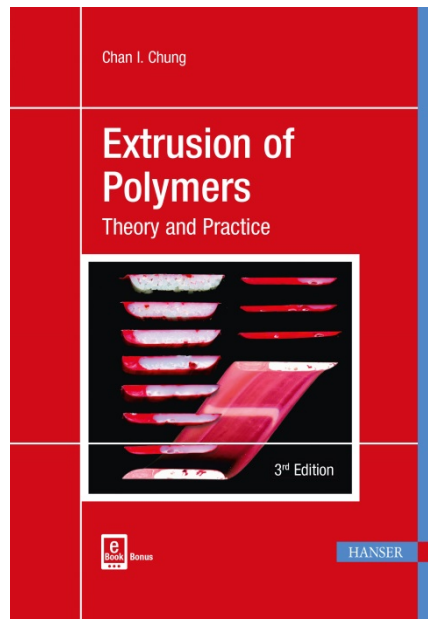


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Chan I. Chung

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Preface

Conceptual understanding and basic analytical skill are sufficient in most cases to deal with practical engineering problems. This philosophy and the contents of this book reflect my industrial, academic, and consulting experience of over 50 years. I have been fortunate to have the opportunity to study the fundamentals of extrusion mechanisms, melt rheology, and polymer physics as well as the opportunity to apply them successfully in commercial practice. My fundamental and practical knowledge of extrusion led to several commercially successful high performance screw designs.

A process engineer must have a good knowledge of the material being processed as well as the engineering aspects of the process in order to fully understand the process and the product. This is especially true for polymers because the properties of a polymer product strongly depend on its processing history. Fundamentals of polymer physics and melt rheology are presented for those who lack previous training. This book starts at a basic level emphasizing conceptual understanding and progresses to an advanced level for ambitious readers. Theoretical models are presented with discussions on their capabilities, assumptions, and limitations. Examples show how the theoretical models can be used in practice. Discussions on disputed or ill-understood topics should be considered as my opinion.

Practical engineering problems are usually too complex to obtain exact mathematical solutions. Approximate solutions with ambiguity are obtained using simplifying assumptions and approximate material properties. The knowledge learned from practical experience is essential to properly interpret the solutions.

I wrote this book to share what I learned through my career with other engineers and scientists. I have tried to present the topics accurately, clearly, and carefully. However, mistakes and ambiguities are inevitable. Your comments will be welcome and appreciated.

Chan I. Chung

About the Author

Chan I. Chung is Professor Emeritus at Rensselaer Polytechnic Institute (RPI). Prof. Chung has been involved in polymer processing, melt rheology, and polymer physics for over 50 years; 11 years as an industrial engineer, 27 years as a professor at RPI, and the past 45 years as an active industrial consultant at numerous companies. His experience includes extrusion modeling, single-screw design, twin-screw configuration, die design, resin development, and compounding. He has authored over 100 papers and holds 12 U.S. patents. The high performance screws based on his patents have been widely used in industry for many years.



Prof. Chung was awarded the prestigious Plastics Engineering/Technology Award of the Society of Plastics Engineers (SPE) in 2004. He was made a fellow of the SPE in 1985. He received the Distinguished Service Award for outstanding contribution to the knowledge of plastics extrusion in 1987, and the Bruce Maddock Award for outstanding achievement in single-screw extrusion in 2000, both from the Extrusion Division of the SPE. Prof. Chung received his B.S. from Seoul National University, M.S. from Stevens Institute of Technology, and Ph.D. from Rutgers University.

Contents

Acknowledgments	VII
Acknowledgments for the Second Edition	IX
Acknowledgments for the Third Edition	XI
Preface	XIII
About the Author	XV
1 Introduction	1
1.1 Polymer Processing	1
1.2 Polymer Extrusion	2
1.3 Types of Extruders	4
1.3.1 Single-Screw Extruders	4
1.3.1.1 Overview of Single-Screw Design Technology	8
1.3.2 Twin-Screw Extruders	9
1.3.2.1 Overview of Intermeshing Co-Rotating Twin-Screw Design Technology	12
1.4 Scale-Up of Single-Screw and Twin-Screw Extruders	14
2 Physical Description of Single-Screw Extrusion	17
2.1 Overall Functions of a Single-Screw Extruder	17
2.2 Feeding Function	23
2.3 Solid Conveying Function	25
2.3.1 Initial Forwarding and Compaction of Pellets	25
2.3.2 Solid Bed Conveying	27
2.4 Melting Function	30

2.4.1	Dissipative Melting	31
2.4.2	Conduction Melting	33
2.5	Metering Function	33
2.6	Melt Quality and Melt Stability	36
2.6.1	Definition of Melt Quality and Melt Stability	36
2.6.2	Melt Pressure	37
2.6.3	Melt Temperature	39
2.6.4	Mixing	41
2.6.5	Effective Residence Time and Residence Time Distribution	43
2.7	Thermodynamic Analysis of Polymer Extrusion	45
2.8	Cooling	49
2.8.1	Barrel Cooling	49
2.8.2	Screw Cooling	49
2.9	Motor Power-Drive Torque Relationship, Screw Torque Strength, and Types of Motors	50
2.9.1	Motor Power-Drive Torque Relationship	50
2.9.2	Screw Torque Strength	52
2.9.3	Types of Motors	53
2.10	Wear	54
2.11	Extruder Size and Instrumentation	55
2.11.1	Extruder Size	55
2.11.2	Instrumentation	55
2.12	Rubbing Mechanisms of Solid Polymer on Metal Surface	56
2.13	Relationships Between Screw Channel Geometries	58
2.14	Variables Controlling Polymer Extrusion	59
3	Fundamentals of Polymers	63
3.1	Introduction to Polymers	63
3.1.1	Polymer Molecules	63
3.1.2	Polymerization Reaction and Common Polymers	65
3.1.2.1	Chain or Addition Polymerization	65
3.1.2.2	Step or Condensation Polymerization	66
3.1.3	Classification of Polymers	68
3.1.3.1	Thermoplastic and Thermoset	68
3.1.3.2	Homopolymer, Copolymer, Block Copolymer, and Graft Copolymers	69
3.1.3.3	Linear Polymer, Branched Polymer, and Crosslinked Polymer	69

3.1.3.4	Amorphous Polymer and Crystalline Polymer	71
3.1.3.5	Chemical Names	71
3.2	Average Molecular Weights and Molecular Weight Distribution	72
3.2.1	Average Molecular Weights	72
3.2.1.1	Number Average Molecular Weight, M_n	72
3.2.1.2	Weight Average Molecular Weight, M_w	73
3.2.1.3	Z-Average Molecular Weight, M_z	73
3.2.1.4	Viscosity Average Molecular Weight, M_v	73
3.2.2	Molecular Weight Distribution	74
3.2.3	Measurements of Average Molecular Weights	75
3.2.3.1	Absolute Methods	76
3.2.3.2	Relative Methods	79
3.3	Molecular Structure and Morphology of Polymer Solid	86
3.3.1	Molecular Structure	86
3.3.1.1	Conformation	86
3.3.1.2	Configuration	87
3.3.2	Morphology of Polymer Solid	89
3.3.2.1	Molecular Orientation	89
3.3.2.2	Amorphous Polymers	90
3.3.2.3	Crystalline Polymers	91
3.3.3	Glass Transition and Melting	100
3.3.4	Phase Separation in Blends, Block Copolymers, and Graft Copolymers	100
3.4	Effects of Processing Variables on Morphology	102
3.4.1	Stress and Strain	102
3.4.2	Temperature	103
3.4.2.1	Thermodynamics of Crystallization	104
3.4.2.2	Nucleation and Growth of Nucleus	105
3.4.2.3	Crystallization Rate and Crystallinity	106
3.4.2.4	Lamellar Thickness as a Function of Crystallization Temperature	107
3.4.2.5	Melting Point of Lamella as a Function of Thickness . .	109
3.4.2.6	Cooling Rate	109
3.4.3	Pressure	110
3.4.4	Annealing	111
3.5	Melt Rheology	111
3.5.1	Types of Fluids	112
3.5.1.1	Viscous Fluid, Viscoelastic Fluid, and Bingham Fluid	112
3.5.1.2	Types of Viscous Fluids	115
3.5.1.3	Behavior of Viscoelastic Fluids	116

3.5.2	Rheological Properties of Polymer Melts	117
3.5.2.1	General Rheological Behavior of Polymer Melts	117
3.5.2.2	Melt Viscosity as a Function of Shear Rate or Shear Stress	118
3.5.2.3	Melt Viscosity as a Function of Temperature	125
3.5.2.4	Melt Viscosity as a Function of Both Temperature and Shear Stress or Shear Rate	129
3.5.2.5	Melt Viscosity as a Function of Pressure	131
3.5.3	Measurement of Melt Rheological Properties	132
3.5.3.1	Capillary Rheometer	133
3.5.3.2	Cone-and-Plate Rheometer	139
3.5.4	Melt Flow Index	145
3.5.5	Extensional Flow and Tensile Viscosity	149
3.5.6	Flow Instability	150
3.5.6.1	Flow Instability in Shear Flow	151
3.5.6.2	Flow Instability in Extensional Flow	156
3.5.7	Flow through Simple Dies	157
3.5.7.1	Circular Tube	157
3.5.7.2	Slit	158
3.5.8	Elastic Memory Effect on Extrudate Shape	165
3.5.9	Effects of Molecular Parameters on Melt Rheological and Physical Properties	166
3.5.9.1	Molecular Weight (MW)	166
3.5.9.2	Molecular Weight Distribution (MWD)	167
3.5.9.3	Molecular Structure	168
3.5.10	Relationships between Melt Rheological Properties and Processability in Extrusion	170
3.5.10.1	Viscosity	170
3.5.10.2	Shear Sensitivity of Viscosity	170
3.5.10.3	Temperature Sensitivity of Viscosity	170
3.5.10.4	Elasticity	171
3.6	Other Polymer Properties and Feed Characteristics Relevant to Extrusion	171
3.6.1	Thermodynamic Properties: Specific Heat, Enthalpy, and Heat of Fusion	171
3.6.2	Flow Temperature and Mechanical Melting	174
3.6.3	Thermo/Mechanical Stability	175
3.6.4	External Friction and Internal Friction	176
3.6.4.1	External Friction	176
3.6.4.2	Internal Friction	178
3.6.5	Bulk Density and Compressibility of Feed	178
3.6.6	Melt Density	180

