NUMERICAL SIMULATION AND EXPERIMENTAL INVESTIGATIONS ON THE EFFECT OF POLYPROPYLENE RHEOLOGY IN THE INJECTION MOLDING PROCESS

by

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DECLARATION

I hereby declare that the work reported in this thesis is the result of my own investigation and that no part of the thesis has been plagiarized from external sources.Materials taken from other sources are duly acknowledged by giving explicit references.

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LIST OF SYMBOLS

SYMBOL	DESCRIPTION	UNITS
English Symbols		
B	Exponential-fitted constant	Pa.s
c_p	Specific heat	J/kg-K
F	Front advancement parameter	-
n	Power law index	-
T	Temperature	K
T	Temperature	°C
T_b	Temperature fitted constant	K
T_{in}	Temperature at inlet	K
T_{wall}	Wall temperature	K
t	Time	s
u	Fluid velocity component in x-direction	mm/s
v	Fluid velocity component in y-direction	mm/s
$\mathrm{v}_{\mathrm{max}}$	Maximum velocity	m/s
w	Fluid velocity component in z-direction	mm/s
$\mathrm{x,y,z}$	Cartesian coordinates	mm

Greek Symbols

η	Viscosity	Pa.s
η_0	Zero shear rate viscosity	Pa.s
ρ	Density	Kg/m^3
τ	Shear stress	Pa
λ	Time constant	s
$\dot{\gamma}$	Shear rate	1/s
τ^*	A parameter that describes the transition region between power law region and zero shear rates of the viscosity curve.	Pa

LIST OF ABBREVIATIONS

		Page
3-D	Three dimensional	xv
ABS	Acrylonitrile-Butadiene-Styrene	3
CAE	Computational Aided Engineering	4
CFD	Computational Fluid Dynamic	4
FDM	Finite difference method	4
FEM	Finite element method	4
FVM	Finite volume method	4
GNF	Generalized Newtonian Fluid	18
N6	Nylon 6	3
PC	Polycarbonate	3
PP	Polypropylene	xvii
VOF	Volume of fluid	16

KAJIAN SIMULASI BERANGKA DAN EKSPERIMEN KE ATAS KESAN REOLOGI POLIPROPILENA DALAM PROSES PENGACUAN SUNTIKAN

ABSTRAK

Reka bentuk dan fabrikasi acuan adalah mahal untuk mesin pengacuan suntikan. Sebelum proses fabrikasi, analisis sebelum pengacuan adalah penting untuk menyiasat kebolehaliran plastik lebur dalam reka bentuk acuan. Analisis sebelum pengacuan dilakukan menggunakan perisian simulasi, bertujuan untuk mengurangkan kos fabrikasi dan masa. Simulasi berangka telah terbukti sebagai alat yang baik dan cara yang kos efektif untuk analisis sebelum pengacuan. Oleh itu, kajian ini memberi tumpuan kepada simulasi tiga dimensi (3D) tak mantap pengisian acuan semasa proses pengacuan suntikan termoplastik dengan menggunakan perisian ANSYS FLUENT 14. Polipropilena gred biasa dan perubatan merupakan bahan yang dipertimbangkan dalam kajian ini. Mesin pengacuan suntikan skru tunggal komersial (Battenfeld TM750 / 210) digunakan untuk mengkaji aliran polipropilena gred biasa pada tekanan suntikan dan suhu cair yang berbeza bagi acuan dulang berongga tunggal. Mesin kapilari reometer GÖTTFERT Rheograph 25 digunakan untuk melaksanakan uji kaji ke atas kelakuan reologi polipropilena (iaitu, kadar ricih dan kelikatan) pada suhu lebur yang berbeza. Keputusan reologi dibandingkan antara reometer kapilari dan data simulasi berangka. Data yang dikumpul antara eksperimen dan simulasi berangka disahkan dan berasas, yang telah menunjukkan pematuhan yang baik. Kajian lanjutan telah dibuat untuk mensimulasikan proses pengisian acuan dalam rongga tong picagari dengan menggunakan polipropilena gred perubatan. Kesan parameter proses (iaitu, tekanan sistem dan suhu cair) dan parameter fizikal (iaitu, bahan, kedudukan salur masuk dan ketebalan picagari) pada proses pengacuan suntikan dipertimbangkan dalam kajian simulasi. Didapati kelikatan menunjukkan

kesan yang besar di mana Lyondellbasell 6331(LB6331) yang mempunyai kelikatan yang lebih rendah mengambil masa yang lebih pendek untuk mengisi acuan berbanding TitanPro SM340 (TP340). Dari pemerhatian, tekanan sistem (tekanan suntikan) merupakan parameter utama yang member kesan terhadap pergerakan aliran PP lebur, di mana tekanan sistem yang tinggi boleh memendekkan masa pengisian. Pada sisi lain, suhu cair menunjukkan pengaruh yang sedikit pada masa pengisian dan aliran di dalam rongga acuan. Salur keluar mesti diletakkan sejauh mungkin dari salur masuk untuk menyalur keluar udara terperangkap dan menampung PP lebur untuk memenuhi rongga acuan. Dalam kajian ini, julat 0.75mm sehingga 1.00mm tebal picagari menunjukkan masa yang lebih pantas pengisian, lebih cepat mengalir dan mempunyai halaju aliran yang lebih tinggi.

