DESIGN OF ROTOR FOR INTERNAL BATCH MIXER AND MIXING ELEMENTS FOR TWIN SCREW EXTRUDER FOR POLYOLEFIN PROCESSING

SHAFAAT AHMED SALAHUDEEN

A thesis submitted in fulfilment of the requirements for the award of the degree of Doctor of Philosophy (Polymer Engineering)

Faculty of Chemical and Energy Engineering Universiti Teknologi Malaysia

FEBRUARY 2017

DEDICATION

This thesis is dedicated to my father Salahudeen, my mother Aathikka Begum for their endless support and encouragement and to all my brothers and sisters

ACKNOWLEDGEMENT

The Allah, Most Merciful and Most Beneficent. This PhD or any think without your help is impossible. I thank you for your help and I would always like to be your obedient servant.

I am most grateful to the support of my supervisor Assoc. Prof. Dr. Abdul Razak Bin Rahmat and his continuous support throughout my PhD research. With his patience and support, this journey becomes unforgettable and I am sincerely apologizing for any of my actions that made him bother during my research.

My sincere thanks to Dr. Othman Alothman and Dr. Rabeh Elleithy for their support both technically and financially and Dr. Yunusa Omar for his moral support.

My heartful thank to my friend Mohammed Ehtesham Ali Mohsin for his support and companionship and technician Khaja Nayeem Uddin for his assistance.

I heartily convey my thanks to my father, mother, sister and wife for their continuous support and encouragement during this journey.

I would like to remember this sentence always, "Things always never travel in the way you want, but patience, hard work and Allah's help brings you to the way you want".

ABSTRACT

Mixing is the key component of polymer processing to achieve homogeneity of final product. Previous researchers have reported poor mixing performance of internal batch mixer (IBM) and twin screw extruder (TSE) due to improper distributive and dispersive mixings. This leads to poor product properties. Hence to overcome the problem, this research aims to design a rotor and mixing element to improve mixing performance of IBM and TSE. The basic rotor design for IBM was developed on the concept of Banbury and roller rotors and this design was then optimized to attain secondary flow. Distributive mixing performance of the optimized rotor was compared with commercial rotors using ANSYS Polyflow, with results showing the new rotor was found to be better than commercial rotors. Based on these results, a prototype of optimized design rotor was developed using Computer Numerical Control machine. Using this prototype rotor, nano calcium carbonate was dispersed in high density polyethylene and its morphology was analysed via scanning electron microscopy (SEM). SEM results showed improved dispersive mixing performance of prototype rotor compared to that of commercial rotor. This prototype rotor design was later modified into two mixing elements namely, Bean-UTM for intermeshing co-rotating TSE and Blade-UTM for intermeshing counter-rotating TSE. The Bean-UTM and Blade-UTM were examined for dispersive mixing (mixing index) and distributive mixing (logarithm of length of stretch, instantaneous efficiency and time average efficiency) and then were compared with commercial TSE mixing elements. The results showed Bean-UTM has better mixing performance than kneader mixing element of Dr. Collin TSE and the Blade-UTM has better mixing performance than screw mixing element of Coperian TSE. The findings of this research will hopefully solve the issue of poor mixing in IBM and TSE.

ABSTRAK

Pencampuran adalah komponen utama pemprosesan polimer untuk mencapai kehomogenan produk akhir. Penyelidik terdahulu telah melaporkan prestasi pencampuran yang tidak memuaskan bagi pencampur kelompok dalaman (IBM) dan penyemperit skru berkembar (TSE) disebabkan oleh campuran taburan dan serakan yang tidak sempurna. Ini menghasilkan sifat-sifat produk yang bermutu rendah. Untuk mengatasi masalah ini, kajian dijalankan bertujuan untuk mereka bentuk rotor dan elemen pencampuran bagi meningkatkan prestasi campuran IBM dan TSE. Reka bentuk asas rotor untuk IBM telah dibangunkan berdasarkan konsep rotor *Banbury* dan penggelek dan seterusnya reka bentuk ini dioptimumkan untuk mencapai aliran sekunder. Prestasi taburan pencampuran rotor yang telah dioptimumkan dibandingkan dengan rotor komersial menggunakan ANSYS Polyflow, dengan keputusan menunjukkan rotor baharu lebih baik daripada rotor komersial. Berdasarkan keputusan ini, reka bentuk prototaip rotor yang telah dioptimumkan dibangunkan menggunakan mesin Kawalan Berangka Komputer. Dengan menggunakan prototaip rotor ini, kalsium karbonat nano telah diserakkan ke dalam polietilena ketumpatan tinggi dan morfologinya dianalisis menggunakan mikroskop elektron pengimbas (SEM). Keputusan SEM menunjukkan peningkatan prestasi serakan campuran prototaip rotor berbanding rotor komersial. Reka bentuk prototaip rotor kemudiannya telah diubahsuai kepada dua elemen campuran iaitu Bean-UTM untuk putaran searus antara jejaring TSE dan Blade-UTM untuk putaran berlawanan antara jejaring TSE. Bean-UTM dan Blade-UTM telah diperiksa untuk campuran serakan (indeks campuran) dan campuran taburan (logaritma daripada panjang regangan, kecekapan serta-merta dan purata kecekapan masa) dan kemudian dibandingkan dengan elemen campuran komersial TSE. Hasil kajian menunjukkan Bean-UTM mempunyai prestasi pencampuran yang lebih baik daripada elemen pencampuran kneader Dr. Collin TSE dan Blade-UTM mempunyai prestasi pencampuran yang lebih baik daripada elemen pencampuran skru Coperian TSE. Hasil kajian ini diharapkan akan dapat menyelesaikan isu pencampuran yang kurang baik di dalam IBM dan TSE.

