Numerical and experimental investigations on cavity roughness effects in micro injection molding

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Numerical and Experimental Investigations on Cavity Roughness Effects in Micro Injection Molding

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ABSTRACT

Injection molding is one of the most common processes for cost-effective mass production of plastic micro parts. In micro injection molding, cavity surface roughness, which is insignificant in conventional (or macro) molding, may play an important role. Although the roughness effects in micro injection molding were mentioned in some research, they were not investigated systematically and understood clearly. In this thesis, the roughness effects on cavity filling in micro injection molding were for the first time mathematically modeled and systematically investigated through experiment and numerical simulation.

To consider the roughness effect on the effective volume of mold cavity, effective cavity wall and effective dimensions were defined and used to represent the geometry of mold cavity, such that the cavities with the same effective dimensions will have the same volume. Several two-dimensional and three-dimensional homogeneous roughness profiles were proposed to represent the physical surface roughness. To consider the roughness effects on heat transfer between polymer melt and the mold, a mathematical formulation was proposed to model thermal conductivity and heat capacity of the roughness layer occupied by both polymer melt and mold material. The thermal conductivity and heat capacity of the roughness layer are determined by the effective roughness height (δ) and the ratio of the volume occupied by the polymer melt to the volume occupied by the mold material (θ). For the proposed roughness profiles, the effective roughness height (δ) can be determined in terms of the average roughness (i.e., R_a or S_a), which is easy to measure.

Experimental investigations of polymer filling into a disk-shaped micro-thickness cavity mold were performed. The effects of different roughness on the filling of the

Abstract

cavity were conclusively demonstrated by using four round core inserts, where each insert consists of two semicircular halves of different roughness. Based on regression analysis, the ratio of the flow area of the rougher half to the entire flow area of the molded part (i.e., the k value), was defined to quantify the significance of roughness effects. For each of the four core inserts, the k values at different mold and melt temperatures were obtained. The dependence of roughness effects on the mold and melt temperatures was identified with the aid of the two-sample t test. The dependence of the roughness effects on the roughness magnitude and cavity thickness was also demonstrated.

A numerical procedure, which utilizes the finite volume and level set methods, and integrates the proposed roughness model, was developed to simulate the axisymmetric filling polymer flow in a thin circular cavity. The numerical procedure was then extended to simulate the pseudo-axisymmetric polymer flow encountered in the experiments by using a newly proposed inlet-velocity iteration approach.

The numerical procedures incorporating the roughness model were validated by comparing numerically predicted quantities with the experimentally measured or analytical quantities. The numerically predicted results were in good agreement with the experimental and analytical data.

Finally, further explorations of the roughness effects on quantities not easily measured experimentally were performed through numerical simulation.

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LIST OF ABBREVIATIONS

ANOVA	Analysis of Variance
BEM	Boundary Element Method
CAE	Computer Aided Engineering
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Levy
CI	Confidence Interval
COC	Cycloolefin Copolymer
EDM	Electrical Discharge Machining
FEM	Finite Element Method
FVM	Finite Volume Method
LCP A	Liquid Crystalline Polymer, Vectra A625 (25% Graphite)
LCP C	Liquid Crystal Polymer, Vectra C950
LIGA	Lithography, Electroplating and Molding
MABS	Methyl Methacrylate/ABS Copolymer
MAC	Marker and Cell
MAPL	Modified Arrhenius Power Law
MC	Modified Cross
MCA	Modified Cross-Arrhenius
MEMS	Micro Electronic Mechanical Systems
MPL	Modified Power Law
NFLV	Near Field Laser Velocimetry
PA	Polyamide
PBT	Polybutylene Terephthalate

List of Abbreviations

PC	Polycarbonate
PDMS	Polydimethylsiloxane
PEEK	Polyetheretherketone
PEI	Polyetherimide
PET	Polyethylene Terephthalate
PFA	Perfluoroalkoxy
PL	Power Law
PML	Porous Medium Layer
PMMA	Polymethylmethacrylate
POM	Polyoxymethylene
PP	Polypropylene
PPE	Polyphenylene Ether
PS	Polystyrene
PSU	Polysulfone
PVT	Pressure Volume Temperature
SBR	Styrene Butadiene Rubber
SBS	Styrene Butadiene Styrene
SE	Standard Error
SIMPLER	Semi-Implicit Method for Pressure-Linked Equations Revised
VOF	Volume of Fluid

LIST OF SYMBOLS

A_r	Flow area of the rougher half of the molded part (mm^2)
A_s	Flow area of the smoother half of the molded part (mm^2)
A_t	Total flow area of the molded part (mm^2)
C_p	Specific heat (J/Kg.K)
d	Diameter (mm)
F	Fractional volume function
H	Height (mm)
H_{app}	Height of mold cavity determined in practical measurement
H_{eff}	Effective height of mold cavity
h	Heaviside function
k	The ratio of flow area of the rougher half to total flow area of the molded part
M_c	Current calculated mass
M_{cor}	Mass correction term
M_o	Original input mass
P	Pressure (Bar)
PL	A percentage value defined to control the inlet velocity iterations
R_a	The average roughness measured in two dimensions (μm)
R_h	The height of roughness elements (μm)
S_a	The average roughness measured in three dimensions (μm)
S_ϕ	Source term
T	Temperature (K)
T_g	Glass transition temperature (K)

List of Symbols

T_{melt}	Temperature of polymer melt at the inlet (K)
T_{mold}	Temperature of the cavity wall (K)
t	time (s)
t'	Pseudo-time used in the re-distancing level set equation
t''	Pseudo-time used in the mass correction procedure
U	Average velocity (m/s)
U_{in}	Velocity at the inlet (m/s)
Vol	Volume of polymer melt (mm^3)
α	Material properties such as density and viscosity
β	The percentage of U_{in}
$\dot{\gamma}$	Shear rate (s^{-1})
Δd	The distance between the mean line of the rougher half and that of the smoother half (mm)
δ	Effective roughness height of the roughness layer (mm)
ε	Factor of the grid spacing
η	Viscosity (Pa.s)
η_0	Viscosity at zero shear rate (Pa.s)
θ	The ratio of the volume occupied by polymer melt to the volume occupied by mold material
κ	Thermal conductivity (W/m.K)
λ_0	Spacing parameter for the two dimensional homogenous roughness profiles
λ_1	Shape parameter for the two dimensional homogenous roughness profiles
ξ	Re-distance function in the level set method

List of Symbols

ρ	Density (kg/m^3)
σ	Surface tension (N/m)
Γ_Φ	Diffusive coefficient
τ	Shear stress (N/m^2)
Φ	Variable such as velocity, temperature, level set function, etc.
φ	Distance function in the level set method
φ_{ref}	Distance function of the reference phase
ω	Dynamic contact angle for surface tension

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Chapter 1 Introduction

In recent years, polymer based micro devices have been extensively used in areas such as medical technology, biotechnology, optics, telecommunication and fluidics. Compared with other materials such as silicon and metal, polymer can offer some unique physical and chemical properties which are desirable in some applications.

Injection molding is one of the most common processes for cost-effective mass production of plastic micro parts. Although the injection molding process is simple, there is however a complex interaction between material properties, processing conditions and molding geometry. The combination of these parameters determines the final quality of the plastic parts. It is this complexity that necessitates the development of simulation software to model the process. Compared with conventional (or macro) molding, micro injection molding normally requires higher injection pressure, injection rate and mold temperature, in order to achieve good quality parts. In addition, evacuation tools are usually needed to avoid short shot and degradation of polymer material caused by the compression of entrapped air. Many researchers have carried out extensive numerical and experimental analysis on the optimization of the process parameters in micro injection molding. Another significant difference between conventional and micro injection molding is that micro scale factors, such as viscous dissipation and cavity surface roughness, which are insignificant in conventional molding, may play an important role in micro molding. However, systematic investigation on the polymer filling of a micro-cavity mold of different surface roughness is lacking.

For cavity roughness, when dimensions of the part, and thus the mold cavity, are small, effects of cavity roughness may become significant as the roughness will affect

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the volume of the cavity and the heat transfer between the polymer melt and the mold. Although the roughness effects in micro injection molding were mentioned in some research, they were not investigated systematically. Thus, the motivation of this research is to investigate the filling of polymer melt into a micro-thickness cavity mold of various surface roughness.

1.1 Objective of work

The objective of this research is to investigate the effects of surface roughness on the filling of polymer melt into a micro-thickness cavity mold. In order to achieve the objective, we focused on the followings:

1. Mathematical modeling of cavity surface roughness.
2. Experimental investigations of polymer filling into a disk-shaped micro-thickness cavity mold. The effects of different roughness on the filling of the cavity are to be demonstrated by using two semicircular halves of the round core insert, with the two halves having different surface roughness.
3. Development of numerical procedures to simulate the filling of the polymer melt into cavities of different surface roughness. The numerical procedure should take into consideration the effects of surface roughness such as the differences in thermal conductivity and effective cavity volumes for different surface roughness.
4. Validation of the roughness model and the numerical procedures by comparing quantities measured experimentally to numerically predicted results.
5. Further exploration of the effects of surface roughness through numerical simulation on quantities not easily measured experimentally.

