the Goddard-Miller constitutive equation, which predicts that $K$ should be unity. However, Bird et al suggested using the above mentioned values of $K$ since the formula is a semi-empirical one.

Further they introduce the following non-dimensional quantities:

**Viscosity**

$$\eta = \frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty}$$  \hspace{1cm} (6.61a)

**Normal stress function**

$$\frac{\pi N_1(\dot{\gamma})}{4K\lambda(\eta_0 - \eta_\infty)}$$  \hspace{1cm} (6.61b)

**Shear rate**

$$\dot{\gamma}$$  \hspace{1cm} (6.61c)

where $\lambda$ is a time constant for the material. They also assumed that the viscosity function can be fitted by the Carreau viscosity eqn. (4.15). Then by combining eqns. (4.15), (6.60) and (6.61), they obtained:

$$\frac{\pi N_1(\dot{\gamma})}{4K\lambda(\eta_0 - \eta_\infty)} = \int_0^\infty \frac{1}{[1 + (\dot{\gamma}^*)^2]^{\frac{n-1}{2}}} - \frac{1}{[1 + (\dot{\gamma}^*)^2]^{\frac{n-1}{2}}} \frac{1}{[\dot{\gamma}^*]^2 - (\dot{\gamma})^2} d(\dot{\gamma})$$  \hspace{1cm} (6.62)

Theoretical prediction from eqn. (6.62) was compared with experimental results and according to Tadmor and Gogos [35] "the agreement is excellent for engineering purposes".

A. PROCEDURE FOR OBTAINING $N_1$ from $\eta$

1. Obtain the viscosity function vs shear rate: the procedure is described in Section 6.3.2(b).

2. Assume $\eta_\infty$ to be zero for melts (for solutions $\eta_\infty$ is equal to the solvent viscosity).

3. Determine $\eta_0$: for the present work $\eta_0$ was selected from capillary data as it has been proposed by Bird et al [34]. However, for a more accurate determination the sandwich viscometer may be used as described by Zakharenko et al in [36,37].

4. Evaluate $\lambda$ and $n$ of the Carreau viscosity equation (4.15) from the viscosity data: the Fletcher and Reeves conjugate gradient optimisation method may be used [30] – see Section 6.2 and Appendix C3. Alternatively one may use the plots provided by Bird et al [34].
5. Once \( \eta_0, \eta, \lambda, \) and \( n \) have been determined, the \( N \) vs \( \gamma \) curve can be estimated either by numerically integrating the integral of eqn. (6.62) or using the master plots provided by Bird et al. Actually their plots have been obtained by numerical integration up to \( \lambda \gamma' = 10^5 \) for \( \lambda \gamma \leq 10^3 \) and for different values of \( n \).

In cases where the viscosity function is known in the form of the power-law model

\[
\eta = m \cdot \gamma^{n-1}
\]  

(4.13a)

the normal stress function can be estimated through eqn. (6.63) below:

\[
N_1 = m' \cdot \gamma^{n'-2}
\]  

(6.63)

The relation between \( n \) vs \( n' \) and \( m \) vs \( m' \) are obtained through figs 6.8 and the relation

\[
\lambda = \left| \frac{m}{\eta_0} \right|^{1/(n-1)}
\]  

(6.63a)

Fig. 6.8: Prediction of melt elasticity from viscosity data:
(a) Relation between power law parameters \( n' \) (in \( N = m' \cdot \gamma^{n'-2} \)) and \( n \) (in \( \eta = m' \cdot \gamma^{n-1} \)); (b) relation of power law parameters \( m' \) and \( m \) as a function of the time constant \( \lambda \) for different values of \( n \).

{Adopted from Abdell-Khalik et al [34]}. 
B. PROCEDURE FOR OBTAINING THE VISCOSITY FUNCTION VS SHEAR RATE

By using the Davenport constant shear rate rheometer, see Section 7.2.4, sets of shear rate/pressure drop raw data were obtained for a series of dies of similar radius but different lengths, over a number of different temperatures. The procedure for correcting these data was as follows:

1. Using eqn. (3.8) obtain the value of Q for each \( \dot{\gamma}_w \) [eqn. (3.8): \( \dot{\gamma}_w = 4Q/\pi R^3 \)].
2. Obtain the dimensionless parameters \( a, b \) and \( c \) from eqn. (3.14) [eqn. (3.14): \( \log \Delta P = a + b \log \dot{Q} + c(\log \dot{Q})^2 \)].
3. Select, arbitrarily, some values of \( \dot{\gamma}_w \) and calculate by means of eqn. (3.8) the corresponding flow rate, \( \dot{Q} \), values.
4. Knowing \( a, b \) and \( c \) from step 2 calculate by means of eqn. (3.14), the pressure drop \( \Delta P \) for each of the calculated values of \( \dot{Q} \) from step 3.
5. Repeat the above steps for all \( L/R \) ratios.
6. Bagnold correction: Plot \( \Delta P \) vs \( L/R \) for each \( \dot{\gamma}_w \) in order to obtain according to eqn. (3.12) [eqn. (3.12): \( \tau_w = \frac{\Delta P}{2(\frac{\dot{\gamma}_w}{L/R} + E)} \)]

\[ \tau_w = \frac{\text{slope}}{2} \]
and
\[ E = \text{intercept on the x-axis (i.e. L/R axis).} \]
7. Using the \( \tau_w \) vs \( \dot{\gamma}_w \) results of step 6, evaluate by means of eqn. (3.15), the dimensionless parameters \( B \) and \( C \) [eqn. (3.15): \( \log \tau_w = A + B \log \dot{\gamma}_w + C(\log \dot{\gamma}_w)^2 \)].
8. Rabinowitsch correction: for each of the selected \( \dot{\gamma}_w \) and knowing \( A, B \) and \( \Gamma \) from step 7, calculate \( n^* \) and \( \dot{\gamma}_{\text{corr}} \) by means of eqns. (3.9) and (3.10) i.e.

\[ n^* = B + 2C \log \dot{\gamma}_w \]  
(3.10)

\[ \dot{\gamma}_{\text{corr}} = \frac{\dot{\gamma}_w}{4} \left[ 3 + \frac{1}{n^*} \right] \]  
(3.9)
9. Melt viscosity: From the known values of \( \tau_w \) and \( \dot{\gamma}_{\text{corr}} \), evaluate the melt viscosity, \( \eta \), from

\[ \eta = \frac{\tau_w}{\dot{\gamma}_{\text{corr}}} \]
10. Repeat the above procedure for all temperatures.

Every time the logarithmic parabola equation \( \log Y = \alpha + \beta \log X + \gamma (\log X)^2 \) was used, measures of goodness of fit and 95% confidence limits on the parameters \( \beta \) and \( \gamma \) were calculated.

6.3.3 Correlation of Shear Stress (\( \tau_{sp} \)) with Pressure

A. CORRELATION OF THE WALL AVERAGE SHEAR STRESS WITH PRESSURE

In order to obtain the wall average shear stress, it seemed necessary to deal with mechanical equilibrium at the duct wall surfaces [38,39]. For steady flow and by referring to Fig. 6.6

\[
H W \Delta P = 4 L \left\{ \int_{-H/2}^{H/2} \tau_w(Y) dY + \int_{-W/2}^{W/2} \tau_w(X) dX \right\}
\]

(6.64)

where \( \tau_w(X) \) and \( \tau_w(Y) \) are the shear stresses at the wall surfaces at \( Y = \pm H/2 \) and \( X = \pm W/2 \), respectively. Rearrange eqn. (6.64) to obtain

\[
\frac{H W \Delta P}{H+W} = \frac{H W}{H+W} \left\{ \int_{-H/2}^{H/2} \frac{\tau_w(Y) dY}{H} + \int_{-W/2}^{W/2} \frac{\tau_w(X) dX}{W} \right\}
\]

(6.65)

where the RHS of eqn. (6.65) is defined as the wall average shear stress \( \tau_{ncd,w} \), the eqn. (6.65) becomes [40]

\[
\tau_{ncd,w} = \frac{\Delta P}{L} \frac{H W}{2(H+W)}
\]

(6.66)

If \( \gamma_{ncd,w} \) is the wall average shear rate of the duct, corresponding to \( \tau_{ncd,w} \), then by analogy to eqn. (6.65)

\[
\gamma_{ncd,w} = \frac{H}{H+W} \left\{ \int_{-H/2}^{H/2} \frac{\gamma_w(Y) dY}{H} + \int_{-W/2}^{W/2} \frac{\gamma_w(X) dX}{W} \right\}
\]

or

\[
\gamma_{ncd,w} = \frac{2}{H+W} \left\{ \int_{-H/2}^{H/2} \frac{\gamma_w(Y) dY}{H} + \int_{-W/2}^{W/2} \frac{\gamma_w(X) dX}{W} \right\}
\]

(6.67)

where \( \gamma_w(Y) \) and \( \gamma_w(X) \) are the shear rates at the wall surfaces at \( Y \) and \( X \) respectively.
Since the shear rate distribution is known from eqn. (6.59), $\dot{\gamma}_{ncd,w}$ can be easily evaluated by integrating numerically [5] each of the bracketed terms of eqn. (6.67).

PROCEDURE

1. Knowing the power-law index $n$ of the material from procedure 6.3.2:B and the range of shear rates over which the extruder can operate, obtain the values of $Q$, $\dot{\gamma}_w(X)$ and $\dot{\gamma}_w(Y)$, $\dot{\gamma}_{ncd,w}$ and $\dot{\gamma}_{ncd,w}$ from eqns. (6.54), (6.59), (6.67) and (6.66) respectively for different pressure gradients.

2. Repeat the same procedure for different aspect ratios $E'$ ($E' = W/H$).

3. Plot $\Delta P$ vs $L/R_H$ (where $R_H$ = hydraulic radius) for each $\dot{\gamma}_{ncd,w}$.

The negative intercept $E$ on the $L/R_H$ axis will give the corrected duct length, something similar to Bagley end correction.

4. Plot $\dot{\gamma}_{ncd,w}$ vs $\dot{\gamma}_{ncd,w}$ and compare it with the $\tau$ vs $\dot{\gamma}$ plot for the capillary.

B. CORRELATION OF PRIMARY NORMAL STRESS FUNCTION, $N_l$, WITH PRESSURE

Han [41] has proposed that for a rectangular duct:

$$\frac{(\tau_{zz}-\tau_{xx})W/2,Y_i,L}{(\tau_{11}-\tau_{22})W/2,Y_i,L} = \frac{P_{W/2,Y_i,L}}{P_{W/2,Y_i,L}}$$  \hspace{1cm} (6.68a)$$

$$\frac{(\tau_{zz}-\tau_{yy})X_i,H/2,L}{(\tau_{11}-\tau_{33})X_i,H/2,L} = \frac{P_{X_i,H/2,L}}{P_{X_i,H/2,L}}$$  \hspace{1cm} (6.68b)$$

where $(\tau_{11}-\tau_{22})W/2,Y_i,L$ and $(\tau_{11}-\tau_{33})X_i,H/2,L$ are, respectively, the normal stress differences along the long and short sides of the rectangle at the exit: $P_{W/2,Y_i,L}$ denotes the exit pressure at $X = W/2$ and $Y = Y_i$, while $P_{X_i,H/2,L}$ denotes the exit pressure at $X = X_i$ and $Y = H/2$. To simplify the nomenclature (refer to Fig. 6.5) eqns. (6.68) may be written as

$$\frac{(\tau_{11}-\tau_{22})A,L}{(\tau_{11}-\tau_{33})A,L} = \frac{P_{A,L}}{P_{A,L}}$$  \hspace{1cm} (6.69a)$$

$$\frac{(\tau_{11}-\tau_{33})B,L}{(\tau_{11}-\tau_{33})B,L} = \frac{P_{B,L}}{P_{B,L}}$$  \hspace{1cm} (6.69b)$$
Since the primary normal stress differences are related to the shear rate by means of eqn. (3.4) i.e.

\[
\tau_{ii} - \tau_{jj} = N_1 \cdot \dot{\gamma}^2_{ij} \tag{3.4}
\]

then eqns. (6.69) may be written as:

\[
P_{A,L} = N_{1,A} \cdot \dot{\gamma}^2_{12} \tag{6.70a}
\]

\[
P_{B,L} = N_{1,B} \cdot \dot{\gamma}^2_{13} \tag{6.70b}
\]

where \(\dot{\gamma}_{12}\) and \(\dot{\gamma}_{13}\) are the wall shear rates at faces A and B, respectively.

From eqn. (A2-C) in Appendix A, it is clear that \(\partial P/\partial z\) is a constant [42], therefore

\[
\left(\frac{\Delta P}{L}\right)_A = \left(\frac{\Delta P}{L}\right)_B
\]

or

\[
\frac{P_{A,O} - P_{A,L}}{L_A} = \frac{P_{B,O} - P_{B,L}}{L_B} \tag{6.71}
\]

where \(P_{A,O}\) and \(P_{B,O}\) are the inlet pressures to the duct at faces A and B, respectively; \(L_A\) and \(L_B\) are the lengths of faces A and B respectively.

Combining eqns. (6.70) and (6.71) to obtain

\[
\frac{L_A}{L_B} = \frac{P_{A,O} - N_{1,A} \cdot \dot{\gamma}^2_{12}}{P_{B,O} - N_{1,B} \cdot \dot{\gamma}^2_{13}} \tag{6.72}
\]

Since the flow has been assumed to be fully developed, then at the inlet the pressure has to be the same i.e. \(P_{A,O} = P_{B,O} = P_{IN}\), thus

\[
\frac{L_A}{L_B} = \frac{P_{IN} - N_{1,A} \cdot \dot{\gamma}^2_{12}}{P_{IN} - N_{1,B} \cdot \dot{\gamma}^2_{13}} \tag{6.72a}
\]

Eqn. (6.72a) indicates clearly that if \(\dot{\gamma}_{12}\) and \(\dot{\gamma}_{13}\) are known, the ratio of the rectangle lengths can be established. Presumably for square ducts where \(\dot{\gamma}_{12} = \dot{\gamma}_{13}\), \(L_A = L_B\).
PROCEDURE

1. Use eqn. (6.59) to obtain the shear rate distribution.
2. Since maximum swell occurs at the centre of each face in the extrudate, select the centre wall shear rates as the reference point.
3. From procedures 6.3.2A and B, find the primary normal stress coefficients $N_{1,A}$ and $N_{1,B'}$ corresponding to each wall shear rate obtained from step 2.
4. Use the exit pressure from the converging section as $P_{IN}$ in conjunction with eqn. (6.72a) to obtain the ratio $L_A/L_B$ of the duct.

It is obvious from the above procedure that a kind of 'physical' singularity arises since the two faces A and B have to meet each other in a common corner. To overcome this difficulty steps (1) - (4) can be repeated for each shear rate moving each time from the reference points towards the common corner where the shear rates are "theoretically" zero. Alternatively, use of the average of the two length values found at the reference points will provide a compromise indication of the duct-length needed to produce uniform swell.

However, since it is practically impossible to avoid swell, an additional technique may be used to further improve the situation which, in basic steps, is as follows:

By using procedure 6.3.1, where the velocity distribution in profile dies is described, select an isovel, say (i) in Fig. 6.9a and enlarge it to the same dimensions as that of the extrudate. This means that the isovel will expand outwards as Fig. 6.9b, shows. Then, mirror (fold) the isovel inwards to the duct, Fig. 6.9c, and this will provide both the height and width of the die lips.

Since the proposed technique is an empirical one, thus needing to follow a trial and error procedure, it is a good practice to start experimenting by using isoveels close to the die walls and then if the isoveels chosen first proved incorrect, move to those remote to the walls. Obviously drawing on the knowledge of an expert die maker would be of great importance here in order to minimise experimentation time while learning to use the technique. A final point is that the technique can be equally applied to any shape where isoveels are available.
Fig. 6.9: Use of the isovels to reduce extrudate swell in non-circular cross-sections
6.4 TRIANGULAR DUCTS

This section deals with triangular ducts where the non-Newtonian flow behaviour (i.e. flow-rate/pressure drop relation) for a generalised incompressible power-law fluid is considered. The performance of the variational principle method described in Section 6.4.1 is compared with the finite difference method described in Section 6.4.2.

6.4.1 Variational Principle Method

For laminar steady flow, through a triangular duct bounded by the straight lines \( y = \pm wx \) and \( x = a \), with the fluid flowing axially in the \( z \)-direction as shown in Fig. 6.10, if it is assumed that eqns (4.18b) and (6.73) hold, then \( v \) will be such that the integral \( J \) is a minimum \([9c, 43, 44]\)

\[
\begin{align*}
& v_x = v_y = 0 \quad \text{(6.73a)} \\
& v = v_z = v_z (x,y) \quad \text{(6.73b)} \\
& \tau_{ij} = m \left( \frac{A_i A_j}{2} \right)^{\frac{n-1}{2}} \Delta_{ij} \quad \text{(4.18b)} \\
& J = \iint_A \left\{ \frac{m}{n+1} \left[ \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] + \frac{\partial p}{\partial z} v \right\} dx dy \quad \text{(6.74)}
\end{align*}
\]

Fig. 6.10: Orientation of the coordinate system in a triangular duct
To apply the variational principle, an assumed function must be found which will minimise the integral. More specifically, a velocity distribution (in this case) must be assumed which can be expressed in terms of a linear combination of basis functions with coefficients to be determined. The trial velocity distribution must satisfy the continuity eqn. (4.4) and the boundary conditions for all values of the arbitrary constants in order to assure convergence of the true solution.

The velocity was assumed to be of the form [9c, 45]

\[ v = \left( \frac{y^2 - wx^2}{wx} \right) (x-a) (b + cx + dx^2 + ex^3 + \ldots) \] (6.75)

where \( b, c, d, e \ldots \) are variational parameters.

For convenience, assume \( c, d, e \ldots \) to be zero and combine eqns (6.74) and (6.75) to give

\[
J = \int_a^b \int_0^{-wx} \left\{ \left( \frac{m}{m+1} \right) b^{n+1} \left[ y^2 - 2 \left( 3w^2 - 2 \right)x^2 - 2x \left( w^2 - 2 \right)x - 2a^2 \right] \right\} dy dx
\]

\[ + \frac{n+1}{2} w^4 x^2 (3x - 2a)^2 \]

\[ + b \frac{dp}{dz} \left( \frac{y^2 - w^2 x^2}{wx} (x-a) \right) dy dx \] (6.76)

Transform the variables to make the integral more suitable [46], thus let

\[
f = \frac{x}{a} \quad \text{and} \quad g = \frac{y}{wx}
\]

then at every point in the region \( 0 \leq f \leq 1 \) and \(-1 \leq g \leq 1\). Also

\[
A_{(x,y)} = \frac{1}{A_{(f,g)}} = \frac{1}{\det \begin{vmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \end{vmatrix}} \text{ for the Jacobian}
\]

Hence

\[
A_{(f,g)} = \det \begin{vmatrix} 1/a & 0 \\ -y/wx & 1/\text{wx} \end{vmatrix} = \frac{1}{awx}
\]

and

\[
A_{(x,y)} = awx
\]
From the theory [5]:

$$\int \int_R v(x,y)dydx = \int \int_S F(f,g) \left[ \frac{\partial (x,y)}{\partial (f,g)} \right] df \; dg$$ \hspace{1cm} (6.78)

where $F(f,g)$ is derived from $v(x,y)$ by substituting for $x,y$ in terms of $f,g$ and $S$ is the region in the $fg$-plane corresponding to $R$ in the $xy$-plane, and where $\frac{\partial (x,y)}{\partial (f,g)}$ is a factor called the Jacobian, see eqn.(6.77).