4	Theories of Single-Screw Extrusion	185
4.1	Three Basic Functions of a Single-Screw Extruder	185
4.2	Solid Conveying Models	187
4.2.1	Frictional Force and Viscous Shear Force	187
4.2.2	Output Rate in Terms of the Solid Conveying Angle	190
4.2.3	Analysis of the Solid Conveying Angle	195
4.2.4	Solid Conveying Model Based on Viscosity	198
4.2.5	Solid Conveying Model Based on Friction	212
4.2.5.1	Isotropic Pressure in the Solid Bed	212
4.2.5.2	Anisotropic Pressure in Solid Bed	219
4.2.6	Elastic Solid Bed	220
4.3	Melting Models	221
4.3.1	Dissipative Melting Models	221
4.3.1.1	Numerical Melting Models	225
4.3.1.2	Analytical Melting Model	233
4.3.1.3	Solid Bed Profile and Melting Capacity	271
4.3.2	Conduction Melting Model	273
4.4	Metering Models	279
4.4.1	Isothermal Newtonian Fluid Model	282
4.4.1.1	One-Dimensional Flow between Parallel Plates	283
4.4.1.2	Two-Dimensional Flow through Rectangular Channel	289
4.4.1.3	Flow through Helical Channel	292
4.4.2	Isothermal Power-Law Fluid Model	293
4.5	Effects of Flight Clearance	299
4.5.1	Solid Conveying Models	300
4.5.2	Melting Models	300
4.5.3	Metering Models	301
4.6	Comprehensive Extrusion Model	302
4.6.1	Computer Simulation	302
4.6.2	Output Rate	303
4.6.3	Motor Power	303
5	Screw Design, High Performance Screws, and Scale-Up	309
5.1	Screw Design	309
5.1.1	General Screw Design Guidelines	309
5.1.2	Scientific Screw Design Method	311
5.2	High Performance Screws	321
5.2.1	Flow Restriction/Mixing Type	322
5.2.2	Barrier-to-Melt Type	332

5.2.3	Barrier between Solid Bed and Melt Pool Type	334
5.2.4	Solid/Melt Mixing Type	341
5.3	Motor Power as a Function of Screw Speed and Size	343
5.4	Melt Temperature as a Function of Screw Speed and Size	347
5.5	Scale-Up Methods	352
5.5.1	Common Scale-Up Method	353
5.5.2	Balanced Scale-Up Method Based on Melting Capacity	356
5.5.3	Scale-Up Method for Heat or Shear Sensitive Polymers	362
6	Gear Pump, Static Mixer, and Dynamic Mixer	365
6.1	Gear Pump	365
6.2	Static Mixer	367
6.3	Dynamic Mixer	369
7	Die Designs	373
7.1	Introduction	373
7.2	An Analytical Model for Coat-Hanger Dies	374
7.2.1	Die Pressure	378
7.2.2	Manifold Inlet Size	379
7.2.3	Manifold Profile	381
7.3	Film and Sheet Dies	383
7.3.1	Introduction	383
7.3.2	Die Types	383
7.3.3	Die Body Materials	385
7.3.4	Manifold Designs	386
7.3.5	Deckling Systems	387
7.3.6	Temperature Control	389
7.3.7	Adjustment Systems	389
7.3.8	Die Operating Information	393
7.3.9	Safety	394
7.4	Coextrusion Dies for Multilayer Flat Films and Sheets	395
7.4.1	Overview	395
7.4.2	Introduction	396
7.4.3	Overview of General Coextrusion Equipment	398
7.4.3.1	Adapter	399
7.4.3.2	Feedblock	402
7.4.3.3	Die	403
7.4.4	Feedblock Designs	404
7.4.5	Coextrusion Systems for Flat Films and Sheets	407

7.4.6	Layer Instabilities or Melt Disturbances	407
7.4.7	Summary	411
8	Viscoelastic Effects in Melt Flow	413
8.1	Introduction	413
8.2	Coextrusion	413
8.3	Viscous Flow Effects	415
8.4	Elastically Driven Flows	418
8.4.1	Background and Theory	418
8.4.2	Numerical Simulations	419
8.4.3	Experimental Procedures	422
8.4.4	Comparison of Experimental and Numerical Results	424
8.5	Viscoelastic Flows	433
9	Special Single-Screw Extruder with Channels on the Barrel	437
9.1	Introduction	437
9.2	HELIBAR® or Extruder with Channeled Barrel	438
9.3	Performance of an Extruder with Channeled Barrel	440
10	Physical Description of Twin-Screw Extruders	449
10.1	Introduction	449
10.1.1	Metered Feeding for Intermeshing Twin-Screw Extruders	451
10.2	Intermeshing Co-Rotating Twin-Screw Extruder	452
10.2.1	Conveying Elements	454
10.2.2	Kneading Blocks	455
10.2.3	Mixing Blocks	457
10.2.4	Sealing Blocks	457
10.2.5	Summary of the Functions and the Design Parameters of Various Screw Elements of Intermeshing Co-Rotating Twin-Screw Extruders	458
10.3	Intermeshing Counter-Rotating Twin-Screw Extruder	459
10.4	Scale-Up of Intermeshing Twin-Screw Extruders	461
10.5	Non-Intermeshing Counter-Rotating Twin-Screw Extruder	462

Appendix: Universal Constants, Unit Conversion Factors, and Prefixes	465
Nomenclature	467
Author Index	475
Subject Index	481

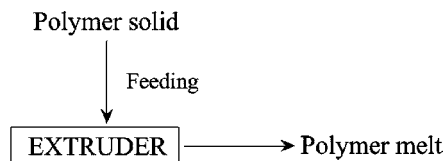
2

Physical Description of Single-Screw Extrusion

■ 2.1 Overall Functions of a Single-Screw Extruder

This chapter is intended to provide an overall physical understanding of the single-screw extrusion operation, including the relevant polymer properties and operating conditions. Although this chapter is quite lengthy, the reader will immediately become familiar with single-screw extrusion and develop further interests to study more details presented in the following chapters. Comprehension of the physical descriptions presented in this chapter alone may prove to be sufficiently beneficial for many readers, and help them to improve their processes and products.

Referring to Chapter 1; Fig. 1.2, an extruder is used to melt a solid polymer and deliver the molten polymer for various forming or shaping processes. The screw is the only working component of the extruder. All other components (motor, gear-box, hopper, barrel and die, etc.) merely provide the necessary support for the screw to function properly. The overall functions of an extruder are depicted below.



Basic functions :

Solid conveying

Melting

Metering

Secondary functions :

Mixing

Shear refining

The feeding function of transferring the feed polymer from the hopper into the screw channel occurs outside of the screw, and it essentially does not depend on the screw design.

The screw performs three basic functions: (1) solid conveying function, (2) melting function, and (3) metering function or pumping function. The three screw functions occur simultaneously over most of the screw length and they are strongly interdependent. The geometric name of a screw section such as feeding section, shown in Chapter 1; Fig. 1.3, does not necessarily indicate the only function of the screw section. For example, the feeding section not only performs solid conveying function, but also melting and metering functions.

The screw also performs other secondary functions such as distributive mixing, dispersive mixing, and shear refining or homogenization. Distributive mixing refers to spacial rearrangement of different components, and dispersive mixing refers to reduction of component sizes as described in Chapter 2; Section 2.6.4. Shear refining refers to homogenization of polymer molecules by shearing.

A single-screw extruder is a continuous volumetric pump without back-mixing capability and without positive conveying capability. What goes into a screw first, comes out of the screw first. A polymer, as solid or melt, moves down the screw channel by the forces exerted on the polymer by the rotating screw and the stationary barrel. There is no mechanism to positively convey the polymer along the screw channel toward the die. The rotating screw grabs the polymer and tries to rotate the polymer with it. Suppose the barrel is removed from the extruder, or perfectly lubricated, such that it gives no resistance to the polymer movement. Then the polymer simply rotates with the screw at the same speed and nothing comes out of the screw. The stationary barrel gives a breaking force to the rotating polymer and makes the polymer slip slightly on the screw surface. The polymer still rotates with the screw rubbing on the barrel surface, but at a slightly lower speed than the screw, because of the slippage. The slippage of the polymer on the screw surface along the screw channel results in an output rate. A lubricated screw surface increases the output rate, but a lubricated barrel surface detrimentally reduces the output rate. It is clearly understandable why commercial screws are highly polished, and why grooved barrels in the feeding section are preferred. Although many commercial practices were developed empirically rather than based on theoretical analyses, they certainly agree with the underlying theoretical concepts.

The mechanisms inside a single-screw extruder are studied by examining the polymer cross-sections along the screw channel taken from “screw-freezing experiments”. In a screw-freezing experiment pioneered by Maddock [1], the screw is run to achieve a steady-state operation. Then, the screw is stopped and water cooling is applied on the barrel (and also on the screw if possible) to freeze the polymer inside the screw channel. The barrel is heated again to melt the polymer, and the screw is pushed out of the barrel as the polymer starts to melt on the barrel sur-

face. Then, the solidified polymer strip is removed from the screw channel and cut at many locations to examine the cross-sections along the screw channel. Some colored pellets are mixed in the feed to visualize the melting mechanism and the flow pattern. The colored pellets retain their shapes if they remained as solid inside the solid bed before the screw stopped, but they are sheared and become streaks inside the melt pool if they were molten before the screw stopped.

Figure 2.1 shows the cross-sections of acrylonitrile-butadiene-styrene copolymer (ABS) strip obtained from a screw-freezing experiment conducted at the Polymer Processing Technology Laboratory of The Dow Chemical Company USA. ABS pellets were extruded using a 63.5 mm (2.5 in) D, $L/D = 21$ conventional screw at 40 rpm. The three barrel zones from the hopper were set at 200, 230, and 250 °C, respectively. The output rate was 34.9 kg/h (77 lbs/h) at 262 °C melt temperature against 7.59 MPa (1,100 psi) head pressure.

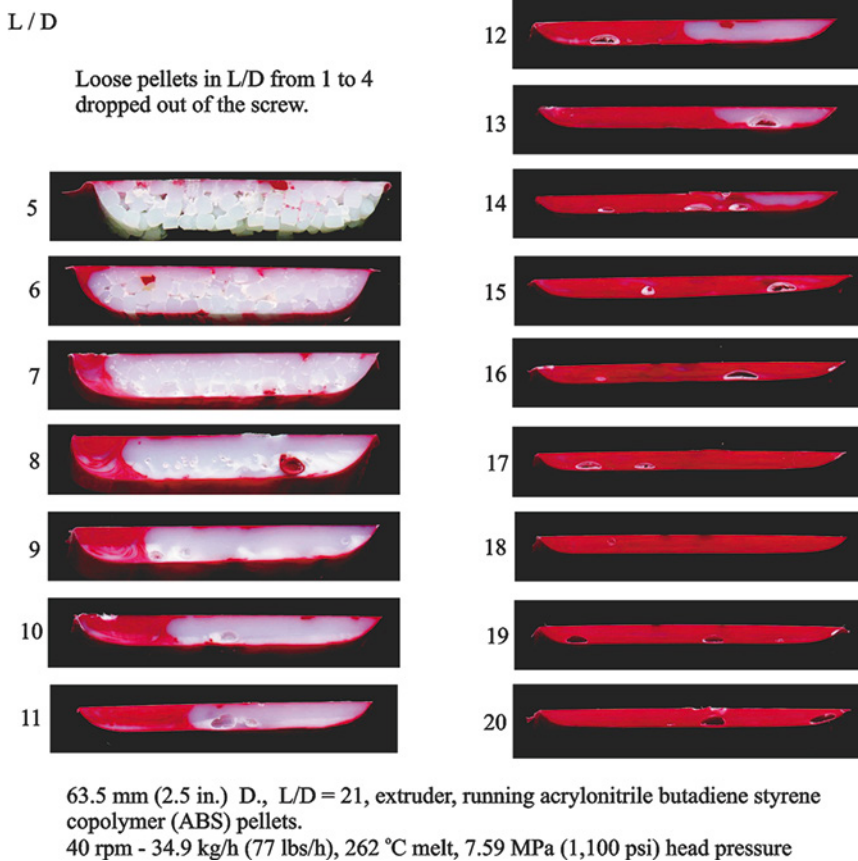
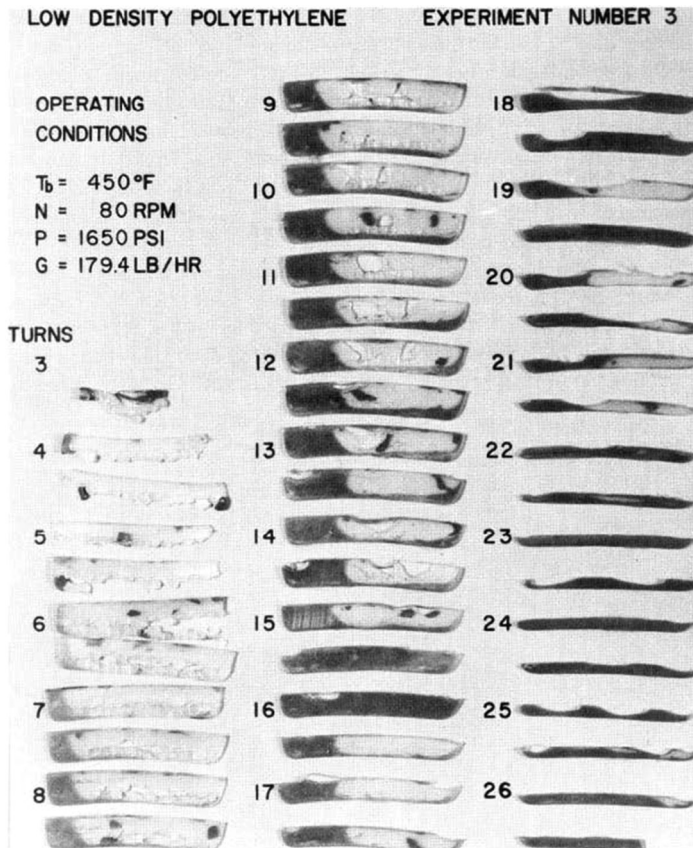