1.2 Methodology of work

Based on literature review, the possible effects of cavity roughness on the flow of polymer melt in micro injection molding were identified, i.e., the effective volume of mold cavity and the heat transfer between the polymer melt and the mold. As illustrated in Figure 1.1, to consider the roughness effect on the effective volume of the mold cavity, effective wall and effective dimensions were defined (e.g., the effective thickness) to represent the geometry of the cavity, such that the cavities with the same effective dimensions will have the same cavity volume. To consider the roughness effect on heat transfer between polymer melt and the mold, several two-dimensional and three-dimensional homogenous roughness profiles were proposed to represent the physical surface roughness. A mathematical formulation was then presented to model the thermal conductivity and heat capacity of the effective roughness layer, which has the homogenous roughness profile. The thermal conductivity and heat capacity of the effective roughness layer are determined by the effective roughness height (δ) and the volume fraction parameter (θ), which is defined as the ratio of the volume occupied by the polymer melt to the volume occupied by the mold material.

Figure 1.1 Polymer melt flow in the cavity with surface roughness

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The effects of different roughness on the filling of the cavity were conclusively demonstrated by using four round core inserts, where each insert consists of two semicircular halves of different roughness. Each core insert was machined and used to form the core wall of the cavity while keeping the cavity wall fixed. The significance of roughness effects was quantitatively represented by the ratio of the flow area on the rougher half to the flow area of the entire molded part. The significance of roughness effects for different mold and melt temperatures was investigated with the aid of the two-sample t test. The dependence of roughness effects on roughness magnitude and cavity thickness was also demonstrated.

For numerical investigations of the roughness effects, a numerical procedure, which utilizes the finite volume and the level set methods, and integrates the proposed roughness model, was developed to simulate the axisymmetric filling of polymer melt into a thin circular cavity. The non-Newtonian viscosity of the polymer melt was modeled using the Cross-WLF law. The variation in polymer density with temperature and pressure was taken into account by using the modified two-domain Tait PVT model. Moreover, the variation in the specific heat of polymer with temperature was also considered. This numerical procedure was then extended to simulate the pseudo-axisymmetric filling flow encountered in the experiments by using a newly proposed inlet-velocity iteration approach. The partial differential equations were solved using the finite volume method. The coupling between the continuity and momentum equations was handled using the SIMPLER algorithm. The resulting algebraic equations were solved using the TriDiagonal Matrix Algorithm.

The proposed numerical procedures and the roughness model were validated by comparing the numerically predicted results with the experimentally measured and analytical data. The numerical procedure for the axisymmetric polymer melt flow was

validated by comparing its numerically predicted results of cavity pressure versus time with the experimentally measured data. Subsequently, the numerically predicted results of average filling flow length versus time were compared with both experimental and analytical data. For further validation, the numerical results of fully developed Newtonian and non-Newtonian modified power law flows were also compared with analytical results. To validate the proposed roughness model and the numerical procedure for the pseudo-axisymmetric polymer flow encountered in the experiments, for each core insert, the numerically predicted results of flow area development on the rougher half versus the increasing total flow area of the molded part were compared with the experimental data. The numerically predicted k values were also compared with those obtained from the experiments.

Finally, the roughness effects on the quantities not easily measured experimentally were further explored by using the proposed numerical procedures. For filling of the cavity having different roughness on its two halves, the roughness effects on the inlet-velocity development on the two halves, as well as the roughness effects for different cavity thicknesses and injection velocities, were investigated. For filling of the cavity of uniform roughness, the roughness effects on the flow profiles of temperature, velocity, viscosity, shear rate, as well as cavity pressure, were studied.

1.3 Contributions

Based on our knowledge, it is the first piece of research work that mathematically models and systematically investigates the roughness effects on cavity filling in plastic micro injection molding (H. L. Zhang et al., 2007a, 2007b, 2008). Effective dimensions were proposed to represent the geometry of mold cavity in the analysis of micro injection molding as opposed to the dimensions used in a conventional analysis. The two and three dimensional homogenous roughness profiles were proposed to

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represent the physical surface roughness. A simple and effective mathematical model for thermal conductivity and heat capacity of the effective roughness layer was proposed with consideration of the effective roughness height (δ) and the volume fraction parameter (θ) (H. L. Zhang et al., 2007a). The effects of different roughness on the filling of the cavity were conclusively demonstrated by using two semicircular halves of the round core insert (H. L. Zhang et al., 2007b, 2008). Two effective numerical procedures were developed for numerical investigations of roughness effects (H. L. Zhang et al., 2006; H. L. Zhang et al., 2007a, 2007c). The observations obtained from the experiments and numerical simulations provide insights on the roughness effects in plastic micro injection molding.

Chapter 2 Literature review

This chapter firstly introduces the typical process of micro injection molding, the fabrication methods for micro mold inserts and the polymer materials widely used in micro injection molding. Secondly, the process parameters, such as mold and melt temperatures, injection rate, injection pressure, holding time and cooling rate, as well as their importance for injection molding, are summarized. The necessity of evacuation and heating components in some operations is highlighted. Thirdly, the micro-factors that are negligible in conventional injection molding but may be significant in micro injection molding, such as viscous dissipation, surface tension, wall slip and mold surface roughness, are evaluated and discussed. Fourthly, the typical interface capturing/tracking techniques and numerical methods for the solution of the governing equations are described. Their advantages and disadvantages are summarized. Finally, the viscosity models for polymer melt flow are summarized and discussed.

2.1 Introduction

Polymer is an important material for mechanical engineering applications. It has many advantages as compared to other materials such as silicon and metal. Firstly, polymer is cheaper. Secondly, there are a wide variety of polymers, some of which can offer unique physical and chemical properties that are not available in other materials.

Polymer based micro devices have been used extensively in areas such as medical technology, biotechnology, optics, telecommunication and fluidics. Examples include clip and bearing caps, glucose and blood pressure sensors, biological micro reactors, optical switches, fiber connectors, micro motors and gears, micro pumps and valves, etc. (Heckele & Schomburg, 2004; Heim & Potente, 2001; S. W. Kim & Turng, 2004;

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Lorenz et al., 1998; Yu et al., 2002). Three definitions can outline the main features of the “micro” parts: (1) the mass of the part is less than a few milligrammes; (2) the part contains dimensions with tolerances in the micrometer range; (3) a product has regions containing details with dimensions of the order of micrometer (Martyn et al., 2004).

Injection molding is one of the most common processes for cost effective mass production of micro plastic parts. A typical micro injection molding process includes the following steps: (1) the mold, equipped with a mold insert containing micro features, is closed, evacuated using a vacuum pump, and heated above a specific temperature; (2) an injection unit heats the polymer melt and pushes the viscous melt into the mold cavity; (3) the mold and the melt are cooled and the part is demolded from the mold cavity. Figure 2.1 demonstrates the injection molding process (Heckele & Schomburg, 2004).

Figure 2.1 Typical process of micro injection molding

In injection molding, mold temperature is usually set lower than the melt temperature to reduce the process cycle time. The non-isothermal nature of the process causes laminar fountain flow, i.e., fluid particles that approach the flow front from the upstream core of the flow are diverted towards the wall (Rose, 1961) and frozen layer forms at the cavity as a result of conductive cooling (Malloy, 1994).

Figure 2.2 shows the flow pattern of filling polymer melt into a channel between parallel plates (Potsch & Michaeli, 1995). Due to the fountain phenomenon, a transverse velocity component exists, which leads to the swelling of the melt front. The fountain effects are important for injection molding. It may significantly influence the micro-structure of the molded parts such as the molecule orientation in thermoplastic, the fiber orientation in fiber filled thermoplastic and the degree of cure in thermoset (R. Y. Chang & Yang, 2001). Moreover, it is one of the causes for the formation of flow marks (Yokoi et al., 2002)

Figure 2.2 Flow pattern in a channel between parallel plates

Figure 2.3 shows a typical development of cavity pressure at different stages in an injection cycle:

$t_A - t_B$: Filling

$t_B - t_C$: Cavity pressure increases dramatically due to complete filling

$t_C - t_D$: Holding

$t_D - t_E$: Holding switch

$t_E - t_F$: Cooling

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Figure 2.3 Cavity pressure at different injection stages

Heat transfer at the filling stage involves convection of filling melt, conduction between melt and mold, and viscous heating due to the deformation of the melt as it flows in the cavity (Kennedy, 1995).

In micro injection molding, when the dimensions of the part, and thus the mold cavity becomes small, micro-scale factors such as viscous dissipation, surface tension, wall-slip and mold surface roughness, which are negligible in conventional injection molding, may play an important role in the flow behavior of polymer melt (Kleinstreuer & Koo, 2004; Li, 2001). Ignoring them in the analysis of micro injection molding may lead to significant inaccuracy.

This chapter reviews previous related work on the injection molding of micro parts and micro structures, including fabrication of micro molding inserts, and the polymer materials widely used in micro injection molding. Also included are process parameters, common defects and their formation causes, factors that are normally neglected in the analysis of conventional injection molding but may become significant in micro injection molding, numerical techniques for the simulation of injection molding and the viscosity models for polymer melts.