TABLE OF CONTENT

CHAPTER		TITLE	PAGE
	DEC	CLARATION	ii
	DEI	DICATION	iii
	ACI	KNOWLEDGEMENT	iv
	ABS	STRACT	v
	ABS	STRAK	vi
	TAI	BLE OF CONTENT	vii
	LIS	T OF TABLES	xii
	LIS	T OF FIGURES	xiii
	LIS	T OF ABBREVATION	xix
	LIS	T OF SYMBOLS	XX
	LIS	T OF APPENDICES	xxii
1	INT	RODUCTION	1
	1.1	Background of Study	1
	1.2	Problem Statement	3
	1.3	Objectives of Study	5
	1.4	Scope of Study	6
2	LIT	ERATURE REVIEW	8
	2.1	Mixing	8
	2.2	Internal Batch Mixer	10
		2.2.1 Intermeshing Type	11
		2.2.2 Non-intermeshing (Tangential) Type	11
	2.3	Single Screw Extruder	14
		2.3.1 Benefit of Twin Screw Extruder Over Single	16

		Screw Extruder	
		2.3.1.1 Remarkable Mixing Capability	16
		2.3.1.2 High level of Process Flexibility	17
		2.3.1.3 Better Control of Process Parameters	17
		2.3.1.4 Higher Process Productivity	17
		2.3.1.5 Why Twin Screw Extruder	18
2.4	Twin	Screw Extruder	18
2.5	Studie	es on Internal Batch Mixer and TSE	21
	2.5.1	Previous Study on Internal Batch Mixer:	
		Numerical Simulation	22
	2.5.2	Previous Study on Internal Batch Mixer:	
		Numerical Simulation and Experimental	
		Verification	24
	2.5.3	Previous Studies on Twin Screw Extruder:	
		Numerical Simulation	26
	2.5.4	Simulation – ANSYS POLYFLOW	29
	2.5.5	Research Studies to Measure the Efficiency of	
		Mixing Using SEM	32
	2.5.6	Simulation – ANSYS POLYFLOW	33
RES	SEARC	TH METHODOLOGY	38
3.1	Resea	rch Methodology Chart	38
3.2	Gener	ation of Material Data of All Simulation	39
	3.2.1	Materials	39
	3.2.2	Experimental Design	39
	3.2.3	Simulation Method	40
3.3	Valida	ation of Simulation with Experimental	
	Verifi	cation for Internal Batch Mixer	40
	3.3.1	Materials	40
	3.3.2	Experimental Procedure of Partical Tracking	
		Method	41
	3.3.3	Simulation Method	42
		3.3.3.1 Geometry and Meshing	42

3

		3.3.3.2	Simulation Step for Particle Tracking	
			Method	42
3.4	Desig	n Proced	are to Develop Secondary Flow at The	
	Cleara	ance		43
	3.4.1	Geomet	ry and Meshing	43
	3.4.2	Simulat	ion Set up	45
3.5	Desig	n of New	Rotor for Internal Batch Mixer	43
	3.5.1	Simulat	ion Method	45
		3.5.1.1	Geometry and Meshing	45
		3.5.1.2	Simulation Setup	46
	3.5.2	Materia	ls	46
	3.5.3	Experin	nental Methods	46
3.6	Co-Re	otating In	termeshing TSE – Simulation Analysis	47
	3.6.1	Simulat	ion Method	47
		3.6.1.1	Geometry	47
		3.6.1.2	Optimization of Meshes	47
		3.6.1.3	Simulation Setup for Co-rotating	
			Intermeshing TSE	48
3.7	Count	ter Rotati	ng Intermeshing TSE – Simulation	
	Analy	vsis		49
	3.7.1	Simulat	ion Method	49
		3.7.1.1	Geometry and Meshing	49
		3.7.1.2	Simulation Setup for Counter rotating	
			Intermeshing TSE	49
3.8	Desig	n of New	Mixing Element for TSE	49
	3.8.1	Geomet	ry and Meshing	49
	3.8.2	Simulat	ion Setup of New Mixing Element for	
		Co-rota	ting Intermeshing TSE	49
	3.8.3	Simulat	ion Setup of New Mixing Element for	
		Counter	Rotating Intermeshing TSE	50
RES	SULTS	AND DI	SCUSSION	51
			ata for The Simulation	5

4

ix

	4.1.1	Experimental Rheological Data of HDPE at	
		Various Temerature	51
	4.1.2	Simulation – ANSYS POLYMAT Curve	
		Fitting	52
	4.1.3	Validation of Simulation using Experimental	
		Verification	53
		4.1.3.1 Velocity Profile	55
4.2	Desig	n Parameter to Develop Secondary Flow in	
	Intern	al Batch Mixer and Extruders	58
	4.2.1	Secondary Flow Design Analysis	60
4.3	Desig	n of New Rotor for Internal Batch Mixer	61
	4.3.1	Simulation Results and Analysis	61
	4.3.2	Experimentail Verification	70
4.4	Co-R	otating Intermeshing TSE – Simulation Results	75
	4.4.1	Geometry	75
	4.4.2	Optimization of Mesh for Twin Screw	
		Extruders	78
	4.4.3	Simulation Results	83
4.5	Count	ter rotating Intermeshing TSE – Simulation	
	Resul	ts	84
	4.5.1	Geometry	84
	4.5.2	Meshing	87
	4.5.3	Simulation Results	87
4.6	Desig	n of New Mixing Element for TSE	87
	4.6.1	Simulation Results for Bean-UTM for Co-	
		rotating Intermeshing TSE	93
	4.6.2	Simulation Results for Blade-UTM for	
		Counter Rotating Intermeshing TSE	97
COI	NCLUS	SION AND RECOMMENDATION	103
5.1	Desig	n Paramenter to Develop Secondary Flow	103
5.2	New 1	Rotor for Internal Batch Mixer	103
5.3	Bean-	UTM Mixing Element for Co-rotating	103

5

	Intermeshing TSE	
5.4	Blade-UTM Mixing Element for Counter Rotating	
	Intermeshing TSE	104
5.5	Recommendation	104
REFERENCES		105

Appendices A - F 111-127

LIST OF TABLES

INDLL NO.	TA	BL	Æ	Ν	О.	
-----------	----	----	---	---	----	--

TITLE

PAGE

2.1	Mixing effeciency of commercial rotor: Cam,	
	Banbury and Roller rotors	25
3.1	List of design geometries for the secondary	
	flow simulation	44
4.1	List of design geometries to optimize secondary flow	62
4.2	List of design geometries to optimize clearance	66