Figure 2.1 Cross-sections of ABS strip along screw channel from screw-freezing experiment (courtesy of Mark Spalding, Kun S. Hyun, and Kevin Hughes, The Dow Chemical Co. USA)

Tadmor and Klein [2], in their book, presented many examples of screw-freezing experiments. Their Fig. 5.2 for branched low density polyethylene (BLDPE) is reproduced in this book as Fig. 2.2. BLDPE pellets were extruded using a 63.5 mm (2.5 in) D, $L/D = 26$ conventional screw at 80 rpm. All barrel zones were set at 232 °C. The output rate was 81.5 kg/h (179.4 lbs/h) against 11.385 MPa (1,650 psi) head pressure.



63.5 mm (2.5 in.) D., $L/D = 26$, extruder, running branched low density polyethylene (BLDPE) pellets.

Figure 2.2 Cross-sections of BLDPE strip along screw channel from screw-freezing experiment (reproduced from Tadmor and Klein [2])

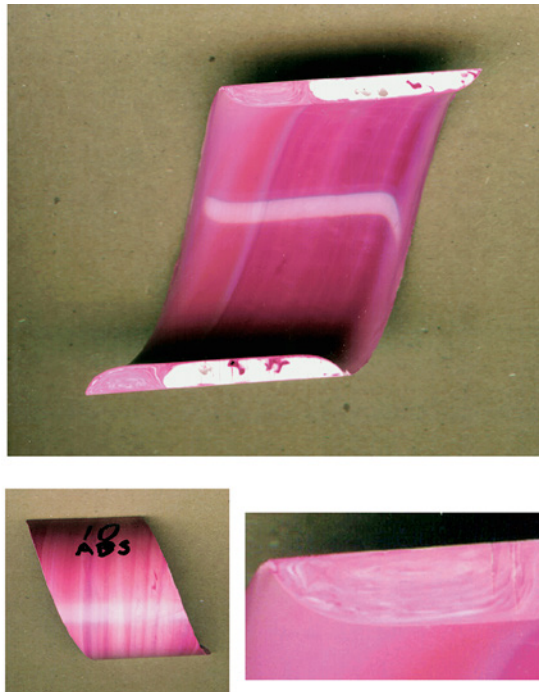
Referring to Figs. 2.1 and 2.2, polymer pellets fed into a screw stay loose over the first 2–4 L/D of the screw from the hopper until they are compacted. Loose pellets drop out of the screw when the screw is removed from the barrel. The pellets are quickly compacted over the next 2–3 L/D into a tightly packed “solid bed”. The solid bed moves down the screw channel as a rigid plug, and no mixing occurs in-

side the solid bed. The solid bed melts mainly by rubbing on the hot barrel surface as it rotates with the screw, and a thin melt film is formed on the barrel surface. The entire barrel immediately after the feed throat is set above the melting point of the polymer, unless an intensively water-cooled barrel section is used in the feeding section. The screw surface of the first several L/D is continuously cooled by cold polymer feed in a steady-state operation. The rest of the screw also becomes hot above the melting point of the polymer because of the heat conducted from hot melt. A melt film also is formed on hot screw surface, and the solid bed becomes surrounded by melt film. The thin melt film on the barrel surface is highly sheared by the rotating solid bed, and a large amount of heat is generated within the thin melt film. The thin melt film is scraped off the barrel surface and collected into a “melt pool” by the advancing flight. The melt pool is sheared and mixed as it is pumped or metered along the screw channel. The melt film on the screw surface is sheared only slightly by the slow movement of the solid bed relative to the screw, and it is not scraped off the screw surface.

The solid bed width gradually decreases and the melt pool width increases as the solid bed melts along the screw, as shown in Fig. 2.1. Melting of the solid bed is complete at about $L/D = 15$ in Fig. 2.1. The solid bed melts primarily by the heat conducted from the thin melt film on the barrel surface. The solid bed also melts on the hot screw surface and at the melt pool interface, but at a sufficiently lower rate to be ignored in comparison to the melting rate on the barrel surface. Melting occurs on the surface of the solid bed, and the interior of the solid bed remains virtually at the feed temperature along the screw. As the screw speed increases, the solid bed remains longer along the screw, as shown in Fig. 2.2, eventually reaching the end of the screw and causing poor melt quality. At high screw speeds, the solid bed and the melt pool coexist over most of the screw length. If the solid bed breaks up into small solid pieces before melting completely, the solid pieces become mixed with the melt pool and slowly melt by the heat conducted from the surrounding hot melt. Thus “solid bed breakup” leads to nonuniform melt temperature. Melting must be completed before the end of the screw and, preferably, the last several L/D of the screw should not contain any solid, in order to achieve uniform melt temperature.

The solid bed is strong under compression, but it can easily split under tension because the pellets in the solid bed are not fused together. The continuous solid bed strip along the screw channel will split if the front part accelerates or the rear part becomes wedged. The surrounding melt under pressure will flow into the broken area of the solid bed once the solid bed splits. Figure 2.2 clearly reveals such “solid bed splitting”. The cross-sections at $L/D = 16$, 18.5, and also 19.5 contain only the melt without any visible solid, but the following cross-sections contain a large solid bed. Solid bed splitting causes pressure fluctuation or surging, resulting in output rate fluctuation.

Figure 2.3 is a typical segment of the solidified polymer strip in the melting section obtained from another screw-freezing experiment running ABS pellets. It shows the melt pool in front of the pushing flight and the solid bed in front of the trailing flight. The solid bed is completely surrounded by a thin melt film on both the barrel surface and the screw surface. The streaks in the melt pool show a circular flow path in the melt pool. Mixing occurs in the melt pool by the circular flow. The colored pellets in the solid bed retain their shapes, and they are not mixed at all with other pellets because the solid bed moves as a solid plug without internal deformation. The streaks on the bottom surface are the direction of the solid bed movement relative to the screw surface, and they have exactly the same helix angle as the flight because the solid bed can move down only along the screw channel. The streaks on the top surface indicate the direction of the solid bed movement relative to the barrel surface, and they have a slightly greater helix angle than the flight. The small difference, about 3° in this case, is the solid conveying angle, which is described further in Chapter 4; Section 4.2.2. The conveying rate of the solid bed, which is the same as the output rate of the extruder, depends on the solid conveying angle. A zero degree solid conveying angle corresponds to a zero output rate.



ABS segment at 10th L/D from 63.5 mm (2.5 in.) D., L/D =21, screw with a square-pitch flight (17.65° helix angle)

Figure 2.3 Segment of ABS strip during melting stage from screw-freezing experiment (courtesy of Kun S. Hyun and Mark Spalding, The Dow Chemical Co. USA)

toring of the operating variables and the extruder performance helps to understand the screw functions and the problems correctly, leading to optimization of the screw design and the operating conditions.

Two additional pressure measurements along the barrel, one called “ P_1 ” at about one-third, and the other called “ P_2 ” at about two-thirds of the barrel length from the hopper, are desired to understand what is happening inside the screw. The three pressure data, P_1 , P_2 , and P_h , provide diagnostic information. An unreasonably low or high value of P_1 indicates insufficient or excessive solid conveying rate, respectively. A low value of P_2 indicates insufficient supply of melt to the metering section in comparison to the pumping capability of the metering section. Severe fluctuations in P_1 or P_2 indicate inconsistent feeding, feed bridging, or wedging of the solid bed in the compression section. If the geometric compression or tapering of the screw channel in the compression section is more than the melting rate, the solid bed cannot go through the screw channel and becomes wedged temporarily until it melts enough to accommodate the geometric compression of the screw channel. If P_1 and P_2 are stable, the head pressure also should be stable.

The head pressure, measured at the end of the screw before the screen pack, slowly increases with time as the screen pack becomes clogged, slowly decreasing the output rate. The die pressure, measured at the adaptor after the screen pack, decreases as the output rate decreases. The die pressure should stay constant at a constant output rate and a constant melt temperature. A widely used feedback control slowly increases the screw rpm to maintain a constant die pressure, as the screen pack becomes clogged, assuring a constant output rate.

■ 2.12 Rubbing Mechanisms of Solid Polymer on Metal Surface

It is well known that feed pellets are compacted into a tightly packed solid bed inside a single-screw extruder. The solid bed rotates with the screw virtually at the same velocity as the screw, rubbing and melting on the barrel surface under high pressures. The solid bed slips slightly on the screw surface as it rotates with the screw, and the slippage of the solid bed on the screw results in the output rate. The extrusion behavior of a polymer depends on the rubbing mechanisms of the solid polymer on the metal surfaces of the barrel and the screw.

Figure 2.18 shows four possible rubbing mechanisms of a solid polymer on a metal surface. At low metal temperatures below the melting (or glass transition) range of the polymer, the rubbing mechanism is “friction”. Friction may occur with or without grinding the polymer. Grinding occurs if the polymer is brittle and the shear

stress τ developed between the polymer and the metal surface is high, exceeding the shear strength of the polymer. Grinding produces fine polymer powders on the metal surface, and it corresponds to a high wear mechanism. τ in friction mainly depends on pressure P . τ is proportional to P in the ideal frictional mechanism, but τ increases less than proportional to P for polymers.