Using the rule from eqn. (6.78)

$$J = \left( \frac{m}{n+1} \right) b^{n+1} \int \int_{0}^{1} \left\{ -2 \right\} y^2 + w^h x^2 (3x-2a)^2 \frac{awx}{a} df \; dg + \frac{dp}{dz} b \int \int_{0}^{1} (y^2 - w^h x^2) (x-a)awx \; dy \; df$$

or

$$J = \left( \frac{m}{n+1} \right) ab^{n+1} w F + I$$ \hspace{1cm} (6.79)

where

$$F = \int \int_{0}^{1} \left\{ w^h a^h b^h - 2 \right\} a w^h a^2 f^2 - 2a w^h a^2 g^2$$

$$+ w^h a^2 f^2 (3f-2a)^2 \frac{awx}{a} df \; dg$$

or

$$F = w^h b^n a^{2n+3} \int \int_{0}^{1} \left\{ z^2 y^2 - 2 \right\} (3f-2) f - \frac{2(f-1)}{w^h} g^2$$

$$+ (3f-2)^2 \frac{n+1}{2} z^n \; df \; dg$$ \hspace{1cm} (6.80)

and

$$I = abw \frac{dp}{dz} \int \int_{0}^{1} \left\{ w^h a^2 f^2 g^2 - a^2 w^h f^2 \right\} (af-a) df \; dg$$

or

$$I = \frac{1}{15} w^h a^5 b \frac{dp}{dz}$$ \hspace{1cm} (6.81)

Combining eqns. (6.79-(6.81)

$$J = \left( \frac{m}{n+1} \right) a^{2n+2} b^{n+1} w^{2n+3} F A + \frac{1}{15} a^5 w^3 b \frac{dp}{dz}$$ \hspace{1cm} (6.82)
where \( FA = \int_0^{n+2} \int_{-1}^{1} \left[ f^2 g^4 - 2 \left( (3f-2)f - \frac{2(f-1)^3}{w^4} \right) g^2 + (3f-2)^2 \right]^{\frac{n+1}{2}} \frac{dg df}{\ln(g)} \) \( (6.83) \)

In order to find the optimum value of \( b \), \( J \) must be minimised, i.e.

\[
\frac{\partial J}{\partial b} = (m) (n+1)b^n a^{2(n+2)} w^{2n+3} FA + \frac{1}{15} a^5 w^3 \frac{dP}{dz}
\]

Since \( \frac{\partial J}{\partial b} = 0 \), \( m b^n a^{2(n+2)} w^{2n+3} FA = -\frac{1}{15} a^5 w^3 \frac{dP}{dz} \)

or \( b = \frac{1}{a^2 w^3} \left[ \frac{a (dP/dz)}{15m FA} \right]^{1/n} \) \( (6.84) \)

The flow rate \( Q \) can now be determined by eqn. (6.85)

\[
Q = \int_{a}^{a'wx} v dy dx \quad (6.85)
\]

Combine eqn. (6.75) with eqn. (6.85) to obtain

\[
Q = \int_{a}^{a'wx} \{y^2-w^2x^2\}(x-a)b dy dx
\]

or \( Q = \frac{1}{15} ba^5 w^3 \) \( (6.86) \)

Substitute eqn. (6.84) into eqn. (6.86) to obtain

\[
Q = \frac{a^3 w}{15} \left[ \frac{a (dP/dz)}{15m FA} \right]^{1/n} \quad (6.87)
\]

To find the volumetric flowrate, \( Q \), the integral \( FA \) has first to be estimated. Numerical means in conjunction with a high speed computer was used. Both the outer integral \( FA \) and the inner integrals \( \ln(g) \) were evaluated by a method, described by Patterson [47,48] of the optimum addition of points to Gauss quadrature formulae. The method uses a family of interlacing common point formulae. Beginning with the 3 point Gaussian rule, formulae using 7, 15, 31, 63, 127 and finally 255 points are derived. Each new formula contains all the pivots of the earlier formulae so that no function evaluations are wasted. Each integral is evaluated by applying
these formulae successively until two results are obtained which differ by less than the specified absolute accuracy.

**Newtonian Fluids**

For Newtonian fluids \((n=1)\) and equilateral triangle \((w=1/\sqrt{3})\), eqns. (6.83 and 6.84) are reduced to

\[
(FA)_N = \frac{8}{30} \quad (6.88a)
\]

and

\[
b_N = \frac{1}{a^2 w^2} \left| \frac{a(dP/dz)}{15\mu (FA)_N} \right| \quad (6.88b)
\]

respectively, where the subscript \(N\) refers to Newtonian fluids.

Combination of eqns. (6.75) and (6.88) yields

\[
v = \left[ \frac{3(dP/dz)}{4a\mu} \right] (y^2 - \frac{x^2}{3}) (x-a) \quad (6.89)
\]

Eqn. (6.89) is the same with the one derived by Bird et al [9c] for Newtonian fluids.

**6.4.2 Finite Difference Method**

![Triangular coordinates](image)

**Fig. 6.11: Triangular coordinates**
The three triangular coordinates \( \theta, \phi \) and \( \psi \)(Fig. 6.11) will be used as a means to locate a point in a plane. A constant ratio \( \psi/\phi \), \( \psi/\psi \) or \( \psi/\theta \) is maintained along the three coordinates, so that only two coordinates are essential.

Assuming the direction \( \theta \) coincident with the x-axis and calling \( \alpha \) and \( \beta \) the angles between \( \phi \) and \( \theta \), and \( \psi \) and \( \theta \), the transformation from Cartesian to triangular coordinates becomes

\[
x = \theta + \phi \cos \alpha + \psi \cos \beta \tag{6.90a}
\]
\[
y = \phi \sin \alpha + \psi \sin \beta \tag{6.90b}
\]

The partial derivatives of \( x \) and \( y \) with respect to \( \theta, \phi \) and \( \psi \) are therefore

\[
\frac{\partial x}{\partial \theta} = 1 \quad \frac{\partial x}{\partial \phi} = \cos \alpha \quad \frac{\partial x}{\partial \psi} = \cos \beta \tag{6.91a}
\]
\[
\frac{\partial y}{\partial \theta} = 0 \quad \frac{\partial y}{\partial \phi} = \sin \alpha \quad \frac{\partial y}{\partial \psi} = \sin \beta \tag{6.91b}
\]

A function \( f(x,y) \) may be considered a function of \( \theta, \phi \) and \( \psi \) through the intermediate functions \( x,y \) defined by eqns. (6.90) and its derivatives may be computed by the rule for the differentiation of composite functions. Thus by eqns. (6.91)

\[
\frac{\partial f}{\partial \theta} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \theta} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \theta} = \frac{\partial f}{\partial x} \tag{6.92a}
\]
\[
\frac{\partial f}{\partial \phi} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \phi} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \phi} = \frac{\partial f}{\partial x} \cos \alpha + \frac{\partial f}{\partial y} \sin \alpha \tag{6.92b}
\]
\[
\frac{\partial f}{\partial \psi} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \psi} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \psi} = \frac{\partial f}{\partial x} \cos \beta + \frac{\partial f}{\partial y} \sin \beta \tag{6.92c}
\]

and 'squaring' these operators

\[
\frac{\partial^2 f}{\partial \theta^2} = \frac{\partial^2 f}{\partial x^2} \tag{6.93a}
\]
\[
\frac{\partial^2 f}{\partial \phi^2} = \frac{\partial^2 f}{\partial x^2} \cos^2 \alpha + 2 \frac{\partial^2 f}{\partial x \partial y} \sin \alpha \cos \alpha + \frac{\partial^2 f}{\partial y^2} \sin^2 \alpha \tag{6.93b}
\]
\[
\frac{\partial^2 f}{\partial \psi^2} = \frac{\partial^2 f}{\partial x^2} \cos^2 \beta + 2 \frac{\partial^2 f}{\partial x \partial y} \sin \beta \cos \beta + \frac{\partial^2 f}{\partial y^2} \sin^2 \beta \tag{6.93c}
\]
Substitute eqn. (6.39a) in eqns. (6.39b) and (6.39c) and eliminating $\partial f/\partial x \partial y$ between these last two equations, $\partial^3 f/\partial y^2$ becomes

$$\frac{\partial^3 f}{\partial y^2} = \frac{\partial^3 f/\partial \beta^2}{2\sin \alpha} \cos \beta \sin (\beta - \alpha)$$

and hence, by eqn. (6.93a)

$$\nabla^2 f = \frac{\partial^3 f}{\partial x^2} + \frac{\partial^3 f}{\partial y^2} = \frac{\partial^3 f}{\partial \beta^2} + \frac{\partial^3 f}{\partial y^2}$$

$$\frac{\partial^2 f}{\partial \beta^2} \sin 2(\beta - \alpha) = \frac{\partial^2 f/\partial \beta^2}{2\sin^2 \beta \sin (\beta - \alpha)}$$

For the equilateral triangle where $\alpha=60^\circ$, $\beta=120^\circ$ and $\beta - \alpha = 60^\circ$

$$\sin \alpha = \sin \beta = \sin (\beta - \alpha) = \sin 2\alpha = \sin 2 (\beta - \alpha) = \frac{\sqrt{3}}{2}$$

$$\sin 2\beta = -\frac{\sqrt{3}}{2}$$

$$\cos \alpha = \frac{1}{2}, \cos \beta = -\frac{1}{2}$$

Eqns. (6.95) and (6.92) reduce to

$$\nabla^2 f = \frac{2}{3} \left[ \frac{\partial^3 f}{\partial \beta^2} + \frac{\partial^3 f}{\partial \phi^2} + \frac{\partial^3 f}{\partial \psi^2} \right]$$

$$\frac{\partial f}{\partial \beta} = \frac{\partial f}{\partial x}$$

$$\frac{\partial f}{\partial \phi} = \frac{1}{2} \frac{\partial f}{\partial x} + \frac{\sqrt{3}}{2} \frac{\partial f}{\partial y}$$

$$\frac{\partial f}{\partial \psi} = -\frac{1}{2} \frac{\partial f}{\partial x} + \frac{\sqrt{3}}{2} \frac{\partial f}{\partial y}$$

Add eqns. (6.98a) and (6.98b) to produce

$$\frac{\partial f}{\partial y} = \frac{1}{\sqrt{3}} \frac{\partial f}{\partial \phi} + \frac{\partial f}{\partial \psi}$$
In Section 6.3.1.3 it has been shown that the flow in a channel of arbitrary cross-section can be expressed through the elliptic equilibrium eqn. (6.46a) and the non-Newtonian viscosity, \( \eta \), through eqn. (6.47a), i.e.

\[
\frac{\partial}{\partial x} (\eta \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y} (\eta \frac{\partial v}{\partial y}) = \left( - \frac{\partial p}{\partial x} \right) \tag{6.46a}
\]

\[
\eta = m \left\{ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right\}^{n-1} \tag{6.47a}
\]

Substitute eqns. (6.96), (6.97) and (6.99) into eqn. (6.46a) to produce

\[
\frac{\partial \eta}{\partial \theta} \frac{\partial v}{\partial \theta} + \frac{1}{3} \left\{ \frac{\partial \eta}{\partial \phi} \frac{\partial v}{\partial \phi} + \frac{\partial \eta}{\partial \psi} \frac{\partial v}{\partial \psi} \right\} + \frac{2}{3} \eta \left\{ \frac{\partial^2 v}{\partial \theta^2} + \frac{\partial^2 v}{\partial \phi^2} + \frac{\partial^2 v}{\partial \psi^2} \right\} = \left( - \frac{\partial p}{\partial z} \right) \tag{6.100}
\]

Similarly combine eqns. (6.97), (6.99) and (6.47a) to yield

\[
\eta = m \left\{ \left( \frac{\partial v}{\partial \theta} \right)^2 + \frac{1}{3} \left( \frac{\partial v}{\partial \phi} + \frac{\partial v}{\partial \psi} \right)^2 \right\}^{n-1} \tag{6.101}
\]

The finite-difference approach to the solution of this problem may be outlined as follows. Fig. 6.12 shows part of a grid in the solution domain. The lines on the grid are uniformly spaced in the \( \theta, \phi \) and \( \psi \) directions, the distance between them being \( \delta \theta = \delta \phi = \delta \psi = h \). The points to be used in the finite-difference analysis are located at the intersection of the grid lines. The point labelled 0 may be regarded as a typical point within the solution domain, and the compass-point labels N, S, E, W, NW, NE, SW and SE are used for the adjacent grid points.

Upon approximation of derivatives by finite difference for grid point 0, see Table 5.1, eqns. (6.100) and (6.101) give, respectively

\[
v_0 = \frac{v_w (3n_w + n_0) + v_E (3n_E + n_0) + (v_{SW} + v_{SE}) [n_{SW} + n_{SE} + 2n_0] + (v_{NE} + v_{NW}) [n_{NE} + n_{NW} + 2n_0]}{3(n_w + n_0) + 2(n_{SW} + n_{SE} + n_{NW} + n_{NE}) + 10n_0} \tag{6.102}
\]

and

\[
\eta_0 = m \left\{ \frac{v_E - v_w}{2h} \right\}^2 + \frac{1}{3} \left\{ \frac{v_{NW} + v_{NE} - v_{SW} - v_{SE}}{2h} \right\}^2 \left( \frac{n-1}{2} \right) \tag{6.103}
\]
Fig. 6.12: Channel of arbitrary cross-section showing part of an equilateral triangular finite difference grid

Fig. 6.13: Finite difference grid in an equilateral triangle
Eqn. (6.102) was solved, iteratively, subject to the boundary conditions that there is no slip at the wall. The over-relaxation technique was used and the mesh points were updated during the iteration process in the light of the current estimates of the velocities. The convergence of the iteration process was accelerated using eqn. (6.53) i.e.

\[ v_{\text{NEW}(I,J)} = v_{\text{OLD}(I,J)} + \omega [v_{\text{C}} - v_{\text{OLD}(I,J)}] \]  

However, application of eqn. (6.102) in the vicinity of the boundaries requires the values of viscosity at the boundaries while its application in the interior boundaries (dotted lines in Fig. 6.13) requires the values of both viscosity and velocity exterior to the interior boundaries. For the latter case, these values were obtained by simply reflecting values across the dotted lines as Fig. 6.13 shows. For the former case, Taylor series expansions were used and for demonstration purposes the boundary mesh point 05 will be selected. With respect to \( \phi \)-axis:

\[ (v)_{23} = (v)_{05} + 2h \frac{\partial v}{\partial \phi} + \frac{(2h)^2}{2!} \frac{\partial^2 v}{\partial \phi^2} + ... \]  

\[ (v)_{14} = (v)_{05} + h \frac{\partial v}{\partial \phi} + \frac{h^2}{2!} \frac{\partial^2 v}{\partial \phi^2} + ... \]

Multiply eqn. (6.104b) by 4 and subtract the resulting eqn. from eqn. (6.104a) to obtain

\[ \frac{\partial v_{14}}{\partial \phi_{05}} = \frac{4(v)_{14} - (v)_{23} - 3(v)_{05}}{2h} + o(h^2) \]  

Repeat the same procedure using Taylor series for \( \frac{\partial v}{\partial \phi_{05}} \) and \( \frac{\partial v}{\partial \phi_{05}} \) and substitute the resulting expressions, together with eqn. (6.105) into eqn. (6.101) to obtain

\[ n_{05} = m \left[ -\frac{1}{12h^2} (4v_{14} - v_{23} + 4v_{13} - v_{21})^2 \right] \]  

(6.106)
6.5 COMMENTS

In Sections 6.3 and 6.4 we concentrated on formulating the non-Newtonian flow behaviour in non-circular ducts using the finite-difference and the variational principle methods. In this section we will discuss the practical aspects of solving the resulting equations, thus we focus our attention on the mathematical side of the problem, leaving the discussion of the results from the physical viewpoint to Chapter 8.

Application of the finite-difference method performs well computationally down to a power-law index, \( n \), of about 0.5, for a tolerance of \( 10^{-6} \), while below \( n=0.5 \), it diverges (for the same tolerance). To overcome this problem, as will be seen later, several qualitative methods were tried.

**Finer mesh**

Although no general guide yet exists which related the magnitude of the discretization error as a function of the mesh length, it is well known \([11, 49]\) that this error usually decreases as the mesh becomes finer. However, use of a finer mesh can result in two problems:

i) an increase in the round-off error, provided that the iteration is continuous without decimal place limitation

ii) an excessive Central Processing Unit (CPU) time in which case the method may become completely uneconomical i.e. the performance of theoretical computations costs as much or more than a practical experiment.

For the present problem a 40x40 mesh was used as the final choice.

**More accurate finite-difference formulae**

The three-point formulae and the five-point formulae were used for the discretization of the first- and second-derivative respectively, thus introducing a truncation error of the order \( O(h^2) \).
To improve the accuracy, through reduction in the truncation error, a higher order finite difference approximation may be used (e.g. nine-point approximation). This means that the number of grid points participating in approximating the derivatives increases. The constraints of this strategy are:

i) more storage space is required in the computer
ii) additional fictitious grid points have to be included when treating points on or near the wall, which in almost all cases destroy the simple tridiagonal form produced by the second order schemes. A possible way to avoid the use of fictitious points is to introduce the concept of one-sided approximations of the same order of accuracy as the rest (see comments below). At this point it is also interesting to see the method proposed by Kreiss [50], who managed to obtain a fourth-order accuracy while retaining the tridiagonal form of the coefficient matrix.

Successive over-relaxation (SOR)

In iterative procedures where the SOR technique is used, the choice of the "right" value of the relaxation factor, \( \omega \), plays a major role, since the choice of an optimum relaxation value, \( \omega_{\text{opt}} \), accelerates quite substantially the rate of convergence. However, the constraint in that respect is the difficulty of estimating \( \omega_{\text{opt}} \) in advance of its use. This is particularly true for complex systems such as the present one as well as for non-uniform net spacing systems. An additional constraint in the choice of \( \omega_{\text{opt}} \) is its dependence on the power-law index.

Forsyth et al [51a] discusses this subject at some length and proposes three practical approaches to determine \( \omega_{\text{opt}} \) stressing also that none of them has yet proved itself to be outstandingly successful. He also recommends [51b] "that it is far better to over-estimate \( \omega_{\text{opt}} \) a little than to under-estimate it by the same amount".