LIST OF FIGURES

. TITLE	PAGE
Schematic illustration of secondary flow (Eddy flow)	
in the velocity profile.	4
Schematic illustration of dispersive and distributive	
mixing mechanisms: Modified reference	
(Manas-zloczower and Tadmor, 1994).	10
Schematic representation of internal batch mixer	
with roller rotor (Thermo-Scientific, 2012).	13
Camera image of Haake Polylab (Germany) Internal	
batch mixer parts: mixing chamber (Top), cam rotor,	
banbury rotor and roller rotor.	14
Schematic representation of single screw extruder.	16
Types of screw rotation in TSE	19
Types of screw arrangement in TSE	19
Mixing Elements of TSE (a) Kneader type Mixing	
Element and (b) Screw Mixing Elements without gap	
(b) (Fard and Anderson, 2013a).	21
Particle tracking results showing the distributive mixing	
of the flow field (a) initially and (b) after 10 revolutions	
(Connelly and Kokini, 2007).	23
Red master batch placed at left most center: Cam Rotor	
(a) after 20 s by simulation (b) after 60 s by simulation	
(c) after 60 s by experiment; Banbury rotor (d) after 20 s	
by simulation (e) after 60 s by simulation (f) after 60 s by	
experiment; Roller rotor (g) after 20 s by simulation	
(h) after 60 s by simulation and (i) after 60 s by	
experiment (Salahudeen et al., 2011).	25
	Schematic illustration of secondary flow (Eddy flow) in the velocity profile. Schematic illustration of dispersive and distributive mixing mechanisms: Modified reference (Manas-zloczower and Tadmor, 1994). Schematic representation of internal batch mixer with roller rotor (Thermo-Scientific, 2012). Camera image of Haake Polylab (Germany) Internal batch mixer parts: mixing chamber (Top), cam rotor, banbury rotor and roller rotor. Schematic representation of single screw extruder. Types of screw rotation in TSE Types of screw arrangement in TSE Mixing Elements of TSE (a) Kneader type Mixing Element and (b) Screw Mixing Elements without gap (b) (Fard and Anderson, 2013a). Particle tracking results showing the distributive mixing of the flow field (a) initially and (b) after 10 revolutions (Connelly and Kokini, 2007). Red master batch placed at left most center: Cam Rotor (a) after 20 s by simulation (b) after 60 s by simulation (c) after 60 s by experiment; Banbury rotor (d) after 20 s by simulation (e) after 60 s by simulation (f) after 60 s by experiment; Roller rotor (g) after 20 s by simulation (h) after 60 s by simulation and (i) after 60 s by

2.10	Color contours of the velocity in z direction for different	
	gap sizes; (a) 0.4, (b) 0.8, (c) 1.2, and	
	(d) 2.4 mm (Fard et al., 2012).	27
2.11	Color contours of the velocity in z direction for different	
	staggering angles; (a) 30, (b) 45, (c) 60, and (d) 90.	28
2.12	Velocity in z direction for SME and a standard conveying	
	element (Fard and Anderson, 2013a).	28
2.13	Secondary flow in the channel, cross sectional view (left)	
	and isometric view (right)	29
2.14	Velocity profiles and direction of shear and elongational	
	flow (Rauwendaal, 1999)	30
2.15	Schematic representation of elongation flow (bottom) and	
	shear flow (top)	30
2.16	Dispersion of particle in the converged channels due to	
	elongational flow (Rauwendaal, 1999)	31
2.17	SEM micrographs of (a) 90% Polymer/10% Nano	
	Calcium carbonate (b) 85% Polymer /15% Nano	
	Calcium carbonate using melt extrusion technique;	
	(c) 90% Polymer/10% Nano Calcium carbonate (d) 85%	
	Polymer /15% Nano Calcium carbonate using melt	
	mixing technique (Modified from Faud et.al, 2010).	32
2.18	Images of good dispersion (left) and poor dispersion (right)	
	with Nano materials (Padmababhan, 2008).	33
3.1	Research Methodology Flowchart	39
3.2	Position of the tracer, (a) Placed at the centre of the mixer,	
	(b) Placed at the left most centre of the mixer	42
3.3	Front view of the modified kneading element of	
	Dr. Collin TSE	44
4.1	Experimental plot of Shear viscosity versus angular	
	frequency at 190 °C, 200 °C, 210 °C and 240 °C	52
4.2	Geometry and meshed view of the internal batch mixer:	
	Front zone - front view of Cam rotor and mixing chambers	
	with mixing zone.	54
4.3	Torque versus Time of HDPE at 9/6 rpm and 190°C.	55

57
58
59
59
60
61
62
63
63
64
65
66
67
67
68
70
70

4.21	Side View of trial 7 rotor	71
4.22	Prototype of Trial 7 rotor design – Right and Left rotors.	71
4.23	Prototype of Trial 7 rotor design – Mounted in the Haake	
	Polylab mixer.	71
4.24	SEM images of commercial rotor Banbury using	
	HDPE + 2% Nano calcium carbonate at 100µm.	73
4.25	SEM images of new rotor using HDPE + 2% Nano	
	calcium carbonate at 100µm.	73
4.26	SEM images of commercial rotor Banbury using	
	HDPE + 2% Nano calcium carbonate at 50μ m.	74
4.27	SEM images of new rotor using HDPE + 2% Nano	
	calcium carbonate at 50µm	74
4.28	SEM images of commercial rotor Banbury using	
	HDPE + 2% Nano calcium carbonate at 10µm.	75
4.29	SEM images of new rotor using HDPE + 2% Nano	
	calcium carbonate at 10µm.	75
4.30	Collin's TSE – Top View.	76
4.31	Collin's TSE – Kneader block mixing section.	76
4.32	Collin's TSE – Die Section.	76
4.33	Collen's TSE – Kneader block mixing section with Die.	76
4.34	Design of mixing element of Dr. Collin's TSE: Front view.	77
4.35	Mixing element of Dr. Collin's TSE: a. isometric view;	
	b. Top view; c. Model of single mixing element.	77
4.36	3D isometric view of Mesh-1 with hexagonal and	
	tetrahedron elements.	78
4.37	Front view of Mesh-1: Mixing chamber with hexagonal	
	and tetrahedron elements.	80
4.38	3D Isometric view of Mesh-1: Mixing Chamber with	
	hexagonal and tetrahedron elements.	80
4.39	3D Isometric view (left) and Front view (right) of Mesh-1:	
	Mixing elements with hexagonal and tetrahedron meshes.	81
4.40	Top view of Mesh-2: Barrel with Screw Elements with	
	only hexagonal elements.	80