2.2 Fabrication of micro molding inserts

Micro mold inserts, which are produced with the aid of ultra precision processes, are usually used to provide micro structures of the molded parts. The micro mold insert is attached to standard molds similar to conventional injection molding (Kemmann & Weber, 2001). It should have smooth side walls to enable good part replication, ease of demolding, and to maintain the tolerance in the micro structures to be molded. Furthermore, the material for the mold insert should be hard but ductile enough to last for many molding cycles and to withstand lateral and normal forces during injection molding (Heckele & Schomburg, 2004; Yu et al., 2002).

There are several techniques available to fabricate the micro mold inserts, e.g., etching, micro-machining, LIGA or LIGA-like, laser ablation, high precision electro-discharge machining (EDM), etc. The technique selected for the fabrication of micro inserts depends on product requirements, e.g., dimensions of the microstructure, accuracy and fabrication cost (Weber & Ehrfeld, 1998). Table 2.1 gives a summary of the different fabrication methods for micro mold inserts (Rotting et al., 2002).

Table 2.1 Summary of different fabrication methods for micro mold inserts
(++ very good, + good, 0 moderate, - bad)

Technology	Choice of geometry	Minimum feature size	Lifetime	Cost	Availability
Wet silicon etching	-	+	+	+	++
Dry silicon etching	+	++	-	0	+
Optical lithography & electroforming	+	++	+	0	0
Laser ablation & electroforming	++	+	+	-	-
LIGA	+	++	+	-	-
Mechanical micro-machining	+	0	++	-	-
Micro-EDM	-	0	++	-	-

2.3 Polymers for micro injection molding

A number of polymer materials have successfully been used for micro injection molding, including not only standard polymers such as PA, PS, PSU, PMMA, POM, PC, PP and COC, but also plastics with high mechanical strength and thermal stability (i.e., the ability of a material to maintain the required properties such as strength, toughness, or elasticity at a given temperature (MacCallum, 1989)) like PEEK, and PET as well as plastics with high chemical resistibility like PFA (Heckele & Schomburg, 2004). In some applications, the choice of materials will significantly affect the quality of the molded parts as well as other properties such as chemical and mechanical properties. Therefore, an appropriate polymer should be selected for specific application and molding conditions to reduce the production cost and shorten the molding cycle time. Shen et al. (2002) studied injection molding of a micro gear with different polymers (i.e. PP, PA, and POM) through numerical simulation and pointed out that different materials should be selected depending on the required optimal conditions. Monkkonen et al. (2002) investigated the molding of micro features with five different amorphous plastic materials (i.e. PC, SBS, PMMA, MABS, and COC) through experiment and found that great differences between the molded materials emerged when the aspect-ratio of the molded part was increased to 2:1.

2.4 Process parameters

Correct process parameters are important for producing high quality molded parts. These parameters include injection pressure, injection rate, melt temperature, mold temperature, holding pressure and time, and cooling time or rate. The optimization of process parameters has been extensively investigated by many researchers. Moreover, the molding machine also has significant influence in the part quality and repeatability (Kelly et al., 2005).

2.4.1 Mold and melt temperatures

Mold and melt temperatures are important parameters in the filling stage of micro injection molding. A higher melt temperature will lead to a lower viscosity of polymer melt, and thus facilitate cavity filling (Monkkonen et al., 2002). Furthermore, melt temperature influences the physical properties of polymer such as specific volume and specific heat. Figure 2.4 illustrates the pressure-volume-temperature (PVT) diagram of polypropylene (PP) (Sato et al., 1997) and the specific heat of polyethylene terephthalate (PET) at different melt temperature (Sridhar & Narh, 2000). It can be observed that the specific volume increases with an increase in temperature and with a decrease in pressure. It can also be observed that the specific heat is temperature dependent and may change steeply within a certain temperature range. The mold temperature influences the solidification speed of polymer melt. A higher mold temperature will prevent melt solidification near the mold wall during cavity filling, and thus prevent the occurrence of short shot. However, higher melt and mold temperatures will increase cooling time and thus increase injection cycle time and therefore reduce production efficiency.

(a)

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(b)

Figure 2.4 Temperature effect on physical properties of polymer melt: (a) pressure-volume-temperature diagram of PP, (b) specific heat diagram of PET

Su et al. (2004) investigated the replication of micro-structures in plastic injection molding. Both simulation and experimental results revealed that mold temperature is a key factor that decisively determines the quality of the molded micro-structures. For an amorphous polymer (e.g., PC), when the mold temperature was 30K to 40K higher than its glass transition temperature, high quality micro-structures can be obtained. Shen et al. (2002) studied the optimization of process parameters for injection molding of a micro gear with different polymers using numerical simulation and Taguchi technique. It was also observed that mold temperature is the most important process parameter and it should be set higher than the glass transition temperature of the polymer material. If mold temperature is not high enough, i.e., below or just a little higher than the glass transition temperature of the polymer, injection short shot may occur even if the melt temperature and injection pressure were set at high values. Yu et al. (2002) carried out numerical and experimental investigations of molding of thin plates with micro features. The importance of mold temperature for mold filling was also identified.

However, it should be pointed out that different polymers demonstrate different sensitivity to mold temperature changes due to their different thermal properties. Sha et al. (2006) performed experiment to investigate the factors affecting the achievable aspect ratios of micro features replicated in PP, ABS and POM. It was observed that an increase in mold temperature leads to a significant improvement of melt flow and achievable aspect ratios only for POM. For PP and ABS, an increase in mold temperature does not have a significant effect on the filling of micro features. Therefore, mold temperature should be applied selectively for improving the filling of polymer melt into micro cavities.

2.4.2 Injection rate

Injection rate defines the volume of polymer melt injected in the mold in a unit time. It is a control parameter at the filling stage. High injection rate will shorten the filling time and thus solidification time during cavity filling when the mold temperature is lower than the glass transition temperature of the polymer. Moreover, higher injection rate will result in higher shear rate, which helps to reduce viscosity through shear thinning effect, and thus benefits the filling of polymer melt. Furthermore, higher injection rate will cause the polymer melt temperature to rise due to viscous heating effect, which lowers the melt viscosity (Knights, 2001; Koh, 2003; B. Xu et al., 2003; Yu et al., 2002). Therefore, high injection rate makes it possible to achieve complete filling with relative lower injection pressure and lower mold temperature. However, too high an injection rate will lead to excessive shear rate that will cause degradation of the polymer. The injection rate should therefore be set appropriately in practice.

2.4.3 Pressure and time

Compared with conventional injection molding, micro injection molding needs higher injection pressure to push the polymer melt through tiny nozzles and flow channels at

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the filling stage (Knights, 2001). After the filling stage, the molding machine switches to holding/packing stage and additional polymer material is packed into the mold cavities at a high pressure to compensate for the material shrinkage caused by cooling and solidification of the polymer melt.

Holding pressure and holding time also have significant effects on the quality of the molded parts. Inappropriate holding pressure and holding time may result in large shrinkage, flash, inaccurate dimensions, and residual stresses of molded parts. Normally, high hold pressure and long holding time provide better replication of parts by eliminating material shrinkage, but they also build in more residual stresses (Huang & Tai, 2001; Yu et al., 2002).

Cooling time (or rate) is another important factor for the build-up of residual stress in plastic parts. High cooling rate typically result in high residual stress. This residual stress can affect dimensional stability of a molded part, its strength, as well as its optical and chemical properties. Therefore, appropriate cooling rate should be selected to achieve minimal residual stress (Daly et al., 1998).

Another factor that has an effect on the part quality is holding profile. Chen and Gao (2003) investigated the influences of different types of holding profiles (i.e., constant, ramp and step change) in part weight, flash, thickness distribution and evenness by using different thin cavity mold inserts. It was observed that part evenness is greatly dependent on the type of the holding profile as well as the pressure level. The ramp-up and step-up profiles cannot produce an even part, while the ramp-down and step-down holding profiles can bring about good evenness in a part. Excessively high holding pressure at the start of the holding stage may cause part flash. Decreasing holding pressure tends to result in large shrinkage, which, however, can be eliminated by increasing the pressure level.

2.5 Evacuation and heating components

Compared with conventional injection molding, micro injection molding usually requires additional auxiliary facilities such as evacuation and heating components (Heckeles & Schomburg, 2004; Kemmann et al., 1999; Su et al., 2004). The evacuation component is used to avoid incomplete filling, as air in micro structures cannot escape quickly when polymer melt is filled in. Without evacuation, air could be trapped and compressed in a tiny cavity while being heated in a mold, which could increase the air temperature to 600°C and thermally degrade the polymer. Therefore, in some situations, air should be removed from the mold cavity right from the start of injection molding.

Heating and cooling components may also be necessary. Without heating of the mold, when polymer melt enters a micro mold cavity with relatively low temperature, heat losses and the melt freezes quickly. The frozen layer near the mold wall will prevent polymer melt from passing through the mold cavity (Huang & Tai, 2001). In addition, due to the decrease in the temperature of polymer melt, the viscosity of polymer melt will increase, further preventing melt flow. Therefore, it is necessary to use some heating devices to keep the mold temperature high enough to avoid these problems. Some researchers (Shen, 2001; Shen & Wu, 2002; Su et al., 2004) suggested that mold temperature be raised to above the glass transition temperature of the polymer material to avoid immediate solidification of polymer melt when it gets into contact with mold cavity wall. The cooling component is sometimes required for facilitating demolding and shortening the cycle time (Heckeles & Schomburg, 2004).