Continuation

A very important factor affecting both the number of iterations needed for an algorithm to converge, as well as the convergence itself, is the choice (quality) of the initial guess at the solution.
For this problem a continuation facility was used where the solution of eqn. (6.49) was obtained for slightly larger values of power-law index, $n$, say for $n_K$, and then this solution was introduced as an initial guess to the eqn. (6.49) for $n_{K+1}$, where

$$n_{K+1} < n_K \quad \text{and} \quad 0 < n \leq 1$$

Such a procedure where the solution for each step ($n=n_{K+1}$) is evaluated by using the solution of its predecessor ($n=n_K$), is known as a Davidenko path procedure [52].

**Treatment of grid points on or near the boundary**

In Section 6.3.1.3, we were faced with the problem as to how to calculate the viscosity (see eqn. (6.51)) in the vicinity of the boundaries, since we required velocity values outside the duct. This problem was overcome by using extrapolation formulae [see eqns. (6.52)]. However, solution of the resulting equations produced results (i.e. the method converges) for values of $n$ down to around 0.5.

An alternative approach was also used, based on the concept of one-side approximation, of the same order of accuracy as the rest of the approximations, u.e. $O(h^2)$. Rather surprisingly (at least to the author), results were obtained. In other words, convergence was achieved for values of $n$ below 0.5 while keeping the tolerance at the same level i.e. $10^{-6}$, or even increasing it at very low power-law indices. It must be stressed here that such an approximation was also used for the triangular section, where extrapolation was impossible due to the awkward shape of the duct near the $60^\circ$ corner - without realising its important application in the square and rectangular ducts. The procedure in deriving this approximation is explained in Section 6.4.2 [see eqns. (6.104)-(6.105)]; however due to the different orientation of the grid points on the rectangular boundary the final form of these approximations is different. These are listed below:
In a subsequent literature survey, it was found that Greenspan [53] made similar remarks after solving the same geometry problem but with a fluid flow governed by the Navier-Stokes equations. His method failed to converge for Reynolds number, Re, between 0 and $10^5$ ($0 \leq Re \leq 10^5$) and grid size, $h$, less than 0.1 ($h < \frac{1}{10}$). He observed that the divergence predominated near the boundaries, so he suggested approximating the normal derivative boundary conditions using grid points on only one side of the boundary as described above (see also Vemure et al [54]).

A final point concerning the calculations in this thesis is that double precision was used throughout except for the evaluation of the thermophysical properties (see Section 8.0) where single precision was used.
REFERENCES


8. See references 29, 37, 40, 55-58, 63, 67 and 69 of Chapter 2.


13. HAMEL, G., Spiralförmige Bewegungen zaher Flüssigkeiten Jahresbericht d Deutschen Mathematiker - Vereinigung 25, 34 (1917). This paper has been translated in the USA under the serial number NACA Technical Memorandum No. 1342, 1953.


CHAPTER 7

EXPERIMENTAL

7.1 MATERIAL

The rubber mix used was based on an ethylene-propylene terpolymer rubber (EPDM) containing 120 parts FEF carbon black, 60 parts of MT carbon black and 100 parts of process oil. It is used in car windscreen seals.

7.2 EQUIPMENT

7.2.1 Mixing

The mixing trials to produce the material necessary to formulate the relationship between extrusion variables and rheological properties were carried out in an upside-down mixing procedure using two mixers:

a) A Farrel-Bridge F80 Banbury, a production scale internal mixer having a mixing chamber volume of 0.08m\(^3\) (80 l). A typical batch weight was about 67 kg at fill factor of 0.7.

b) A Francis-Shaw K2A mixer having a chamber volume of 0.027m\(^3\) (27 l), with a batch capacity of 27 kg (calculated for specific gravity = 1.0).

7.2.2 Extrusion

The extrusion trials were performed using a Farrel-Bridge 38 mm (1.5") extruder having a 12:1 length to diameter ratio NRM plastiscrew, based on the Maillefer design. The barrel was divided into three zones for temperature control purposes and the head and the die were heated separately. A Dynisco, model PT460E-10M-6, 0-10,000 psi pressure transducer was sited in the extruder head, before the flow convergence (or divergence) to the die. Signals from the pressure transducer were amplified and relayed to a 'Servoscribe' chart recorder.

7.2.3 Dies

1. To determine the extruder operation curve a special die of circular cross-section with a conical lead in, was devised. The die was fitted with an adjustable flow restrictor, a pressure transducer and a thermocouple. The pressure transducer position was carefully chosen...
to determine the pressure prior to the start of divergent flow to the die exit. The thermocouple was passed through the hollow flow restrictor to measure the temperature of the melt once it had reached the end of the screw.

II. To test the validity of the model developed for the converging channels and non-circular ducts of rectangular, square and triangular shape, a number of dies of the shapes mentioned were reconstructed, with dimensions shown in Table 7.1 below.

**TABLE 7.1: Approach channels and dies used**

<table>
<thead>
<tr>
<th>Cone</th>
<th></th>
<th>Length (mm)</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Half angle in degrees</td>
<td>Rectangular</td>
<td>Square</td>
<td>Equilateral</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Height = 5.5mm</td>
<td>Height = 8.0mm</td>
<td>Height = 8.0mm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Width = 15 mm</td>
<td>Width = 8.0mm</td>
<td>Side = 13.92 mm</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>4.0</td>
<td>4.0</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>12.5</td>
<td>12.5</td>
<td>12.5</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>25</td>
<td>25</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7.2.4 Flow Properties

Flow data were obtained by using a Davenport capillary constant shear-rate rheometer. The rheometer consists of an electrically thermostated barrel in the bottom of which one of a number of interchangeable dies was inserted. Polymer melt in the barrel was driven by a plunger at preselected constant shear rates. Plunger speeds ranging from about 1.25 mm/min to 200 mm/min were available but only the range of 2.5 mm/min to 150 mm/min was covered as fulfilling the usual industrial extrusion shear rates range of 100-1000 s⁻¹. The pressure drops in the capillary were measured using a Dynisco PT, model 460E-10N-6, 0-10,000 psi pressure transducer sited at the end of the barrel and before the entry to the die. Signals from the pressure transducer were amplified and relayed to a chart recorder. Since the available control system fitted to the rheometer was unable to achieve temperatures below 100°C, a separate controller was connected to the rheometer for this purpose. Conventional and electric 'Comark' thermometers were also used to ensure controllable temperature within ±0.1°C. The capillaries and the temperatures used are listed in Table 7.2.
TABLE 7.2: Capillary dimensions and temperatures used for flow data
(diameter of the barrel = 9.5 mm)

<table>
<thead>
<tr>
<th>Temperature of Measurement (°C): 80, 90, 100, 110, 120</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of Capillary (mm)</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>2</td>
</tr>
</tbody>
</table>

7.2.5 Thermophysical Properties

1. Thermal diffusivity: a Moore compression moulding press was used in
   conjunction with cured rubber sheets and an electric Comark thermo-
   meter.

2. Specific heat: the Differential Scanning Calorimeter (DSC) was used
   for the measurement of specific heat.

7.2.6 Miscellaneous

Some other items of equipment which have been used throughout this
work are:

A. Two-roll mills: the first one was provided by Hubron Company to
   sheet the material dumped from the F80 Banbury mixer and the other
   one was provided by the Francis-Shaw Company.

B. A 'Betol' puller, model No 1005, of the caterpillar type was used
   to draw away the extrudate at a constant and controllable rate.

7.3 PROCEDURE

7.3.1 Extrusion

I. Two sets of extrusion trials were carried out:
   Trials to determine the extrusion operation curve where the following
   four extrusion variables were selected: screw speed, back pressure,
   head temperature/barrel temperature and die temperature. The Rotat-
   able Centre Composite Factorial Design was used to explore the
   extruder performance and the design matrix of Table 5.2 was followed.
   The relation between the absolute values of the extruder variables
   and the code values in Table 5.2 is given in Table 7.3.
TABLE 7.3: Absolute values of the extrusion variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Code Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Screw speed (rpm)</td>
<td>-2  -1  0</td>
</tr>
<tr>
<td>Die temperature (°C)</td>
<td>20  30  40</td>
</tr>
<tr>
<td>Head factor [Y₁]/</td>
<td>90 100 110</td>
</tr>
<tr>
<td>Barrel factor [Y₃]</td>
<td>20%/40% 15%/30% 10%/20% 5%/10% 0</td>
</tr>
<tr>
<td>Back pressure (MPa)</td>
<td>3.45 7.76 12.1 16.4 20.7</td>
</tr>
</tbody>
</table>

The scaling factors used in Table 7.3 were set up according to Fig. 7.1 where:

Head temperature = Die temperature * (1-Y₁)
Barrel temperature = Die temperature * (1-Y₃)

The above variables, as well as their upper and lower limits, were selected by reference to commercial practice, machine capabilities and previous experience.

Fig. 7.1: Relation between the scaling factors of the head/barrel temperature ratio and the die temperature

The procedure for running the extruder was as follows: when thermal equilibrium had been established in the barrel zones, head and die, the motor was switched on and the extruder was fed with material while the screw speed was slowly increased to the required level. Enough time was allowed for the extruder to reach steady-state conditions, once the flow restrictor had been adjusted so that the back pressure would reach its set value. Readings of the following dependent variables (or responses) were taken:
a) Extrudate temperature (using a needle pyrometer)
b) Temperature of the melt before entering the diverging die (using a thermocouple)
c) Mass output rate by weighing the amount of material produced over a period of time, usually 1-2 minutes operation.

Note that the extrusion trials were run in random order to avoid systematic time-varying effects confusing the results.

II. Trials to assess the validity of the model, where the different converging sections and dies of Table 7.1 were interchanged, in order to obtain pressure drop measurements. In addition, the extrudate temperature was measured as well as the mass output rate by weighing the amount of material produced over a period of time. Also one sample was selected for extrudate swell measurements. In each case the following extrusion settings were used:

Screw speed = 40 rpm
Barrel: zone 1 = 40°C
zone 2 = 60°C
zone 3 = 80°C
Head temperature = 100°C
Die temperature = 110°C

7.3.2 Rheological Tests

I. Capillary

After the die was inserted into the barrel and the retaining nut was tightened, enough time was allowed for the set temperatures to be reached and become steady. Once thermal equilibrium had been established, the rheometer barrel was filled with material and tamped down with the tamping tool provided. Then by using the driven ram, a small pressure was applied to compress the heated material in order to ensure a porosity-free extrudate. During this period the applied pressure was decreased reaching a steady value. When the heating period was completed, the ram was switched on and the speed was adjusted to 2.5 mm/min. Once the pressure was steady the speed was changed to 5 mm/min and again some time was allowed until a steady pressure was obtained. This procedure was continued until all the required speed/pressure drop data were obtained. When the ram was cut off by the safety stops the motor was reversed, thus allowing for the ram to
be extracted from its housing. Then the die was removed and the barrel was cleaned before continuing with a new die, thus minimising the possibility that thermally degraded material adhering to the barrel walls would be mixed with the new material. Since some extrudate swell data were necessary, samples at each speed were taken immediately after the extrudate emerged from the capillary. Efforts were made to avoid any draw-down effects due to the extrudate weight, so a beaker with hot water was placed directly underneath the capillary to accept the emerging extrudate.

II. Thermophysical properties

A: Thermal diffusivity: a thermocouple was placed between two rubber sheets of known thickness and the assembled stack was placed between the press plates, clamping them lightly. The increase in temperature was recorded with respect to time in order to obtain the heating curve which will provide information about the value of thermal diffusivity.

B: Specific heat: the rate of heat input of a small sample (22.6 mg) of the EPDM compound was compared with that of a reference material (aluminium) for the same rate of temperature rise. The displacement in the Y-axis for the area under the resulting curve coupled with the equation provided by the DSC manual gave the value of the specific heat of the compound.
CHAPTER 9
ANALYSIS AND DISCUSSION OF RESULTS

This chapter deals with the presentation, analysis and discussion of the results obtained experimentally and analytically. Their sequential order (labelling) will be that of Figure 6.1. Further, two more sections will be included: section 8.0, which in a brief form presents and comments on the rheological and thermophysical properties of the compound used; and section 8.3.0, which deals with the preliminary extrusion runs, where the adjustable flow restrictor was used and the results were analysed by statistical means.

8.0 THERMOPHYSICAL AND RHEOLOGICAL PROPERTIES

8.0.1 Thermal Diffusivity

Following the procedure of section 7.3.2-II/A, Table 8.1 was constructed showing the heat transfer data obtained for the evaluation of thermal diffusivity:

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>15</th>
<th>30</th>
<th>45</th>
<th>60</th>
<th>90</th>
<th>120</th>
<th>160</th>
<th>180</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>118.0</td>
<td>123.5</td>
<td>127.5</td>
<td>130.2</td>
<td>135.0</td>
<td>138.5</td>
<td>142.0</td>
<td>143.3</td>
</tr>
<tr>
<td></td>
<td>210</td>
<td>240</td>
<td>280</td>
<td>300</td>
<td>330</td>
<td>360</td>
<td>390</td>
<td>420</td>
</tr>
<tr>
<td></td>
<td>145.5</td>
<td>146.8</td>
<td>148.8</td>
<td>149.8</td>
<td>150.8</td>
<td>152.0</td>
<td>153.0</td>
<td>153.8</td>
</tr>
<tr>
<td></td>
<td>480</td>
<td>510</td>
<td>540</td>
<td>570</td>
<td>660</td>
<td>155.5</td>
<td>156.2</td>
<td>156.8</td>
</tr>
</tbody>
</table>

The analysis of the data is outlined in Appendix D1 and is based briefly on:

i) the Fourier partial differential equation for the case of unsteady-state conduction

ii) negligible surface resistance to heat transfer.

The value of thermal diffusivity was found to be \((6.92) \times 10^{-8} \text{ m}^2/\text{s}\).
8.0.2 Specific Heat

Using the Differential Scanning Calorimetry (DSC) as described in Section 7.3.2-II/B, the value of the specific heat was found to be

\[
2.32 \frac{\text{kJ}}{\text{kg °C}}
\]

8.0.3 Rheological Properties

Table 8.2 below contains the experimental data obtained from the capillary rheometer following the procedure of Section 7.3.2-I. To achieve generality the data were corrected for end effects, (Bagley correction), and for the non-Newtonian velocity profile (Rabinowitsch equation) by the method described in Section 6.3.2-B.

**TABLE 8.2: Capillary Raw Data**

<table>
<thead>
<tr>
<th>Temperature °C:</th>
<th>80</th>
<th>90</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>L/R [R=1mm] :</td>
<td>0</td>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>V_p (mm/min)  :</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure (psi)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>232</td>
<td>530</td>
<td>797</td>
</tr>
<tr>
<td>5.0</td>
<td>252</td>
<td>603</td>
<td>894</td>
</tr>
<tr>
<td>10</td>
<td>280</td>
<td>693</td>
<td>1003</td>
</tr>
<tr>
<td>20</td>
<td>337</td>
<td>775</td>
<td>1100</td>
</tr>
<tr>
<td>25</td>
<td>357</td>
<td>812</td>
<td>1148</td>
</tr>
<tr>
<td>50</td>
<td>447</td>
<td>930</td>
<td>1293</td>
</tr>
<tr>
<td>75</td>
<td>505</td>
<td>1026</td>
<td>1402</td>
</tr>
<tr>
<td>100</td>
<td>556</td>
<td>1079</td>
<td>1500</td>
</tr>
<tr>
<td>125</td>
<td>590</td>
<td>1130</td>
<td>1570</td>
</tr>
<tr>
<td>150</td>
<td>615</td>
<td>1173</td>
<td>1626</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature °C:</th>
<th>110</th>
<th>120</th>
</tr>
</thead>
<tbody>
<tr>
<td>L/R [R=1mm] :</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>V_p (mm/min)  :</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure (psi)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>150</td>
<td>372</td>
</tr>
<tr>
<td>5.0</td>
<td>169</td>
<td>450</td>
</tr>
<tr>
<td>10</td>
<td>193</td>
<td>517</td>
</tr>
<tr>
<td>20</td>
<td>226</td>
<td>595</td>
</tr>
<tr>
<td>25</td>
<td>242</td>
<td>624</td>
</tr>
<tr>
<td>50</td>
<td>290</td>
<td>712</td>
</tr>
<tr>
<td>75</td>
<td>332</td>
<td>777</td>
</tr>
<tr>
<td>100</td>
<td>363</td>
<td>837</td>
</tr>
<tr>
<td>125</td>
<td>391</td>
<td>874</td>
</tr>
<tr>
<td>150</td>
<td>411</td>
<td>909</td>
</tr>
</tbody>
</table>
Note that the pressure drop raw data of Table 8.2 are expressed in psi since this is the input form used in the computer program to obtain the necessary rheological properties. A simplified flowchart is given in Appendix C4.

The processed results are shown in conventional manner in Figures D1 and D2 in Appendix D2. For comparison the raw data were also treated using the two-point method, while the processed results are shown in Figures D3-D6 in Appendix D2.

Although it is not the chief concern of this thesis to concentrate on the study of capillary flow, a few observations and comments cannot be omitted:

1. Figure D1 shows that as temperature increases the flow data obtained were approximated better to a polynomial fit.

2. For temperatures 80-110°C, the data for shear rate vs viscosity can be approximated to a single expression for shear rates in the region 100 s\(^{-1}\) to 1000 s\(^{-1}\), while for temperature 120°C the material tends to show a transition to Newtonian shear flow at shear rates below 0.1 s\(^{-1}\).

3. The end correction is in general large and shows the same trend for all temperatures i.e. if decreases as shear rate increases, reaching a minimum at around 70 s\(^{-1}\) and then starts to increase with shear rate. Perhaps this unexpected result is the reason that the curves of (log \(\eta\) vs log \(\dot{\gamma}\)) Figure D2 coincide in the shear rates mentioned in (2) above.

4. When pressure data were plotted against L/R for different shear rates, straight lines resulted. Although such a result is encouraging in that the pressure effect on viscosity is minimal, as has already been assumed, its true validity must be accepted with some reservations, unless it is also verified at large L/D capillaries [1,2].

Possible reasons for some of the unexpected observations above include: possible operational error and definite misbehaviour of the capillary rheometer, especially at low speeds.
When the TMS biconical rotor rheometer was used for the estimation of the power-law index and the consistency index, the values of 0.216 and 102 kPa s were obtained respectively [3]. Note that the TMS rheometer used was operated at a temperature of 100°C, and shear rates of between 0.1 and 40 s⁻¹. For the temperature of 100°C, the consistency index from the capillary is 105 kPa s, which is in excellent agreement with the TMS. The fact that the power-law index increases as the shear rate decreases tends to justify the result obtained from the TMS. However, some questions may arise about the validity of TMS as "processability tester" since at processing conditions high shear rates are normally encountered.

Though the figures displayed in Appendix D2 were fitted to a logarithmic parabola equation the power-law model was used for convenience, as a means to provide indices for use in subsequent calculations. Their values at 110°C are:

\[ \text{Power-law index (n)} = 0.1521 \]
\[ \text{Consistency index (m)} = (9.51) \times 10^4 \text{ Pa.s} \]

8.1 CONVERGING SECTION

8.1.1 Motion Equations

Table 8.3 summarises and compares the experimentally measured die pressure drops with those predicted by the theoretical model developed in Sections 6.1.1-6.1.4 and expressed by equation 6.12b.