NUMERICAL SIMULATION AND EXPERIMENTAL INVESTIGATIONS ON THE EFFECT OF POLYPROPYLENE RHEOLOGY IN THE INJECTION MOLDING PROCESS

ABSTRACT

The design and fabrication of the mold are costly for the injection molding machine. Prior to the fabrication process, the prior to molding analysis is important to investigate the flowability of molten plastic in the mold design. The pre-molding analysis is carried out using simulation software, with the purpose to reduce the fabrication cost and time. Numerical simulation has been proven as a good tool and cost effective way for pre-molding analysis. Therefore, this research focuses on the unsteady three-dimensional (3D) simulation of mold filling during the thermoplastic injection molding process using ANSYS FLUENT 14 software. Common Polypropylene (PP) and medical grade materials are considered in the study. Commercial single screw injection molding machine (Battenfeld TM750/210) is used to study the flow front advancement of the common polypropylene at different injection pressures and melt temperatures of a single cavity of the tray. GÖTTFERT Rheograph25 Capillary Rheometer machine is employed to perform the experiments on the rheological behavior of the polypropylene (i.e., shear rate and viscosity) at different melt temperatures. The rheological results are compared with those obtained by numerical simulation. The data collected from experiment and numerical simulation are verified and substantiated showing a good conformity. Further studies have been made to simulate the mold filling process in the syringe barrel cavity using medical grade polypropylene. The effects of process parameters (i.e., system pressure and melt temperature) and physical parameters (i.e., material, inlet position and syringe thickness) on injection molding process are considered in the simulation studies. It is found that viscosity shows a significant effect with LyondellBasell 6331 (LB6331) having a lower viscosity takes shorter time to fill the mold compared to TitanPro SM340. System pressure (injection pressure) is observed to be the main parameter that affected the flow movement of the molten PP, where higher system pressure can shorten the filling time. On the other side, melt temperature shows a slight influence on the filling times and flow front advancement in the mold cavity. The outlet vent must be located as far as possible from the inlet to channel out the entrapped air and accommodate the molten PP to occupy the mold cavity. In the present study, the range of 0.75 mm to 1.00 mm of syringe thickness showed faster filling time, faster flow front advancement and higher flow velocity.

CHAPTER 1

INTRODUCTION

1.1 General injection molding

Injection molding is basically a high temperature and high pressure casting process (An et al. , 2008). There are various types of injection molding processes such as conventional injection molding, gas assisted injection molding, water assisted injection molding, micro injection molding, etc. Dissimilar cases of injection molding have different melt mechanisms or machine components. The differences are primarily because of different requirements for the product itself. Although there many types of injection molding, they still follow the same working principle. The most commonly used is conventional injection molding.

The conventional injection molding machine consists of several parts, which are hopper, screw barrel, heaters, injection unit, clamping unit and mold. Figure1.1 shows the diagram of basic injection molding machine. It has mold filling, packing, and cooling stages (Jiang et al. , 2007; Ozcelik et al. , 2006). The machines are usually classified by their injection pressure and clamping force capability. Prior to the process of injection molding, the raw material is preheated in the hopper to remove moisture. Then, the polymer becomes hot and melts after feeding through the screw barrel equipped with heaters. This hot mixture is injected into the mold to form the shape based on the design of the mold cavity.

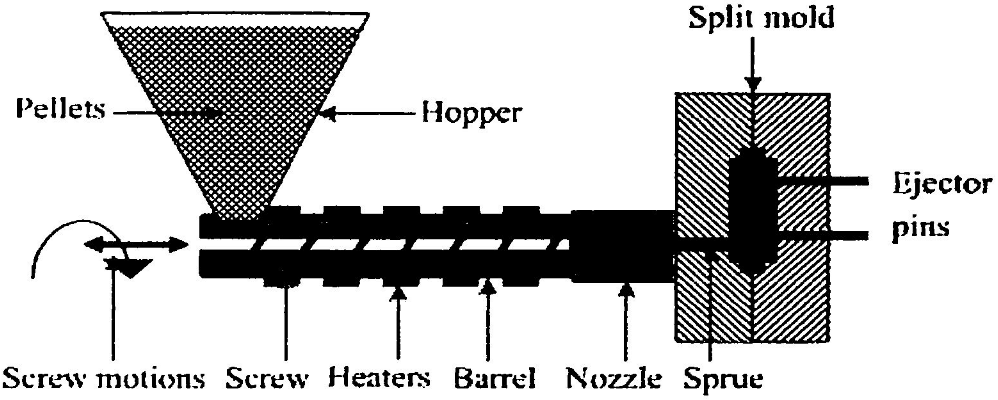


Figure 1.1: Diagram of basic injection molding machine (Kopeliovich, 2012).

Mold is one of the essential parts in the injection molding machine, to form the melting feed stock to the desired product design. Mold is mainly consisting of core, cavity, former ring and molding (He, 2011). The cavity is very important in getting the form and surface of the desired product. The mold must be designed to allow the molten material easily fills and flow at all parts of the cavity. It also has its own cooling channels to control the mold surface temperature so that the molten polymer can be cool at a cooling phase in the required temperature. The proper cavity pressure will produce products with precise dimensions. Improper flow of melt material in the mold cavity will affect the product quality. For example, incomplete mold filling because of insufficient injection pressure, high injection time due to low injection pressure and the feed material freezing before completing the mold cavity because of low melt temperature. The correct determination of polymeric materials with suitable rheological properties and correct parameter can prevent these problems.