4.41	Top view of Mesh-2: Screw Elements with only	
7.71	hexagonal elements.	81
4.42	Front view of Mesh-2: Barrel and fluid domain with only	01
7.72	hexagonal elements.	82
4.43	3D Isometric view (left) and Front view (right) of	02
4.43	Mesh-2: Mixing elements with only hexagonal meshes.	82
4 4 4		
4.44	Mesh-1; Shear rate at 9 rpm, time step at 10 sec.	83
4.45	Mesh-2, Shear rate at 9 rpm, time step at 10 sec	83
4.46	Coperion TSE - equipment view.	84
4.47	SME Type mixing element of Coperion intermeshing TSE.	84
4.48	Dimensions of the SME type mixing element: Front view.	85
4.49	Dimensions of the SME type mixing element: Side view.	86
4.50	Top view of the right and left SME Type mixing element.	86
4.51	Mesh for Coperion intermeshing TSE Mixing Elements.	87
4.52	Reference mixing element design from Trial 7 rotor of	
	internal batch mixer.	88
4.53	Overlapping of mixing element in TSE.	88
4.54	Dimensions of the two wing mixing element	
	(Bean-UTM): Front view.	90
4.55	Dimensions of the three wing mixing element	
	(blade-UTM): Front view	90
4.56	Bean-UTM Mixing element for co-rotating	
	intermeshing TSE: a. Isometric view of mixing region;	
	b. Top view of mixing region; c. isometric view of	
	single mixing element.	90
4.57	Isometric view of meshed Bean-UTM Mixing Elements.	91
4.58	Blade-UTM Mixing element for counter rotating	
	intermeshing TSE: a. Isometric view of mixing region;	
	b. Top view of mixing region; c. isometric view of	
	single mixing element.	92
4.59	Meshed view of Blade-UTM mixing element	
	a) side view b) front view.	93
	u, she from 0, hold from.	5

4.60	Mixing index at 10 sec of kneader mixing element of	
	Dr. Collin TSE at 9 rpm (right) and Bean-UTM mixing	
	element TSE at 9 rpm (left) - At Z plane = 30 mm.	93
4.61	Mixing index at 10 sec of kneader mixing element of	
	Dr. Collin TSE at 9 rpm (right) and Bean-UTM mixing	
	element TSE at 9 rpm (left) - At X plane center.	94
4.62	Maximum mixing index verses time curve at 9 rpm for	
	kneader mixing element of Dr. Collin TSE and	
	Bean-UTM mixing element TSE.	95
4.63	Mean value of Natural logarithm of stretching verses	
	time chart of Collin TSE and Bean-UTM TSE at 9 rpm.	96
4.64	Instantaneous efficiency verses time chart of Collin	
	TSE and Bean-UTM TSE at 9 rpm.	96
4.65	Mean Time average efficiency verses time chart of	
	Collin TSE and Bean-UTM TSE at 9 rpm.	97
4.66	Mixing index at 10 sec of SME mixing element of	
	Coperian TSE at 9 rpm (right) and Blade-UTM mixing	
	element TSE at 9 rpm (left) - At Z plane = 30 mm.	98
4.67	Mixing index at 10 sec of SME mixing element of	
	Coperian TSE at 9 rpm (right) and Blade-UTM	
	mixing element TSE at 9 rpm (left) - At X plane center.	100
4.68	Maximum mixing index verses time curve at 9 rpm for	
	SME mixing element of Coperian TSE and	
	Blade-UTM mixing element TSE.	100
4.69	Mean value of Natural logarithm of stretching verses	
	time chart of SME Coperian TSE and Blade-UTM	
	TSE at 9 rpm	100
4.70	Mean value of Instanteneous Efficiency verses time	
	chart of SME Coperian TSE and Blade-UTM TSE	
	at 9 rpm.	101
4.71	Mean Time average efficiency verses time chart of	
	SME Coperian TSE and Blade-UTM TSE at 9 rpm.	10 3

LIST OF ABBREVIATION

CFD	-	Computational fluid dynamics
CPU	-	Central process unit
EVA	-	Ethyl vinyl acetate
FEM	-	Finite element method
HDPE	-	High density polyethylene
L	-	Left rotor
LDPE	-	Low density polyethylene
LLDPE	-	Linear low density polyethylene
PET	-	Polyethylene terephthalate
PS	-	Polystyrene
R	-	Right rotor
RPM	-	Rotation per minute
SME	-	Screw Mixing Element
SSE	-	Single screw extruder
TSE	-	Twin screw extruder

LIST OF SYMBOLS

β	-	Compression factor
$ ho_{f}$	-	Fluid density
Cpf	-	Fluid heat capacity
$r_{\rm f}$	-	Fluid heat source
$\mathbf{k}_{\mathbf{f}}$	-	Fluid thermal conductivity
ρ_s	-	Density of the moving part
c _{ps}	-	Heat capacity of the moving part
r _s	-	Heat source of the moving part
ks	-	Thermal conductivity of the moving part
\mathbf{Q}_{g}	-	Viscous dissipation
Q_{out}	-	Hear-transfer rate
k	-	Heat conductivity of polymer melt
VΤ	-	Temperature gradient
А	-	Total surface area of the mixer
e_{λ}	-	Local efficiency of mixing
λ	-	Length of stretch of a material
Р	-	Pressure
D	-	The rate-of-deformation tensor
f	-	Body force
Т	-	Extra – stress tensor
v	-	Velocity
γ	-	Local shear rate
ρ	-	Fluid density
H(T)	-	Arrhenius Law
η _o	-	Zero shear-rate viscosity
η_∞	-	Infinite shear-rate viscosity
Κ	-	Natural time

Т Temperature - T_{α} Reference Temperature -The ratio of the activation energy to the thermodynamic content Α -Clearnace between mixing element and mixing chamber α -W The vorticity tensor. λ_{MZ} Mixing index

LIST OF APPENDICES

APPENDIX

TITLE

PAGE

A	Simulation Steps for Curve Fitting	111
В	Simulation Setup for Particle Tracking Method	113
С	Simulation Setup to Develop Secondary Flow at The	
	Clearance	117
D	Simulation Setup for Optimization of Meshes	120
E	Simulation Setup for Co-Rotating Intermeshing Tse	123
F	Simulation Setup for Counter Rotating Intermeshing Tse	127

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Mixing is the most important step in polymer processing industries and it determines the homogeneity of the final end product (Rauwendaal, 2001; Tatterson *et al.*, 1991). A mixing process involves two mechanisms, dispersive and distributive mixing. In general, mixing begins with a 'distributive' step (drops are deformed passively), followed by a 'dispersive' one (drops break up into smaller droplets), and finally by the distribution of the droplets in the flow (Osswald and Hernandez-Ortiz, 2006).