The significant points are:

i) the model underestimates the true pressure drop value with an average error ranging from -4% to -28%.

ii) the prediction is of the right magnitude at low angles and the error increases as the taper angle increases.

Two possible reasons can be identified as being responsible for this discrepancy: elongational effects and the accelerating shear component. Until now no mention has been made of elongational effects. Although the author is aware of the importance of these effects, especially in converging flows, their exclusion was deliberate for two reasons:
TABLE 8.3: Comparison of predicted and experimental results for the convergent section

<table>
<thead>
<tr>
<th>Cone Half-Angle (degrees)</th>
<th>Cone Length (cm)</th>
<th>Volumetric Flowrate $\mu\text{m}^3/\text{s}$</th>
<th>Pressure [MPa]</th>
<th>Error $^*$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Theoretical</td>
<td>Experimental</td>
</tr>
<tr>
<td>10</td>
<td>9.68</td>
<td>4.174</td>
<td>5.06</td>
<td>5.29</td>
</tr>
<tr>
<td>20 (R)</td>
<td>4.68</td>
<td>4.174</td>
<td>2.81</td>
<td>3.04</td>
</tr>
<tr>
<td>20 (S)</td>
<td>4.68</td>
<td>4.300</td>
<td>2.82</td>
<td>3.28</td>
</tr>
<tr>
<td>20 (T)</td>
<td>4.68</td>
<td>4.307</td>
<td>2.82</td>
<td>2.94</td>
</tr>
<tr>
<td>30 (R)</td>
<td>2.96</td>
<td>4.209</td>
<td>2.07</td>
<td>2.63</td>
</tr>
<tr>
<td>30 (S)</td>
<td>2.96</td>
<td>4.389</td>
<td>2.08</td>
<td>2.73</td>
</tr>
<tr>
<td>30 (T)</td>
<td>2.96</td>
<td>4.143</td>
<td>2.07</td>
<td>2.41</td>
</tr>
<tr>
<td>45 (R)</td>
<td>1.73</td>
<td>4.288</td>
<td>1.71</td>
<td>2.37</td>
</tr>
<tr>
<td>45 (S)</td>
<td>1.73</td>
<td>4.276</td>
<td>1.71</td>
<td>2.54</td>
</tr>
<tr>
<td>45 (T)</td>
<td>1.73</td>
<td>4.273</td>
<td>1.71</td>
<td>2.26</td>
</tr>
</tbody>
</table>

$^*$ Error $= \frac{\text{Experimental} - \text{Theoretical}}{\text{Experimental}}$.

$^{*\dagger}$ Negative error means that the model underestimates the true value.

$^{*\dagger\dagger}$ Average value.

* R, S and T mean that the cone exit was shaped in a rectangular, square and triangular form respectively.
1. In order to test the performance of the viscous shear flow predictions, which are much better understood than the extensional flows.

2. The uncertainty among researchers as to how categorical one can be about the extensional behaviour of rheologically complex fluids [4]. This is partially due to the difficulty in making accurate measurements of elongational viscosity over a sufficient wide range of extensional strain rates in the existing extensional rheometers; as well as the uncertainty that these instruments do in fact give the data they are designed to provide. Cogswell [5] reflects the situation best where in a review paper he outlines that "each author who has taken this course (i.e. elongational effects) has approached it from a different route generating different equations which have to some extent, obscured the picture".

Walters [4] considers that the main difficulty with extensional flow is the correct interpretation of data from experiments which are relatively easy to perform (e.g. converging flows) and the practical construction, if possible, of those experiments which are fairly easy to interpret.

The fact also that elongational flow has to be introduced through a constitutive equation causes two more problems:

i) to choose the right constitutive equation which will describe the material adequately

ii) if such an equation exists, to incorporate it into the transport equations in a form that a solution of the problem under consideration may be visible.

An alternative way is to split the viscoelasticity of the material into its two parts: the viscous part and the elastic part; then deal with them separately adding their effects at the end. However, strictly speaking, such a distinction is not justifiable because the two effects may interact in a complicated way.
The other possible factor responsible for the discrepancy was attributed to the assumption of creeping flow i.e. ignoring any contribution from accelerating shear flow. Although the creeping flow concept is appealing in the sense that:

i) it reduces the mathematical complexity of the problem
ii) it is partly justified, at least physically, from the fact that the melt under consideration is very viscous

but it does not rest on a sound mathematical basis as it has been outlined in Section 6.1.7.

Although the above concepts are still under investigation, what seems to be well established is that the effects due to elongation and acceleration increase as the angle increases. This observation seems to fulfill the picture of Table 8.3 where the error in the predicted pressure drop values increases with angle. The fact also that at small angles the contribution of the axial pressure gradient resulting from extensional flow is negligible (or at least very small) compared to that due to shear flow has been justified experimentally by Worth et al [6,7]. Therefore, the proposed model appears to be adequate for engineering design applications, especially if one considers the lack of experimentally proven models. This is best emphasised by Forsyth [8], who in a review of converging flow in polymers states that "Despite the analytical success in examining the flow of viscoelastic fluids in converging dies, applications of these results have been infrequent and isolated".

8.1.2 Energy Considerations

It is well established that most of the heat put into the melt during extrusion is worked into it through frictional processes and through dissipation accompanying the shear deformation of the polymer.

If the angle of convergence is small, this means that the shear rate in the flow channel is nearly uniform through the whole axial length of the channel (unless there is a severe restriction at the exit), but uniform \( \dot{\gamma} \) implies uniform \( \dot{\gamma} \) provided of course that there is no temperature difference over the channel length. Since the product of \( \tau \) and \( \dot{\gamma} \) is the mean of the viscous dissipation rate, it means that
the melt at the die will be at a uniform temperature - a situation highly desirable for best control of extrudate shape and dimensions.

At high shear stresses, when the applied pressure is high, all the pressure energy is converted into heat, thus raising the melt temperature. Since the \( \dot{\gamma} \) and \( \tau \) are greatest at the die wall - ranging from that maximum value down to zero at the centre - and the rate of conversion of pressure energy into heat is proportional to the product of \( \dot{\gamma} \) and \( \tau \), heat production is at its highest level near the die wall and lowest near the centre. This in turn, results in substantial lowering of viscosity near the wall, thus causing the flow rate to increase, as well as altering the velocity distribution profile, making it more pluggish and therefore distorting the flow in general.

Obviously this dissipation effect becomes more pronounced as the converging channel narrows, since the heat can only be transferred to a limiting extent to:

1. the isothermal wall
2. the colder melt in the centre of the die
due to the low thermal conductivity of the melt.

Having said that, it appears from Figure 8.1, which shows the temperature distribution between the centre and the wall at the exit of the converging section, that the viscous dissipation effect is either negligible due to the short residence time (short lengths), or if it is present, it serves to flatten the velocity profile due to lowering of viscosity near the wall.

It is not surprising that the curve of the lower angle (i.e. \( \alpha=10^\circ \)) appears to lie above those of the larger angles, since this has to do with the axial length of the cones, \( l \) (i.e. \( l_{100^\circ} > l_{200^\circ} > l_{300^\circ} > l_{450^\circ} \)). see Table 8.3. In order to justify this point further, both the flow-rate and the axial length were kept at the same level for each angle while the die wall temperatures were varied. Figures 8.2 illustrate this variation. For clarity only the two extreme angles are shown, with the others lying in between them.
Fig. 8.1: Temperature distribution at the outlet for converging sections of different half-angle
Fig. 8.2: Temperature profile at the outlet for converging sections of different half-angle: (a) $T_{\text{wall}} > T_{\text{centre}}$
(b) $T_{\text{wall}} < T_{\text{centre}}$
In order to compare the results, the Newtonian curve was also included (see Figure 8.1), based on the same flow rate and axial length as the 10° convergent section. The temperature distribution shows a temperature maximum near the wall. This can be attributed to the viscous dissipation effect because as this effect builds up heat is transferred to the main body of the die but owing to the poor fluid thermal diffusivity, the temperature builds up until it actually peaks. The greater influence of viscous dissipation effect on Newtonian fluid compared to a non-Newtonian one can be also deduced from the dissipation function \((\tau_1 \nabla \nabla)\) included in the energy eqn. (4.24) and expressed by eqn. (A3-B) in Appendix A - which is directly proportional to the velocity gradient raised to the power \(\left(\frac{n+1}{2}\right)\).

Experimental results, whereby using a pyrometer the temperature of the emerging extrudate was measured, indicated a temperature of around 110°C for each angle. However it is rather difficult to assess the validity of such indication since the cross section of the extrudate was small and therefore it was very difficult to define precisely where the actual reading was taken (i.e. near the wall or near the centre). It should also be noted that all calculations were based on a constant average inlet temperature of 100°C, see Section 7.2.3-I.

8.2 ESTIMATION OF THE PREFORM SECTION BASED ON MEMORY EFFECTS

Some of the concepts discussed in Section 6.2 are illustrated in Figures 8.3 obtained using capillary data. Study of the curves leads to the following conclusions:

i) swelling decreases strongly at first and then not to such a decided extent (minimum) as the length of the capillary is increased

ii) a direct proportionality exists between shear rate and swell

iii) the eqn (6.30) selected for representation of swelling index vs L/R capillary data has been justified according to Figure 8.3; of course there is a large variety of other equations to fit the same data, some with more apparent theoretical justification [9], but the exponential form is probably the simplest that can be justified theoretically.
Fig. 8.3a: Swelling index vs capillary L/R at different shear rates

Fig. 8.3B: Variation of the decay rate constant, K, with shear rate
Following the procedure proposed in Section 6.2, Table 8.4 and Figure 8.3 were obtained. To find the wall average shear rate for each of the three sections, a typical output of \(10^{-6} \text{ m/s}\) was used from the results of Tables 8.3, 8.8 and 8.10.

**TABLE 8.4: Preform section results**

<table>
<thead>
<tr>
<th>Section</th>
<th>(E') (or (\alpha))</th>
<th>(a)</th>
<th>(b)</th>
<th>(\gamma^*) (sec⁻¹)</th>
<th>(K)</th>
<th>(L) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rectangle</td>
<td>5.5/15</td>
<td>0.276</td>
<td>0.768</td>
<td>124.5</td>
<td>7.868</td>
<td>6.16</td>
</tr>
<tr>
<td>Square</td>
<td>1</td>
<td>0.212</td>
<td>0.677</td>
<td>24.6</td>
<td>2.833</td>
<td>7.29</td>
</tr>
<tr>
<td>Triangle</td>
<td>30</td>
<td>0.188</td>
<td>0.646</td>
<td>89.2</td>
<td>6.088</td>
<td>7.83</td>
</tr>
</tbody>
</table>

* For definition of quantities, see Section 6.2.

It must be realised that the procedure can be regarded as providing only an estimate for non-circular geometries due to:

i) it is based on 1-D analysis (thus it is more applicable to simple profiles)

ii) it separates the two possible effects responsible for extrudate swell i.e. reversible deformation and rearrangement of the velocity profile taking into account only the former cause, so the length which it calculates must be considered as the minimum length necessary to avoid the effects

iii) it uses average values.

The length needed to avoid the effect referred to in (ii) can be added physically to the die land as a preform section.

In the absence of completely accurate methods for the calculation of extrudate swell, which take into consideration both causes of its existence, it is hoped that the method used, although approximate will at least allow some predictive design and will contribute to a reduction in empiricism. This is very important when working with rubber materials compared to plastics. The reason being that while a number of tabulated empirical values are used in practice for correcting extrudate swell in specific dies, thermoplastics and operating conditions [10a-12], the situation with rubber is completely different due to the vast number of compounds used.
Although no direct experimentation was used to test the validity of the prediction of preform length, the extrusion trials (Sections 8.1.1, 8.3 and 8.4) indicate that the dimensions obtained are viable. This can be demonstrated by evaluating the pressure drop across each preform length of Table 8.4 using the theory of Section 6.2 and then comparing the findings with the experimental ones for lengths close to those of the preform sections.

Combining eqns. (6.34), (6.35) and (6.40) yields:

\[
\Delta p = \frac{m_C L n}{A \gamma_w} \quad (8.1)
\]

Use of eqn. (8.1) in conjunction with the data provided by Table 8.4 result in the following pressure drops for each duct:

- \( \Delta p_{\text{rectangular}} = 0.61 \text{ MN/m}^2 \)
- \( \Delta p_{\text{square}} = 0.56 \text{ MN/m}^2 \)
- \( \Delta p_{\text{triangular}} = 0.73 \text{ MN/m}^2 \)

8.2.0 Extrusion

Table 8.5 shows the raw data obtained from the extrusion trials carried out in order to determine the extrusion operation curves. The results were then treated by multi-variate regression analysis using the statistical package designated GLIM (a typical output is shown in Appendix D3, for the flowrate Q). From the resulting information, the table of significance 8.6 was constructed, defining the significance of each independent variable with respect to the responses. To further assist the understanding of the results, graphical means, in the form of contour plots, were used. The computer program developed

- reads the polynomial coefficients for every response from a data file
- sets the two independent variables at any required code value i.e. +2, or +1, or ..., -2, while it varies the other two, simultaneously, between +2 and -2.
- calculates the response of each combination, which is then printed on each contour line of the contour plots.
TABLE 8.5: Extrusion results using the flow restrictor

<table>
<thead>
<tr>
<th>Expt. No</th>
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<tbody>
<tr>
<td>-----------</td>
</tr>
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</tr>
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<td>29(4)</td>
</tr>
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<td>30(15)</td>
</tr>
</tbody>
</table>

* Temperature of the melt at the end of the screw tip before it enters the diverging section of the flow restrictor.
### TABLE 8.6: Polynomial coefficients for the extrusion results of Table 8.5

<table>
<thead>
<tr>
<th>Polynomial Terms</th>
<th>Volumetric flow rate ($\mu m^3/s$)</th>
<th>Melt Temperature ($^\circ C$)</th>
<th>Extrudate Temperature ($^\circ C$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b_0$ (grand mean)</td>
<td>3.28*</td>
<td>118.70*</td>
<td>113.70*</td>
</tr>
<tr>
<td>$b_1(S)$</td>
<td>0.83*</td>
<td>4.88*</td>
<td>3.71*</td>
</tr>
<tr>
<td>$b_2(D)$</td>
<td>-0.01</td>
<td>7.38*</td>
<td>7.04*</td>
</tr>
<tr>
<td>$b_3(R)$</td>
<td>0.05</td>
<td>7.21*</td>
<td>5.63*</td>
</tr>
<tr>
<td>$b_4(P)$</td>
<td>-0.08</td>
<td>0.88*</td>
<td>1.63*</td>
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<tr>
<td>$b_{11}(SS)$</td>
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<td>-0.59</td>
<td>0.03</td>
</tr>
<tr>
<td>$b_{22}(DD)$</td>
<td>-0.07</td>
<td>0.16</td>
<td>0.16</td>
</tr>
<tr>
<td>$b_{33}(RR)$</td>
<td>0.05</td>
<td>-0.34</td>
<td>-0.22</td>
</tr>
<tr>
<td>$b_{44}(PP)$</td>
<td>0.08</td>
<td>0.03</td>
<td>-0.22</td>
</tr>
<tr>
<td>$b_{12}(SD)$</td>
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<td>0.06</td>
<td>0.69</td>
</tr>
<tr>
<td>$b_{13}(SR)$</td>
<td>-0.05</td>
<td>-0.19</td>
<td>-0.31</td>
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<tr>
<td>$b_{14}(SP)$</td>
<td>0.04</td>
<td>-0.06</td>
<td>1.19</td>
</tr>
<tr>
<td>$b_{23}(DR)$</td>
<td>-0.10</td>
<td>0.31</td>
<td>1.31*</td>
</tr>
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<td>$b_{24}(DR)$</td>
<td>0.05</td>
<td>0.19</td>
<td>-0.02</td>
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<tr>
<td>$b_{34}(RP)$</td>
<td>-0.03</td>
<td>-0.06</td>
<td>1.06</td>
</tr>
</tbody>
</table>

* Indicates coefficient significance > 95% (in t-distribution tables)
In order to reduce the amount of information requiring detailed consideration, due to the large number of contour plots resulting from all combinations, it is sensible to select only those responses associated with statistically significant coefficients, or at least the ones of primary interest. To further save space, as well as to establish optimum operating windows, the responses can be superimposed. The discussion here will be mainly concerned with the screw speed vs pressure effect on each response, shown in Figures 8.4-8.8. A point worth mentioning here is that by using the adjustable flow restrictor (see Section 7.2.3-I) the back pressure is no longer a dependent variable, as it has been treated until now, but it appears as an independent variable.

According to Table 8.6, the output shows a strong dependence on screw speed; an expected fact but also verified by the relevant figures 8.4-8.8. However, what seems to be rather surprising is the independence of flow rate on pressure. This neutral effect is also supported by the results of Table 8.3 where the experimental extrusion-die runs are tabulated and which clearly show that whatever the increase of the pressure drop, $\Delta P$, the flowrate is nearly unaffected. The fact also that the melt temperature at the end of the screw was not affected as well, see Table 8.6 and Figures 8.4-8.8, makes any interpretation, through consideration of rise in melt temperature - as a consequence of increase in $\Delta P$ - difficult. A possible experimental error, to that extent, must also be rejected because the differences between $Q$ vs $\Delta P$ were also trivial for any die length tried. On the basis of the foregoing, the only possible explanation it can be given is through the leakage effect; where any increase in back pressure results in an increase in leakage flow which in turn reduces the net flow rate.

The only effect that pressure appears to have is on extrudate temperature though it is only a weak one. One would expect this effect to be at its maximum when the die temperature is at its maximum, but as Figure 8.8 indicates, this happens when the barrel/head temperature ratio is at its maximum.