The raw materials that can be used for injection molding are thermosets, thermoplastics, metals, glasses, confections, elastomers and composites. Different materials used have different requirements for the injection machine and the mold itself. The most widely used material for injection molding is thermoplastic.

1.2 Thermoplastic injection molding

The polymeric materials have been widely used to produce the everyday life product for centuries. The use of polymer materials includes the automotive, home appliances, electronics, medical and others. Several processes can produce the polymer products such as injection molding, extrusion, roll forming and etc. The famous and widely used process is an injection molding (Bikas et al. , 2002; Oktem et al. , 2007; Shen et al. , 2007) which is often used in the production of polymer products for low cost, versatility and efficiency. Polymers are inserted in the shape of granule or pallet. Polymers from thermoplastic group are one of commonly used in injection molding process. Polypropylene (PP), Acrylonitrile-Butadiene-Styrene (ABS) Polycarbonate (PC) and Nylon 6 (N6) are commonly used as thermoplastic in injection molding process. The choice of material is based on the function and strength of the materials. Differences in the use of materials require different process parameter settings and probably the mold also have to be setup differently.

Injection molding has also been used in manufacturing of medical devices (Chang et al. , 2001). Syringe, connectors and test tube are some examples of the medical devices that produce from injection molding process. The material selections of the medical device are strictly, because the manufacturers must be specialized to maintain the appropriate certification with U.S. Food and Drug Administration (FDA). Medical thermoplastic usually has special requirement depends on the usage of the medical device. Common requirements include the ability to withstand high temperature, not corrosive to certain chemical, not chemically active to blood,etc.

Even though injection molding is widely used and matured technology, it still encounters the defect problem in the process. Examples of defects in a thermoplastic process are silver streak, burn marks, weld lines, short shot, etc. Some of the defects are cosmetic defect (e.g., burn mark), affect the mechanical strength of the part (e.g., weld line) and not noticeable until the stage of test run.

Fabrication of mold consumes a plenty of time and money. The difficulty depends on the design of the cavity itself. Additional tooling process and parts are required for complex shape and unique surface cavity. The conventional mold design method is based on experience and trial-and-error methods. If a defect occurs, the trial and error approaches are used to find the root cause and solution. This can cause high repair cost and time consuming process including high usage of raw material wasted. The high cost of tooling and mold development causing a proper and most cost effective pre-molding analysis need to be conducted. Alternatively, with the aids of virtual modeling tools, the engineer and mold designer can easily understand the filling problem and identify the best design of the cavity.

1.3 Numerical simulation

Computer-aided engineering (CAE) tools can be used for mold design and optimize the processes (Pazos et al. , 2003; Qiao, 2006). CAE has proven to be a cost effective tool for pre-molding analysis (Makinouchi et al. , 1991). For flow analysis, usually Computational Fluid Dynamic (CFD) software is used (Ferng et al. , 2007). CFD usually uses the Finite Element Method (FEM), Finite Difference Method (FDM) and Finite Volume Method (FVM) for the numerical solutions. In the injection molding process, each parameter change will influence other parameters. Computer-aided analysis will facilitate to tackle the crucial parameter causing problems with the quality of the part. The defects that affect the quality of the product cannot be detected earlier but the defect precautions can be taken before the fabrication of the mold. The earlier precaution step can save the cost of mold modification. Besides, it also avoids the mold that could not be used properly after the fabrication, which could raise the manufacturing cost of a new mold. Experimental approach to find an optimized solution requires a longer time compared to numerical solution that consumes shorter research cycle time (Smith et al. , 2008).

The reliability of numerical simulation on computer-aided techniques mainly depends on the rheological characteristics (Bariani et al. , 2007). Viscosity model is important for the flow modeling in numerical simulation. Reliable result can be assured with the proper viscosity model for the simulation of injection molding process (Koszkul et al. , 2004). The capability of viscosity model to predict material behavior at different shear rates, pressure and temperature during the process is crucial to the accuracy of numerical simulation (Gou et al. , 2011).

1.4 Problem statement

Research on molding using the experimental method is costly and time consuming. The conventional trial-and-error techniques in the experiment consume a plenty of time and waste of materials. The interchange of material, physical form and parameters require extra setup and time for running the experiment. Costs will soar if any physical modification of the mold is involved. The cavity design and the location of the sprue influence the flowability of the molten plastic during the injection molding. The understanding of the molten plastic flow behavior is important to the designer and engineer prior to fabricate the mold. However, plastic flow behavior in the mold cannot be visualized because of the non-transparent mold and it is closed during the injection molding process. This situation creates the difficulties for the study of the flow in terms of flow profile, temperature, pressure and possible part defect during the injection process.The effect of processing parameter and physical parameter to the medical grade thermoplastic and differences of flow behavior between common and the medical grade thermoplastic need to be studied and investigated. Numerical simulation needs to be validated with the experimental works to prove its capability to simulate filling process of the thermoplastic injection molding. In addition, the study of injection molding process for the medical syringe by considering the medical grade thermoplastic is still not reported in the literature. Thus, the present study aims to fill this research gap using the simulation analysis technique.