2.6 Demolding

Demolding is a critical step to obtain good-quality molded parts. Most problems in micro injection molding are not caused by the filling of the mold, but by demolding

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(Hecke & Schomburg, 2004). If the design of micro parts is not appropriate or molding parameters are not properly selected, the micro parts may be deformed or destroyed during demolding. Although it is possible to demold micro parts with vertical side walls, an inclination of just 2° can reduce demolding forces significantly and is even more important than the roughness of the side walls (Kemmann et al., 1999). It is also important to demold orthogonal to the substrate surface so that lateral forces, which could damage the structures, are minimized. An important factor in demolding is the shrinkage of the polymer. The demolding forces are a function of the orientation of the micro structures relative to the direction of shrinkage and the placement of critical micro structures relative to the center of shrinkage.

2.7 Molding defects

2.7.1 Shrinkage and warpage

Part shrinkage and warpage are problems frequently experienced in injection molding. Many factors can affect the shrinkage and warpage of the parts, such as the type of polymer material, the type of machine, the geometrical shape of the molded part, the design of runner systems, flow path and process parameters (Choi & Im, 1999; Huang & Tai, 2001; Weber et al., 1996; Yokoi et al., 2002).

Weber et al. (1996) performed some experiments and observed that the shrinkage and warpage of the part are material dependent. Amorphous thermoplastics are less prone to warpage than crystalline polymers. Moreover, the direction of the warpage is either negative or positive depending on the material used. Huang and Tai (2001) performed analysis of variance (ANOVA) to determine the relative significance of the factors causing warpage. It was found that packing pressure, melt temperature, mold temperature, and packing time are the significant factors. Filling time and the gate dimensions are not significant parameters. Choi and Im (1999) developed an

integrated injection molding analysis program for predicting residual stress, shrinkage, and warpage coupled with filling and post-filling stages.

2.7.2 Surface roughness of molded parts

For some precise parts such as lenses and waveguide, surface roughness is an important quality parameter. Weber (1996) investigated surface roughness of the parts molded with different polymer materials, i.e., liquid crystalline (LCP), semi crystalline (PBT, PEEK and POM) and amorphous (PPE and PEI). The experimental results indicated that the parts molded with semi-crystalline polymer have the smallest roughness as well as the smallest variation. Yoshii and Kuramoto (1993) studied the relationship between molding conditions and surface roughness of parts molded with polycarbonate (PC). The flow marks formed due to the cooling of molten polymer as it flows, particularly the cooling of polymer at the advancing front was investigated. It was found that low melt and mold temperatures and low injection rate will result in higher surface roughness of the molded parts. Optimization of molding conditions can help achieve smooth surfaces.

2.7.3 Flow marks

Prevention of the occurrence of flow marks is critical in some applications such as the production of optical lenses, substrates for optical discs and mirrors. The formation of flow marks is because molten polymer near the mold wall at its advancing front is cooled to its non-flow temperature before it comes into contact with the mold wall (Yoshii & Kuramoto, 1993). Figure 2.5 shows the typical micro flow marks in injection molding. Yoshii et al. (1996) investigated the process parameters affecting the occurrence of micro flow marks by heat transfer analysis. It was found that melt and mold temperatures and injection rate are the most important factors in the

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formation of micro flow marks. Higher melt and mold temperatures and injection rate will decrease the depth of flow marks.

Figure 2.5 Typical micro flow marks in injection molding

2.8 Effects of micro-scale factors

There has been evidence indicating that polymeric flow and heat transfer characteristics in micro channels are remarkably different from those in conventional size channels (Li, 2001; Qu et al., 2000; Yao & Kim, 2002; Yu et al., 2004). This section evaluates the micro-scale factors that are normally negligible in conventional injection molding but may be important in micro injection molding, including viscous dissipation, surface tension, wall slip and mold surface roughness.

2.8.1 Viscous dissipation

Viscous dissipation is caused by the shear heating effect. It is normally negligible in conventional injection molding. However, when the dimensions of mold cavity become small (e.g., in the order of micrometer), it may lead to significant increase in melt flow temperature, and thus reducing the viscosity of polymer melt. Koo and Kleinstreuer (2004) studied the effects of viscous dissipation on temperature field

with the aid of dimensional analysis and numerical simulations. It was observed that viscous dissipation is a strong function of the channel aspect ratio, Reynolds number, Eckert number, Prandtl number and conduit hydraulic diameter. Ignoring viscous dissipation could significantly affect simulation accuracy. Xu et al. (2003) investigated the effects of viscous dissipation on water flow in micro channels. It was pointed out that the effect of viscous dissipation presents itself in different levels. In some cases, it is significant, but in other cases, it is small enough to be negligible. The significance of viscous dissipation in flows can be analyzed based on the temperature rise in the inlet and the outlet.

2.8.2 Surface tension

Surface tension is a result of a microscopic, localized surface force which exerts itself at the interface between two fluids and has components in both the normal and tangential directions, dependent upon the curvature of the free surface (Abdullah & Gethin, 1998). Figure 2.6 shows a schematic diagram of a pressure-driven filling flow.

Figure 2.6 Schematic diagram of a pressure-driven filling flow from: (a) side view, (b) top view

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The pressure drop caused by surface tension can be evaluated using Yang-Laplace equation (D. S. Kim et al., 2002)

$$\Delta p = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \quad (2.1)$$

where, σ is the surface tension of the fluid, and R_1 and R_2 are the principal radii of curvature of flow front shape. When the pressure of air in the channel is assumed to be zero, the pressure imposed on the flow front can be calculated as

$$p = -2\sigma \cos \omega \left(\frac{1}{W} + \frac{1}{H} \right) \quad (2.2)$$

where, W and H are the width and height of the channel respectively, and ω is the dynamic contact angle between the fluid and the channel wall. For a thin cavity geometry ($W \gg H$), the surface tension effect in the width direction could be neglected in comparison with that in the thickness direction since $1/R_1 \gg 1/R_2$. As a result, the pressure on the flow front can be calculated as

$$p = -\frac{2\sigma \cos \omega}{H} \quad (2.3)$$

where, H is the thickness for parallel plates, and radii for circular pipes.

In some applications, the effect of surface tension on flow in micro channels may be significant (D. S. Kim et al., 2002). However, it is not significant in micro injection molding. As the surface tension of polymer melt is normally much less than 1N/m (e.g., about 0.033N/m for polystyrene), it can be estimated that the maximum pressure drop caused by surface tension in a 1 μ m height channel is approximately 2000Pa for a flow with $\sigma=1$ N/m. This pressure drop is very small as compared to the typical pressure involved in injection molding that typically falls between several MPa to hundreds MPa (Yao & Kim, 2002).

2.8.3 Wall slip

In the analysis of conventional injection molding, it is usually assumed that the relative velocity between polymer melt and the solid wall is zero, i.e., no wall-slip occurs (Kennedy, 1995). This assumption is supported by experimental evidence at macro scales. However, it is yet to be justified at micro scales. Various studies (Awati et al., 2000; Henson & Mackay, 1995; Piau & Agassant, 1996; Yao & Kim, 2002) indicated that the non-slip boundary condition may not be applied to the polymer melt flow in micro channels. The polymer melts may slip over solid surfaces when the wall shear stress exceeds a critical value. Wall slip can be explained by the polymer viscoelastic characteristics and microscale viscosity. Hervet and Leger (2003) conducted direct measurements of the interfacial velocity by use of the near field laser velocimetry (NFLV) technique. Their experiment clearly demonstrated that the polymer fluids can exhibit flow with slip at the smooth wall, and the non-slip boundary condition postulated in most hydrodynamics investigations may not be fulfilled. To consider wall slip during the filling of polymer melt, Yao et al. (2002) proposed a modified power-law slip model. In the simulation, mold temperature was set the same as melt temperature (i.e., 530K). The numerical results showed that when wall-slip is considered, the predicted pressure is 20% - 30% higher than that otherwise. Wall slip for polymer melt (i.e., PS) flowing through micro-channels was also investigated by Chien et al. (2005). The mold temperature was set the same as melt temperature in the experiment. It was observed that the ratio of slip velocity to mean velocity increases with decreasing size of the micro-channels and the wall slip seems to play a dominant role when melt flows through micro-channels and would result in a greater percentage in apparent viscosity reduction when the size of the micro-channel

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was decreased. Moreover, it was found that wall-slip becomes more significant when the melt temperature increases.

To account for wall-slip during mold filling, two models have been proposed. The modified power-law slip model was proposed by Rosenbaum & Hatzikiriakos (1997):

$$u_s = \frac{a}{1 + (\tau_c / \tau_w)^j} \tau_w^i \quad (2.4)$$

where, τ_c and τ_w are critical shear stress and wall shear stress respectively, j is a large power (e.g., 10) such that the factor $1/[1+(\tau_c/\tau_w)^j]$ basically zeros the slip velocity for stresses less than τ_c and becomes about one for shear stress slightly greater than τ_c , i is a power-law index, and “a” is a scalar coefficient.

Robin boundary condition can also be used to consider the wall slip (Haagh & Vosse, 1998; Medale & Jaeger, 1997), which was written as:

$$au_t + \tau_t = 0 \quad (2.5)$$

where, u_t is the tangential velocity, τ_t is the shear stress, and “a” is “Robin penalty parameter”, which scales with η/H .