The break-up of agglomerates or liquid cluster into small particles or droplets is termed as dispersive mixing. This has been studied by many researchers using shear and elongation stresses (Manas-zloczower and Tadmor, 1994; Rauwendaal, 1999). The distribution of compounds such as small particles or droplets into the polymer melt matrix is termed as distributive mixing (Ottino, 1989). This has been studied by many researchers using logarithm of length of stretch (Cheng and Manas-zloczower, 2004; Connelly and Kokini, 2004, 2007).

There are two types of polymeric mixers, batch mixer (internal batch mixer) and continuous mixers (single screw and twin screw extruder). Internal batch mixer is again of two types, intermeshing rotors and non-intermeshing rotors. Intermeshing rotors work in synchronizing style with similar rotational speed. While, non-intermeshing rotors work with both similar or at different rotational speeds.

However, most of the polymer industries use different rotational non-intermeshing type (Dick and Annicelli, 2001). Therefore, for batch mixer, this research work will focus on the use of non-intermeshing type internal batch mixer with different rotational speeds.

Numerous experimental and numerical research studies have been published related to internal batch mixer (Bai *et al.*, 2011; Flaherty, 1988; Hutchinson *et al.*, 1999; Jongen, 2000; Salahudeen *et al.*, 2011). Notably, Salahudeen *et al.*(2011) studied the batch mixer using numerical simulation and verified the data experimentally. Salahudeen *et al.* (2011) identified the poor mixing region in commercial mixer such as cam, banbury and roller batch mixer. They explained that this poor mixing region decreased the overall distributive mixing efficiency of internal batch mixer. Also they reported the generation of secondary flow between the rotor edge and mixing chamber by banbury rotor. They predicted that this secondary flow was created due to some design features of banbury rotor. Interestingly, overall dispersive mixing performance of banbury rotor was better than cam rotor and roller rotor. As for distributive mixing, roller rotor performance was considered better than cam rotor and banbury rotor.

Therefore, in order to improve the distributive and dispersive mixing performance of internal batch mixer, this study will focus on developing a new rotor design with the features of banbury rotor and roller rotor for internal batch mixer. Additionally, the reason for generation of secondary flow will be analyzed in this research.

As for continuous mixer, single screw extruder is not considered for this research work. The mixing capacity of a single screw extruder is considered weak. On industrial scale; twin screw extruders (TSE) are used for compounding and mixing purpose (Clextral, 2015; Connelly and Kokini, 2007; Rathod and Kokini, 2013). Therefore, twin screw extruders were used for this research. Similar to batch mixer, TSE has two types, intermeshing and non-intermeshing. Based on screw rotation it has two types, co-rotating and counter rotating TSE. On industrial scale; intermeshing co-rotating TSE and intermeshing counter-rotating TSE are commonly

used (Manas-Zloczower, 2009). As for TSE, this research work covered intermeshing co-rotating TSE and intermeshing counter-rotating TSE.

Numerous experimental and numerical research studies have been published related to twin screw extruders (Bakalis and Karwe, 1999; Barrera et al., 2008; Bertrand et al., 2003; Bigio and Wang, 1996; Cheng and Manas-zloczower, 2004; Connelly and Kokini, 2007; Fard and Anderson, 2013b; Fard et al., 2012; Ishikawa et al., 2000; Sämann, 2008; Vyakaranam et al., 2012a; Zhang et al., 2009). Notably, Fard et al. (2012) and Fard and Anderson (2013) studied the mixing in twin screw extruders using kneader mixing element (co-rotating TSE) and Screw mixing element (SME) (counter rotating TSE). Fard et al. (2012) identified the poor mixing zones in the twin screw extruders. Fard and Anderson (2013) provided solution for poor mixing with an increase in the gap size between the mixing elements and between the mixing element and the barrel. The radial mixing (cross-sectional mixing) was improved due to the increase in amount of back flow. However, it decreased the axial mixing due to decrease in positive transport. In order to improve the axial mixing and overall mixing performance of TSE, this study focused on to develop new mixing element to replace kneader mixing element and SME for TSE. In this research, base design of new mixing element was adopted from the new rotor design of internal batch mixer. Similar approach was used to develop kneader mixing element for TSE from the base design of cam roller geometry of internal batch mixer by Kiani and Burbank (2000).

1.2 Problem Statement

This research covered two important pieces of polymer mixing equipment i.e. internal batch mixer and twin screw extruders. In internal batch mixer, Salahudeen et al. (2011) identified the poor mixing region in commercial mixers such as cam, banbury and roller batch mixer. This poor mixing region overall decreased the distributive mixing efficiency of internal batch mixer. Comparatively, they identified roller rotor has better distributive mixing performance than cam rotor and banbury rotor. They identifed that banbury rotor has better dispersive mixing performance compared to cam and roller rotor. Interestingly, they noticed secondary flow at the rotor edge of banbury rotor and it helped to improve the dispersive mixing performance of banabury rotor. They predicted that improved dispersive mixing was due to this secondary flow as shown in Figure 1.1.

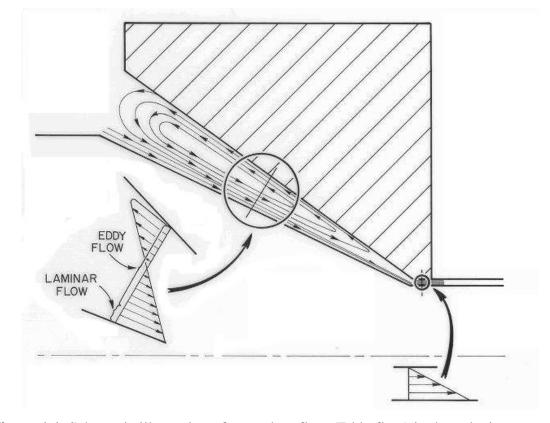


Figure 1.1 Schematic illustration of secondary flow (Eddy flow) in the velocity profile (Avitzur, 1983).

In order to improve the distributive and dispersive mixing performance of internal batch mixer (Salahudeen et al., 2011), this study considered to develop new rotor design with the combined features of roller rotor (distributive mixing) and banbury rotor (dispersive mixing) for internal batch mixer. The reason behind the generation of secondary flow in banbury rotor was unknown. In order to unveil the secret, design procedure to develop secondary flow between rotor edge and mixing chamber was studied. The result of the secondary flow study was implemented directly on the new rotor as well as in further studies on twin screw extruders. Design procedure to develop secondary flow in internal batch mixer and twin screw extruder is an one of the major contribution of this research. This design procedure can be used in any types of polymer mixing equipments.