1.5 Objective

The general objective of the research is to investigate the flow behavior of the medical grade PP during the filling stage of injection molding process for a medical syringe barrel. In order to achieve this aim, 3D numerical simulation is use and four main objectives were set out as mentioned below:

- To validate numerical simulation capability to predict the flow of molten thermoplastic in the mold cavity compared to experimental and the ability to predict material behavior at different shear rate, temperature and pressure.
- To investigate the effects of processing parameter of injection pressure and melt temperature on the medical grade thermoplastic flow behavior and characteristics.

- To study the influence of different physical parameters (i.e., thickness and inlet position) to the flow characteristics and behavior of molten medical grade thermoplastic.
- To identify the difference of flow behavior of two types of thermoplastic (medical grade and common grade) with different viscosity profiles.

1.6 Scope of the study

The general purpose of this study is to investigate the effect of PP rheology in the injection molding process. In this study, the PP being study is the medical grade PP. The chosen medical grade PP is special for syringe barrel. The medical grade polypropylene will undergo viscosity and shear rate measurement using off-line capillary rheometer. Cross-viscosity model's values were taken from the Capillary Rheometer and the values were used as viscosity model input for numerical simulation analysis. The experiments were conducted for the validations at different melt temperatures and different injection pressures using a tray shape mold cavity. The validation was done by comparing flow front advancement between experiment and numerical simulation results.

The study was extended to an injection molding of a syringe barrel shape cavity. The study will focus on the flow behavior at different process parameters, physical parameters and materials. The physical parameters are varied with different inlet positions and different thicknesses of syringe cavity. The different process parameters are the melt temperature and injection pressure. The injection molding process consists of mold filling, packing, and cooling stages but this study only considers at the mold filling stage.

1.7 Thesis outline

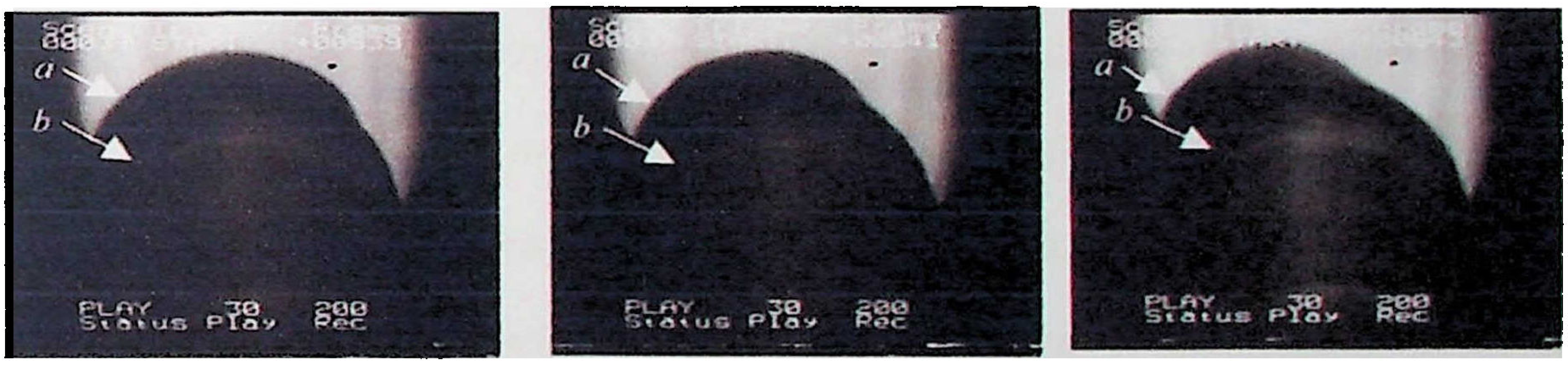
This thesis consists of five chapters. Chapter 1 covers general and a brief presentation about injection molding, thermoplastic injection molding, simulation modeling, problem statement, objectives and scope of research. Chapter 2 covers literature review on numerical simulation in the injection molding process. The mathematical model, experiment, the numerical simulation method and validation of simulation compared with experimental results are covered in Chapter 3. Meanwhile, Chapter 4 describes the studies of molten PP flow behavior in the syringe barrel cavity. Chapter 5 represents the findings of this study and future work recommendation.

CHAPTER 2

LITERATURE REVIEW

2.1 Experimental investigation

Multifarious experimental studies of injection molding process had been reported in the literature. Yokoi et al. (2002) used two-axis tracking system using high-speed camera to observe the flow front area, which tracks the flow automatically and measure the flow front position. This system is able to capture pictures of flow marks and silver streaks generation. High injection rates on PP causing asymmetrical fountain flow without formation of flow marks and silver streak it is the result of air bubble that expand to the surface of the cavity. Figure 2.1 shows the flow front advancement captured using high-speed camera at different filling times.



(1) 1.195ms (2) 1.205ms (3) 1.215ms

Figure 2.1: Observation of flow front advancement using high speed camera (Yokoi et al. , 2002).

Chen et al. (2003) studied the effect of different packing profiles, types on shrinkage, thickness distribution, part weight, flash and evenness in the injection molding process. They used reciprocating screw injection molding machine with four different inserts and different pressure settings to create different packing profiles.