Use of the GLIM results, see Table 8.6, shows that the effect of barrel/head temperature ratio and/or die temperature on output is minimal.
Fig. 8.4: Red contour height = volumetric flowrate (m³/s)
Green contour height = melt temperature (°C)
Blue contour height = extrudate temperature (°C)

X-axis = screw speed
Y-axis = pressure

Die temperature is kept at level: -2
Head Temperature is kept at level: 0
Barrel Temperature is kept at level: 0
Fig. 8.5: Red contour height = volumetric flowrate (m$^3$/s)
Green contour height = melt temperature (°C)
Blue contour height = extrudate temperature (°C)

X-axis = screw speed
Y-axis = pressure
Die temperature is kept at level: 0

Head Temperature is kept at level: 0
Barrel Temperature is kept at level: 0
Fig. 8.6: Red contour height = volumetric flow rate \( \frac{m^3}{s} \times 10^{-8} \)
Green contour height = melt temperature (°C)
Blue contour height = extrudate temperature (°C)

X-axis = screw speed
Y-axis = pressure

Die temperature is kept at level: 2
Head Temperature is kept at level: 0
Barrel Temperature is kept at level: 0
Fig. 8.7: Red contour height = volumetric flow rate (m$^3$/s)
Green contour height = melt temperature (°C)
Blue contour height = extrudate temperature (°C)

X-axis = screw speed
Y-axis = pressure
Die temperature is kept at level: 0
Head Temperature is kept at level: -2
Barrel Temperature is kept at level: -2
Fig. 8.8: Red contour height = volumetric flowrate \( (m^3/s) \)
Green contour height = melt temperature \( (^\circ C) \)
Blue contour height = extrudate temperature \( (^\circ C) \)

X-axis = screw speed
Y-axis = pressure
Die temperature is kept at level: 0

Head Temperature is kept at level: 2
Barrel temperature is kept at level: 2
It seems therefore that the only alternative to increase output is through screw speed which, also increases the extrudate temperature as Figures 8.4-8.8 shows. However, the situation becomes very sensitive if the material contains curatives, due to the possibility of premature vulcanisation (scorch). The uniformity of the extrudate is another factor which must be viewed very carefully. Thus, an optimum valance between output/extrudate temperature has to be chosen and the contour plots, with the responses superimposed, enables the selection of an operating window. The criteria for selecting the operating window in this work were based on the capabilities of the system to achieve simultaneously:

a) maximum output
b) extrudate temperature between 100-110°C
c) melt temperature between 100-110°C (in extruder head).

The conditions are met in Figure 8.7 in the area enclosed by the curves:

a) output $\approx (4.5) \times 10^{-6} - (5) \times 10^{-6}$ m$^3$/s
b) extrudate temperature = 105°C - 108°C
c) melt temperature = 107°C - 110°C.

The best performance is the intersection point of the following settings:

Screw speed $\approx 57.5$ rpm (±1.75)
Pressure $\approx 3.45$ MPa (±2.0)
Head temperature = 88°C ±2.0
Barrel temperature = 66°C
Die temperature = 110°C (±0)

which results

output $= (5) \times 10^{-6}$ m$^3$/s
extrudate temperature $\approx 105°C$
melt temperature $= 108°C$
8.3 SQUARE AND RECTANGULAR SECTIONS

Computed results for the square and rectangular ducts are shown together with the experimental results in Tables 8.7 and 8.8 respectively while a simplified flow chart in respect to the computer program used is shown in Appendix C5. The tables are self-explanatory, so only a few observations will be outlined; these are:

i) both net*- and total* - theoretical pressure drops underestimate the corresponding experimental values

ii) although there is no specific pattern in the change of the net error either with duct length or with the cone angle, the total error seems to increase with both the duct length and the cone angle

iii) from the heat transfer point of view there would appear to be no significant advantage to be gained by treating the systems as non-isothermal.

Possible explanations for the discrepancies outlined in (i) and (ii) can be given as arising from the following three factors:

a) experimental error

b) inadequacy of the power-law model

c) inaccuracy of the finite difference method at low power-law indices.

Accurate experimental data are essential, if one expects to draw firm conclusions about the adequacy of the model. Tables 8.7 and 8.8 show that errors are present if one examines the fluctuations in the output. The only way to reduce (and possibly eliminate) these errors is to run the extruder for considerable time before taking any measurements, but then we are faced with the problem of material-availability. The possible inadequacy of the power-law model has been discussed in great length throughout this work (see Section 4.3B) so it will not be considered further. However some attention will be given to the possible inaccuracy of the finite-difference method used to model the process.

To obtain solutions at low power-law indices the Davidenko path procedure (see Section 6.5) was followed; and this obviously introduced

* For definition of net- and total-theoretical pressure drop see comments in Table 8.7.
### TABLE 8.7: Comparison of predicted and experimental results for square ducts

<table>
<thead>
<tr>
<th>Cone Half-Angle (degrees)</th>
<th>Length of the Square (mm)</th>
<th>Temperature of the Extrudate (°C)</th>
<th>Volumetric Flow rate (μm³/s)</th>
<th>Pressure (MPa)</th>
<th>Error Net (%)</th>
<th>Error Total (%)</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>Experimental</td>
<td>Total†</td>
<td>Calculated by the model for the land section</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Experimental</td>
<td>Net‡</td>
<td>Sum of pressures in the converging and non-circular sections estimated by the models</td>
</tr>
<tr>
<td></td>
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<td>Theoretical</td>
<td>Net*</td>
<td>**</td>
</tr>
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<td></td>
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<td>Theoretical</td>
<td>Total**</td>
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† Measured by the pressure transducer
‡‡ Difference between total experimental pressure drop and that due to the converging section (see Table 8.3)
* Calculated by the model for the land section
** Sum of pressures in the converging and non-circular sections estimated by the models
TABLE 8.8: Comparison of predicted and experimental results for rectangular ducts*

<table>
<thead>
<tr>
<th>Cone Half-Angle (degrees)</th>
<th>Length of the Rectangle (mm)</th>
<th>Temperature of the Extrudate (°C)</th>
<th>Volumetric Flow rate (µm³/s)</th>
<th>Pressure (MPa)</th>
<th>Error Net (%)</th>
<th>Error Total (%)</th>
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<td>Experimental Net</td>
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<td>6.570</td>
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</table>

* Same comments apply as in Table 8.7
additional errors to that of the iterative procedure. To reduce these errors double precision arithmetic was used, thus improving the number of significant figures used in the computations. Further, to improve the accuracy of the relaxation method, a fine mesh was used, also bearing in mind that as the mesh becomes finer the computational time increases while the rate of convergence decreases. To obtain some idea of the inaccuracy of the computed results, Table 8.9 has been constructed, in which the results of this thesis are compared with the results of other workers at different power-law indices. The product of friction factor, \( f \), and Reynolds number, \( Re \), \( f.Re \) is used as a comparison basis. The calculation of \( (f.Re) \) was done using eqn. (8.2), provided by the analysis of Yound et al \([13,14]\), i.e.

\[
f.Re = 2 \left[ \frac{1}{\lambda(n)} \right]^n
\]  

(8.2)

where \( \lambda(n) \) is the dimensionless volumetric flow rate [see eqn. (6.56)].

The deviation of the results expressed in % error using the results of Wheeler and Wissler \([14]\) as a basis, may be attributed to:

i) the accuracy of the methods used in each paper referred to

ii) the difference of convergence criterion in the iterative techniques used

iii) the difference in the mesh points over which the integral was taken to calculate the dimensionless flow rate, \( \lambda(n) \), and consequently the \( f.Re \) product.

The lack of data below \( n=0.4 \) limits a more rigorous comparison. However, use of the data provided by Al-Kharafi and Evans \([15,16]\) show that the two methods, i.e. finite-difference and finite-element, start to diverge at a power law index of about 0.4, until the case of \( n=0.15 \) is reached where the divergence is at its maximum. It is the author’s opinion that the value of \( f.Re \) obtained by Al-Kharafi and Evans must be in error, at least, for \( n=0.15 \) for the following three reasons:

i) it does not follow the decreasing pattern of \( f.Re \) with respect to \( n \)
TABLE 8.9: Friction factor - Reynolds number product for typical values of $n$ in a square duct estimated by various methods

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>57.08 (0.298%)</td>
<td>56.91</td>
<td>56.92 (0.018%)</td>
<td>56.97 (0.105%)</td>
</tr>
<tr>
<td>0.9</td>
<td>-</td>
<td>47.62</td>
<td>47.56 (-0.126%)</td>
<td>47.53 (-0.189%)</td>
</tr>
<tr>
<td>0.8</td>
<td>-</td>
<td>39.66</td>
<td>39.69 (0.076%)</td>
<td>39.66 (-)</td>
</tr>
<tr>
<td>0.75</td>
<td>36.34 (0.331%)</td>
<td>36.22</td>
<td>36.25 (0.083%)</td>
<td>36.21 (-0.028%)</td>
</tr>
<tr>
<td>0.7</td>
<td>-</td>
<td>33.07</td>
<td>33.10 (0.091%)</td>
<td>33.04 (-0.091%)</td>
</tr>
<tr>
<td>0.6</td>
<td>-</td>
<td>27.53</td>
<td>27.56 (0.109%)</td>
<td>27.44 (-0.327%)</td>
</tr>
<tr>
<td>0.5</td>
<td>23.02 (0.568%)</td>
<td>22.89</td>
<td>23.12 (1%)</td>
<td>22.54 (-1.529%)</td>
</tr>
<tr>
<td>0.4</td>
<td>-</td>
<td>18.97</td>
<td>20.53 (8.22%)</td>
<td>18.25 (-3.795%)</td>
</tr>
<tr>
<td>0.3</td>
<td>-</td>
<td>-</td>
<td>17.10</td>
<td>14.32</td>
</tr>
<tr>
<td>0.2</td>
<td>-</td>
<td>-</td>
<td>14.18</td>
<td>10.45</td>
</tr>
<tr>
<td>0.15</td>
<td>-</td>
<td>-</td>
<td>0.29</td>
<td>8.18</td>
</tr>
</tbody>
</table>

* Ritz and Galerkin
** Over-relaxation
*** Finite element
ii) incorporation of their $f_\text{Re}$ value into eqn. (8.2) produces a dimensionless flow rate having a value of $(3.94) \times 10^5$ which must be most certainly in error if one compares it with the analogous values of $\lambda(n)$ at higher indices; for example when $n$ is equal to 0.2 and 0.3 the $\lambda(n)$ values are $(5.58) \times 10^{-5}$ and $(7.83) \times 10^{-4}$.

iii) graphical representations displayed by the authors [15,16] show that the dimensionless velocity profile for power-law indices of 0.25 and 0.17625 has a curvature inwards and opposite to the mean flow direction at the centre of the duct (see Figure 8.9) while one expects the profile to be pluggish at such low indices (Fig. 8.10).

In order to illustrate how the behaviour of the flow varies with $n$, velocity profiles are superimposed (Fig. 8.10) for various values of $n$ at $\hat{x} = 0.5$ or $\hat{y} = 0.5$ (since the flow patterns are symmetrical around these two lines).

8.4 TRIANGULAR SECTION

Table 8.10 gives both the theoretical- and experimental-pressure drops in triangular ducts for various ducts-lengths. Note that the theoretical values were calculated based on the variational principles method.

It appears that there is no specific pattern as far as the net error is concerned and this must be in response to the inconsistent pattern of the output, as Table 8.10 shows. Obviously this inconsistency is due to experimental error, although all the necessary precautions were taken and the method recommended by Griff [10b] for one minute output-collection was most certainly followed. However when both the converging and triangular sections are coupled together, the (total) error seems to follow a specific pattern, in that an increase in die length results in an increase in the error. Two points worth observing are that:

i) for small lengths the models tend to underestimate the pressure drop; actually this underestimation tends to increase as the converging angle increases

ii) the prediction is better for large angles than for small ones.
Fig. 8.9: Superposition of dimensionless velocity profiles at 
\( x = 0.5 \) or \( y = 0.5 \) for: (a) \( n = 1.0, 0.75, 0.5, 0.25, 0.17625 \); (b) \( n = 0.25, 0.17625 \) with \( y \)-axis scale in 
(a) reduced 200 times; (c) \( n = 0.17625 \) with \( y \)-axis scale 
in (b) reduced 10 times (Reproduced from Al-Kharafi et al [15,16])
Fig. 8.10: Superposition of dimensionless velocity profile at $x = 0.5$ or $y = 0.5$ for: (a) $n=1.0, 0.5$ and 0.15; (b) $n=0.15$ with velocity-axis scale enlarged
<table>
<thead>
<tr>
<th>Cone Half-Angle (degrees)</th>
<th>Length of Triangle (mm)</th>
<th>Temperature of the Extrudate (°C)</th>
<th>Volumetric Flow rate (μm³/s)</th>
<th>Pressure (MPa)</th>
<th>Error Net (%)</th>
<th>Error Total (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Experimental Total</td>
<td>Experimental Net</td>
<td>Theoretical Net</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.276</td>
<td>0.336</td>
<td>0.377</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.780</td>
<td>0.840</td>
<td>1.181</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.285</td>
<td>1.345</td>
<td>1.559</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.621</td>
<td>1.681</td>
<td>2.370</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.891</td>
<td>1.951</td>
<td>2.740</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.562</td>
<td>2.622</td>
<td>3.487</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.898</td>
<td>2.958</td>
<td>3.942</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.752</td>
<td>0.342</td>
<td>0.380</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.444</td>
<td>1.034</td>
<td>1.186</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.482</td>
<td>1.072</td>
<td>1.498</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.217</td>
<td>1.807</td>
<td>2.322</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.722</td>
<td>2.312</td>
<td>2.708</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>5.293</td>
<td>2.883</td>
<td>3.474</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.562</td>
<td>3.152</td>
<td>3.906</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.604</td>
<td>0.344</td>
<td>0.375</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.108</td>
<td>0.848</td>
<td>1.187</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.511</td>
<td>1.251</td>
<td>1.566</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.978</td>
<td>1.718</td>
<td>2.367</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.419</td>
<td>2.159</td>
<td>2.740</td>
</tr>
<tr>
<td></td>
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<td></td>
<td></td>
<td>5.058</td>
<td>2.798</td>
<td>3.523</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.394</td>
<td>3.134</td>
<td>3.897</td>
</tr>
</tbody>
</table>

* Same comments apply as in Table 8.7.
These two points seem to be in line with the fact that the underestimated values of the converging section (see Table 8.3) are coupled together with the overestimated predictions of the triangular duct (see net error), the net result (expressed as total error in Table 8.3) reflects this compensation.

From the temperature viewpoint, the assumption of isothermal flow seems not to be precisely fulfilled in lengthy dies: however the error introduced does not violate the assumption to a significant extent.

Application of the finite-difference method to the present case, where $n = 0.1521$, must be ruled out. The reason being that in order to obtain the velocity profile at this value of $n$, the tolerance must be of the order of $10^{-9}$ (at least), to avoid the wall effects, in which case the solution diverges. Satisfactory solutions, however, were obtained - assuming that the variational principles method represents the 'true' flow rate values - for $0.4 \leq n \leq 1.0$. Table 8.11 compares the two methods based on arbitrarily selected pressure gradients.

**TABLE 8.11: Predictions by variational principle vs finite difference for triangular sections**

<table>
<thead>
<tr>
<th>$n$</th>
<th>$Q_{\text{var}}$</th>
<th>$Q_{\text{fd}}$</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{m}^3/\text{s}$</td>
<td>$\text{m}^3/\text{s}$</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$(4.2738)10^{-6}$</td>
<td>$(4.4291)10^{-6}$</td>
<td>3.6</td>
</tr>
<tr>
<td>0.9</td>
<td>$(6.4100)10^{-6}$</td>
<td>$(6.586)10^{-6}$</td>
<td>2.7</td>
</tr>
<tr>
<td>0.8</td>
<td>$(4.4656)10^{-6}$</td>
<td>$(4.5476)10^{-6}$</td>
<td>1.8</td>
</tr>
<tr>
<td>0.7</td>
<td>$(7.5379)10^{-6}$</td>
<td>$(7.6083)10^{-6}$</td>
<td>0.9</td>
</tr>
<tr>
<td>0.6</td>
<td>$(1.3875)10^{-5}$</td>
<td>$(1.3871)10^{-5}$</td>
<td>-0.03</td>
</tr>
<tr>
<td>0.5</td>
<td>$(3.6016)10^{-5}$</td>
<td>$(3.536)10^{-5}$</td>
<td>-1.8</td>
</tr>
<tr>
<td>0.4</td>
<td>$(1.5004)10^{-4}$</td>
<td>$(1.4685)10^{-4}$</td>
<td>-2.1</td>
</tr>
</tbody>
</table>

* Volumetric flow rate based on the variational principles method
** Volumetric flow rate based on the finite-difference method and tolerance $= 10^{-6}$

Note that for the finite-difference case the volumetric flow rate, $Q_{\text{fd}}$, was calculated from eqn. (8.3) below (see also Figure 6.13).
\[ Q_{\text{fd}} = 6 \ A \ \frac{V_{13} + V_{14} + V_{22}}{3} \]  

(8.3)

where \( A \) is the area of each small triangle and the factor 6 accounts for the whole duct since only 1/6 of the total duct was used for the analysis due to the symmetry of the system.

As far as the numerical investigation of eqn. (6.83) is concerned, Table 8.12 has been constructed, in order to show the variation of the integral, \( FA \), with respect to the power-law index, \( n \), the maximum absolute permissible accuracy and the number of function evaluations.

<table>
<thead>
<tr>
<th>( n )</th>
<th>Integral, ( FA ) (eqn.(6.83))</th>
<th>Accuracy (absolute)</th>
<th>No. of functions evaluations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>((26.6667)10^{-2})</td>
<td>(10^{-17})</td>
<td>633</td>
</tr>
<tr>
<td>0.9</td>
<td>((28.0371)10^{-2})</td>
<td>(10^{-7})</td>
<td>4777</td>
</tr>
<tr>
<td>0.8</td>
<td>((29.5174)10^{-2})</td>
<td>(10^{-6})</td>
<td>2009</td>
</tr>
<tr>
<td>0.7</td>
<td>((31.1189)10^{-2})</td>
<td>(10^{-6})</td>
<td>4361</td>
</tr>
<tr>
<td>0.6</td>
<td>((32.8542)10^{-2})</td>
<td>(10^{-5})</td>
<td>1637</td>
</tr>
<tr>
<td>0.5</td>
<td>((34.7378)10^{-2})</td>
<td>(10^{-5})</td>
<td>1821</td>
</tr>
<tr>
<td>0.4</td>
<td>((36.7859)10^{-2})</td>
<td>(10^{-5})</td>
<td>1953</td>
</tr>
<tr>
<td>0.3</td>
<td>((39.0166)10^{-2})</td>
<td>(10^{-5})</td>
<td>1977</td>
</tr>
<tr>
<td>0.1521</td>
<td>((42.6956)10^{-2})</td>
<td>((2)10^{-5})</td>
<td>1945</td>
</tr>
</tbody>
</table>

### 8.5 COMMENTS

#### 8.5.1 Feeding

Since extrusion is a continuous process, the long-term consistency in the output depends on the consistency of feeding the extruder. This statement was strongly supported by the present experimentation and it was found that a few times force feeding was necessary to overcome the consistency problem.

Erratic feeding can be the result of two factors:

i) due to the slipping action between material and screw surface

ii) due to the discontinuity in the form of the feeding material.
Factor (i) was overcome by lowering the temperature of the barrel in the feeding section while for factor (ii) the material was fed to the extruder in a form of a continuous strip.

Certain speculations arise as to whether strip feeding must be superseded by alternative ways of feeding, such as pellet or power feeding, since at its present state it is
a) labour intensive
b) affects the flow rate
c) increased the power requirements
d) cannot cope successfully with the automatic and continuous operations which have to be introduced in the industry.

8.5.2 Limitations

A. Assumptions

Presumably, the accuracy of the models described in Section 6 depends upon the validity of the various assumptions made. A comprehensive discussion of these assumptions can be found in Section 4.8 as well as in the discussion of the results; however the most important appear to be:

i) no-slip at the wall
ii) elongational effects in the convergent section at large angles
iii) split of the elastic and viscous part of the behaviour of the viscoelastic fluids
iv) use of the power-law constitutive equation.