In the investigations of wall-slip as mentioned above, the mold temperature was set the same as the melt temperature. Most importantly, the surface roughness in the channel was small or negligible. However, the occurrence of wall-slip were seldom reported when the mold temperature was lower than the melt temperature or when the surface roughness of the channel was high. Conversely, Smialek and Simpson (1998) observed that the increase of cavity surface roughness can prevent slippage during the filling stage. Griffiths (2007) pointed out that wall-slip was not observed during filling of polymer melt into the cavity with considerable surface roughness. Hervet and Leger (2003) also mentioned that the surface roughness have effect on the level of wall slip. Therefore, in this thesis, considering the fact that the mold temperature is

normally lower than the melt temperature, and the surface roughness is high, it is reasonable to assume that wall-slip does not occur.

2.8.4 Cavity surface roughness

With the decrease of dimensions for the mold cavity, cavity surface roughness may have a significant effect on cavity filling. With an increase in surface roughness, the contact area between polymer melt and mold wall increases, therefore, heat transfer between them is enhanced as heat transfer rate is proportional to the contacted surface area (Theilade et al., 2003). Although not many investigations of roughness effects on micro injection molding were performed, many researchers have studied the roughness effects on fluid flow in micro channels, conduits and tubes. Hu et al. (2003) studied the pressure-driven liquid flow in microchannels with rough rectangular prism elements on the surfaces. The three-dimensional numerical solution showed significant effects of surface roughness in terms of rough elements' height, size, spacing, and the channel height on both flow velocity distribution and pressure drop. Croce and Agaro (2004) investigated the roughness effect on heat transfer and pressure loss of the steady-state flow in microscale tubes and channels through a finite element code. Surface roughness was explicitly modeled through a set of random generated peaks along the ideal smooth surface. Different peak shapes and distributions were taken into consideration. A significant increase in Poiseuille number (i.e., the product of friction factor and Reynolds number) was detected while the effect of roughness on heat transfer rate was small and highly dependent on the tube shape. Koo and Kleistreuer (2003; 2005) treated surface roughness as a porous medium layer (PML) and performed analysis based on the available PML theory. It was found that the roughness effect on heat transfer is dependent on the Reynolds

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number of the flow. Mala and Li (1999), as well as Qu et al. (2000), accounted for roughness effect by using a roughness dependent viscosity model.

In these prior investigations, the fluid was normally Newtonian. Moreover, the Reynolds number of the flow were much higher than that encountered in micro injection molding. Therefore, a good insight on the roughness effects in micro injection molding cannot be obtained based on these previous work.

For injection molding, the surface roughness effects have been investigated by only a few researchers. Smialek and Simpson (1998) found that an increase in cavity surface roughness can prevent slippage during the filling stage, and lead to a more appealing surface for the molded parts. Griffiths et al. (2007) investigated the flow behavior of the polymer melt in micro cavities with different surface roughness levels through experiment and Taguchi technique. Polypropylene (PP), acrylonitrile butadiene styrene (ABS) and polycarbonate (PC) were selected for the experiments. The experimental results showed that mold surface roughness has influence in the level of turbulence in the melt flow. However, its effect on the slip-stick phenomena was not observed. Theilade et al. (2003) performed experiment to study the effects of mold surface roughness on linear part shrinkage through injection molding of polystyrene (PS) and polypropylene (PP). A two-cavity tool, each cavity of which has different surface topographies, was used. The experimental results showed that a rough surface yields a lower linear shrinkage for either PP or PS.

2.9 Duplication of micro features

Molding of micro features is one of the most important technological issues addressed recently in the micro injection molding community. The significance of process parameters for precise duplication of micro features was investigated by many researchers. Yu et al. (2002) found that the injection rate and mold temperature

greatly affect the replication accuracy of the micro structures on the mold inserts. Sha et al. (2006) investigated the effects of five process parameters (i.e., barrel temperature, mold temperature, injection rate, holding pressure and presence of evacuation) and one size factor (i.e., the sizes of micro features) on the achievable aspect ratios, and the role these factors play in producing micro components in different polymer materials. It was observed that the melt temperature and injection rate are the key factors affecting the aspect ratios achievable for all three materials investigated, namely PP, ABS and POM. However, the effect of mold temperature depends on the polymer material used in injection molding. The use of evacuation could increase the replication quality. However, it could also reduce the surface temperature in micro channels, which could have a detrimental effect on the melt flow. Xu et al. (2005) carried out experimental and numerical studies of the filling length of micro-features in micro injection molding. The mold/melt heat transfer coefficient was found to be a critical factor in determining the filling length. The use of a local heat transfer coefficient in the simulation could provide a much better agreement than a constant heat transfer coefficient. Young (2007) presented a simplified analytical model to investigate the effects of mold temperature, injection rate, heat transfer coefficient and micro-channel dimension on the filling length. It was observed that the filling length is strongly dependent on the value of the heat transfer coefficient. A lower value of heat transfer coefficient will result in a larger filling length. For a constant heat transfer coefficient, a higher mold temperature will result in a longer filling length.

2.10 Simulation techniques

Thus far, several commercial packages are available to assist in the design of plastic products. Among them, Moldflow Plastics Insight (MPI) is widely used in industries

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for in-depth simulations to validate part and mold designs. It allows analyzing CAD solid models of thin-walled parts directly. Moreover, it allows three-dimensional flow simulations on parts that tend to be very thick and solid in nature as well as those that have extreme changes from thin to thick sections. However, MPI is mainly for the analysis of conventional injection molding. The micro-scale factors that may be significant in micro injection molding were not taken into consideration (Piotter et al., 2002). Therefore, it is not applicable for micro injection molding. To conduct numerical analysis of micro injection molding, it is necessary to develop in-house codes that can account for the micro-scale factors such as mold surface roughness.

2.10.1 Techniques for capturing/tracking flow front

Numerical simulations of mold filling especially have difficulty to accurately predict the advancing polymer-air interface of complex topology. Much effort has been devoted to developing numerical models to predict the moving polymer-air interface in the last two decades (R. Y. Chang & Yang, 2001). In general, two different formulations can be employed for this purpose, i.e., Lagrangian formulation and Eulerian formulation, each of which leads to very different numerical models. Simulation of flow front advancement using Lagrangian formulation is called interface “tracking”, and that using Eulerian formulation is called interface “capturing”.

In the Lagrangian formulation or interface tracking technique, the computational space grid deforms as the flow field calculation proceeds such that a line of nodes always coincides with the interface. In this formulation, the moving interface is sharply defined and it is easy to impose the necessary boundary conditions. However, Lagrangian methods require mesh refinement or re-meshing for large deformations of the moving interface, which is computational intensive. Furthermore, the Lagrangian

approach becomes difficult to implement when the finite element method is used (Khayat et al., 2000; J. Zhang & Khayat, 2001).

In the Eulerian formulation or interface capturing technique, the grid points remain stationary or move in a predetermined manner. Typically, the fluid moves in and out of the computational cells. The moving interface is not explicitly tracked, but implicitly captured by solving a transport equation of a scalar, which is used to identify the interface. The Eulerian methods can handle arbitrarily large interface deformations without loss of accuracy. Its main disadvantage, however, is the lack of sharp definition of the moving interface, and thus leading to difficulty in imposing the kinematic and dynamic boundary conditions on the moving interface (R. Y. Chang & Yang, 2001; Hetu et al., 1998; Medale & Jaeger, 1997). Figure 2.7 shows the schematic diagrams of Lagrangian and Eulerian formulations (Voller & Peng, 1995).

Figure 2.7 Formulations for interface tracking/capturing: (a) Lagrangian, (b) Eulerian

As the Eulerian methods have been widely used for modeling the mold filling problems due to their topological robustness and computational efficiency, the interface capturing techniques based on the Eulerian methods are discussed in more details, including the marker and cell (MAC) method (Harlow & Welch, 1965), the

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volume-of-fluid (VOF) method (Hirt & Nichols, 1981) and the level set method (Osher & Sethian, 1988).

The MAC method uses particles with no mass nor energy, distributed in the whole fluid volume to trace the free surface (see Figure 2.8). Cells with marker particles and no empty neighbors are considered to be filled with fluid. The markers do not track interface directly, but instead track fluid volumes. Interfaces are simply the boundaries of the volumes, and in this sense interfaces may appear, merge or disappear as volumes break apart or coalesce. One great advantage of the MAC method is its ability to handle complex and general situations as breaking interface, dam breaking, splash, or fluid detachment. However, this method is computationally prohibitive for large scale three-dimensional applications because it needs to use a large number of continually redistributed particles in order to capture the free surface shape properly. Moreover, it can lead to mass dissipation, especially with stable fluid style advection. Furthermore, even with a large number of markers, it is difficult to determine the orientation of the surface in a cell. Therefore, the MAC method is primarily used for two-dimensional simulations (M. S. Kim & Lee, 2003).