They found the shrinkage, thickness distribution, part weight and evenness were mainly affected by packing profiles. Meanwhile, over-pack at the start of the packing process causing the flash problem.

Postawa et al. (2005) used amorphous polystyrene (PS) and semi-crystalline polyoxymethylene (POM) to study the weight, longitudinal and perpendicular shrinkage. The influences of clamp pressure, injection speed, mold temperature, cooling time and injection temperature were tested. It was found that injection temperature and clamp pressure are the most important parameters that influence processing shrinkage and mass.

Tang et al. (2007) fabricated a thin plate mold with a thickness of 1mm for warpage testing. The most affecting factor of warpage was the melt temperature. A comparison between in-line slit die that mounted as a mold on a commercial injection molding machine with a commercial capillary rheometer was studied by Bariani et al. (2007) to evaluate the accuracy of the in-line slit die.

Demirer et al. (2007) compared a hot runner system with the conventional runner system. Two-cavity mold that compatible with both systems was designed so that all experimental work can be done on the same mold. ABS and PP was used as base polymers. The observation found a hot runner system required lesser injection pressure when using the higher sample weight. The shrinkage and warpage decreased when higher injection pressure was applied. However, the use of higher process temperature increases the shrinkage and warpage.

Boronat et al. (2009) evaluated flow properties of reprocessed and virgin materials of two ABS grade thermoplastic polymers with low and high viscosity grade. The effects of reprocessing on the processability of both types ABS were investigated. Capillary rheometer was employed to study the flow properties for both

ABS grades. This study revealed the temperature and shear rate significantly influence the flow behavior of the material.

Tsai et al. (2009) studied the quality characteristics of optical lenses based on waviness, light transmission and surface finish using the injection molding process. It was found that melt temperature, packing pressure and mold temperature significantly affect the surface waviness. However, the surface finish and light transmission were slightly affected by the injection process parameters.

Kurt et al. (2009) investigated the significance of cavity pressure and mold temperature in the injection molding process. The cavity pressure and mold temperature were measured using pressure and temperature-pressure sensors that attached to the mold. The quality of the parts was being observed to study the influence of both parameters. The results indicated that cavity pressure and mold temperature were the dominant factors to the part quality.

Ozcelik et al. (2010) studied the effects of packing pressure, cooling time, melt temperature and injection pressure to the ABS's mechanical properties. Aluminum 2000 series and AISI 1020 were used as the mold materials in the experiments. The mechanical properties such as tensile strength and tensile strain at yield, elasticity module, flexural modules, tensile strain at break and impact strength were considered. For a steel mold, melt temperature affects the elasticity module, tensile strength and tensile strain at break, tensile strain at yield. Injection pressure affects the flexural module. In aluminum case, melt temperature affects the tensile strain at yield and flexural module. Injection pressure affects elasticity module, tensile strength at yield and impact limit. Besides, tensile strain at break was found affected by the packing pressure.

PP and PS were used by Altan (2010) to study the effects of injection pressure, packing pressure, packing time and melt temperature on shrinkage. Both materials were injected into a rectangular-shaped cavity mold. Packing pressure and melt temperature were found as the most significant parameter that affects shrinkage for both materials. The least affecting parameter for shrinkage was injection pressure.

Aho et al. (2011) studied the polymer melts rheological properties using an injection molding machine that being attached with a slit die. The in-line slit die can be set to three different slit heights by having three exchangeable inserts. Two grades of PP and PS were used and compared with the results from off-line capillary rheometer and rotational rheometer. The results showed a good agreement by using the in-line slit die and the off-line rheometers for both polymers.

Kovács et al. (2011b) developed a new measurement method for the deformation analysis by using a V–top mold. The method was used to investigate the effect of glass fiber content of the material (PP), gate type and location, holding pressure and mold temperature difference. From the data, it concludes that mold temperature and fiber content strongly effecting warpage.

Recently, the dynamic visualization system with a flow visualization mold was used by Xie et al. (2014) to study the mold filling phenomena with different processing parameters and gate sizes. Larger gate size has smaller residual stress and faster cavity filling time. It was also found that injection rate and nozzle temperature had a significant effect on the filling time and residual stress.

Gruber et al. (2014) presented a novel methodology that can evaluate the visual perceptibility of sink marks. ABS was used as the testing material. Holding pressure was varied and the results obtained were close to human vision by using this method.