B. Statistical Design

A disadvantage of the statistical design method used is the limitation that it should not be used to extrapolate or extend the results outside the experimental region. However the use of the flow restrictor described in Section 7.2.3.I helps to overcome this problem since

i) it is easy and cheap to construct
ii) once it has been made it can be used in conjunction with a number of extruders and elastomeric compounds to support the design of a range of dies.
C. **Numerical Method**

The method of finite-difference is computationally satisfactory for solving the elliptic equations derived in Chapter 6, provided that the tolerance is kept at a satisfactorily high level; but this happens at relatively high power-law indices. Once the wall effects start to become more effective - and this happens at low n - convergency problems start to appear; and in order to obtain solutions one has to compromise in tolerance (i.e. reduce it relatively to the dimensionless velocity values).

D. **Variational Method**

Although the method is an elegant one when compared to the finite difference method in that one obtains analytical expressions rather than tabulations of numerical results, its application is limited because there exist many fluids for which a variational principle cannot be written.

E. **Material Range**

The availability of data for one compound only does not allow one to rule out spurious effects conclusively. However, at this point it has to be stressed that the compound used represents a material with production applications; in actual fact it is being used for the production of car windscreen seals. This is very important if one compares related studies where with most of them the experimental verification of the proposed models has been based on rather idealised cases, i.e. the materials used for testing were either dilute polymer solutions or polymer melts with high power law indices. Although such investigations add a great deal to the body of knowledge, it would be more helpful to concentrate these studies in polymers with low power law index. This results from the fact that all rubber compounds and most of the widely used thermoplastics whose consumption accounts for more than 70% of the total polymer consumption have power-law indices less than 0.5 (see Table 8.13).
TABLE 8.13: Market share and power-law index for some bulky polymers

<table>
<thead>
<tr>
<th>Polymer</th>
<th>Market Share* [18]</th>
<th>n [19]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyethylene</td>
<td>39%</td>
<td>0.3-0.6</td>
</tr>
<tr>
<td>Polypropylene</td>
<td>13%</td>
<td>0.2-0.4</td>
</tr>
<tr>
<td>Polyvinyl chloride</td>
<td>19%</td>
<td>0.2-0.5</td>
</tr>
</tbody>
</table>

* USA, Western Europe, Japan

F. Preform Length

The method proposed for the evaluation of the preform length is not fully suitable for extrudates passing through cooling baths since the temperature of the bath influences the geometry of the extrudate and the method is only valid for isothermal conditions.

G. Computing Time

Approaching the problem from the computational viewpoint, it was realised that the machine computing time was an important factor. However, the situation with computers has changed so rapidly recently, so the usual choice between accuracy and computational cost favours the priority of accuracy. Preference in accuracy is also reinforced by the flow appearance of alternative computational procedures such as "parallel processing" where the computational time has drastically been reduced. In fact, there is a move towards the use of "parallel processing" for applications of this kind of problem [20].

8.5.3 Summary of Equations for Each Section

This sub-section serves as a quick guide for the use of the equations derived and explained at some length in Chapter 6.

A. Converging section, Fig. 6.2:

1. Motion equation \((6.9)\)
2. Boundary conditions equation \((6.10)\)
3. Volumetric flow rate \((6.6b)\)
4. Pressure drop \((6.12)\)
5. Energy equation \((6.23), (6.26)\) and \((6.27)\).
Procedure:

i) Solve (1) in conjunction with (2)

ii) Obtained from step (i) the f(0) value which will satisfy the known flow rate value as it is expressed by (3)

iii) Obtain pressure drop from (4)

iv) Once the f(θ) and f'(θ) values are known from step (ii), use (5) to obtain the temperature distribution.

B. Preform section:

i) See procedure in Section 6.2.

ii) Use eqn. (8.1) [or combine eqns. (6.34)-(6.35) and (6.40)] in conjunction with step (i) to obtain the pressure drop.

C. Rectangular and Square Sections, Fig. 6.6

1. Velocity distribution - (6.49)
2. Viscosity distribution - (6.51)
3. Boundary conditions - (6.44)
4. Extrapolated velocities - (6.52)
5. Extrapolated viscosities - (6.51) and (6.52)
6. Volumetric flow rate - (6.55)
7. Shear rate - (6.59)

Procedure:

i) Set (3)

ii) Initialise the system

iii) Find (4)

iv) Estimate (1)

v) Accelerate process

vi) Compute (2) and (5)

vii) Calculate (6) and (7).

8. Wall average shear stress - see procedure in Section 6.3.3A.

9. Primary normal stress difference as a function of pressure - see procedures in Sections 6.3.2A, 6.3.2B and 6.3.3B.
Notes:

a) If one-sided approximation has been used, neglect (4) and in place of (5) use eqns. (6.107).

b) For the rectangular section integrate eqn. (6.55) between 
   $0 \leq \hat{x} \leq w/h$ and $0 \leq \hat{y} \leq 1$

c) For the square section (9) is not applicable.

D. Triangular section, Fig. 6.10

I. Variational principles:

Procedure: (i) Integrate numerically eqn. (6.83)
   (ii) Use eqn. (6.87) in conjunction with (i) to obtain
        the pressure drop

II. Finite difference:

1. Velocity distribution - (6.102)
2. Viscosity distribution - (6.103)
3. Viscosity at the boundaries - (6.106)
4. Volumetric flow rate - (8.3)

Procedure: See procedure in C.

8.5.4 Example

An example will be given next, to demonstrate how the theory may
be applied to the design of an equilateral triangular die. The follo-
wing data are given:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power-law index, $n$</td>
<td>0.1521</td>
</tr>
<tr>
<td>Consistency index, $m$</td>
<td>$(0.95)10^5$ N.s$^n$/m$^2$</td>
</tr>
<tr>
<td>Extruder diameter</td>
<td>$(3.81)10^{-2}$ m (1\frac{1}{4}&quot;&quot;)</td>
</tr>
<tr>
<td>Extrudate side</td>
<td>20 mm</td>
</tr>
<tr>
<td>Volumetric output</td>
<td>$(5)10^{-6}$ m$^3$/s</td>
</tr>
<tr>
<td>Converging angle</td>
<td>$30^\circ$</td>
</tr>
</tbody>
</table>

Solution:

Area of the extrudate = $\frac{\sqrt{3}}{4} [(2)10^{-2}]^2 = (1.732)10^{-4}$ m$^2$

Hydraulic radius = $\frac{(2)(1.732)10^{-4}}{(3)(20)10^{-3}} = (5.77)10^{-3}$ m
A. Converging section

From the geometry of the system (see Fig. 6.2)

\[ r_{1,30} = (1.155)10^{-2} \text{m} \quad \text{and} \quad r_{1,00} = 10^{-2} \text{m} \]

\[ r_{2,30} = (3.8)10^{-2} \text{m} \quad \text{and} \quad r_{2,00} = (3.3)10^{-2} \text{m} \]

Following the procedure 8.5.3A(i)-(iii)

\[
\Delta P(r_2 - r_{1,30}) = -\frac{(0.951)10^{-5}}{(3)(0.1521)} \left[ \frac{0.1521}{(2.9212)10^{-5}} \right] [\cos 30 + \\
(0.1521) \left( \frac{5.4644}{{2.9212}10^{-5}} \right) \left[ \frac{1}{(3.8)10^{-2}0.4563} \right] - \left[ \frac{1}{(1.155)10^{-2}0.4563} \right] \\
\]

or \( \Delta P(r_2 - r_{1,30}) = \Delta P_c = 0.63 \text{ MN/m}^2 \)

Similarly \( \Delta P(r_2 - r_{1,00}) = \Delta P_c = 0.524 \text{ MN/m}^2 \)

B. Preform section

Since for an equivalent triangle, \( 2a = 60° \), use of Table 6.1 provides the following constants

\[ a = 0.1875 \]
\[ b = 0.6462 \]

Evaluate \( \dot{\gamma}_w \) from eqn. (6.40) i.e.

\[
\dot{\gamma}_w = \frac{0.1875+(0.64652)(0.1875)}{0.1521} \left( \frac{(2)(3)(20)10^{-3}}{(1.732)10^{-4}} \right)^2 (5)10^{-6}
\]

or \( \dot{\gamma}_w = 37.6 \text{ s}^{-1} \)

For the value of \( \dot{\gamma}_w \) calculated, obtain \( K \) by means of Fig. 8.3b, i.e.

\[ K = 3.489 \]
Use of eqn. (6.29) will provide the preform length, i.e.

\[ L \geq (8.28) \times 10^{-3} \text{m} \]

This length represents the value of the preform section necessary to minimise the reversible deformation effects responsible (partly) for the swell of the extrudate.

To obtain the pressure drop across the preform length, use eqn. (8.1), i.e.

\[ \Delta P_L = \frac{(0.951) \times 10^5 (3) (20) \times 10^{-3} (8.28) \times 10^{-3}}{(1.732) \times 10^{-4}} \times (37.6) \times 0.1521 \]

or

\[ \Delta P_L = 0.474 \text{ MN/m}^2 \]

C. Triangular section

Numerical integration of eqn. (6.83) for power-law index, \( n = 0.1521 \) yields:

\[ \Delta A = (42.7) \times 10^{-2} \]

The pressure gradient, \( \left( \frac{\Delta P}{L} \right)_T \), can now be obtained from eqn. (6.87):

\[ \left( \frac{\Delta P}{L} \right)_T = \frac{(30)(0.951) \times 10^5 (42.7) \times 10^{-2}}{\sqrt{3} (20) \times 10^{-3}} \left[ \frac{(40)(5) \times 10^{-6}}{(20) \times 10^{-3}^3} \right] \times 0.1521 \]

or

\[ \left( \frac{\Delta P}{L} \right)_T = 57.4 \text{ MN/m}^3 \]

It was discussed in Section 8.3.0 that the optimum pressure-operating setting for the extruder was 3.45 MPa. Therefore

\[ \Delta P_C + \Delta P_L + \Delta P_T = 3.45 \text{ MPa} \]

or

\[ \Delta P_T = 2.346 \text{ MPa} \]

Hence the length of the triangular section must be about 41 mm.
REFERENCES


17. SCHECHTER, R.S., AIChe J., 7 (3), 445 (1961).


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CHAPTER 9
CONCLUSIONS AND RECOMMENDATIONS

9.1 CONCLUSIONS

The overall objective of this thesis was to seek efficient methods of predicting polymer melt flow behaviour through dies of conical and non-circular shape. The approach used towards this objective was to develop theoretical models capable of predicting such flow behaviour and to contrast them with experimental results. A summary of the main conclusions resulting from the investigation can be stated as follows:

1. For the convergent section the model provides sufficiently accurate predictions, especially at low angles where the agreement appears to be excellent. Extensional effects have a significant effect towards higher angles. Clearly these effects require investigation but some difficulty arises in:
   a) measuring them precisely
   b) incorporating them into the transport equations.

   Viscous dissipation was found to be an insignificant factor in these systems; thus the isothermal assumption may be regarded as not constituting a source of error.

2. Statistical experimental design, multi-variable regression analysis and graphical representation of the results using contour plots has been shown to be a very useful and effective method for optimising extrusion performance. The reason being that it can accommodate processes with interactive independent variables as well as providing an operating window for the selection of optimum working conditions, which in turn may be used as a linkage method for the extruder-die combination.

3. Incorporation of a preform section in the die has been proven to be essential if the effects of the prior history, i.e. of the converging- and inlet-section, on the geometry of emerging profile is to be avoided. A quantitative method has been suggested which, although simple in its nature - since it is based on average values and 1-D analysis, has proven itself when compared with experimental results.
4. Finite difference is an attractive method for the solution of flow through dies due to its simplicity when compared to finite element methods. The results of the numerical simulation for non-circular dies are in fair agreement with experimental observations, and in general tend to underestimate the 'true' pressure drop values. The convergence of the iterative scheme for low power-law indices, while keeping the tolerance in a confidence level of accuracy, remains a major difficulty. An alternative approach, to that used previously [1] for the estimation of the viscosities at the boundaries, based on the concept of one-sided approximation, has been proven to be a powerful tool for both the improvement of the convergence rate and the convergency itself. Comparison of the dimensionless product of friction factor and Reynolds number (fRe) between this work and other related investigations, showed a close agreement. However, extension of this comparison between the finite-element method and finite difference method for values of power-law index below 0.4 showed a discrepancy between the predicted f.Re values by the two methods.

5. Use of the variational principle method provided answers for the pressure drop in triangular ducts for any power-law index, in contrast to the finite-difference methods which failed to produce satisfactory results for low power-law indices (n<0.4). However, a comparison between the two methods at higher power law indices but with sufficient non-Newtonian behaviour showed a close agreement. Theoretical predictions for the pressure drop are found to be in a fair agreement with experimental results.

6. Experimental evidence showed that the assumed isothermal flow, for all three non-circular sections investigated, was grossly accurate.
9.2 RECOMMENDATIONS

From the fact that research in the rubber industry in this area is trivial, compared to the plastics industry, it appears that every effort in nearly every aspect constitutes a recommendation. Possible suggestions include the following areas:

1. Repetition of this exercise either with a compound having completely different rheological characteristics and/or with a compound being susceptible to mastication.

2. More utilisation of processability testers such as capillary and slit rheometers since the traditional way of measuring processability such as, for example, Mooney viscosity can only provide a single point assessment of the material behaviour plus the fact that it operates far below the usual processing shear rates.

3. Possible incorporation of the wall slip condition, though it is realised that the problem in hand will become more complicated from the computational point of view.

4. Need to incorporate the elongational effects, at least in the converging section at large angles. Possible ways of achieving this include the addition of the pressure drop due to elongational flow to that derived by the author, although such an addition may lack theoretical justification. Recommended procedures to obtain elongational pressure drops, at present, include those proposed by Gibson et al [2,3].

5. More utilisation of statistical based techniques, for the reasons explained in 9.1. This is particularly helpful to the industry where techniques such as 'Evolutionary Operation' or 'EVOP' may be applied on the full-scale plant on a day-to-day basis; thus supplying useful information as for example 'how to improve the product while it is being obtained' or 'how to obtain the best operating conditions of the processing equipment'.

6. Use of more realistic constitutive equations due to the limitation of the power law model. A possible incorporation of an effective model describing fluid-memory effects is highly desirable.
7. It will be an attractive idea to think of a transformation that can be utilized to reduce the non-linear formulation of the problem to a linear one; it has recently come to the author's notice that such transformation has been achieved but not yet published [4].

8. Having realised the difficulties encountered in the design of dies from both the mathematical and computational point of view, and the rather simplified view taken here in comparison to the complexity of the problem in hand, it appears that the specialised knowledge of an expert is also essential. This as a consequence raises the question of a possible use of an expert system in this field. Such an approach is also supported by the fact that since the method in designing dies until now has been based solely on gained experience stretching over a considerable number of years, this accumulated knowledge can be transferred into programs constructed to perform these tasks i.e. knowledge engineering.

9. If recommendation (8) is unacceptable as being not feasible, then there is a great need for relying on more rigorous mathematical treatments, realising of course the complicated nature of the problems but on the other hand the increasing impetus of the market demand. The fact that this kind of problem offers a great area of research for mathematicians [5,6] proves that there is a need either for researchers with an excellent "grasp" of engineering mathematics or for collaboration between polymer scientists and mathematicians. This is especially true if one considers the increasing application of more sophisticated approaches such as the finite element and boundary integral equation methods. In our University this can be viewed as a collaboration between the Institute of Polymer Technology and the Engineering Mathematics Department.
REFERENCES

4. Professor D.J. EVANS, Computer Studies Department, Loughborough University of Technology, Private communication, UK, 1983.
6. See references 13, 15-17 in Chapter 8.
APPENDIX A

THE EQUATION OF CONTINUITY IN TWO COORDINATE SYSTEMS

COMPONENTS OF
THE EQUATION OF MOTION
THE FUNCTION \( \frac{\Delta \xi \Delta}{2} \) AND
THE RATE-OF-STRAIN TENSOR IN
TWO COORDINATE SYSTEMS

SUMMARY OF DIFFERENTIAL OPERATIONS INVOLVING THE
\( \nabla \)-OPERATOR
TABLE A1: Continuity equation in two coordinate systems based on eqn (4.4)

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

\[
(\nabla \cdot \mathbf{u}) = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \quad \text{(A)}
\]

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

\[
(\nabla \cdot \mathbf{u}) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (u_r \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} \quad \text{(B)}
\]

TABLE A2: Motion equations in terms of \(\tau\) based on eqn (4.6)

Rectangular coordinates

x-component:
\[
- \frac{\partial p}{\partial x} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \quad \text{(C)}
\]

y-component:
\[
- \frac{\partial p}{\partial y} = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \quad \text{(C)}
\]

z-component:
\[
- \frac{\partial p}{\partial z} = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} - \{ \rho \left[ \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right] \} \quad \text{(C)}
\]

Spherical coordinates

r-component:
\[
- \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (r \sin \theta \tau_{r\theta}) + \frac{1}{r \sin \theta} \frac{\partial \tau_{r\phi}}{\partial \phi} -\frac{\tau_{\theta \phi}}{r} \quad \text{(D)}
\]

\(\theta\)-component:
\[
\frac{1}{r} \frac{\partial p}{\partial \theta} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{r\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\tau_{\theta \theta} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \tau_{\theta \phi}}{\partial \phi} + \frac{\tau_{\phi \theta}}{r} \quad \text{(E)}
\]

\(\phi\)-component:
\[
- \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{r\phi}) + \frac{1}{r} \frac{\partial \tau_{\phi \phi}}{\partial \phi} + \frac{1}{r \sin \theta} \frac{\partial \tau_{\phi \theta}}{\partial \theta} + \frac{\tau_{\phi \phi}}{r} \quad \text{(F)}
\]
TABLE A3: The function \( \frac{\Delta \Delta}{2} \) for rectangular and spherical coordinates

Rectangular coordinates

\[
\frac{\Delta \Delta}{2} = 2 \left[ \left( \frac{\partial u_x}{\partial x} \right)^2 + \left( \frac{\partial u_y}{\partial y} \right)^2 + \left( \frac{\partial u_z}{\partial z} \right)^2 \right] + \left( \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right)^2 + \left( \frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z} \right)^2 \\
+ \left( \frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z} \right)^2
\]  
(A)

Spherical coordinates

\[
\frac{\Delta \Delta}{2} = 2 \left[ \left( \frac{\partial u_r}{\partial r} \right)^2 + \left( \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r} \right)^2 + \left( \frac{\partial u_\phi}{\partial \phi} + \frac{u_\theta}{r} + \frac{u_\phi \cot \theta}{r} \right)^2 \right] \\
+ \left[ \frac{r}{\partial r} \left( \frac{\partial u_\theta}{\partial r} \right) + \frac{1}{r} \frac{\partial u_\phi}{\partial \theta} \right]^2 + \left[ \frac{\sin \theta}{r} \frac{\partial u_\phi}{\partial \phi} + \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} \right]^2 \\
+ \left[ \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + r \frac{3}{\partial r} \left( \frac{u_\phi}{r} \right) \right]^2
\]  
(B)