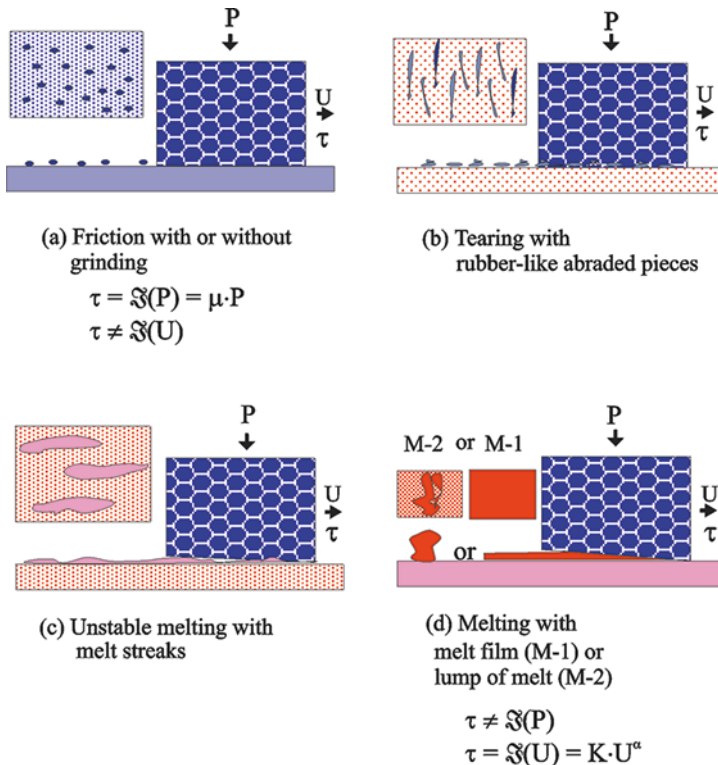


Figure 2.18 Possible rubbing mechanisms of solid polymer on metal surface

At high metal temperatures well above the melting range of the polymer, the rubbing mechanism is “melting” and a thin melt film is formed between the polymer and the metal surface. The melting mechanism forming a smooth melt film on the metal surface is denoted by M-1 in Fig. 2.18d. The melting mechanism forming lumps of the melt on the metal surface is denoted by M-2 in Fig. 2.18d. The M-2 mechanism may result from poor adhesion of melt on metal surface, high melt elasticity, or melt instability at the high shear rates in the thin melt film. The shear stress τ in the melting mechanism mainly depends on rubbing velocity (U), increasing exponentially with increasing U , similar to the dependence of melt viscosity on shear rate. Rigid, highly crystalline polymers, such as polyesters, nylons, polypropylene, and high density polyethylene, and rigid amorphous polymers

(glassy polymers), such as polystyrene and polycarbonate, make a distinct transition from the frictional mechanism to the melting mechanism with increasing metal temperature.

Soft, semi-crystalline polymers with a broad melting range, such as low density polyethylenes, exhibit intermediate rubbing mechanisms between friction and melting. “Tearing” and “unstable melting” are two representative intermediate rubbing mechanisms. Tearing occurs when the polymer at the metal temperature behaves like an elastomer, and it produces rubber-like, abraded polymer pieces on the metal surface. Unstable melting combines the tearing and melting mechanisms, producing melt streaks on the metal surface. High shear stresses are developed in tearing and unstable melting.

The rubbing mechanism of a solid polymer on a metal surface depends on the thermodynamic, mechanical, and melt rheological properties of the polymer over the temperature range from the polymer temperature to the metal temperature. These properties, in turn, depend on the molecular and morphological characteristics of the polymer.

All barrel zones of an extruder, except the first zone next to the hopper, are set at temperatures far above the melting point of the polymer in most cases, and the rubbing mechanism on the extruder barrel will be melting. The first zone is set at a lower temperature, but still well above the melting point of the polymer, to avoid the sticking problem of the feed materials on the feed throat and the screw. A barrel temperature below the start of melting mechanism, where grinding, tearing, or unstable melting mechanism occurs, should be avoided because an unnecessary high torque would be required without effectively melting the polymer.

■ 2.13 Relationships Between Screw Channel Geometries

Referring to Chapter 1; Fig. 1.3, the pitch P and the helix angle ϕ of a flight are related. Figure 2.19 shows one turn of the flight removed from the screw root and unwrapped on a flat surface. The following relationship is found:

$$\tan\phi = \frac{P}{\pi D}$$

$$\phi = \tan^{-1}\left(\frac{P}{\pi D}\right)$$
(2.13)

For the square-pitch with $P = D$, $\phi = 17.65^\circ$ is found using Eq. 2.13.

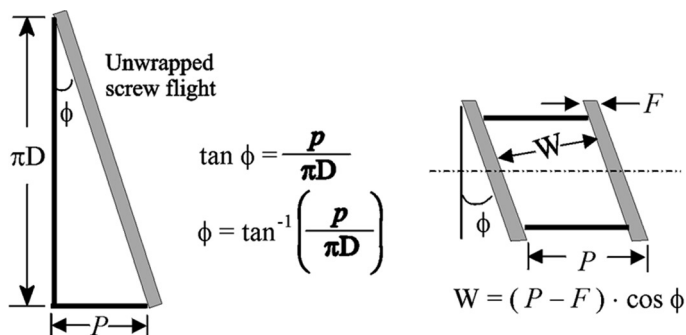


Figure 2.19 Relationships between screw channel geometries of a single-flighted screw

The cross-sectional area of the screw channel used for flow rate calculations is equal to (the channel depth H) \times (the channel width W measured perpendicular to the flights). The relationship given below between the pitch P and the channel width W of a single-flighted screw is also shown in Fig. 2.19.

$$W = (P - F) \cdot \cos\phi \quad (2.14)$$

or

$$W = \pi D \cdot \sin\phi - F \cdot \cos\phi \quad (2.15)$$

where F = flight width measured along the screw axis.

■ 2.14 Variables Controlling Polymer Extrusion

The performance of an extruder for a polymer depends on polymer properties, feed characteristics, screw design parameters, and operating conditions, as discussed previously. Also, feeding conditions assuring a consistent feeding rate are essential. Table 2.1 summarizes these variables. Descriptions of the polymer properties relevant to processing are presented in Chapter 3.

Table 2.1 Variables Controlling Polymer Extrusion

Polymer properties
Thermodynamic properties
Melting characteristics – melting range
Heat capacities and thermal conductivities of solid and melt, heat of fusion
Melt rheological properties
Viscosity; elasticity; shear sensitivity; temperature sensitivity

Table 2.1 Variables Controlling Polymer Extrusion (*continued*)

Mechanical properties
Modulus; yield strength
Solid density and melt density
External friction on metal surface
Thermomechanical stability
Additives
Feed characteristics
Size and shape of feed pellets, and their distribution
Bulk density of feed pellets
Internal friction of feed pellets
Feeding conditions
Feed temperature – preheating or drying of the feed
Gravity, forced or metered (starved) feeding
Constant feeding rate, in weight
Consistent composition if more than one component feed
Recycling
Screw design parameters
Pitch (or lead)
Number of parallel flights
Feeding section depth and length
Compression (or transition) section length
Taper or reduction rate of the channel area in compression section
Metering section depth and length
Compression ratio (CR)
Mixing section design
Special channel geometry
Single or multiple stages
Operating conditions
Screw rpm
Barrel temperature settings
Head pressure
Die design; screen pack; breaker plate; adaptor
Screw temperature control

3.5.8 Elastic Memory Effect on Extrudate Shape

A polymer melt is viscoelastic with a characteristic relaxation time (see Section 3.5.1.1), and it has a memory of the stress/strain condition during a time period longer than the relaxation time after a stress/strain condition was applied. The relaxation time for a highly viscous and highly elastic polymer melt, such as high molecular weight-high density polyethylene (HMW-HDPE) and rigid polyvinyl chloride, can be very long, on the order of minutes.

The shape and layer structure, if coextruded, of an extrudate exiting a die are influenced by the previous stress/strain history leading to the die exit, and they may be quite different from the shape of the die opening or the feedblock structure [67]. Such elastic memory effect is pronounced for polymers with a long relaxation time and a large recoverable shear strain. A drastic example of the memory effect is shown in Fig. 3.46. A HMW-HDPE was fed radially into a long circular tube with 19.05 mm (0.75 in) diameter at four corners at about 18 kg/h (39.6 lbs/h). The cross-sectional shape of the extrudate exiting the circular orifice was initially circular, but it slowly changed to more or less square with four corners corresponding to the four feed ports. A picture of the final extrudate cross-section is shown. The molecules were oriented radially at the feed port and they recoil upon leaving the die, swelling at the four inlet corners.

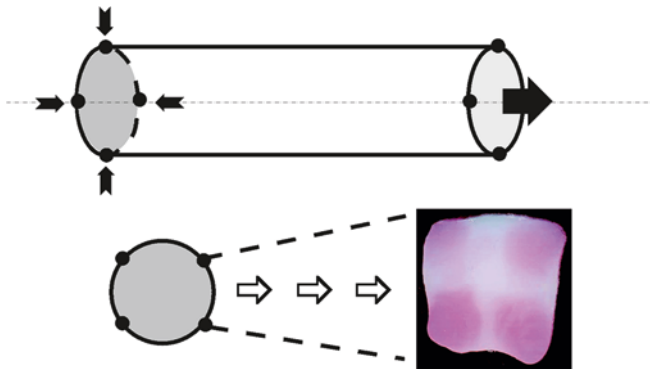


Figure 3.46 Elastic recovery of HMW-HDPE melt
Observation by C. Chung and J. Dooley at the Processing Technology Laboratory of The Dow Chemical Company USA

The elasticity of a polymer melt has pronounced effects on the flow of the polymer melt. The extrudate may show surface irregularities or distorted shapes caused by the elasticity at high extrusion speeds as discussed in Section 3.5.6. The flow through a die may develop undesirable profiles caused by the elasticity, giving incorrect extrudate shapes or structures. The elastic effects in polymer melt flow are further discussed in Chapter 8.

3.5.9 Effects of Molecular Parameters on Melt Rheological and Physical Properties

3.5.9.1 Molecular Weight (MW)

Both the melt rheological and physical properties of a polymer are correlated best to the weight average MW. Physical properties improve and viscosity increases with increasing weight average MW.

The dependence of viscosity on weight average MW for linear polymers, shown in Fig. 3.31b in Section 3.5.2.2, can be expressed by the following equation [1, 69, 70]:

$$\eta = K_T \cdot M_w^\alpha \quad (3.89)$$

where

η = viscosity of a polymer melt

M_w = weight average molecular weight

K_T = temperature-dependent constant

$\alpha = 1.0$ for $M_w < M_c$

$\alpha = 3.4$ for $M_w > M_c$ at zero shear rate, decreasing to 1.0 at infinite shear rate

M_c is the critical MW for entanglement, and its value depends on the polymer. It is noted again that Eq. 3.89 is applicable only to linear polymers.

The relationship between viscosity and MW for branched polymers is not completely developed. The following equation is proposed for branched low density polyethylene [13, 68]:

$$\eta = L_T \cdot (M \cdot g)_w^\beta \quad (3.90)$$

where

M = molecular weight

g = branching parameter < 1.0 , defined by the ratio of the radii of gyration of branched molecule to linear molecule with the same MW

$(M \cdot g)_w$ = weight average of $(M \cdot g)$ of all molecules

L_T = temperature-dependent constant

The uncertainty of Eq. 3.90 arises from the high experimental value of $\beta = 6.6$ – 6.8 at zero shear rate [13, 68], which is about twice of $\alpha \approx 3.4$ for linear polymers.