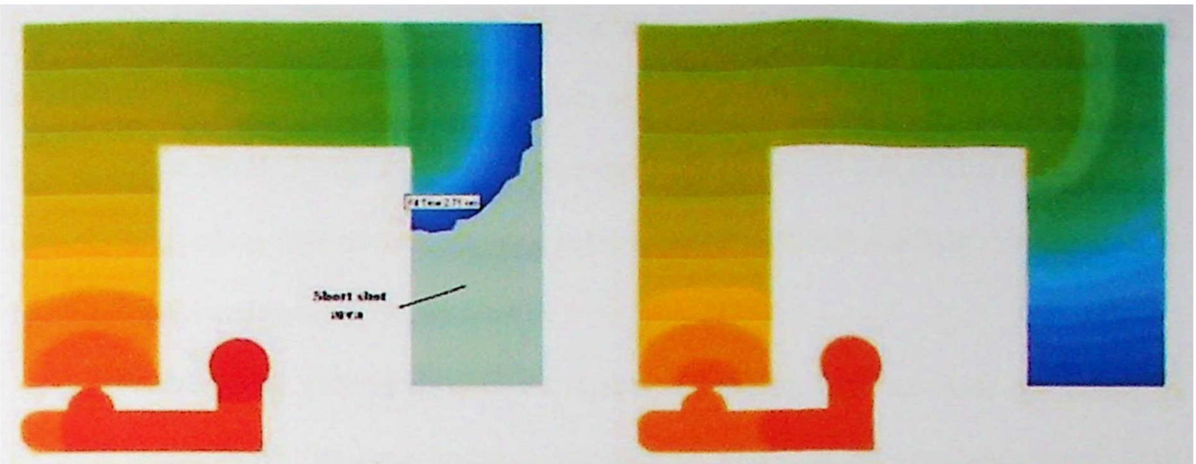
2.2 Simulation analysis

A number of simulation modeling had been carried out in the injection molding process. Simulation analysis is vital to provide detailed phenomenon and understanding of the molten plastic during the process. Different software had been utilized in the previous works with different discretization methods.

Chun (1999) reported the visualization and identification of the problem during the injection molding process. MOLDFLOW was used to visualize the polymer flow pattern, weld line, and bubble formation during the cavity filling.

Kumar et al. (2002) employed computer simulation to simulate injection molding of low density polyethylene (LDPE) at a constant flow rate for cylindrical shape part. Their simulation considered isothermal and non-isothermal conditions. The Power Law viscosity model was used for non-zero shear rate zone. However, "zero-shear viscosity" value was used when the shear rate is zero. They applied FDM to solve the governing differential equations.

An injection mold was designed and fabricated by Ozdemir et al. (2004) that allows images to be obtained from the plastic flow. Molten HDPE and PP filling and flow behavior were recorded at different injection pressures and velocities. The experimental results of flow front advancement were compared with the predictions of MOLDFLOW 5.0 software. They reported that MOLDFLOW software is capable to predict the accurate flow profile but could not estimate the exact filling time. Figure 2.2 illustrates the predicted flow profile by MOLDFLOW software.



T_{mold} = 34° C
T_{melt} - 215° C
Injection Pressure = 20 MPa

T_{mold} 34° C
T_{melt} - 215° C
Injection Pressure = 25 Mpa

Figure 2.2: Melt front advancement for PP using MOLDFLOW 5.0 (Ozdemir et al., 2004).

Spina (2004) studied the fabrication of medium size car's plastic arm of the body interior. Spina evaluated the product configuration, gating and hot runner systems. FEM analysis was used to study the process filling, post-filling and cooling phases. A deeper investigation of strain distribution and thermal stress was conducted for defect predictions.

Wang et al. (2005) used C-MOLD software with a finite element model to study the residual stress behavior on different process conditions such as packing pressure, filling time, mold temperature and melt temperature. In their study, the size of the core region and residual stress were affected by mold temperature. The high-packing pressure was found to be insensitive to the residual stress.

Stress and flow patterns of two different rib designs ("X" and "V") for composite clutch pedal was studied by Imihezri et al. (2006). The stress of "X" and "V" rib patterns were evaluated by using LUCAS, a finite element analysis (FEA) software and Moldflow Plastic Insight (MPI).

Tang et al. (2006) studied the thermal residual stress in warpage testing specimen mold. Unigraphics Version 13.0, computer aided design software was used to design the mold. Tang et al. developed thermal residual stress analysis model due to uneven cooling and the model was solved using LUCAS Analyst Version 13.5, finite element analysis software.

Pantani et al. (2007) carried out injection molding tests to study the effect of packing pressure to the morphology distribution. The results were compared with previous works that apply to lower holding pressure. The molding test then simulated using code from University of Salerno. The results revealed the molecular orientation increased with the increase of holding pressure.

Song et al. (2007) used experimental method and numerical simulation to study the influence of injection pressure, metering size, part thickness, injection rate and melt temperature at the filling time of ultra-thin wall plastic injection molding process. Part thickness was the process significant parameter in their study. Injection rate and metering size were the principal factors while injection pressure and melt temperature were considered as the secondary factors. Higher injection pressure and melt temperature were necessary in this process.

Moldflow simulation software was employed by Shen et al. (2008) to simulate numerical simulations of three-dimensional thin-walled product of PC+ABS materials. Control volume finite element method was used to discretize the governing differential equations.

Smith et al. (2008) utilized FLUENT 6.3 simulation software to analyze the injection molding process on the cooling phase. The final model was compared with earlier experimental results. The final model in FLUENT 6.3 indicated the model is a useful tool for further studies of optimizing injection molding process on cooling phase. The numerical model could provide the additional information that could not be assessed or deduced experimentally relating to condition changes.

A time-dependent three dimensional (3D) analysis was reported by Hassan et al. (2009a) to investigate the cooling of polymer by considering three different gate locations. The numerical model was solved by a FVM. The validation between numerical and analytical results showed a good agreement for both solutions.

Rudert et al. (2009) compared the cavity filling time and filling flow pattern of viscoplastic Carbopol gel between the experimental and numerical simulations. A front and rear transparent mold was used to visualize the viscoplastic flow. The numerical solution using FVM and Volume of Fluid (VOF) method with shear-thinning behavior, yielding point and effect of the gel were described by Herschel-Bulkley model. FLUENT software and Open Source code OpenFOAM were employed to solve the governing equations. Experimental and simulation showed a good agreement for a cavity filling time and filling flow pattern.