Figure 2.8 MAC method: (a) real interface, (b) MAC representation

The Volume of Fluid (VOF) method is another interface capturing technique and perhaps the most widely adopted approach to model the mold filling problems (Rajupalem et al., 1997; Swaminathan & Voller, 1994; Voller & Peng, 1995; Yang et al., 2003). The VOF method can be applied to problems where several fluids with different densities are present. It can handle complex physical situations such as breaking surfaces, splash and fluid detachment. In the VOF method, a function F is introduced (see Eq. (2.6)). Its value is one at any point occupied by fluid and zero otherwise. The average value of F in a cell will then represent the fractional volume of the cell occupied by the fluid. In particular, $F = 1$ corresponds to cell filled with fluid, $F = 0$ to a cell with no fluid at all, and $0 < F < 1$ to cell containing the free surface. Figure 2.9 illustrates the volume fraction representation of the real interface.

$$\frac{\partial F}{\partial t} + \nabla \cdot (uF) = 0 \quad (2.6)$$

(a)

0.3	0.0	0.0	0.0
0.95	0.44	0.0	0.0
1.0	0.99	0.52	0.02
1.0	1.0	1.0	0.92

(b)

Figure 2.9 VOF method: (a) real interface, (b) volume fraction representation

One disadvantage of the VOF method is that it is difficult to accurately compute local curvatures from volume fractions due to the sharp transition of the volume fractions in regions of the interface (Sussman & Puckett, 2000). Thus, surface tension effect is difficult to take into account. Moreover, the VOF method requires the use of

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meshes with rectangle cells and it is not suitable to be utilized for complex geometry. To overcome this problem, the pseudo-concentration method (Thompson, 1986), which is based on the VOF method, was developed. Hetu et al. (1998), as well as Haagh and Vosse (1998), employed the pseudo-concentration method to capture the advancing flow front. In this method, the governing equations are solved on a fixed grid that covers the entire mold cavity so that elaborate re-meshing can be avoided. The air downstream of the polymer flow front is represented by a fictitious fluid. The main property of this fictitious fluid is that its viscosity can be set to a value at least 10^{-3} times smaller than that of polymer melt, exceeding the real value of air viscosity by several orders of magnitude. However, the contribution of the fictitious fluid to the pressure build-up in the mold cavity during filling is negligible. By using the fictitious fluid instead of air, the stability and convergence of the numerical solution can be enhanced without sacrificing significant accuracy. The pseudo-concentration method has also been used in the context of molding filling by others (Lewis et al., 1995; Medale & Jaeger, 1997).

The level set method (Osher & Sethian, 1988) was developed in recent years and has been widely used for capturing multiple-interface. In this method, a level set function, ϕ , which represents a signed distance between a point and the interface, is defined to represent fluid phases, e.g., $\phi < 0$ stands for the first phase, $\phi > 0$ for the second phase, and $\phi = 0$ for the two-phase interface. ϕ is transported by the Eq. (2.7) to capture the interface.

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (u\phi) = 0 \quad (2.7)$$

In the level set method, the fluid field is solved in the entire computational domain, without the necessity of special coding for the free boundary (i.e., the phase interface). Therefore, the level set method is efficient in describing complex interfaces

with changing topology. In addition, by incorporating the boundary conditions at the interface into governing equations, it is not necessary to locate the position of the interface separately as in VOF or MAC method. The level set method can handle complex physical situations like breaking waves, droplets, fluid detachment, etc. The curvature of the interface can be easily obtained via finite differences of the level set function, and thus surface tension can be easily included in the momentum equation. However, one disadvantage of the level set method is that discretization of the transport equation has a tendency to lose or add mass. Special consideration is therefore needed to ensure mass preservation. Sussman (2000) proposed a coupled level set and volume of fluid method to avoid mass loss. Comparable mass conservation properties as with other second order VOF advection methods were obtained.

Based on the above discussions, it can be judged that the pseudo-concentration method and the level set method are preferred to others because of their easy implementation, computational efficiency and capability for complex geometries.

2.10.2 Solution methods for governing equations

At the filling stage in injection molding, polymer melt flow is governed by the mass, momentum and energy conservation equations, which are also called governing equations (Kennedy, 1995). For a complicated geometry, to obtain the closed form analytical solution of the general governing equations, together with proper initial and boundary conditions, is impossible. Therefore, numerical solutions are always used to solve these equations.

The numerical methods generally require discretizing the entire physical geometry into finite sub-domains and the temporal domain into small time steps. Through discretization, the continuous governing equations as well as the initial and boundary

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conditions are converted into a set of discretized algebraic equations to be solved by the use of computers. Several solution methods for solving the governing equations of viscous fluid have been developed and used successfully over the years, e.g., the vorticity-stream function approach (Fromm & Harlow, 1963), the direct method (Turek, 1999), the artificial compressibility method (Chorin, 1968), the penalty method (Hughes et al., 1979), the pseudo-compressibility method (Quarteroni & Valli, 1994), the projection method (Chorin, 1968), and the pressure-correction method, i.e., the SIMPLE family of methods (Patankar & Spalding, 1972).

The vorticity-stream function approach (Fromm & Harlow, 1963), which is a non-primitive variable solution, has been a popular method when it comes to solving the two-dimensional incompressible Navier-Stokes equations. One of the major attractive features of this method is that it does not involve the solution of the pressure field. Pressure is completely eliminated by cross-differentiation of the momentum equations. Another advantage of this method is that the governing equations for stream function and vorticity constitute a second order elliptic system whose properties are well understood. Therefore, it is easy to construct numerical schemes for the solution of stream function and vorticity, which are highly robust and stable.

The direct method (Turek, 1999) obtains a coupled system of equations from direct discretization of the governing equations, and solves them by using nonlinear iteration techniques (e.g. Newton-Raphson) or predictor-corrector techniques. This method is usually computationally expensive, especially for three-dimensional applications. However, for parallel computations, it can be attractive if the number of processors used is large enough so that a direct solution of the algebraic system is possible on each processor.

The artificial compressibility method (Chorin, 1968), penalty method (Hughes et al., 1979) and Petrov-Galerkin elliptic pressure regularization (Quarteroni & Valli, 1994) were developed primarily for compressible flows.

The projection method (Chorin, 1968) and the pressure-correction method (Patankar & Spalding, 1972) are uncoupled type solutions. They separate the computation of the velocity from the computation of the pressure for solving the incompressible Navier-Stokes equations.

2.10.3 Spatial discretization techniques

Independent of each of the previous solution methods mentioned above, a discretization method has still to be chosen in order to transform the continuous problem into a discrete one. Four discretization techniques have globally gained acceptance in the CFD community, i.e., Finite Difference Method (FDM), Finite Element Method (FEM), Boundary Element Method (BEM) and Finite Volume Method (FVM). Each of these methods has its own advantages and disadvantages. Therefore, one may be preferred for certain type of process and geometry.

The FDM is a relatively simple and efficient method for solving the partial differential equations. In this method, the physical domain is discretized in the form of finite difference grids. A set of algebraic equations are generated as the derivatives of the partial differential equations are expressed by finite difference of the variable values at the grid points. When the boundary conditions are applied, the algebraic equations can be solved numerically. As a result, the approximate solution of the continuous partial differential equations is obtained (Kennedy, 1995).

The BEM only requires that the boundary or surface of the physical domain be discretized. Discretization is derived through the application of the weighted-residual method, with the weighting function taken to be the fundamental solution, and

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integrating by parts, converting the volume (surface) integral of the residual to surface (line) integrals and single-point function values. Consequently, the number of unknowns and the effort for computation and mesh generation are reduced significantly, which is the main advantage of this method. The resulting algebraic equations are dense and non-axisymmetric (Halpern & Gaver, 1994; S. W. Kim & Turng, 2004).

The FVM applies the conservation principles to a fixed control volume, and the integral forms of the governing equations are solved in the physical domain. The domain is subdivided into small control volumes, and the field variables over a control volume are evaluated either as averaged values of the variables at the centre of the control volume or as values at the faces of the control volume (S. W. Kim & Turng, 2004).

FEM has become the basis for most commercial software for structural dynamics and fluid flow simulation. This method requires discretizing the physical domain into finite elements. The element fields are expressed by shape functions and nodal values over each finite element. Using residual minimization techniques, e.g. the Galerkin method, the partial differential equations are transformed into discretized algebraic equations, which can be solved numerically when applied with boundary conditions (Kennedy, 1995).

Each of these four techniques has their own advantages and disadvantages. The FDM is simple in discretization grid construction and easy to implement in solution procedure. However, it has poor capacity in representing complex geometries due to the necessity of rectangular discretization. The BEM is more efficient in generation and modification of mesh as the BEM discretization is restricted to the boundary. However, it is inefficient for non-linear problems and therefore it is seldom used in

simulation of plastic injection molding, which involves strong non-linearity. FVM is a particular type of FDM, but has an advantage over FDM as it can be applied to highly irregular and complicated domains using arbitrary small cells. FEM has excellent flexibility in treating complex geometries and irregular boundaries. FEM has proved to be ideal for simulating mold filling processes, fiber orientation, shrinkage and warpage of thin plastic parts, although the numerical implementation of the FEM requires large memory and computing time.

Among the four techniques, the FVM and FEM are the prevailing methods used for simulation of injection molding due to their capability of handling complex geometries and non-linear problems (S. W. Kim & Turng, 2004; Yu et al., 2004).