TABLE A4: Components of the rate of strain tensor \( \Delta \)

Rectangular coordinates

\[
\Delta_{xx} = 2 \frac{\partial u_x}{\partial x} ; \quad \Delta_{yy} = 2 \frac{\partial u_y}{\partial y} ; \quad \Delta_{zz} = 2 \frac{\partial u_z}{\partial z} \\
\Delta_{xy} = \Delta_{yx} = \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} ; \quad \Delta_{yz} = \Delta_{zy} = \frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z} ; \quad \Delta_{xz} = \Delta_{zx} = \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}
\]  
(A)

Spherical coordinates

\[
\Delta_{rr} = 2 \frac{\partial u_r}{\partial r} ; \quad \Delta_{\theta\theta} = 2 \left[ \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r} \right] ; \quad \Delta_{\phi\phi} = 2 \left[ \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + \frac{u_\theta}{r} + \frac{u_\phi \cot \theta}{r} \right] \\
\Delta_{r\theta} = \Delta_{\theta r} = r \frac{\partial u_\theta}{\partial r} \left( \frac{1}{r} \right) + \frac{1}{r} \frac{\partial u_r}{\partial \theta} ; \quad \Delta_{r\phi} = \Delta_{\phi r} = \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + r \frac{3}{\partial r} \left( \frac{u_\phi}{r} \right)
\]  
(C)

(D)
\[ \Delta \theta \phi = \Delta_{\phi\theta} = \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left( \frac{u_\phi}{\sin \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial u_\theta}{\partial \phi} \]  

\[ \text{(E)} \]

**TABLE A5: Summary of differential operations involving the \( \nabla \) operator**

**Rectangular coordinates**

\[ (\nabla . u) = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \]  

\[ (\nabla^2 u) = \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \]  

\[ (u . \nabla T) = u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \]  

\[ \text{(A)} \]

\[ \text{(B)} \]

\[ \text{(C)} \]

**Spherical coordinates**

\[ (\nabla . u) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 u_r \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( u_\theta \sin \theta \right) + \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} \]  

\[ (\nabla^2 u) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial u_r}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial u_\theta}{\partial \theta} + \frac{1}{r^2 \sin \theta} \frac{\partial^2 u_r}{\partial \phi^2} \right) \]  

\[ (u . \nabla T) = u_r \left( \frac{\partial T}{\partial r} \right) + u_\theta \left( \frac{1}{r} \frac{\partial T}{\partial \theta} \right) + \frac{u_\phi}{r \sin \theta} \frac{\partial T}{\partial \phi} \]  

\[ \text{(D)} \]

\[ \text{(E)} \]

\[ \text{(F)} \]

**Reference**

Tables A1, A2, A3, A4 and A5 have been abstracted from Tables 3.1-1 (p.83), 3.4-2/3.4-4 (p.84/86), 3.4-5/3.4-7 (p.88/90), 3.4-8 (p.91) and 10.2-2/A.7-1/A.7-3 (p.318/739A/739C) respectively, of Transport Phenomena by R.B. Bird, W.E. Stewart and E.N. Lightfoot, Wiley, New York, 1960.
APPENDIX B
PRESSURE DROP OF NON-NEWTONIAN FLUIDS DUE TO AN ENTRANCE REGION OF ARBITRARY CROSS-SECTION

B1. INTRODUCTION

Following the review of the hydrodynamic entrance-region flow of fluids in Section 3.2, the present research constitutes a comprehensive theoretical investigation of laminar flow of non-Newtonian fluids through arbitrary cross-sections. The derivation of the necessary equations is based on the approach of Lundgren et al [1] whose ideas - originally applied to Newtonian fluids, are here extended further to non-Newtonian fluids.

The purpose is to obtain a relationship which will give the incremental pressure drop factor at the entrance region of a duct. The method involves the linearization of momentum equations to obtain an approximate solution.

B2. ANALYSIS
B2.1 Pressure Drop Based on Momentum

The axis of the duct is assumed to be along the positive z-direction, while x and y axes are the cross-sectional coordinates. Assume, also, the $u_z$ represents the axial velocity component (which for convenience will be approximated by $u$) while $u_x$ and $u_y$ are the cross-sectional velocity components (Fig. B1).

---

Fig. B1: Coordinates and velocity components configuration
If the fluid density is considered as constant, and the longitudinal shear component $\partial \tau_{zz}/\partial z$ is neglected, then combination of equations (A1-A) and (A2-C) from Appendix A gives

$$\frac{\partial (uu_x)}{\partial x} + \frac{\partial (uu_y)}{\partial y} + \frac{\partial u_z}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \frac{1}{\rho} \left[ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} \right]$$  (1)

Integration of equation (1) over the cross-section area $A$ gives:

$$\int_A \left[ \frac{\partial (uu_x)}{\partial x} + \frac{\partial (uu_y)}{\partial y} + \frac{\partial u_z}{\partial z} \right] dA + \frac{1}{\rho} \int_A \frac{\partial p}{\partial z} dA = \frac{1}{\rho} \int_A \left[ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} \right] dA$$  (2)

At the wall the no-slip assumption implies that $u_x = u_y = u = 0$, then from the divergence theorem [2a] it follows that

$$\int_A \left[ \frac{\partial (uu_x)}{\partial x} + \frac{\partial (uu_y)}{\partial y} \right] dA = 0$$  (3a)

and

$$\frac{1}{\rho} \int_A \left[ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} \right] dA = \frac{1}{\rho} \int_C \tau_{xz} dy - \tau_{yz} dx$$  (3b)

where the symbol $\int_C$ indicates that the integration is carried over a closed curve, and $C$ is the circumference of the duct.

With the help of equations (3) the integrated form of equation (2) becomes

$$\rho \int_A \frac{\partial u_z}{\partial z} dA + \int_A \frac{\partial p}{\partial z} dA = \int_C \tau_{xz} dy - \tau_{yz} dx$$  (4)

For a fluid whose flow behaviour could be described by an Ostwald-de-Waele power-law model, the stresses and the rate of strain tensors are related by a functional relation of the type (see Section 4.3D)

$$\tau_{xz} = m \left[ \frac{\Delta : \Delta'}{2} \right]^{n-1} \Delta_{xz}$$  (5a)

$$\tau_{yz} = m \left[ \frac{\Delta : \Delta'}{2} \right]^{n-1} \Delta_{yz}$$  (5b)
where \[ \left[ \frac{\Delta_1}{2} \right] \] is given by equation (A3-A) in Appendix A;

and \[ \Delta_{xz} = \frac{\partial u}{\partial x} = \Delta_{yz} = \frac{\partial u}{\partial y} \] are given by equation (A4-B) in Appendix A.

The RHS of equation (4) in conjunction with eqns (5) can now be written as

\[
\int_{xz} \tau_{xz} \, dy - \tau_{yz} \, dx = \phi \left[ \frac{\Delta x}{2} \right]^n \left\{ \frac{\partial u}{\partial x} \right\} \, dy - \left( \frac{\partial u}{\partial y} \right) \, dx
\]

\[
= \phi \left[ \frac{\Delta x}{2} \right]^n \left\{ \frac{\partial u}{\partial x} \right\} \, ds \quad \text{(see Ref. 2b)}
\]

\[
= \phi \left[ \frac{\Delta x}{2} \right]^n \left\{ \frac{\partial u}{\partial y} \right\} \, ds
\]

\[
= - \int_{c} \tau_{w} \, ds
\]

The negative sign indicates that \( \tau_{w} \) acts in a direction opposite to that of \( \tau_{xz} \) and \( \tau_{yz} \). Combining eqns. (4) and (6) to obtain

\[
\rho \int_{A} \frac{\partial u^2}{\partial z} \, dA + \int_{A} \frac{\partial P}{\partial z} \, dA = - \int_{c} \tau_{w} \, ds \quad \text{(7)}
\]

Integration w.r.t. \( z \) between the entrance region where \( z = z_o = 0 \) and any other axial locations where \( z = z \) gives

\[
- \frac{1}{\rho} \int_{z_0}^{z} \frac{dP}{dz} \, dz = \frac{1}{A} \left\{ \int_{z_0}^{z} \frac{d}{dz} \left( \int_{A} u^2 \, dA \right) \, dz \right\} + \frac{1}{\rho A} \int_{z_0}^{z} \phi \tau_{w} \, ds \, dz
\]

or

\[
- \frac{P - P_o}{\rho} = \frac{1}{A} \left[ \int_{A} u^2 \, dA \right]^{z_o} - \frac{1}{A} \left[ \int_{A} u^2 \, dA \right]^{z_o}_{z} + \frac{1}{\rho A} \int_{z_0}^{z} \phi \tau_{w} \, ds \, dz
\]

where \( P_o = \) pressure at the entrance where \( z = z_o = 0 \)

\( P_z = \) pressure at any axial location \( z \).

According to this analysis, any velocity profile is permissible at the entrance region, so if it is assumed that flow is plugged, i.e. flat velocity profile, at \( z_o \) and if the velocity at this point is represented by the average velocity \( \bar{u} \) the middle term of the RHS of equation (8) may be written as:
\[-\frac{1}{A} \left[ \int_A u^2 dA \right]^{z_0} = -\frac{1}{A} \int_A \bar{u}^2 dA = -\bar{u}^2 \]

which in the case of equation (8) takes the form

\[
\frac{P_0 - P}{\rho} = \frac{1}{A} \int_A u^2 dA - \bar{u}^2 + \frac{1}{\rho A} \int_{z_0}^z dz \int_c \tau_w ds
\]

Multiply eqn. (9) by 2 and then divide it by \( \bar{u}^2 \); also consider that the velocity \( u \) at the fully developed region can be represented by \( u_\infty \), then

\[
\frac{P_0 - P}{\frac{1}{2} \rho u^2} = 2 \left[ \frac{1}{A} \int_A \left( \frac{u_\infty}{u} \right)^2 dA \right] - \frac{2}{\rho A u^2} \int_{z_0}^z dz \int_c \tau_w ds
\]

If the fully developed wall shear stress \( \tau_{w(\infty)} \) is being introduced, equation (9a) becomes, after some rearrangement:

\[
\frac{P_0 - P}{\frac{1}{2} \rho u^2} = \frac{2}{\rho A u^2} \int_{z_0}^z dz \int_c \tau_{w(\infty)} ds + 2 \left[ \frac{1}{A} \int_A \left( \frac{u_\infty}{u} \right)^2 dA \right] - \frac{2}{\rho A u^2} \int_{z_0}^z dz \int_c \left[ \tau_w - \tau_{w(\infty)} \right] ds
\]

Pressure drop at the fully developed region

Pressure drop at the entrance region based on the momentum equation

Alternatively, equation (10a) may be written as:

\[
\frac{P_0 - P}{\frac{1}{2} \rho u^2} = C_f \frac{Z}{D_e} + K_m(z)
\]

where

\[
C_f \frac{Z}{D_e} = \frac{2}{\rho A u^2} \int_{z_0}^z dz \int_c \tau_{w(\infty)} ds
\]

\[
K_m(z) = \frac{1}{A} \int_A \left( \frac{u_\infty}{u} \right)^2 dA - \frac{2}{\rho A u^2} \int_{z_0}^z dz \int_c \left[ \tau_w - \tau_{w(\infty)} \right] ds
\]

\[C_f = \text{fully developed friction factor}\]
\[z = \text{axial distance measured from the inlet section of the duct}\]
\[\text{where } z = z_0\]
\[D_e = \text{equivalent diameter}\]
$K_m(z) = \text{incremental pressure drop term due to entrance region (or loss coefficient) which is a correction term consisting of two parts: (a) the excess energy loss due to the gain of kinetic energy, and (b) the accumulated wall shear increment (higher viscous friction) between a developing and fully developed flow.}$

**B2.2 Pressure Drop Based on Mechanical Energy**

An alternative equation for the pressure drop may be derived based on the mechanical energy equation (or microscopic mechanical energy equation), and since the mechanical energy equation (12) results from the momentum equation (A2-C) of Appendix A by multiplying the latter equation by $u$ (i.e. $u=uz$) one may expect, presumably, the same result for the pressure drop, independent to the equation which is used as a basis. However, from the fact that the analyses include a number of approximations then it would not be surprising if the end results were different.

$$
\rho \left[ u \begin{array}{c} \frac{3u}{3x} + uu \frac{3u}{3y} + u^2 \frac{3u}{3z} \end{array} \right] = -u \begin{array}{c} \frac{3P}{3z} + u \end{array} \left[ \frac{3\tau_{xz}}{3x} + \frac{3\tau_{yz}}{3y} \right] (12)
$$

Proceeding with equation (12) in the same way as with momentum equation (A2-C), the incremental pressure drop $K_e(z)$ is derived as being

$$
K_e(z) = \left\{ \frac{1}{A} \int_A \left[ \frac{u_{\infty}}{u} \right]^3 dA - \frac{2}{\rho A u^2} \int^z_0 dz \int_A \left[ \frac{u}{u} \left( \frac{3\tau_{xz}}{3x} + \frac{3\tau_{yz}}{3y} \right) \right] \right\} (13)
$$

As in equation (10), the first term on the RHS of equation (13) represents the difference between the kinetic energy of the fully developed and entering flow, while the rest (bracketed) term of the equation represents the accumulated increment in friction work between a developing and fully developed flow.
B2.3 Evaluation of Pressure Correction Term, K

Comparison of eqns. (11b) and (13) shows that the first bracketed term in both equations is the same and can be easily evaluated once the fully developed velocity, \( u_\infty \), is available. The last term in both equations appears to depend on the developing velocity profile and in order to be determined, a knowledge of the entrance region velocity distribution (i.e. \( u(x,y) \)) is required. To relate these two dissimilar bracketed terms, linearisation of the inertial terms in the momentum equation (A2-C) of Appendix A is carried out, according to the equation (14)

\[
\varepsilon u \frac{\partial u}{\partial z} = F(z) + \frac{1}{\rho} \left( \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} \right)
\]

(14)

where \( \varepsilon = \) free constant which facilitates the selection of a proper weighting of \( \bar{u} \)

\( F(z) = \) unknown function of \( z \) which includes the pressure gradient \( \frac{1}{\rho} \frac{dP}{dz} \) as well as the residual of inertia terms

The \( F \)-function is found by integrating equation (14) over the cross-section and employing the condition \( \frac{\partial}{\partial z} \int_A u dA = 0 \),

\[
F(z) = -\frac{1}{\rho A} \int \left[ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} \right] dA
\]

(14a)

The last term of equation (14a) can be treated in the same way as that of equation (2), where according to eqns (3b), (5) and (6), it proves to be equal to \( \int_c \tau_w ds \), then

\[
F(z) = \frac{1}{\rho A} \int_c \tau_w ds
\]

(14b)

Eqns. (14) and (14b) may also be applied to the fully developed flow, so

\[
O = F(\infty) + \frac{1}{\rho} \left[ \frac{\partial \tau_{xz}(\infty)}{\partial x} + \frac{\partial \tau_{yz}(\infty)}{\partial y} \right]
\]

(15)

and since \( \frac{\partial u_\infty}{\partial z} = O \),

then

\[
F(\infty) = -\frac{1}{\rho} \left[ \frac{\partial \tau_{xz}(\infty)}{\partial x} + \frac{\partial \tau_{yz}(\infty)}{\partial y} \right]
\]

(15a)
where $\tau_{ij}(\omega)$ are the shear stresses at the fully developed region.

Following the same procedure as for that of equation (14b), one may prove that

$$F(\omega) = \frac{1}{\rho A} \int_C \tau_{i\omega}(\omega) \, ds \tag{15b}$$

Multiply eqn. (14) by $u_\omega$ and eqn. (15) by $u$, then, upon subtracting the second from the first, it follows

$$u_\omega \frac{\partial u}{\partial z} = u_\omega F(z) - uF(\omega) + \frac{1}{\rho} \left[ u_\omega \left( \frac{\partial \tau_{xz}(\omega)}{\partial x} + \frac{\partial \tau_{yz}(\omega)}{\partial y} \right) - u \left( \frac{\partial \tau_{xz}(\omega)}{\partial x} + \frac{\partial \tau_{yz}(\omega)}{\partial y} \right) \right] \tag{16}$$

Integrate eqn. (16) over the cross-sectional area, $A$, and substitute eqns. (14b) and (15a) into the integrated eqn. (16) to obtain

$$\varepsilon u \frac{\partial u}{\partial z} \int_A u_\omega u \, dA = \frac{u}{\rho} \int_C \left[ \tau_{i\omega} - \tau_{i\omega}(\omega) \right] \, ds + I \tag{17}$$

where $I = \frac{1}{\rho} \int_A \left[ u_\omega \left( \frac{\partial \tau_{xz}(\omega)}{\partial x} + \frac{\partial \tau_{yz}(\omega)}{\partial y} \right) - u \left( \frac{\partial \tau_{xz}(\omega)}{\partial x} + \frac{\partial \tau_{yz}(\omega)}{\partial y} \right) \right] \, dA \tag{17a}$

Integrating eqn. (17) with respect to $z$ from $z = z_0 = 0$ to $z = z = \infty$

$$\frac{2}{\rho A} \int_0^\infty dz \left[ \tau_{i\omega} - \tau_{i\omega}(\omega) \right] \, ds = 2\varepsilon \left[ \frac{1}{A} \int_A \frac{u_\omega}{u} \, dA - 1 \right] - \frac{2}{A u^3} \int_0^\infty I \, dz \tag{18}$$

The second bracketed term of eqn. (11b) is the same with the left-hand side of eqn. (18), then

$$K_m(z) = 2 \left[ \frac{1}{A} \int_A \frac{u_\omega}{u} \, dA - 1 \right] + 2\varepsilon \left[ \frac{1}{A} \int_A \frac{u_\omega}{u} \, dA - 1 \right] - \frac{2}{A u^3} \int_0^\infty I \, dz$$

or

$$K_m(z) = (2+2\varepsilon) \left[ \frac{1}{A} \int_A \frac{u_\omega}{u} \, dA - 1 \right] - \frac{2}{A u^3} \int_0^\infty I \, dz \tag{19}$$

Using similar steps to the ones used for derivation of eqn. (19), $K_e(z)$ is determined to be
\[ K_e(z) = \frac{1}{A} \int_A \left( \frac{u_\infty}{u} \right)^3 dA + \frac{\epsilon}{A} \int A \left( \frac{u_\infty}{u} \right)^2 dA - \left( 1 + \epsilon \right) - \frac{2}{\text{Au}^3} \int_0^\infty I dz \quad (20) \]

As it has already been mentioned, \( K_m(z) \) and \( K_e(z) \) should be equal to each other. If one equates expressions (19) and (20) and then solves for the velocity scale factor, \( \epsilon \)

\[ \epsilon = \frac{1 - \frac{2}{\text{A}} \int_A \left( \frac{u_\infty}{u} \right)^2 dA + \frac{1}{A} \int A \left( \frac{u_\infty}{u} \right)^3 dA}{\frac{1}{A} \int A \left( \frac{u_\infty}{u} \right)^2 dA - 1} \quad (21) \]

the pressure correction for the entrance region then takes the form

\[ K_m = K_e = K = \frac{2}{A} \int_A \left[ \left( \frac{u_\infty}{u} \right)^3 - \left( \frac{u_\infty}{u} \right)^2 \right] dA - \frac{2}{\text{Au}^3} \int_0^\infty I dz \quad (22) \]

Eqn. (22) expresses the pressure correction for the entrance region for both Newtonian and non-Newtonian fluids. For Newtonian fluids, \( I=0 \) when the components of the stress tensor in Cartesian co-ordinates are substituted in eqn. (17a), so that eqn. (22) becomes the same as that derived by Lundgren et al [1]. For the non-Newtonian case, the situation is slightly different because \( I \) appears to depend on the developing velocity profile hence raising a difficulty in solving eqn. (22).