Numerical simulation using Moldflow software and experiments were conducted by Chen et al. (2009) to reduce warpage variation in a thin-shell plastic parts of injection molding process using the statistical techniques. Both simulation and experimental results indicated that melt temperature and packing pressure have a significant effect on the warpage.

Hassan et al. (2009b) used finite volume approach to perform a cyclic cooling analysis. T-mold plastic part consists of four cooling channel design was analyzed. The study was focused on the cooling channels form and location effect on the mold temperature distribution and the solidification degree of polymer.

Ozcelik & Sonat (2009) studied the production of thin shell cell phone by using PC and ABS. MOLDFLOW plastic insight (MPI) 4.0 was used to examine the injection parameters that affect the warpage for different thicknesses.

Khor et al. (2010) used an ABS material in the investigation of numerical and experimental of polymer rheology of the miniature injection molding process. The Cross model was used to describe the viscosity of molten ABS. The numerical predicted viscosity-shear rate from FLUENT 6.3 was substantiated by the experimental results obtained from Davenport High Shear Viscometer with injection nozzle. ABS melts front were tracked by using the Volume of Fluid (VOF) method in their simulation analysis. The flow front profile was in good agreement for both simulation and experimental results. In the investigations, they compared the numerical simulation and experimental results in terms of flow profile, where the molding experiments were conducted by using a simple square mold that attach to a modified rheometer.

Hassan et al. (2010a) utilized FVM to study the effect of different shapes of cooling channel with the same cross-sectional area. Two thicknesses of cuboids mold were used in their study.

Wang et al. (2010) used arbitrary Lagrangian-Eulerian (ALE) FEM for the numerical simulation scheme. The scheme used three-dimensional non-Newtonian fluid flow. Pressure-stabilized fractional step algorithm was used to solve incompressible Navier–Stokes equations.

Gou et al. (2011) obtained the Polypropylene rheological data from the online and offline measurement as an input data for the simulation of injection molding process by using Mold-flow software. The data were used to predict shrinkage and warpage.

Kovács et al. (2011a) used MOLDFLOW Insight 2011 to analyze the development of heat flow in the mold. The study was concentrated on the warpage at the corners of injection parts. This phenomenon was attributed to the asymmetrical cooling of the mold.

Sin et al. (2012) investigated the process ability of polyvinyl alcohol (PVOH) blending with starch in the injection molding process. The process ability was analyzed by using Moldflow software. Two percents of starch mixture were considered in the studies of the injection temperature, injection pressure, frozen layer fraction and volumetric shrinkage.

Ozcelik et al. (2012) used finite element analysis to study the effect of molecular orientation on PP mechanical properties for weld line defect. Three obstacles with different angles, which located at the center of the mold contributes to the weld line. MOLDFLOW was used for the simulation analysis.

Recently, Fernandez et al. (2014) attached a measuring device at the nozzle of the plasticizing injection unit. The apparent viscosity at different shear rates was calculated from the in-line measurement of the temperature and pressure drop. The results were corrected using SIM-Fit software to obtain the constants of Carreau-WLF rheological model. The material model constants were then inputted to the Cadmould 3D-F simulation software. The simulation results were compared with the injection molding experimental results.

2.3 Generalized Newtonian Fluid (GNF)

Computational analysis of the injection molding process requires material properties of the polymer. GNF is often used in engineering and science field (Chai et al., 2011) . GNF behavior is about the same to Newtonian fluid but the difference is on viscosity change where GNF follows the aspect of non-Newtonian fluid (Duffy et al. , 2014). GNF viscosity depends on the shear rate of the fluid. There are a number of viscosity model of GNF used in previous studies. A viscosity model is required to model the molten polymer behavior in the injection molding process.

Koszkul et al. (2004) used different rheological models to investigate the injection molding process. The simulation analysis was performed using MOLDFLOW INSIGHT ver.1.1. Four parameters (i.e., volumetric flow rate, shear rate, shear stress and temperature) were plotted versus process time for different viscosity models. Power Law model, MOLDFLOW second order model, Carreau Model and Cross model were considered in their study. Their study revealed that the values of Carreau Model and Cross model are close to each other rather than the Power Law model, which had higher values. However, MOLDFLOW second order model showed the lowest result for all parameters.

Carreau model and Cross model were compared for shear rate dependence by Hieber et al. (1992). The comparison used five different materials, namely nylon, ABS, polystyrene, PC and poly (methylmethacrylate). They reported that Cross model could accurately describe the shear-rate dependence compared with Carreau model.

Hassan et al. (2010b) used Cross model to describe the rheological behavior of polymer. They considered the pressure and temperature in the study. The physical model was solved by the FVM. The validation showed a good agreement between the numerical solution and literatures for the temperature distributions. Besides, Khor et al. (2010) also used the Cross model and finite volume based software FLUENT 6.3 to visualize the flow front profile during the meso-scale injection molding process. The simulated flow front profile showed a good agreement with experimental.