2.10.4 Time discretization techniques

To discretize the temporal term in the governing equations, time stepping schemes are required. Time stepping schemes are usually divided into two main groups: explicit and implicit schemes. The explicit scheme allows for an arbitrary order of temporal accuracy. It is easy to implement. Moreover, the prescription of boundary condition is relatively simple. However, the time step is limited by stability constraints such as the Courant-Friedrichs-Levy (CFL) condition.

The implicit scheme can maintain stability over much larger time step. Hence, fewer time steps are required to make calculation over a given time interval. However, implicit schemes are more difficult to implement than explicit ones. Larger time steps will also result in large truncation error. Furthermore, implicit scheme requires more memory storage than explicit one.

2.11 Viscosity models

Polymer melt flow is non-Newtonian in nature. Many mathematical viscosity models have been proposed to describe its viscosity. To select the appropriate model that can

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accurately predicted the viscosity of polymer melt during mold filling, several viscosity models for polymer flow are reviewed and their capabilities are evaluated (Kennedy, 1995; Koh, 2003).

2.11.1 Power-Law (PL) model

$$\eta = m |\dot{\gamma}|^{n-1} \quad (2.8)$$

where, η is the viscosity (Pa.s), $\dot{\gamma}$ is the shear rate (s^{-1}), m and n are the fluid consistency coefficient and the flow behavior index respectively, which can be obtained by curve fitting to the experimental data. For shear-thinning fluids like polymer melt, $n < 1$.

From Eq.(2.8), the viscosity will become infinite with vanishing shear rate for shear-thinning fluid where $n < 1$, which will lead to instability in numerical simulation. This problem can be avoided by modification of Eq. (2.8) as shown below,

$$\eta = \begin{cases} \eta_0 & \dot{\gamma} < 0.01 \\ m |\dot{\gamma}|^{n-1} & \text{else} \end{cases} \quad (2.9)$$

where, η_0 is the viscosity at zero shear rate.

2.11.2 Modified Power-Law model (MPL)

$$\eta = \frac{\eta_0}{1 + \frac{\eta_0}{K} \dot{\gamma}^{1-n}} \quad (2.10)$$

where, $\dot{\gamma}$ is the shear rate and η_0 is the viscosity at zero shear rate, respectively. K and n are constants which can be obtained through curve fitting to the experimental data. MPL eliminates the limitation of the PL model through consideration of the viscosity at zero shear rates.

2.11.3 Modified Arrhenius Power Law (MAPL) model

$$\eta = \frac{\eta_0(T)}{1 + \frac{\eta_0(T)}{K} \dot{\gamma}^{1-n}} \quad (2.11)$$

$$\eta_0 = B e^{cT}$$

where, $\dot{\gamma}$ is the shear rate and η_0 is the viscosity at zero shear rate, respectively. K and n are constants. B is a structural component of viscosity, which mainly describes the effects of channel length. c is the temperature sensitivity of the polymer material.

2.11.4 Modified Cross-Arrhenius (MCA) model

$$\eta = \frac{\eta_0(T)}{1 + \left(\frac{\eta_0 \dot{\gamma}}{\tau^*} \right)^{1-n}} \quad (2.12)$$

where, τ^* is the shear stress at the transition between Newtonian and power law behavior.

2.11.5 Modified Cross (MC) model

$$\eta = \frac{\eta_0(T, P)}{1 + \left(\frac{\eta_0 \dot{\gamma}}{\tau^*} \right)^{1-n}} \quad (2.13)$$

$$\eta_0(T, P) = D_1 \exp \left\{ -\frac{A_1(T - T^*)}{A_2 + (T - T^*)} \right\}$$

$$T^* = T_g(P) = T_0 + D_3 P$$

where, T^* is the pressure-dependent glass-transition temperature. T_0 is the glass transition temperature at ambient pressure. D_3 specifies the linear pressure dependence of the glass transition temperature. n, τ^*, D_1, A_1, A_2 are constants.

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2.11.6 Cross-Exp model

$$\eta(T, \dot{\gamma}, P) = \frac{\eta_0(T, P)}{1 + (\eta_0(T, P) \cdot \dot{\gamma} / \tau^*)^{1-n}} \quad (2.14)$$

$$\eta_0(T, P) = B \cdot \exp(T_b / T) \cdot \exp(\beta P), \text{ for } T > T_g$$

$$\eta_0(T, P) = \infty, \text{ for } T < T_g$$

where, η_0 is the zero-shear-rate viscosity, $\dot{\gamma}$ is the shear rate, T is the temperature, P is the pressure, T_g is the glass transition temperature, n , τ^* , β , T_b are constants. The value of T_b , which represents the temperature sensitivity of η_0 , is a strong function of temperature.

2.11.7 Cross-WLF model

$$\eta(T, \dot{\gamma}, P) = \frac{\eta_0(T, P)}{1 + (\eta_0(T, P) \cdot \dot{\gamma} / \tau^*)^{1-n}} \quad (2.15)$$

$$\eta_0(T, P) = D_1 \cdot \exp\left\{-\frac{A_1 \cdot (T - T^*)}{A_2 + (T - T^*)}\right\}$$

$$T^*(P) = D_2 + D_3 P$$

$$A_2 = \tilde{A}_2 + D_3 P$$

where, n , τ^* , D_1 , D_2 , D_3 , A_1 and $\tilde{A}_2$ are constants.

Among the viscosity models mentioned above, the Power Law (PL) and the Modified Power Law (MPL) are not quite accurate for modeling the viscosity of polymer melt as the temperature effect on the viscosity is not taken into consideration. The MAPL model accounts for the effects of shear rate and temperature on the viscosity. However, the structural component and the temperature sensitivity parameters in the model are difficult to determine. Furthermore, pressure effect is not considered. The other viscosity models take into account the effects of shear rate, temperature and pressure on viscosity.

The MCA model is not sensitive to pressure and is therefore not applicable to micro injection molding, where high pressures are present. Conversely, the MC model is too sensitive to pressure influence, i.e., the viscosity predicted by the MC model will become very small at very high pressures, which may lead to inaccuracy and instability in numerical simulation.

Compared to the other models, the Cross-Exp and the Cross-WLF models are more accurate. However, the Cross-WLF model is superior to the Cross-Exp model as the temperature and pressure sensitivities of the zero-shear-rate viscosity are better represented. Therefore, the Cross-WLF model should be used in numerical simulation to accurately predict the non-Newtonian viscosity of polymer melt during mold filling in micro injection molding.

2.12 Concluding remarks

This chapter gave a brief review of the related research conducted in injection molding. Compared with conventional (or macro) injection molding, micro injection molding normally requires higher injection pressure, injection rate and mold temperature in order to achieve good quality parts. Evacuation tools are usually necessary to avoid short shot and degradation of polymer material due to compression of trapped air. Moreover, heating and cooling facilities are usually required.

The micro-scale factors such as viscous dissipation and cavity surface roughness which are negligible in conventional injection molding, may play an important role in micro injection molding. However, surface tension is not significant in micro injection molding. Although wall-slip was observed in some circumstances (e.g., when the mold temperature is the same as the melt temperature and the channel roughness is small), it was not observed in the filling of polymer melt into the mold cavity of high surface roughness.

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The roughness effects on fluid flow in micro conduits, tubes and channels have been investigated by some researchers. However, the fluids involved in these investigations were normally Newtonian, in steady state and with high Reynolds numbers, which is different from the polymer melt flow encountered in micro injection molding, which is non-Newtonian, transient and with low Reynolds number (in the order of 0.1). Therefore, a good insight on the roughness effects in micro injection molding cannot be obtained based on the previous investigations.

Although commercial package such as MoldFlow has been widely used for the analysis of conventional injection molding, it is not appropriate for micro injection molding as micro-factors such as mold surface roughness are not taken into consideration. It is therefore necessary to develop in-house codes to numerically investigate the effects of micro-factors in micro injection molding.

The interface tracking and capturing techniques for the prediction of advancing flow front were reviewed. To accurately predict the advancing flow front, the Eulerian formulations, especially the pseudo-concentration method and the level set method, which are based on fixed meshes, are preferred to others for modeling the mold filling problem due to their easy implementation, topological robustness and computational efficiency.

The solution methods, as well as the spatial and temporal discretization techniques, for solving the governing equations were summarized. Their advantages and disadvantages were discussed.

Finally, several viscosity models for polymer flow were summarized and their capabilities were evaluated. The Cross-WLF model was identified as the most appropriate model for the polymer flow in micro injection molding.

Chapter 3 Modeling of surface roughness

This chapter presents the mathematical formulation for modeling the roughness effects in micro injection molding. Firstly, possible effects of surface roughness in micro injection molding were identified based on the previous related work. The effective dimensions were proposed to represent the geometry of the mold cavity. Several two and three dimensional homogeneous roughness profiles were proposed to represent the physical surface roughness. The thermal conductivity and heat capacity of the homogenous roughness layer were modeled in terms of the effective roughness height (δ) and the volume fraction parameter (θ). For each homogenous roughness profile, the explicit link between the effective roughness heights and the average roughness (R_a or S_a) was given. Finally, the roughness model was validated by comparing the analytical results obtained using this model with the numerical results obtained directly using commercial software for a steady state heat conduction problem.