In twin screw extruder, Fard *et al.* (2012) and Fard and Anderson (2013) studied the mixing in twin screw extruders using kneader mixing element (corotating TSE) and Screw mixing element (SME) (counter rotating TSE). Fard *et al.* (2012) identified the poor mixing zones and Fard and Anderson (2013) provided solution to remove the poor mixing regions. However, this solution increased the radial mixing, but decreased the axial mixing. In order to improve the axial mixing, the focus of this research was to develop a new mixing element for TSE. In this research, new rotor design of internal batch mixer was adopted as a basic design for new mixing element of intermeshing co-rotating TSE and intermeshing counter rotating TSE. Please note that results of the design procedure to develop secondary flow was implemented on new mixing elements.

The questions that needed to be answered in this research are:

- i. What is the general design parameter to develop secondary flow in internal batch mixer and TSE?
- ii. What is the best feasible rotor design for internal batch mixer based on distributive and dispersive mixing performance?
- iii. What is the effect of new TSE mixing element, developed based on the design of new rotor for internal batch mixer with kneader mixing element in intermeshing co-rotating TSE.
- iv. What is the effect of new TSE mixing element, developed based on the design of new rotor for internal batch mixer with screw mixing element in intermeshing counter rotating TSE.

1.3 Objectives of Study

The objective of this research was to develop a suitable rotor design for internal batch mixer with improved dispersive and distributive mixing performance than commercial rotor such as cam rotor, roller rotor and banbury rotor. Additionally, mixing elements for intermeshing co-rotating TSE and intermeshing counter-rotating TSE was developed using new rotor design of internal batch mixer. Therefore, the specific objectives can further be classified as:

- i. To develop the general design procedure for secondary flow in internal batch mixer and TSE.
- ii. To determine the best feasible rotor design for internal batch mixer based on distributive and dispersive mixing performance experimentally and numerically.
- iii. To simulate the effect of new TSE mixing element developed based on the design of new rotor for internal batch mixer with Kneader mixing element in intermeshing co-rotating TSE using ANSYS Polyflow.
- iv. To simulate the effect of new TSE mixing element developed based on the design of new rotor for internal batch mixer with screw mixing element in intermeshing counter rotating TSE using ANSYS Polyflow.

1.4 Scope of Study

Materials used for this work are High density polyethylene (HDPE- injection molding grade), red master batch (Injection molding grade) and Nano Calcium carbonate (approximately 20 nm).

The following equipment and softwares were used for the model design purpose. Equipments such as internal batch mixer (Haake Polylab, Germany) with different rotors; cam, banbury and roller rotors, kneader mixing element for intermeshing co-rotating TSE from COLLIN Twin-screw Extruder, Germany, Screw mixing element (SME) for Intermeshing counter-rotating TSE from COPERION Twin-screw Extruder, Germany were used. Softwares such as- ANSYS POLYFLOW and supportive applications - ANSYS DESIGN MODELER, ANSYS MESHING, ANSYS POLYDATA, ANSYS POLYMAT, ANSYS POLYSTAT, ANSYS CFX and ANSYS POLYCURVE were used. ANSYS DESIGN MODELER was used to create a base geometry for the simulation. ANSYS MESHING was used to create meshes on the geometry. ANSYS POLYDATA was used to perform simulation task on the meshed geometry. ANSYS POLYMAT was used to generate material data from the experimental rheological data. ANSYS POLYCURVE was used to draw XY curve plots. ANSYS POLYSTAT was used to generate raw data and curves from the result files of POLYDATA. ANSYS CFX was used to graphically visualize the result files of POLYDATA.

The rheological data was generated experimentally using AR-G2 Rheometer (TA Instrument). For simulation, this shear –viscosity data was used as a polymer (melt domain) material data.

Experimental methods - Injection molding grade HDPE was melted in internal batch mixer, followed by injection of red master batch for specific period of time at 20 sec and 60 sec. The constant temperature of 190° C was maintained. The result was recorded via digital camera.

Experimental methods – Injection molding grade HDPE was melted in internal batch mixer, followed by injection of 2% of nano calcium carbonate for 5 min. The result was analyzed using scanning electron microscopy (SEM).

Simulation methods – For internal batch mixer, constant speed ratio of 9 rpm (left rotor) / 6 rpm (right rotor) and constant temperature of 190° C were used. As for intermeshing co-rotating TSE and intermeshing counter-rotating TSE, constant speed of 9 rpm was maintained. ANSYS supporting software's such as ANSYS POLYMAT, ANSYS POLYCURVE and ANSYS CFX were used for result analysis.

REFERENCES

- Ansys. (2007a). Polyflow User's Manual, Version 3.12.0. Place del'Universite 16, B-1348 Louvain-la-Neuve, Belgium: Ansys.
- Ansys. (2007b). *Polyflow Mixing User's Manual, Version 3.12.0.* Place del'Uni¬versite 16, B-1348 Louvain-la-Neuve, Belgium.: Ansys.
- Avitzur, B. (1983). Handbook of metal-forming processes. New York :: Wiley.
- Bai, Y., Sundararaj, U., and Nandakumar, K. (2011). Nonisothermal Modeling of Heat Transfer Inside An Internal Batch Mixer. *AIChE Journal*, 57(10), 2657-2669.
- Bakalis, S., and Karwe, M. V. (1999). Measuring of Velocity Distributions in the Nip Region of a Co-Rotating Twin-Screw Extruder. *Trans IChemE*, 77(Part C).
- Banbury, F. H. (1916). USA Patent No. 1,200,070 U.S. Patent.
- Barrera, M. A., Vega, J. F., and Martínez-Salazar, J. (2008). Three-Dimensional Modelling of Flow Curves in Co-rotating Twin-Screw Extruder Elements. *Journal of Materials Processing Technology*, 197(1–3), 221-224.
- Berk, Z. (2009). Food Process Engineering and Technology: Elsevier Science.
- Bertrand, F., Tanguy, P. A., and Thibault, F. (1997). A Three-Dimensional Fictitious Domain Method for Incompressible Fluid Flow Problems. *International Journal of Numerical Methods in Fluids*, 25, 719-736.
- Bertrand, F., Thibault, F., Delmare, L., and Tanguy, P. A. (2003). Adaptive Finite Element Simulations of Fluid Flow in Twin-screw Extruders. *Computers and Chemical Engineering*, 27, 491-500.
- Bigio, D., and Wang, K. (1996). Scale-up Rules for Mixing in a Non-intermeshing Twin-screw Extruder. *Polymer Engineering and Science*, 36(23), 2832 – 2839.
- Bigio, D. I., Boyd, J. D., Erwin, L., and Gailus, D. W. (1985). Mixing Studies in the Single Screw Extruder. *Polymer Engineering & Science*, 25(5), 305-310.
- Bird, R. B., Stewart, W. E., and Lightfoot, E. N. (2004). *Transport Phenomena* (second ed.). New York: John Wiley & Sons.