2.4 Tracking melt front: Volume of Fluid (VOF)

VOF is a numerical technique that is typically used in CFD to track the multiphase fluid advancement. The function of the technique is for free surface tracking and locating (Albadawi et al. , 2014; Aniszewski et al. , 2014; Jabbari et al. , 2014). A numerical method had been developed by Shin et al. (2000) and being applied to mold filling simulation. The development of the numerical method was to simulate the incompressible viscous flow with moving free surface. Besides, finite element method was also used to solve the volume of fluid (VOF) equation in the simulation.

Luoma et al. (2000) used the method that unifies many of VOF methods with an explicit scheme for flow front tracking during the polymer mold filling. Besides, Khor et al. (2010) used VOF for melt front tracking of ABS in meso-scale injection molding simulation. Molten ABS was injected at different melt temperatures to fill a mold cavity. Moreover, Tutar et al. (2010) used parallel computing approach to simulate the injection molding process for a single and multi cavity mold. FVM and VOF were used to simulate injection molding filling stage.

2.5 Summary

The use of injection molding in plastic industry is very common in this era. Versatile product development process is one of the factors why the process is often used in the manufacture of plastic products. This process is moving toward production of smaller and higher accuracy parts. Medical sector also shows a tendency of producing products using the injection molding process but in present, lack of paper discuss on the application of injection molding in medical product. Good part production is not easy as one thinks. Various factors must be taken into account to produce a good part and to prevent defects from occurring. Past practice in the manufacture of mold is to use the technique of trial-and-error and cost consuming in terms of material and time. CAE is proven to be one of the best solutions in doing the pre-analysis for the fabrication of a mold. More cost effective and the ability to study the flow behavior that cannot be seen in an experiment making it as a very good method for mold fabrication.

Various parameters, methods, materials and mold design had been considered in the previous researches. Khor et al. (2010) had carried out the numerical simulation and experimental investigations on a miniature injection molding by comparing the flow profile. The experimental works were conducted on a modified rheometer for the injection process, which not on a commercial injection molding machine. Their investigation only focuses on the effect of melt temperature. However, in the current study, the validations were conducted between numerical simulation and experiment using commercial injection molding machine. The comparisons include the injection pressure and melt temperatures. The material used in this study was PP from the thermoplastic polymer group. The study than furthered to injection syringe barrel injection molding process using medical grade PP. This study covers the aspects of the injection pressure, melt temperature, injection position, the thickness of the part and the material used during the injection molding process.

Cross model was considered in the current simulation of injection molding process as it was proven by Hassan et al. (2010a) and Khor et al. (2010), whereas Cross model can predict and model the behavior of polymer that close to the experimental results. Besides, Cross model will be used in the validation process of the tray part and the extended study for the syringe barrel.

FEM method is commonly used in the previous studies. However, FEM consumes more computing time and memory. Low computing time is highly desired by the engineer and researcher to reduce the research cycle time. Hence, FVM based software FLUENT 14.0 was selected for the current study. Besides, VOF technique was utilized to track the melt front of the molten polymer using FLUENT 14.0.

CHAPTER 3

METHODOLOGY

3.1 Introduction

Simulation study was conducted using CFD software, ANSYS FLUENT 14. Numerical simulation involves mathematical model to solve the complex fluid motion. Conservation of mass, momentum and energy are used as the basic principles in fluid flow analysis. The Cross viscosity model was used in the numerical simulation to describe the viscosity behavior of the polymer flow. In the experiment, a tray shaped part was injected using a commercial injection molding machine and rheolgical data of molten PP were taken from a capillary rheometer. Then, numerical simulation results will be validated with the experimental results to confirm its capability in solving the injection molding filling process.

3.2. Numerical method

The Navier - Stokes approach was used in the current study for the injection molding process. The assumptions for this approach are:

- The fluid (molten PP) is Generalized Newtonian Fluid (GNF).
- The fluid is three-dimensional, laminar (refer Appendix A) and incompressible flow.
- The density of the fluid is constant.
- The process is a non-isothermal process.

By using these assumptions, the fluid motion of molten PP, where it was injected into the mold cavity can be described by the governing equations of conservations of mass, momentum and energy.

The conservation of mass or continuity equation is:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \tag{3.1}$$

Eq. (3.1) is the mass conservation equation, which valid for incompressible flow.

Conservation of momentum in *x*-, *y*- and *z*- direction is written as:

(*x*-direction) $$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial P}{\partial x}+\eta\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) \tag{3.2}$$

(*y*-direction) $$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=-\frac{\partial P}{\partial y}+\eta\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right) \tag{3.3}$$

(*z*-direction) $$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=-\frac{\partial P}{\partial z}+\eta\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right) \tag{3.4}$$

where, P is the static pressure, $\rho$is density, η is the viscosity and u, v, w is the velocity in *x*-,*y*- and *z*- direction.

The energy equation can be described as:

$$\rho c_p\left(u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}\right)=k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)+\eta\dot{\gamma} \tag{3.5}$$

where k is the thermal conductivity, T is the temperature, η is the viscosity and $\dot{\gamma}$ is the shear rate, respectively.

3.3 Viscosity model - Cross Model

Cross model is a most appropriate model to describe the rheological behavior in the injection molding process (Hassan et al. , 2010; Khor et al. , 2010). The description of the molten PP is assumed as GNF by using the Cross model with Arrhenius temperature dependence.