A possible alternative is to assume that \( I = 0 \) (i.e. Newtonian fluid) and to obtain the loss coefficient \( K \) using only the first bracketed term of eqn. (22) i.e.

\[ K = \frac{2}{A} \int_A \left[ \left( \frac{u_\infty}{u} \right)^3 - \left( \frac{u_\infty}{u} \right)^2 \right] dA \quad (23) \]

However, in order to proceed with such an assumption its validity must be firstly justified; and since no experimentation has been carried out by the author, one has to rely on literature sources.

B.3 COMPARISON WITH OTHER STUDIES

B.3.1 Circular Ducts

According to McKelvey [3], the fully developed velocity \( u_\infty \) is related to the average velocity, \( \bar{u} \) by
\[
\frac{u_\infty}{u} = (\frac{3n+1}{n+1}) \left[ 1 - \left( \frac{r}{R} \right)^n \right]
\]  

(24)

Substituting this eqn. in eqn. (23)

\[
K_c = \frac{2}{A} \int_A \left[ (\frac{3n+1}{n+1}) \right]^2 \left[ 1 - (\frac{r}{R})^n \right] \left\{ \left[ (\frac{3n+1}{n+1}) (1 - (\frac{r}{R})^n) \right] - 1 \right\} dA
\]

\[
= \frac{4}{R^2} (\frac{3n+1}{n+1})^2 \left[ \frac{nR^2}{n+1} - (\frac{n}{3n+1})^2 R^2 + (\frac{8n+2}{n+1})^2 \frac{R^2}{4n+2} \right]
\]

\[
- (\frac{3n+1}{n+1}) (\frac{n}{5n+3}) R^2
\]

or

\[
K_c = 4 (\frac{n}{n+1}) (\frac{3n+1}{n+1}) \left[ 1 - (\frac{7n+1}{3n+1}) + (\frac{4n+1}{2n+1}) - (\frac{3n+1}{5n+3}) \right]
\]  

(25)

B3.2 Parallel Plates (slit)

The fully developed velocity, \( u_\infty \), for parallel plates is given by McKelvey [3]

\[
\frac{u_\infty}{u} = (\frac{2n+1}{n+1}) \left[ 1 - \left( \frac{r}{R} \right)^n \right]
\]  

(26)

Following the same procedure as for circular ducts, the loss coefficient, \( K_p \), is obtained in a straightforward manner:

\[
K_p = 2 (\frac{n}{n+1}) (\frac{2n+1}{n+1})^2 \left[ 1 - (\frac{4n+1}{2n+1}) + (\frac{5n+2}{3n+2}) - (\frac{2n+1}{4n+3}) \right]
\]  

(27)

Using eqns. (25) and (27) Table B1 can be constructed.

| TABLE B1: K-values for circular and slit ducts |
| n   | 0     | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
| K_c | 0     | 0.457 | 0.782 | 1.018 | 1.196 | 1.333 |
| K_p | 0     | 0.2267 | 0.391 | 0.515 | 0.610 | 0.686 |
The values of Table B1 are plotted in Fig. B2 in conjunction with the theoretical results of Collins and Schowalter [4,5], Bogue [6] and Tomita [7] and the experimental results of Bogue and RamaMurthy [8] for power-law fluids flowing in the entrance region of circular and slit ducts.

B.4 DISCUSSION

The discussion will be very brief and concentrated on the usefulness and limitations of this procedure rather than seeking to demonstrate and discuss its application in this work.

Examination of Fig. B2 clearly indicates that there is a close agreement between the results of this analysis, and that of other investigators. Mention must be made at this point that while all comparison studies fulfil the assumption of flat velocity profile of the entrance, Bogue's [6] analysis is not clear at this point. This perhaps may be the reason that his results show a discrepancy in comparison with the rest.

Although the reliability of eqn. (23) has been justified for non-Newtonian fluids, some caution must be exercised about its validity, due to a number of limitations such as:

i) The inclusion of inertia terms in the equations indicates that the work described in this section is essentially valid for high Reynolds number flows and becomes increasingly invalid at low Reynolds number.

ii) The use of a power law model during the analysis makes this work valid for purely viscous fluids and possibly for moderately elastic fluids. Its validity for highly elastic and viscoelastic fluids must be questionable, especially if one takes into account that at the entrance phenomena such as elasticity, and circulating vortices are present as has been noted by some investigators [9,10]. Of course, the procedure could be easily extended for fluids obeying other rheological models as well.

iii) The assumption that the velocity profile at the entrance of the duct is flat holds only for fluids with small pseudoplasticity index. Actually, for n=0, the velocity distribution is completely flat, even in a fully developed case, but it becomes steeper as n increases.
Fig. B2: Power-law index, $n$, vs loss coefficient, $K$: (a) for circular sections, $K_c$ and (b) for slit sections, $K_p$.

- Present work
- Collins et al [4, 5]
- Tomita [7]
- Bogue [6]
- Booger et al [8]
In spite of these restrictions, the final result devised by the method appears to be quite simple with relatively little computational effort, thus useful in engineering design.

REFERENCES

APPENDIX C

APPENDIX C1: SUBROUTINE USED IN CONJUNCTION WITH NAG D02RAF TO EVALUATE THE VOLUMETRIC FLOWRATE IN THE CONVERGING SECTION

APPENDIX C2: LOGIC FLOWCHART FOR ENERGY CALCULATIONS IN CONVERGING SECTIONS

APPENDIX C3: FLETCHER AND REEVES LOGIC DIAGRAM

APPENDIX C4: LOGIC FLOWCHART FOR THE CORRECTION OF CAPILLARY DATA USING BAGLEY AND RABINOWITSCH CORRECTIONS

APPENDIX C5: LOGIC FLOWCHART FOR NON-NEWTONIAN FLOW IN NON-CIRCULAR DUCTS
APPENDIX C1
---------------------------
SUBROUTINE USED IN CONJUNCTION WITH NAG D02RAF TO EVALUATE
---------------------------
THE VOLUMETRIC FLOWRATE IN THE CONVERGING SECTION
---------------------------

SUBROUTINE FCN(X,EPS,Y,F,M)
DOUBLE PRECISION EPS,X,NC,AC1,AC2,AC3,AC4,AC5,AC6,AC7,
& F(M), Y(M)
INTEGER M
F(1)=Y(2)
F(2)=Y(3)
IF (X .EQ. 0) GOTO 10
NC = 0.1521D0
AC1=Y(2)*(12*(1-NC)*EPS+9*EPS*EPS*(NC-1)*(NC-1)
& +3*EPS*(NC-1)-6+1/(DSIN(X)**2))
AC2=Y(3)*(DCOS(X)/DSIN(X))
AC3=12*Y(1)*Y(1)+Y(2)*Y(2)
AC4=(NC-1)*EPS*(12*(1-Y(1)+Y(3))*Y(2))
& - (12*(1-NC)*EPS*Y(1))
AC5=12*(NC-1)*EPS*(Y(2)**3)
AC6=(((1-NC)*(1-NC)*EPS-EPS-2*(NC-1)*EPS)*Y(2)*Y(2)
& +Y(2)*(12*Y(1)+Y(3)))/(12*Y(1)+Y(3))/AC3
AC7=12*Y(1)*Y(1)+EPS*(NC*EPS)*Y(2)*Y(2)
F(3)=((AC1-AC2)*AC3+AC4-AC5-AC6)/AC7
RETURN
10 F(3)=0.0
RETURN
END
APPENDIX C2: LOGIC FLOW CHART FOR ENERGY CALCULATIONS IN CONVERGING SECTIONS

1. Initialise Constants
   - Read Data
   - Set boundary conditions
   - Start iteration loop along r-axis for each theta-point
     - Eqn 6.26a
     - Eqn 6.26b
   - Close iteration loop
     - Print results
     - Stop

Call subroutine Thomas to solve the system of tridiagonal equations.
FLETCHER AND REEVES LOGIC DIAGRAM

APPENDIX C3

Pick Starting Point

Determine Direction of Steepest Descent

Conduct One Dimensional Search in Steepest Descent Direction

Determine Conjugate Direction Components

Conduct One Dimensional Search in Conjugate Direction

Yes

No

Yes

Convergence Obtained?

Stop

No

Yes

Search in N+1 Directions?

No
APPENDIX C4:

LOGIC FLOWCHART FOR THE CORRECTION OF
CAPILLARY DATA USING BAGLEY AND RABINOWITSCH CORRECTIONS

Nomenclature

DP = Pressure
G = Shear rate (= f(V))
G_⊥ = Shear rate arbitrarily selected
G_corr = Shear rate after Rabinowitsch correction
L/R = Length/radius for each die
n* = Flow behaviour index
Q = Volumetric flow rate
T = Temperature
V = Plunger speed (mm/min)
FLOW CHART

- INITIALISE CONSTANTS
  - READ $c_1$

  READ $T$

  READ L/R

  READ RAW DATA (I.E. $v$ AND $dp$)

  - CALCULATE $c$
    - CALCULATE $q$ (EQN 3.8)

  YES ANOTHER $v$

  NO

  CALCULATE CONSTANTS USING
  LOGARITHMIC PARABOLA
  SUBROUTINE (EQN 3.14)

ESTIMATE $q$ AND $dp$
  FOR EACH $c_1$

  YES ANOTHER L/R

  NO

  BARLET CORRECTION

  ESTIMATE SS
  (EQN 3.15)

  CALCULATE FOR EACH $c_2$
  (1) $n$ (EQN 3.9)
  (2) $\delta_{m, c_2}$ (EQN 3.10)
  (3) VISCOITY

  YES ANOTHER $T$

  NO

  STOP
APPENDIX C5

LOGIC FLOWCHART FOR NON-NEWTONIAN FLOW IN NON-CIRCULAR DUCTS

- INITIALISE CONSTANTS
- SET BOUNDARY CONDITIONS

INITIALISE VISCOSITY AT BOUNDARIES AND VELOCITY AT THE INTERIOR POINTS

START ITERATION LOOP

ESTIMATE VELOCITY PROFILE (EQN 6.49)

ACCELERATE (EQN 6.53)

COMPUTE VISCOSITY DISTRIBUTION (EQN 6.51)

- CONVERGENCE CRITERION
  - UPDATE VELOCITY

IMPROVE VISCOSITY DISTRIBUTION AT BOUNDARIES (EQN 6.107)

CLOSE ITERATION LOOP

CALCULATE DIMENSIONLESS FLOWRATE (EQN 6.57)

CALCULATE PRESSURE GRADIENT (EQN 6.59)

ESTIMATE SHEAR RATE DISTRIBUTION (EQN 6.59)

STOP
APPENDIX D

APPENDIX D1: EVALUATION OF THERMAL DIFFUSIVITY

APPENDIX D2: TREATMENT OF CAPILLARY DATA USING -

(a) Bagley and Rabinowitsch corrections (Figures D1 and D2)

(b) Two-point method (Figures D3-D6)

APPENDIX D3: GLIM OUTPUT FOR THE EXTRUSION VOLUMETRIC FLOWRATE RESPONSE
APPENDIX D1
EVALUATION OF THERMAL DIFFUSIVITY

The basic Fourier equation for unsteady-state conduction is expressed by [1]

$$\frac{\partial T}{\partial t} = \alpha \frac{T}{L^2}$$

where $\frac{\partial T}{\partial t}$ = the rate of temperature with time

L = thickness of the slab

$\alpha$ = thermal diffusivity (= $K/\rho C_p$)

Solution of the above equation for the case of an infinite slab heated from both surfaces with negligible resistance to heat transfer is given by the converging series

$$\frac{T_s - T_x}{T_s - T_0} = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin[(2n-1)\pi x/2L]}{2n-1} \exp\left[-\frac{(2n-1)^2 \pi^2 \alpha t}{4L^2}\right]$$

which after expansion gives

$$\frac{T_s - T_x}{T_s - T_0} = \frac{4}{\pi} \left[ \sin \frac{\pi x}{L} - \pi^2 x + \frac{1}{3} \sin \frac{3\pi x}{L} - 9\pi^2 x + \frac{1}{5} \sin \frac{5\pi x}{L} - 25\pi^2 x + \ldots \right]$$

where $T_s$ = temperature of the heating medium and slab surface

$T_0$ = initial temperature of the slab

$T_x$ = temperature at a plane, distance x from the slab surface

$L = L/2$ = half-thickness of the slab

$t$ = heating time

$X = \alpha t/4L^2$

The temperature at the centre of the slab heated from both sides can be obtained from the above equation which is reduced to

$$Y = \frac{T_s - T}{T_s - T_0} = \frac{4}{\pi} \left[ \pi^2 x - \frac{1}{3} \pi^2 x - 9\pi^2 x + \ldots \right]$$

where $T$ is the temperature at the centre plane of the slab.
Generally the first term of this series is sufficient, since other terms have a negligible effect after a short time in the heat cycle i.e. \( \alpha t^2/4Y^2 \geq 0.06-0.08 \), therefore

\[
\ln \left( \frac{\pi Y}{4} \right) = -\frac{\pi^2 \alpha}{4Y^2} \cdot t
\]

A plot of \( t \) vs \( \left( \frac{4Y^2}{\pi^2} \ln \left( \frac{\pi Y}{4} \right) \right) \) yields a straight line with slope equal to thermal diffusivity.

Reference

Fig. D1: Shear rate vs shear stress at various temperatures

Fig. D2: Shear rate vs viscosity at various temperatures (legend as in Fig. D1)
Fig. D3: Shear rate vs shear stress at various temperatures using the two-point method

Fig. D4: Shear rate vs viscosity at various temperatures using the two-point method (legend as in Fig. D3)
**Fig. D5:** Shear rate vs shear stress at various temperatures using the two-point method

<table>
<thead>
<tr>
<th>Symbol</th>
<th>L/R</th>
<th>Temp.</th>
<th>Colour</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>5</td>
<td>100°C</td>
<td>Red</td>
</tr>
<tr>
<td>o</td>
<td>10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>+</td>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>*</td>
<td>5</td>
<td>110°C</td>
<td>Green</td>
</tr>
<tr>
<td>□</td>
<td>10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>○</td>
<td>15</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Fig. D6:** Shear rate vs viscosity at various temperatures using the two-point method (legend as in Fig. D5)
APPENDIX D3

GLIM OUTPUT FOR THE EXTRUSION VOLUMETRIC FLOWRATE RESPONSE

```
glim -file extrusion 1
GLIM 3.12 (c)1977 Royal Statistical Society, London
$units 30
$data s d r p q t e
$dinput 1
$cal ss=s*s
$cal dd=d*d
$cal rr=r*r
$cal pp=p*p
$cal sd=s*d
$cal sr=s*r
$cal sp=s*p
$cal dr=d*r
$cal dp=d*p
$cal rp=r*p
$yvar q
$fit s, d, r, p, ss, dd, rr, pp, sd, sr, sp, dr, dp, rp
$display d e r
  cycle deviance df
  1 0.1928E-11 15

deviance = 0.1928E-11 df = 15

  estimate  s.e.  parameter
  1  0.3282E-05  0.1464E-06  %gm  
  2  0.8275E-06  0.7318E-07  s   
  3  -0.1417E-07  0.7318E-07  d   
  4  0.4667E-07  0.7318E-07  r   
  5  -0.8083E-07  0.7318E-07  p   
  6  -0.7813E-07  0.6845E-07  ss  
  7  -0.7063E-07  0.6845E-07  dd  
  8  0.4937E-07  0.6845E-07  rr  
  9  0.8313E-07  0.6845E-07  pp  
 10  0.2500E-07  0.8962E-07  sd  
 11  -0.5125E-07  0.8962E-07  sr  
 12  0.3875E-07  0.8962E-07  sp  
 13  -0.1013E-06  0.8962E-07  dp  
 14  0.5375E-07  0.8962E-07  rp  
 15  -0.3000E-07  0.8962E-07  

scale parameter taken as 0.1285E-12

  unit observed  fitted  residual
  1  0.4180E-05  0.3980E-05  0.2004E-06  
  2  0.3870E-05  0.4016E-05  -0.1462E-06  
  3  0.4230E-05  0.4251E-05  -0.2125E-07  
  4  0.4380E-05  0.4168E-05  0.2121E-06  
  5  0.4120E-05  0.4053E-05  0.6708E-07  
  6  0.4090E-05  0.4305E-05  -0.2146E-06  
  7  0.4160E-05  0.3920E-05  0.2404E-06  
```
$c a l \; r e=q-7 . l p$
$\text{plot } r e7 . l p$
$\text{display}$

\begin{verbatim}
6 0.3840E-05 0.4051E-05 -0.2112E-06
9 0.2260E-05 0.2300E-05 -0.3958E-07
10 0.2380E-05 0.2491E-05 -0.1112E-06
11 0.2710E-05 0.2366E-05 0.3438E-06
12 0.2120E-05 0.2438E-05 -0.3179E-06
13 0.2390E-05 0.2473E-05 -0.8292E-07
14 0.2650E-05 0.2880E-05 -0.2296E-06
15 0.2030E-05 0.2135E-05 -0.1046E-06
16 0.2350E-05 0.2421E-05 -0.7125E-07
17 0.4500E-05 0.4624E-05 -0.1242E-06
18 0.1560E-05 0.1314E-05 0.2458E-06
19 0.2850E-05 0.2971E-05 -0.1208E-06
20 0.3270E-05 0.3027E-05 0.2425E-06
21 0.3790E-05 0.3572E-05 0.2175E-06
22 0.3290E-05 0.3386E-05 -0.9583E-07
23 0.3090E-05 0.3453E-05 -0.3625E-06
24 0.4260E-05 0.3776E-05 0.4842E-06
25 0.3200E-05 0.3282E-05 -0.8167E-07
26 0.3800E-05 0.3282E-05 0.5183E-06
27 0.3490E-05 0.3282E-05 0.2083E-06
28 0.3030E-05 0.3282E-05 -0.2517E-06
29 0.3490E-05 0.3282E-05 0.2083E-06
30 0.2680E-05 0.3282E-05 -0.6017E-06
\end{verbatim}

---- current display inhibited