The shear sensitivity of viscosity increases with increasing MW. However, the temperature sensitivity of viscosity or the apparent flow activation energy does not depend on MW for commercial polymers with high MWs (see Section 3.5.2.3).

Measured at a constant shear stress, the recoverable shear strain or extrudate swell ratio of a polymer melt increases with increasing MW at low MW, but becomes constant above a very high MW that is much higher than the critical MW for entanglement [69]. However, the shear stress measured at a constant shear rate

continuously increases with increasing MW because the viscosity increases with MW. Consequently, the recoverable shear strain measured at a constant shear rate continuously increases with increasing MW.

3.5.9.2 Molecular Weight Distribution (MWD)

The MWD or polydispersity of a polymer is usually defined by the ratio of weight average MW to number average MW (see Section 3.2.2). Broader MWD indicates more low MW molecules and more high MW molecules. MWD strongly influences the shear thinning behavior and the elasticity of a polymer melt [3, 69, 70] as well as the physical properties. Physical properties generally deteriorate with increasing MWD at the same weight average MW because of the weakness of low MW molecules.

The effect of MWD on shear thinning behavior is shown in Fig. 3.47 for two polymers with the same weight average MW or $[MI]$. The polymer with broad MWD starts the shear thinning behavior at a lower shear rate than a polymer with narrow MWD. For the usual processing range of shear rate, the polymer with broad MWD is more shear thinning than the polymer with narrow MWD. When two polymers with the same $[MI]$ are compared, the one with broader MWD will have lower viscosity at the high shear rates of processing, consuming less torque and developing lower melt temperature.

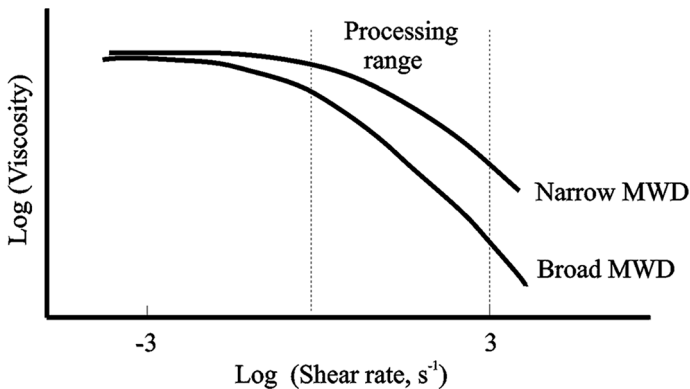


Figure 3.47 Dependence of shear sensitivity on molecular weight distribution

The apparent flow activation energies of commercial polymers with high MWs does not depend on MWD because apparent flow activation energy is independent of MW at high MWs.

The recoverable shear strain or extrudate swell ratio of a polymer melt is affected more by high MW molecules than low MW molecules, and it is sensitive to the z-average MW. The extrudate swell ratio can be significantly increased by a small

amount of very high MW molecules. Measured at a constant shear stress, the extrudate swell ratio increases with increasing MWD.

3.5.9.3 Molecular Structure

The physical and the melt rheological properties of a polymer as well as the morphology of the polymer strongly depend on the molecular structure. Various polyethylenes with different molecular structures, shown in Fig. 3.48, are widely used, and they provide an excellent example to study the effects of molecular structure [5].

A perfect polyethylene (PE) crystal with orthorhombic unit cell structure has 0.9972 g/cm^3 density at $30 \text{ }^\circ\text{C}$ with a melting point at about $141 \text{ }^\circ\text{C}$ [71], and it is a hard solid at room temperature (RT). Amorphous PE has 0.855 g/cm^3 at $30 \text{ }^\circ\text{C}$ [71] with a glass transition temperature at about $-120 \text{ }^\circ\text{C}$, and it behaves as a soft elastomer at RT. PE molecules cannot crystallize completely because of structural irregularities such as chain ends, short chain branches (SCB), and long chain branches (LCB), as well as the chain folding behavior. A branch is considered a LCB if it has a sufficiently long length for entanglement. The crystallinity decreases as the amount of SCB or LCB increases, resulting in a lower density and a lower modulus.

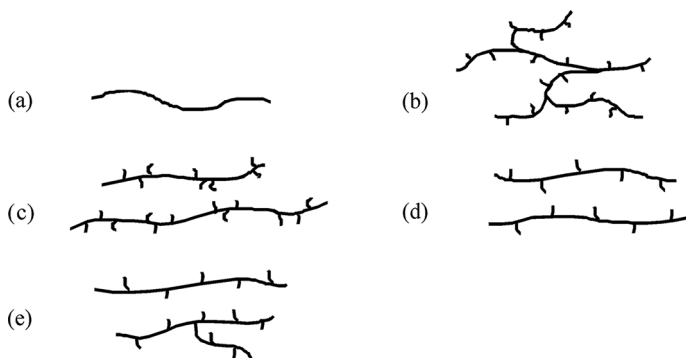


Figure 3.48 Molecular Structures of Various Polyethylenes: (a) Linear or high density polyethylene (HDPE); (b) Branched low density polyethylene (LDPE); (c) Ziegler-Natta or heterogeneous linear low density polyethylene; (d) Metallocene or homogeneous linear low density polyethylene; (e) Homogeneous linear low density polyethylene with occasional long chain branches

High density polyethylene (HDPE), shown in Fig. 3.48a, is a homopolymer of ethylene with a linear molecular structure. HDPE crystallizes to a high degree, reaching about 80 wt.% crystallinity, resulting in a high density around 0.950 g/cm^3 , as the name indicates.

4.2.3 Analysis of the Solid Conveying Angle

A small segment of a solid bed with a segmental length ΔZ along the screw channel is shown in Fig. 4.7, together with various forces acting on the solid bed segment. These forces and the resulting torque are at equilibrium and control the movement of the solid bed segment relative to the barrel and the screw. It is a three-body dynamic problem with a stationary barrel, a rotating screw, and a floating solid bed. The movement of the solid bed relative to the screw, that is, the slippage of the solid bed on the screw, results in solid conveying.

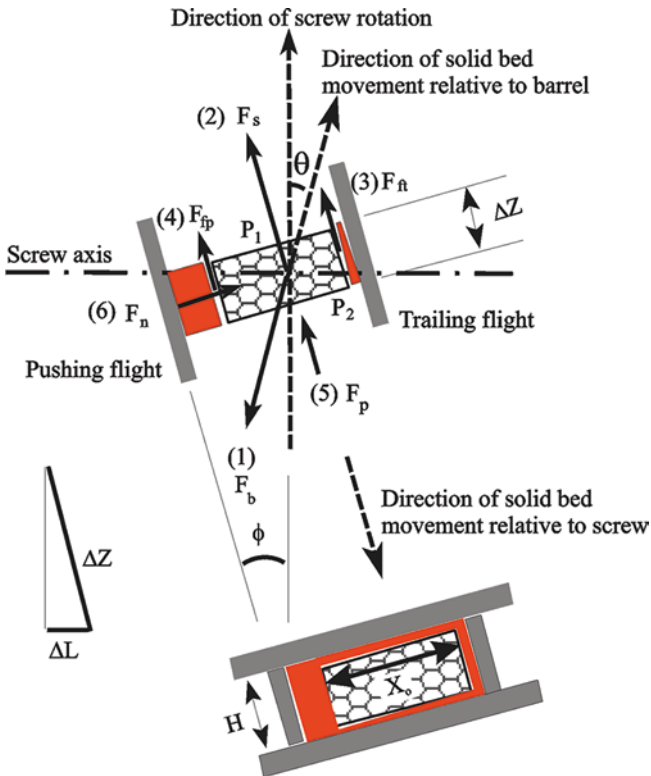


Figure 4.7 Segment of solid bed in melting section and six forces acting on the segment: (1) Force on the barrel; (2) Force on the screw root; (3) Force on the trailing side of the flight; (4) Force on the pushing side of the flight; (5) Force caused by the pressure; (6) Kinetic force on the pushing side of the flight

There are six forces acting on the solid bed segment:

1. F_b is the force on the barrel resisting the solid bed movement on the barrel in the θ -direction. This force acts in the negative θ -direction at a distance R from the screw axis.

2. F_s is the force on the screw root resisting the movement of the solid bed relative to the screw. This force acts in the screw channel ϕ -direction toward the hopper at a distance $(R - H)$ from the screw axis.
3. F_{ft} is the force on the trailing side of the flight resisting the movement of the solid bed relative to the screw. This force acts in the screw channel ϕ -direction toward the hopper at an average distance $(R - \frac{1}{2}H)$ from the screw axis.
4. F_{fp} is the force on the pushing side of the flight resisting the movement of the solid bed relative to the screw. This force acts in the screw channel ϕ -direction toward the hopper at an average distance $(R - \frac{1}{2}H)$ from the screw axis.
5. F_p is the force caused by the pressure increase along the screw channel. This force pushes the solid bed segment in the screw channel ϕ -direction toward the hopper at an average distance $(R - \frac{1}{2}H)$ from the screw axis.
6. F_n is the kinetic force acting on the solid bed segment by the pushing flight in the direction perpendicular to the pushing flight. This force acts at an average distance $(R - \frac{1}{2}H)$ from the screw axis.

The above six forces must be at equilibrium in a steady-state operation, canceling out each other without any residual force or torque. Referring to Fig. 4.7, the solid conveying angle θ in a steady-state operation is calculated from the dynamic equilibrium force and torque balances among the various forces acting on the solid bed segment.

Taking the die direction as positive, the force balance along the screw axis is

$$-F_b \cdot \sin\theta - (F_s + F_{fp} + F_{ft} + F_p) \cdot \sin\phi + F_n \cdot \cos\phi = 0 \quad (4.8)$$

The torque balance in the direction of screw rotation is

$$\begin{aligned} -F_b \cdot \cos\theta \cdot R + F_s \cdot \cos\phi \cdot (R - H) + (F_{fp} + F_{ft} + F_p) \cdot \cos\phi \cdot \left(R - \frac{1}{2}H\right) \\ + F_n \cdot \sin\phi \cdot \left(R - \frac{1}{2}H\right) = 0 \end{aligned} \quad (4.9)$$

F_b , F_s , F_{fp} , and F_{ft} are the shear forces, and they can be expressed in terms of the corresponding shear stress and acting area.

$$F_b = \tau_b \cdot X_o \cdot \Delta Z_b \quad (4.10)$$

$$F_{ft} = \tau_{ft} \cdot H \cdot \Delta Z \quad (4.11)$$

$$F_s = \tau_s \cdot X_o \cdot \Delta Z_s \quad (4.12)$$

$$F_{fp} = \tau_{fp} \cdot H \cdot \Delta Z \quad (4.13)$$

Referring to Fig. 4.6, the length of the solid bed segment measured along the screw channel is ΔZ_b on the barrel surface and ΔZ_s on the screw root because of the curvature of the screw channel. The average length of the solid bed segment is

$$\Delta Z = \frac{1}{2} (\Delta Z_b + \Delta Z_s) \quad (4.14)$$

F_p is caused by the increased pressure $\Delta P = P_2 - P_1$ along the solid bed segment, and it can be expressed as

$$F_p = \Delta P \cdot X_o \cdot H \quad (4.15)$$

P_1 and P_2 are the average pressure in the screw channel at Z_1 and Z_2 , respectively. It is possible that the pressure varies across the screw channel at a given Z .