- Cheng, H., and Manas-zloczower, I. (2004). Distributive Mixing in Conveying Elements of a ZSK-53 Co-rotating Twin Screw Extruder. *Polymer Engineering Science*, 38, 626–635.
- Cheng, J. J., and Manas-Zloczower, I. (1990). Flow Field Characterization in a Banbury Mixer. *International Polymer Processing*, *3*, 178-183.
- Clextral. (2015). Benefits of twin screw extrusion. from <u>http://www.clextral.com/technologies-and-lines/technologies-et-</u> <u>procedes/benefits-of-twin-screw-extrusion/</u>
- Connelly, R. K., and Kokini, J. L. (2003). 2-D Numerical Simulation of Differential Viscoelastic Fluids in a Single Screw Continuous Mixer: Application of Viscoelastic Finite Element Methods. *Advances in Polymer Technology*, 22(1), 22-41.
- Connelly, R. K., and Kokini, J. L. (2004). The Effect of Shear Thinning And Differential Viscoelasticity on Mixing in a Model 2d Mixer As Determined Using Fem With Particle Tracking. J. Non-Newtonian Fluid Mech, 123, 1-17.
- Connelly, R. K., and Kokini, J. L. (2007). Examination of the Mixing Ability of Single and Twin Screw Mixers Using 2d Finite Element Method Simulation with Particle Tracking. *Journal of Food Engineering* 79, 956-969.
- Cooke, R. T. (1934). UK Patent No. 431,012. British Patent.
- Coperion. (2016). ZSK twin screw extruder
- Dick, J. S., and Annicelli, R. A. (2001). *Rubber Technology: Compounding and Testing for Performance*: Hanser Publishers.
- Dr.Collin. (2012). Laboratory Twin-Screw Kneader ZK 25. In Collin (Ed.). Ebersberg: Plastima.
- Elemans, P. H. M. (2016). Polymer Twin-Screw Extrusion: Melting, Mixing and Screw Design. In *Reference Module in Materials Science and Materials Engineering*: Elsevier.
- Fard, A. S., and Anderson, P. D. (2013a). Simulation of distributive mixing inside mixing elements of co-rotating twin-screw extruders. *Computers & Fluids*, 87, 79-91.
- Fard, A. S., and Anderson, P. D. (2013b). Simulation of Distributive Mixing Inside Mixing Elements of Co-rotating Twin-screw Extruders. *Computers & Fluids*, -(Accpeted).

- Fard, A. S., Hulsen, M. A., Meijer, H. E. H., Famili, N. M. H., and Anderson, P. D. (2012). Tools to Simulate Distributive Mixing in Twin-Screw Extruders. *Macromolecular Theory and Simulations*, 21(4), 217-240.
- Flaherty, W. F. (1988). The Acquisition and Application of Data Obtained During the Mixing Cycle of an Internal Batch Mixer. *RubberWorld*, *198*(4), 14-18.
- Fuad, H. Z., Mohd. Ishak, Azman Hassan. (2010). Polypropylene/calcium carbonate nanocomposites – effects of processing techniques and maleated polypropylene compatibiliser. *Express Polymer Letter*, 4(10), 611-620.
- Garmabi, H., and Kamal, M. R. (1999). Improved Barrier and Mechanical Properties of Laminar Polymer Blends. *Journal of Plastic. Film Sheeting*, *15*(2), 120–130.
- Ghoreishy, M. H. R. a. N., V. (1997). Modeling the transient flow of rubberr compunds in the dispersive section of an internal mixer with slip-stick boundary conditions. *16*(1), 45-68.
- Harnby, N., Edwards, M. F., and Nienow, A. W. (1992). *Mixing in the Process Industries* (second ed.). Oxford: Butterworth/Heinemann Ltd.
- Hétu, J. F., and Ilinca, F. (2013). Immersed boundary finite elements for 3D flow simulations in twin-screw extruders. *Computers & Fluids*, 87, 2-11.
- Hrymak, A. N., Bravo, V. L., Khalfalla, Y., and Benyounis, K. Y. (2016). Polymer Melt Mixing in Twin Screw Extruders. In *Reference Module in Materials Science and Materials Engineering*: Elsevier.
- Hutchinson, B., Rios, A. C., and Osswald, T. A. (1999). Modeling the Distributive Mixing in an Internal Batch Mixer. *Int. J. Polym. Proc* 16(315).
- Ishikawa, T., Kihara, S.-I., and Funatsu, K. (2000). 3-D Numerical Simulations of Nonisothermal Flow in Co-rotating Twin Screw Extruders. *Polymer Engineering* & Science, 40(2), 357-364.
- Jongen, T. (2000). Characterization of Batch Mixers Using Numerical Flow Simulations. *AIChE Journal*, *46*(11), 2140-2150.
- Kiani, A., and Burbank, F. R. (2000). Mixing element for screw extruder: Google Patents.
- Kohlgrüber, K. (2008). Co-Rotating Twin-Screw Extruders: Hanser.
- Kwon, T. H., Joo, J. W., and Kim, S. J. (1994). Kinematics And Deformation Characteristics As A Mixing Measure In The Screw Extrusion Process. *Polymer Engineering & Science*, 34(3), 174-189.

- Manas-Zloczower, I. (2009). *Mixing and Compounding of Polymers: Theory and Practice*: Carl Hanser GmbH.
- Manas-zloczower, I., and Tadmor, Z. (1994). *Mixing and Compounding of Polymers* - *Theory and Practice*. New York: Carl Hanser Verlag.

Millauer, C. (1978). Kneading and mixing machine: Google Patents.