The reduced channel depth k is defined by

$$k = \frac{H}{R} \quad (4.16)$$

The following dimensionless geometric constants are defined to simplify the equations, and they are further related to k using the geometry of the screw channel.

$$C_1 = \frac{\Delta Z_b}{\Delta Z} = \frac{R}{\left(R - \frac{1}{2}H\right)} = \frac{1}{\left(1 - \frac{1}{2}k\right)} \quad (4.17)$$

$$C_2 = \frac{\Delta Z_s}{\Delta Z} = \frac{(R - H)}{\left(R - \frac{1}{2}H\right)} = \frac{(1 - k)}{\left(1 - \frac{1}{2}k\right)} \quad (4.18)$$

C_1 and C_2 are close to unity for large screws with negligible channel curvature or very shallow screw channel with $H \ll R$. Substituting Eqs. 4.10 to 4.18 into Eqs. 4.8 and 4.9, and further eliminating the elusive kinetic force F_n by combining the resulting equations, the following equation is obtained:

$$\begin{aligned} \frac{\Delta P}{\Delta Z} = & \frac{C_1}{H} \cdot \tau_b \cdot (C_1 \cdot \cos\theta \cdot \cos\phi - \sin\theta \cdot \sin\phi) \\ & - \frac{C_2}{H} \cdot \tau_s \cdot (\sin^2\phi + C_2 \cdot \cos^2\phi) - \frac{1}{X_o} (\tau_{fp} + \tau_{ft}) \end{aligned} \quad (4.19)$$

It is noted that $\cos\theta$ decreases and $\sin\theta$ increases almost proportionally to θ as θ increases for small values of θ in the range of 2–5° found for actual extrusion operations.

There are two interdependent unknowns in Eq. 4.19:

1. Pressure gradient, $\Delta P / \Delta Z$
2. Solid conveying angle, θ

One of them must be known or assumed to calculate the other. Eq. 4.19 was derived without making any assumption crucial to its validity. Eq. 4.19 is in a simple format, and several important points can be learned for the effects of operating conditions and screw design on the solid conveying rate by examining this simple equation. The most important point is that, for a given pressure gradient along the screw, the solid conveying angle (i.e., the solid conveying rate) increases as the shear stress on the barrel (τ_b) increases or as the shear stress on the screw (τ_s) decreases, as shown in Fig. 4.8.

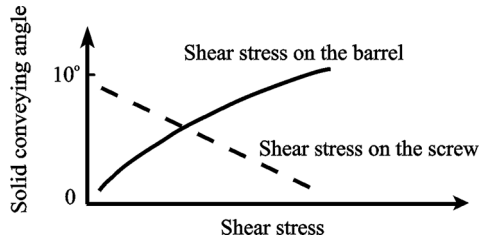


Figure 4.8 Solid conveying angle as a function of the shear stress acting on barrel or the shear stress acting on screw

4.2.4 Solid Conveying Model Based on Viscosity

All barrel zones starting immediately after the throat section are set well above the melting point of a polymer in most cases, and the solid bed is surrounded by the melt film and the melt pool, as shown in Chapter 2; Figs. 2.6, and Figs. 4.1 and 4.7. The forces acting between the solid bed and the surrounding hot metal surfaces are viscous shear forces. A solid bed conveying model for this situation was developed by Chung [1].

The following six assumptions and simplifications are made in Chung's model based on viscosity:

1. The solid bed is surrounded by melt film on all four sides: the barrel, the screw root, the pushing side, and the trailing side of the flight.
2. The solid bed moves along the screw channel as a solid plug, and the stresses involved in internal deformation of the solid bed are ignored.
3. The internal pressure of the solid bed changes only along the screw channel.
4. There is a kinetic force F_n acting on the pushing flight resulting from the advancing movement.
5. The slight difference in the helix angle of the flight from the bottom to the top of the flight is neglected.
6. The clearance between the flight and the barrel is negligible.

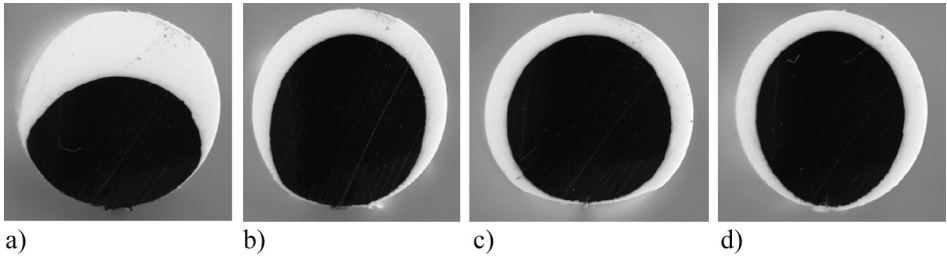


Figure 8.7 Layer interface deformation for a coextruded structure of polyethylene A resin in the cap layer and polyethylene D resin in the substrate layer flowing through a circular channel. Section (a) is from near the entry of the channel while section (d) is from near the exit of the channel

■ 8.4 Elastically Driven Flows

The previous section described how differences in viscosities in different layers in a multilayered structure can produce a flow field that leads to “viscous encapsulation” that produces layer non-uniformities. This section will cover elastic effects in polymer melt flow and how they produce different flow patterns that can also affect layer uniformity in coextruded structures.

8.4.1 Background and Theory

It has been shown previously that non-Newtonian flows in a straight pipe of non-circular cross-section are subject to secondary recirculations, with velocity components orthogonal to the primary axial flow. When a non-Newtonian fluid is sheared, it may experience two normal stress differences:

$$N_1(\dot{\gamma}) = \tau_{11} - \tau_{22} = \Psi_1(\dot{\gamma})\dot{\gamma}^2 \quad (8.1)$$

$$N_2(\dot{\gamma}) = \tau_{22} - \tau_{33} = \Psi_2(\dot{\gamma})\dot{\gamma}^2 \quad (8.2)$$

where $\dot{\gamma}$ is the shear rate and Ψ_1 and Ψ_2 are the first and second normal stress coefficients.

Directions 1, 2, and 3 are the flow, velocity gradient, and the neutral directions, respectively [20]. The stress components in the transverse plane are ultimately responsible for the secondary flow. But geometry plays a key role as well, and no secondary flow occurs in a circular pipe. The normal stresses are usually said to represent fluid “elasticity”, even though they actually stem from the nonlinearity of the constitutive equation and do not imply an elastic relaxation time. Although the magnitude of viscoelastic secondary flow is typically orders of magnitude lower

than the primary flow, it may produce significant effects by introducing flow across the otherwise rectilinear streamlines. For example, it is known to greatly enhance heat transfer in pipe flows [21, 22]. In bicomponent coextrusion, secondary flows produce considerable interface deformation over an axial distance $\approx 100 D$, D being the characteristic dimension of the cross-section [23–27].

Because of its fundamental and practical importance, the secondary flow of non-Newtonian fluids in non-circular pipes has received numerous investigations since the 1950s. Experimentally, several groups have observed secondary flows of polymer solutions and melts in pipes of elliptic [28] and square cross-sections [23, 24, 26, 27, 29, 30]. For an elliptic cross-section, four recirculation areas occupy the four symmetric quadrants, flowing from the center toward the wall along the minor axis and back to the center along the major axis. For a square cross-section, eight recirculation areas are demarcated by the symmetry lines, going from the center of the sides toward the corners. Theoretically and computationally, a larger number of studies have been devoted to secondary flows in those geometries, using different constitutive models: Reiner-Rivlin [21, 28, 31, 32], Criminale-Ericksen-Filbey (CEF) [22, 29, 30, 33, 34], co-rotational Maxwell [35], Phan-Thien-Tanner (PTT) [36], modified PTT (MPTT) [37], Giesekus [25, 27], and Leonov [38]. For square and elliptic cross-sections, all predict the correct number of recirculation zones and the general flow pattern.

8.4.2 Numerical Simulations

The momentum and continuity equations for the steady-state flow of an incompressible viscoelastic fluid are given by

$$-\nabla p + \nabla \cdot \mathbf{T} = 0 \quad (8.3)$$

$$\nabla \cdot \boldsymbol{\nu} = 0 \quad (8.4)$$

where p is the pressure field, \mathbf{T} is the viscoelastic extra-stress tensor, and $\boldsymbol{\nu}$ is the velocity field.

Inertial and volume forces are assumed to be negligible.

If a discrete spectrum of N relaxation times is used, then \mathbf{T} can be decomposed as follows:

$$\mathbf{T} = \sum_{i=1}^N \mathbf{T}_i \quad (8.5)$$

where \mathbf{T}_i is the contribution of the i -th relaxation time to the viscoelastic extra-stress tensor.

For the extra-stress tensor \mathbf{T}_i , a constitutive equation must be chosen. For example, the Giesekus constitutive equation takes the form

$$\mathbf{T}_i \left[\mathbf{I} + \frac{\alpha_i \lambda_i}{\eta_i} \mathbf{T}_i \right] + \lambda_i \overset{\nabla}{\mathbf{T}}_i = 2\eta_i \mathbf{D} \quad (8.6)$$

where \mathbf{I} is the unit tensor, λ_i are the relaxation times, η_i are the partial viscosity factors, \mathbf{D} is the rate of deformation tensor, and the symbol $\overset{\nabla}{\mathbf{T}}$ stands for the upper-convected time derivative operator.

In Equation 8.6, α_i are additional material parameters of the model, which control the ratio of the second to the first normal stress difference. In particular, for low shear rates, $\alpha_1 = -2 N_2/N_1$, where α_1 is associated with the highest relaxation times λ_i .

The rate of deformation tensor \mathbf{D} can be written as:

$$\mathbf{D} = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \quad (8.7)$$

The finite element technique was used to solve the set of equations described. Depending on the number of relaxation times used, the computational resources required to solve the problem can be extremely large. When more than a single relaxation time was required, the elastic viscous split stress (EVSS) algorithm was used. This method divides the viscoelastic extra stress tensor into elastic and viscous parts as follows:

$$\mathbf{T}_i = \mathbf{S}_i + 2\eta_i \mathbf{D} \quad (8.8)$$

Using this algorithm, the equations expressed in terms of \mathbf{S}_i , \mathbf{D} , \mathbf{v} , and p can be solved. A post-calculation then gives the total viscoelastic extra-stress tensor \mathbf{T} . A quadratic interpolation is used for \mathbf{v} , while a linear interpolation is used for \mathbf{S}_i , \mathbf{D} , and p .

The numerical simulations of the flow of the polystyrene resin in this study were performed using a Giesekus model with five relaxation times. Figure 8.8 shows the secondary flow patterns predicted by the simulation for flow in the square channel. Because of the symmetry of the channel shape, there are two secondary flow patterns in each quadrant resulting in a total of eight secondary flow zones.

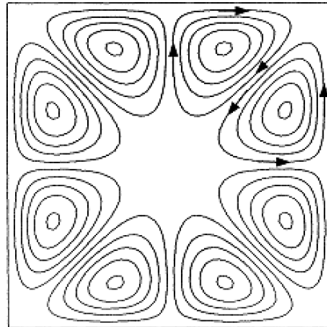


Figure 8.8 Simulation results for square channel

Figure 8.9 shows the results from a similar simulation using the triangular channel rather than the square channel. Note that the symmetry of this geometry produces a total of six secondary flow zones compared to the eight seen in the square channel.

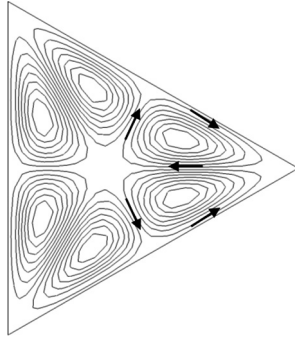


Figure 8.9 Simulation results for triangular channel

One common misconception is that the secondary flows observed in the square and triangular channels are due to the sharp corners present in these geometries. In actuality, the secondary flows are caused by second normal stress differences produced in non-radially symmetric geometries. This implies that flow through a non-radially symmetric geometry with no corners, such as an oval, would still produce secondary flows. This result is illustrated in Fig. 8.10 showing the predicted secondary flow patterns in an oval channel. Note that there are only four secondary flow regions in this geometry.

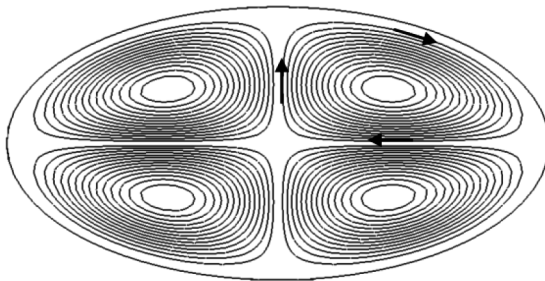


Figure 8.10 Simulation results for oval channel

Figure 8.11 shows the simulation results for a rectangular channel with 4:1 aspect ratio. These results are similar to the results from the square channel since there are eight total secondary flow areas (two per quadrant). The results are different from the square channel, however, because the strength and location of the sec-

ondary flow areas have changed. Note that the secondary flow areas near the short channel wall are much smaller than those near the long channel wall.

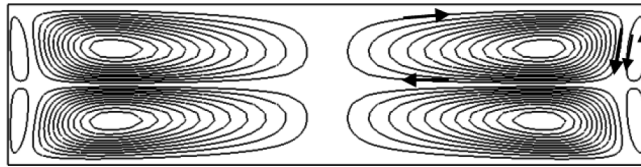


Figure 8.11 Simulation results for rectangular channel

Figure 8.12 shows the simulation results for a rectangular channel in which one end has been rounded into a semi-circular shape. These results show that rounding one end of the rectangular channel has eliminated two of the secondary flow areas, reducing the total number from eight to six.

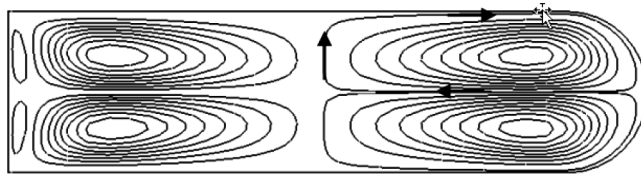


Figure 8.12 Simulation results for rounded rectangular channel

8.4.3 Experimental Procedures

The resin chosen for this study was a high impact polystyrene resin manufactured by The Dow Chemical Company. The rheological properties of this resin have been described previously [24]. This resin was chosen because it has exhibited significant viscoelastic properties in previous studies.

The equipment and experimental procedures used in these experiments were the same as those described previously in Section 8.3. The normal extrusion rate was approximately 2.5 kg/h for the polystyrene resin at 200 °C, which would give a wall shear rate of approximately 10 s^{-1} .

The first major difference in these experiments was that an identical polymer was used in the individual layers such that all the layers had the same viscosity. Thus, the viscous encapsulation phenomenon would be minimized and only the elastic effects would be present.

The second major difference was that the feedblocks were designed to produce specific coextruded structures with alternating layers or strands of the same polystyrene pigmented black or white. A series of experiments were conducted that

Author Index

A

Agassant, J.-F. 152, 184
Alfrey, Jr., T. 412, 435
Armstrong, R. C. 435
Arpaci, V. S. 316
Avalosse, T. 436
Avenas, P. 184

B

Bagley, E. B. 154, 182
Baird, D. G. 154, 182
Ballman, R. L. 435
Barr, R. A. 61, 307, 337, 339, 340,
363 – 372
Beek, W. J. 306
Benbow, J. J. 154, 182
Bernhardt, E. C. 15, 61
Berry, G. C. 181
Billmeyer, Jr., F. W. 184
Bird, R. B. 435
Birks, A. M. 154, 182
Blyler, Jr., L. L. 156, 182
Booy, M. L. 316
Boudreaux, E. 182
Bowden, F. P. 61, 176, 184
Bowles, W. A. 183
Bradley, N. L. 412
Brandrup, J. 183
Brzoskowski, R. 182
Bueche, F. 181, 184
Butler, T. I. 184

C

Cabot, I. M. 182
Cannon, M. A. 184
Carley, J. F. 280, 306, 364, 380, 412
Carreau, P. J. 184
Casale, A. 181
Caton, J. A. 435
Chabot, J. F. 15
Chapman, F. M. 15, 181, 184
Charley, R. V. 182
Cheng, C. Y. 183, 184, 263, 306
Cheremisinoff, N. P. 15
Chisholm, D. S. 414, 435
Christensen, R. E. 156, 183
Choi, M. K. 447
Chung, C. I. 15, 61, 165, 180, 181, 184, 198,
233, 305 – 307, 339, 340, 363, 364,
376, 412, 447
Chung, K. H. 306
Clark, J. C. 181
Cleereman, K. J. 435
Clegg, P. L. 182
Cloeren, P. F. 399 – 403, 406, 412
Cohen, B. R. 184
Cooper, Jr., A. R. 184
Cowie, J. M. G. 184
Cox, W. P. 181
Cross, M. M. 121, 181
Cuculo, J. A. 182

D

Darnell, W.H. 212, 219, 220, 305, 447
Dealy, J. M. 156, 182, 183
Debbaut, B. 436
DeBoo, R. V. 363
DeFornasari, E. 181
Denn, M. M. 154, 156, 182, 183
Desmond, R. M. 364
Dillon, R. E. 151, 181
Dodson, A. G. 436
Donnelly, G. J. 157, 183
Donovan, R. C. 306
Dooley, J. 15, 165, 183, 363, 383, 412, 413,
435, 436
Drda, P. A. 156, 183
Dreval, V. E. 183
Dulmage, F. E. 322, 324, 363, 369
Duvdevani, I. J. 305
Dyer, D. F. 317

E

Eaton, L. E. 184
Eirich, F. R. 182, 184
Elias, H.-G. 184
Etemad, S. G. 436
Everage, A. E. 435

F

Ferguson, J. 181
Ferry, J. D. 125, 181
Finch, C. R. 435
Finger, F. L. 183
Flory, P. J. 180, 184
Fox, T. G. 181
Freese, Jr., J. A. 182
Fritz, H.-G. 447

G

Gale, G. M. 372
Gao, S. X. 436
Garvey, B. S. 182
Geiger, K. 364

Gerson, P. M. 306
Gervang, B. 436
Geyer, P. 336, 363
Giachetti, E. 181
Gogos, C. G. 15, 61, 184, 263, 306
Gould, R. J. 61
Graessley, W. W. 181
Green, A. E. 436
Griffin, O. M. 233, 306
Griffith, R. M. 307
Gruenschloss, E., 364, 447
Grukke, E. A. 15
Gunning, L. 447
Guo, Y. 363
Gurnee, E. F. 435

H

Han, C. D. 157, 183, 435
Han, M. H. 182
Hart, Jr., A. C. 156, 182
Hartnett, J. P. 436
Hasegawa, T. 183
Hashemabadi, S. H. 436
Hassager, O. 435
Hatzikiriakos, S. G. 156, 182
Haward, R. N. 181
Heard, C. B. 363
Heisler, M. P. 306
Hennessey, W. J. 184, 447
Hensen, F. 15
Hill, D. A. 61, 156, 183
Hilton, B. T. 435
Hong, B. K. 306
Hogan, T. A. 306
Hsu, J. S. 337, 363
Hughes, K. 19, 183, 305, 372, 436
Hyun, J. C. 157, 183
Hyun, K. S. 15, 19, 22, 61, 176, 181, 183,
184, 219, 220, 264, 305, 306, 363, 436

I

Iemoto, Y. 436
Immergut, E. H. 183

Inn, Y.-W. 183
Ishihara, H. 183
Ivanova, L. I. 155, 183

J

Jackson, J. B. 180, 184
Janssen, L. P. B. M. 463
Jenkins, S. R. 184
Johnson, J. F. 181

K

Kaghan, W. S. 182
Kalika, D. S. 154, 182
Karlekar, B. V. 364
Kase, S. 156, 183
Khan, A. A. 435
Kim, E. K. 463
Kim, H. S. 184, 306
Kim, H. T. 338 – 340, 363
Kim, Y. S. 181
Kim, Y. W. 157, 183
Kirkpatrick, D. E. 184
Klein, I. 20, 61, 305
Knight, G. W. 183
Kramer, W. A. 61, 372
Kroesser, F. 307
Kruder, G. 363, 447
Kuo, S. H. 184, 306
Kurtz, S. J. 154, 182

L

Lacher, F. K. 336, 363
Lai, S. Y. 181, 183
Lamb, P. 154, 182
Landel, R. F. 125, 181
Larsen, P. S. 436
Lau, H. C. 156, 183
Lee, B. L. 435
Lee, T. S. 181
Leonov, A. I. 419, 436
LeRoy, G. 363
Lodge, A. S. 182

Lohkamp, D. T. 376, 412
Lupton, J. M. 155, 182

M

Maddock, B. 18, 61, 307, 322, 333, 334
Mai-Duy, N. 436
Maillefer, S. A. 336, 363
Mallouk, R. S. 306, 307
Manaresi, P. 181
Marschik, C. 364
Marshall, D. I. 305
Martelli, F. 463
Martin, G. 364
Matheson, A. J. 181
Matovich, M. A. 156, 183
Matsubara, Y. 412
Matsuo, T. 156, 183
Mavridis, H. 412
McClelland, D. E. 305
McKelvey, J. M. 61, 306, 307, 364
Mehta, A. K. 183
Meissner, J. 182
Mendelson, R. A. 181, 183, 180
Merz, E. H. 181
Meyers, J. A. 372
Michaeli, W. 412
Middleman, S. 61, 307
Miethlinger, J. 364
Mol, E. A. J. 212, 219, 305, 447
Mooney, M. 155, 182
Morton-Jones, D. H. 15
Mount III, E. M. 184, 306, 395, 412, 447

N

Naganawa, T. 436
Naitove, M. H. 372
Nakajima, N. 182
Narkis, M. 307
Nason, H. K. 181
Nichols, R. J. 363

O

Oliver, G. 375, 383, 412

P

Parnaby, J. 183
Pearson, J. R. A. 156, 183, 233, 306
Penwell, R. C. 181
Petrie, C. J. S. 156, 182
Phan-Thien, N. 419, 436
Plumley, T. A. 363
Porter, R. S. 181
Pouncy, H. W. 435
Protasov, V. P. 183