- Muzzio, F. J., Alexander, A., Goodridge, C., Shen, E., Shinbrot, T., Manjunath, K., Dhodapkar, S., Jacob, K. (2004). Solids Mixing. In E. L. Paul, V. A. Atiemo-Obeng and S. M. Kresta (Eds.), *Handbook of Industrial Mixing: Science and Practice*. Hoboken, NJ, USA: John Wiley & Sons, Inc.
- Nassehi, V., and Ghoreishy, M. H. R. (2001). Modeling of mixing in internal mixers with long blade tips. *Advances in polymer technology*, *20*(2), 132-145.
- Osswald, T., and Hernandez-Ortiz, P. (2006). *Polymer Processing Modeling and Simulation*. Ohio: Hanser Gardner Publication.
- Ottino, J. M. (1989). *The Kinematics of Mixing: Stretching, Chaos and Transport*. Cambridge: Cambridge University Press.
- Padmanabhan, B. (2008). Understanding the Extruder Processing Zone: the heart of a twin screw extruder. *Plastics, Additives and Compounding, 10*(2), 30-35.
- Pinto, G., and Tadmor, Z. (1970). Mixing And Residence Time Distribution In Melt Screw Extruders. *Polymer Engineering & Science*, 10(5), 279-288.
- Qiu, G., Zhang, P., Pan, J., Xie, Y., and Zhoa, S. (2003). Mechanical Properties and Morphology of Polypropylene Toughened with Metallocine Polymerized Polyethylene Elastomers. *Polymer Plastics Technology and Engineering* 42(1), 33–44.
- Qu, F., Jiang, Z., and Lu, H. (2015). Effect of Mesh on Springback in 3D Finite Element Analysis of Flexible Microrolling. *Journal of Applied Mathematics*, 2015, 7.
- Ralf, S., Martin, B., Thomas, P., and Stephan, H. (2012). Droplet based microfluidics. *Reports on Progress in Physics*, 75(1), 016601.
- Rathod, M. L., and Kokini, J. L. (2013). Effect of mixer geometry and operating conditions on mixing efficiency of a non-Newtonian fluid in a twin screw mixer. *Journal of Food Engineering*, 118(3), 256-265.
- Rauwendaal, C. (1987). Scale-up of Single Screw Extruders. *Polymer Engineering & Science*, 27(14), 1059-1068.

- Rauwendaal, C. (1999). New Dispersive Mixers Based on Elongational Flow. *Plastics, Additives and Compounding, 1*(4), 21-23.
- Rauwendaal, C. (2001). *Polymer Extrusion* (Fourth ed.). Cincinnati: Hanser publications.
- Rauwendaal, C. (2002). New Directions for Extrusion: Compounding with Single Screw Extruders. *Plastics, Additives and Compounding, 4*(6), 24-27.
- Rauwendaal, C. (2012). The Role of Screw Design in Efficient Extrusion of Medical Devices. *Plastics Technology*.
- Rauwendaal, C. (2014a). 8 Extruder Screw Design. In C. Rauwendaal (Ed.), Polymer Extrusion (Fifth Edition) (pp. 509-652): Hanser.
- Rauwendaal, C. (2014b). 10 Twin Screw Extruders. In C. Rauwendaal (Ed.), *Polymer Extrusion (Fifth Edition)* (pp. 697-761): Hanser.
- Rauwendaal, C. J., Gramann, P. J., Davis, B. A., and Osswald, T. A. (2000). Screw extruder with improved dispersive mixing elements: Google Patents.
- SABIC® HDPE Injection Molding M300054, (2013).
- Salahudeen, S. A., Elleithy, R., AlOthman, O., and AlZahrani, S. M. (2011). Comparative Study of Internal Batch Mixer Such as Cam, Banbury and Roller: Numerical Simulation and Experimental Verification *Chemical Engineering Science*, 66(12), 2502-2511
- Sämann, H.-J. (2008). Screw Elements for Co-rotating, Closely Intermeshing, Twin-Screw Extruders. In K. Kohlgrüber (Ed.), *Co-rotating Twin-screw Extruder* (pp. 215-235): Hanser.
- Shengwei, M. (2011). Top 5 misunderstandings on (good) mesh.
- Tatterson, G. B., Brodkey., R. S., and Calabrese, R. V. (1991). Move Mixing Technology into the 21st Century. *Chemical Engineering Progress*, 87(6), 45-48.
- Thermo-Scientific. (2012). Haake Rheomix* QC for the Haake PolyLab* QC System.
- Vyakaranam, K. V., Ashokan, B. K., and Kokini, J. L. (2012a). Evaluation of Effect of Paddle Element Stagger Angle on the Local Velocity Profiles in a Twin-Screw Continuous Mixer with Viscous Flow Using Finite Element Method Simulations. *Journal of Food Engineering*, 108, 585-599.
- Vyakaranam, K. V., Ashokan, B. K., and Kokini, J. L. (2012b). Evaluation Of Effect Of Paddle Element Stagger Angle On The Local Velocity Profiles In A Twin-

Screw Continuous Mixer With Viscous Flow Using Finite Element Method Simulations. *Journal of Food Engineering*, *108*(4), 585-599.

- Wagner Jr, J. R., Mount Iii, E. M., and Giles Jr, H. F. (2014). 11 Twin Screw Extruder Equipment. In J. R. W. M. M. F. Giles (Ed.), *Extrusion (Second Edition)* (pp. 125-148). Oxford: William Andrew Publishing.
- Wiedmann, W. M., and Schmid, H. M. (1982). Optimization of Rubber Mixing in Internal Mixers. *Rubber Chemistry and Technology*, 55(2), 363-381.
- Yang, H.-H., Wong, T. H., and Manas-Zloczower, I. (1994). Flow Field Analysis of a Banbury Mixer. In I. Manas-Zloczower and Z. Tadmor (Eds.), *Mixing and Compounding of Polymers: Theory and Practice* (pp. 187-223). New York: Carl Hanser Verlag.
- Yobas, L., Martens, S., Ong, W.-L., and Ranganathan, N. (2006). High-performance flow-focusing geometry for spontaneous generation of monodispersed droplets. *Lab on a Chip*, 6(8), 1073-1079.
- Zhang, X.-M., Feng, L.-F., Chen, W.-X., and Hu, G.-H. (2009). Numerical Simulation And Experimental Validation Of Mixing Performance Of Kneading Discs In A Twin Screw Extruder. *Polymer Engineering & Science*, 49(9), 1772-1783.