R

Radford, J. A. 435
Ram, A. 307
Ramamurthy, A. V. 154, 155, 182
Rauwendaal, C. 15, 61, 372
Regester, J. W. 155, 182
Reinhart, C. 412
Richardson, M. J. 189, 184
Rivlin, R. S. 419, 436
Rodriguez, F. 184
Roland, W. 364
Rudolph, L. 435, 436

S

Saha, P. 412
Schippers, H. 363
Schott, H. 182
Schowalter, W. R. 156, 183
Schreiber, H. P. 182
Schrenk, W. J. 412, 414, 435
Schuele, H. 447
Schultz, J. 184
Schut, J. H. 372
Semmekrot, G. J. M. 372
Shah, Y. T. 183
Shroff, R. N. 412
Siline, M. 436

Somers, S. A. 363
Sonia, J. 435
Southern, J. H. 435
Spalding, M. A. 15, 19, 22, 61, 184, 219,
220, 264, 305, 306, 363, 364, 372
Speed, C. S. 183
Spencer, R. S. 151, 181
Sperling, L. H. 184
Speziale, C. G. 436
Squires, P. H. 306
Stehling, F. C. 183
Strub, R. A. 306
Sundstrom, D. W. 234, 306
Syrjala, S. 436

T

Tabor, D. 61, 176, 184
Tadmor, Z. 15, 20, 61, 225, 232, 305, 447
Tanner, R. I. 419, 436
Tanoue, S. 436
Terry, B. W. 180, 184
Thangam, S. 436
Thomka, L. M. 435
Todd, D. B. 449, 463
Tordella, J. P. 151, 154, 182
Townsend, P. 436
Trudell, B. C. 183
Tung, L. H. 181
Tusim, M. H. 184, 447
Tzoganakis, C. 412

U

Underwood, E. E. 306

V

Vermeulen, J. R. 233, 306
Vinogradov, G. V. 155, 183
Vlachopoulos, J. 15
Vlcek, J. 412

W

Wagner, J. R. 15, 412
Walters, K. 436
Wang, J-S. 181
Wang, N. 306
Wang, S.-Q. 156, 183
Waterhouse, W. M. 436
Watson III, J. G. 184, 306
Weinberger, C. B. 157, 183
West, D. C. 182
Westerman, L. 181
Westover, R. F. 181
White, J. L. 182, 435, 463
Whitlock, M. H. 182
William, M. L. 181
Wissbrun, K. F. 183
Woodward, A. E. 95, 96, 184
Worth, R. A. 183
Wright, B. 181

X

Xue, S.-C. 436

Y

Yang, K. 180, 184
Yoon, D. S. 447
Yoshimoto, Y. 156, 183
Young, C. C. 306
Young, R. J. 184

Z

Zatloukal, M. 412

Subject Index

Symbols

2-lobe (or bi-lobe) design 11
3-lobe (or tri-lobe) design 11

A

adapter 399
adiabatic operation 46
air entrapment problem 24, 26
alternating copolymer 69
amorphous polymer 71
analytical melting model 224
angle of repose 178
annealing 111
apparent flow activation energy 126
apparent shear rate 136
apparent viscosity 137
Arrhenius equation 126
ASTM 68
atactic configuration 88
average molecular weights 72

B

Banbury® 449
barrel cooling 49
barrier screws 334
Barr ring mixer (BRM) 371
Barr sleeve mixer (BSM) 372
biaxial extensional flow 149
Bingham fluid 114
block copolymer 69

branched polymer 69
bulk density 6, 24, 178
Buss Ko-Kneader® 449

C

capillary rheometer 133
cavity transfer mixer (CTM) 371
chain folding 91, 94
chain or addition polymerization 65
chain re-entry 94
channel depth 59
channel width 59
channeled barrel 438
choker bars 375
coat-hanger dies 374
coextrusion dies 395
common scale-up method 353
compaction factor 263
compatibility 100
complex dynamic shear modulus 141
complex dynamic viscosity 142
compressibility 178
compression ratio (CR) 6
compression section 5
conduction melting 33
conduction melting model 273
cone-and-plate rheometer 133
configuration 87
conformation 86
consistent feeding rate 24
conveying element or screw bushing 452

cooling rate 109
copolymer 69
Couette viscometer 133
crammer feeder 23
CRD mixer 372
critical molecular weight for
 entanglement 85
critical nucleus size 105
critical shear stress 152
cross-channel drag flow 35
crosslinked polymer 69
crystalline polymer 71
crystallization rate 106
crystallization temperature 105
curvature factors 292

D

dead spot 5
deckling systems 387
die swell 89, 138
dilatant fluid 115
dispersion 41
dispersive mixing 41
dissipative melting 31
dissipative melting models 221
distributive mixing 41
domain 101
down-channel drag flow 35
drag flow 34
drag flow rate 284
draw ratio 156
draw resonance 156
drive torque 51
Dulmage mixing section 322
dynamic friction coefficient 176
dynamic loss shear modulus 141
dynamic loss viscosity 142
dynamic mechanical test 140
dynamic mixers 369
dynamic shear modulus 141
dynamic viscosity 142

E

effective residence time 43
elastic memory 165
elution volume 82
enthalpy 173
ET (Energy Transfer)-Screw 341
extensional flow 149
extensional rheometer 149
external friction 24, 176
extrudate swell 90, 138
extruder size 55

F

Farrel continuous mixer (FCM) 449
feedback control 56
feed binding 29
feed bridging 26
feedblock 402
feeding 18
feeding depth 5
feeding section 5
first normal stress difference 145
flight 6
flight clearance 31
flight interchange 339
flow instability 119, 150
flow rate ratio 147
flow segregation 24
flow temperature 174
friction 56
fringed micelle 95
fully oriented chain 86
functional groups 66

G

gear pump 365
glass transition 100
glass transition temperature (T_g) 71
glassy polymer 71
graft copolymer 69
grinding 56
gross melt fracture 151
growth of nucleus 106

H

hand-squeeze test 178
head pressure 5
heat of fusion 174
Helibar 438
helical coil 91
helix angle 58
heterogeneous copolymer 69
high load [MI] or 10X-[MI] 147
high performance screw 321
homogeneous copolymer 69
homopolymer 69

I

infinite shear viscosity 119
in-line mixer 367
instrumentation 55
interlamellar ties 64, 95
intermeshing co-rotating twin-screw
extruder 9, 452
intermeshing counter-rotating twin-screw
extruder 10, 459
internal friction 24, 178
intrinsic viscosity (IV) 79
isotactic configuration 88
isothermal Newtonian fluid model 282
iterative numerical melting model 224

K

Kenics KM mixer 368
kneading element or block 452
Koch SMX mixer 369

L

lamella 64, 95
lateral stress ratio 219
layer instability 407
layer interface 417
L/D ratio 5, 55
lead 6
light scattering 77
linear polymer 69

linear viscoelastic (LVE) 113
long chain branches (LCB) 69
loss-in-weight feeder 23

M

Maddock (or Union Carbide) mixing
section 333
manifold 374
manifold profile 381
Mark-Houwink equation 80
matrix 101
mechanical energy efficiency 46
mechanical melting 174
melt breakage 156
melt disturbances 407
melt film thickness 223
melt flow index 145
melt fracture 119, 151
melt index 145, 147
melt indexer 145
melting 2, 57, 100
melting efficiency 237
melting function 18
melting models 221
melting rate 223
melting section 5
melting temperature 71
melt pool 21
melt pressure drift 39
melt rheology 111
melt temperature drift 39
melt temperature fluctuation 39
melt viscosity 85
metered feeding device 10
metering depth 5
metering efficiency 295
metering function 18
metering models 279
metering section 5
microphase morphology 101
miscibility 100
mixing element or block 452
mixing-pin types 322
molecular entanglements 64

molecular orientation 1, 89
molecular weight distribution 74
molecular weight 72
monodisperse 74
morphology 1, 89
motor power 51, 303

N

Newtonian fluid 115
non-intermeshing counter-rotating twin-screw extruder 10, 462
non-Newtonian fluid 115
nucleation of crystal 105
number average molecular weight 72
numerical melting model 225

O

optical birefringence 90
osmotic pressure 76

P

packing density (PD) 93
phase angle 140
phase separation 100
pineapple mixing section 322
pitch 6
planar extensional flow 149
planar zig-zag 91
plasticating 2
plug flow 44
polydispersity 74
polymer extrusion 4
polymerization reaction 65
polymorphism 91
power-law equation 121, 377
pressure flow 34
pressure flow rate 284
pressure fluctuation 21
pseudoplastic fluid 115
pumping function 18
pumping section 5
purely viscous fluid 112

purging 23
pushing flight 22

Q

quenching 103

R

Rabinowitsch equation 136
race track 404
random coil 86
random copolymer 69
reduced channel depth 197
reduced pressure gradient 206
reduced screw length 201
reduced solid bed width 271
relaxation time 114
residence time distribution 43
residence time or dwell time; average residence time 43
retention time 82
retention volume 82
rheological mechanical spectrometer 139
rheopectic or anti-thixotropic fluid 115
rubbing mechanism 56

S

scale-up methods 352
scale-up of extruders 14
scientifically designed pineapple mixer 326
screw configuration 452
screw cooling 6, 49
screw design 309
screw elements 452
screw-freezing experiments 18
screw root 58
screw simulator 234
screw speed 7
screw torque strength 52
semi-crystalline polymers 71
shape factors 289
shear mixer 334

shear modulus G 112
shear rate 102
shear rate at the wall 136
shear strain 102
shear stress 56, 102
shear stress at the wall 135
short chain branches 69
side-feeding 8
single crystal 94
single-screw design technology 8
single-screw extruders 3
slip-stick mechanism 154
solid bed 20
solid bed breakup 21, 33
solid bed profile 271
solid bed splitting 21
solid conveying angle 22, 191
solid conveying efficiency 207
solid conveying function 18
solid conveying models 187
specific heat 171
specific output rate 309
spherulite 96
square-pitch 6
static friction coefficient 176
static mixer 367
step or condensation polymerization 66
stereoregularity 88
strain 102
stress 102
stress efficiency 237
super-cooling 105
surface melt fracture 151
surging 21, 38
syndiotactic configuration 88

T

tacticities 88
tearing 58
tensile stress 102
tensile viscosity 149
thermal shrinkage 90
thermomechanical history 1
thermo/mechanical stability 175

thermoplastics 68
thermosets 68
thixotropic fluid 115
trailing flight 22
transition section 5
transverse flow 35
true viscosity 137
Twente sleeve mixer (TSM) 371
twin-screw design technology 12
twin-screw elements 452
twin-screw extruder 9, 449
twin-screw scale-up 461
two-stage screw 7

U

uniaxial extensional flow 149
unit cell 91
unsaturated bond 65
unstable melting 58

V

viscoelastic 113
viscoelastic effects 413
viscoelastic fluid 113
viscosity 112
viscosity average molecular weight 73
viscous shear stress 223
volumetric feeder 23

W

wall slip 155
Wave-Screw 341
weight average molecular weight 73
Williams-Landel-Ferry (WLF) equation 125

X

X-ray diffraction 90

Z

Z-average molecular weight 73
zero shear viscosity 118