3.1 Mathematical modeling of surface roughness

Based on our current knowledge, there is no mathematical model proposed for modeling the roughness effects in micro injection molding. However, some investigations have been carried out for the roughness effects on fluid flow (e.g., water) in micro channels, conduits and tubes. In summary, three methods have been used to consider the roughness effects:

1. The use of some regular (normally rectangle) roughness elements (Hu et al., 2003) or irregular and randomly distributed roughness elements (Croce & Agaro, 2004) in the computation domain to simulate the physical rough walls.

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2. The roughness layer was considered as a porous medium layer (PML) (Kleinstreuer & Koo, 2004; Koo & Kleinstreuer, 2003, 2005) and analysis was performed based on the available PML theory.
3. The roughness effect was included into the viscosity model (Mala & Li, 1999; Qu et al., 2000).

Based on these prior investigations, the following conclusions can be drawn:

- Higher roughness will enhance heat transfer whilst keeping the other conditions constant (Croce & Agaro, 2004; Kandlikar et al., 2003; Koo & Kleinstreuer, 2005).
- The roughness effect on heat transfer is dependent on the Reynolds number of the flow (Kandlikar et al., 2003; Koo & Kleinstreuer, 2003, 2005).
- For fluid flow with low Reynolds number ranging from 0.001 to 10, roughness has a negligible effect on pressure drop under isothermal conditions (Hu et al., 2003).
- When Reynolds number is above 100, roughness affects the friction factor and hence the flow parameters (Kleinstreuer & Koo, 2004).

However, the existing models for the investigation of surface roughness have the following limitations:

- A number of researchers used the height of roughness elements or the relative roughness (R_h) to describe the roughness amplitude in their models (see Figure 3.1). In practice, however, the value of R_h is difficult to determine due to a lack of explicit link between R_h and the measurable roughness parameter such as average roughness (R_a). This limits the practical application of those models. From a practical standpoint, the roughness amplitude parameter used in a

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roughness model (as proposed in this thesis) should be easy to determine in terms of the measurable roughness parameter such as R_a or S_a .

Figure 3.1 Roughness amplitudes in terms of roughness elements' height (R_h) and the average roughness (R_a)

- Although the porous medium layer (PML) was used to model the roughness effects by some researchers, the volume porosity and permeability of the roughness layer are difficult to determine in practical applications. Moreover, significant modifications will be required for numerical implementation of the existing algorithms for injection molding.
- The fluids used in the previous investigations were mostly Newtonian and isothermal, without interaction between flow field and thermal field. The effect of roughness on heat transfer was therefore not taken into account. In micro-injection molding, however, the effect of roughness on heat transfer is crucial due to the non-Newtonian and non-isothermal nature of polymer flow. The importance of roughness for heat transfer in micro injection molding cannot be reflected by the previous models.
- In some of the previous investigations, the roughness effect was modeled in terms of the Reynolds number of flow. However, the Reynolds number of the polymer flow involved in micro injection molding is typically in the order of 0.1, which will lead to negligible roughness effect predicted by those models.

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Therefore, the roughness models in terms of the Reynolds number are not suitable to account for the roughness effects in micro injection molding.

- Although the roughness-viscosity model was used to account for the roughness effects in some studies, it is not sensitive to roughness at low Reynolds number. Moreover, the contribution of temperature effects was not taken into account.

As such, there are deficiencies in the existing approaches to account for the effects of surface roughness for micro-injection molding, where the non-Newtonian nature of a polymer melt, and the heat transfer between the melt and the mold are important. In this present investigation, a new mathematical model was proposed to consider the effects of mold surface roughness on the physical volume of mold cavity and heat transfer between the polymer melt and the mold wall.

A cavity having two parallel plates is used as an illustration (see Figure 3.2a) to model the effects of surface roughness. In practice, the distance between the roughness peaks of the lower and the upper walls is usually measured to represent the height of the cavity (i.e., H_{app}) as normal measurements are determined by the peaks of the roughness. Indeed, as shown in Figure 3.2a, the values of H_{app} will be different at different measurement locations due to the randomness of surface roughness. In the conventional analysis of injection molding, H_{app} is usually used to represent the real height of the cavity and mold surface roughness is neglected as seen in Figure 3.2b. However, when mold surface roughness is comparable to H_{app} , the volume of the melt for filling the rough region (i.e. the region consisting of roughness peaks and valleys) will become significant and cannot be neglected. In such situation, ignoring surface roughness by employing H_{app} could result in significant inaccuracy in the calculation of the cavity volume as compared to the physical cavity volume. Therefore, it is

necessary to use effective cavity height, instead of H_{app} , to account for the roughness effects.

Figure 3.2 Mold cavities: (a) physical cavity with surface roughness, (b) simplified cavity in conventional analysis

To consider the effect of surface roughness on the physical volume of the cavity, we consider a cross-section of the cavity shown in Figure 3.3. The effective wall should be at the mean plane (also called “center plane”) of the surface roughness. This is to ensure that the volume between the two effective walls (i.e., mean planes) will correspond to the volume of the physical cavity as the cross-sectional area/volume subtended between the roughness profile and the mean plane has to have an equal value above and below (Whitehouse, 2004). Thus, instead of H_{app} , the effective cavity height, H_{eff} , which is defined as the distance between the mean plane of the roughness

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elements at the lower and the upper walls (see Figure 3.3), should be employed in the analysis.

Figure 3.3 Cavity with surface roughness

To model the effect of surface roughness on heat transfer, surface roughness can be considered as a homogenous roughness layer characterized by its thermal conductivity, heat capacity and effective height, δ . Based on a simple rule of mixture, the thermal conductivity within the roughness layer (see Figure 3.4) is modeled as:

$$\kappa(y) = \theta(y)\kappa_1 + (1-\theta(y))\kappa_2 \quad (3.1)$$

where, κ_1 and κ_2 are the thermal conductivities of the melt and the mold respectively, and $\theta(y)$ is the volume fraction occupied by the polymer melt at the cross-sectional plane of y , which is parallel to the roughness mean plane.

Similarly, the heat capacity (in term of density and specific heat) of the roughness layer is modeled as:

$$\rho C_p(y) = \theta(y)\rho_1 C_{p1} + (1-\theta(y))\rho_2 C_{p2} \quad (3.2)$$

where, $\rho_1 C_{p1}$ and $\rho_2 C_{p2}$ are the heat capacities of the melt and the mold respectively.

Figure 3.4 Schematic diagram for determination of thermal properties of roughness layer

For the two-dimensional homogenous triangle or rectangle roughness profiles as illustrated in Table 3.1, the volume fraction, θ , can be expressed in a general form as:

$$\theta(y) = (\lambda_1 - \lambda_0) \cdot \frac{y}{\delta} + \lambda_0 \quad 0 \leq y \leq \delta \quad (3.3)$$

where, λ_0 is the ratio between the volume occupied by the polymer melt and the total volume of the mean plane (i.e., the effective wall), λ_1 is the ratio between the volume occupied by polymer melt and the total volume of the top plane of the roughness layer (i.e., the plane of $y = \delta$) and δ is the effective roughness height of the roughness layer (i.e., the distance from the roughness peaks to the mean plane).

By using the three parameters, λ_0 , λ_1 and δ , the proposed roughness model takes into account the roughness height, spacing, and geometrical shape of the two dimensional homogenous triangle or rectangle roughness profile. Table 3.1 gives the values of λ_0 , λ_1 and δ in terms of the average roughness (R_a) for the two-dimensional homogeneous triangle and rectangle roughness profiles.

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Table 3.1 The values of λ_0 , λ_1 and δ for the two-dimensional homogeneous triangle and rectangle roughness profiles

Profile	Schematic diagram	λ_0	λ_1	θ	δ
1		0.5	1	$0.5y/\delta + 0.5$	$2R_a$
2		0.75	1	$0.25y/\delta + 0.75$	$4R_a$
3		0.5	0.5	0.5	R_a
4		0.25	0.25	0.25	$2R_a$

Taking the first triangle profile in Table 3.1 as an example, the roughness effective height (δ) in terms of the average roughness (R_a) is obtained through the following calculation. As shown in Figure 3.5, according to the definition of the roughness mean line, the area of region B (A_B) equals to that of region C (A_C). According to the definition of the average roughness (i.e., the average deviation from the mean line or arithmetical average),

$$R_a = \frac{A_B + A_C}{2a} = \frac{A_B}{a} \quad (3.4)$$

The area of region B can also be expressed as

$$A_B = \frac{1}{2} a \delta \quad (3.5)$$

Therefore, δ can be expressed in terms of R_a as $\delta = 2R_a$. Similarly, δ in terms of R_a can be obtained for the other roughness profiles.

Figure 3.5 Schematic diagram for calculation of effective roughness height (δ) in terms of average roughness (R_a)

For three dimensional homogeneous roughness profiles, the determination of the volume fraction (θ) and the effective roughness height (δ) in terms of average roughness (S_a) is more complicated. Here, two simple three-dimensional homogeneous roughness profiles are discussed, i.e., the square column profile and the pyramid profile.

For three-dimensional roughness profiles, the average roughness (S_a) is defined as:

$$S_a = \frac{\iint_{\Omega} |z(x,y)| dx dy}{A} \quad (3.6)$$

where, $|z(x,y)|$ is the distance from the evaluated point to the mean plane, A is the area of the evaluated region. According to this definition, for the square column profile as shown in Figure 3.6, the average roughness (S_a) can be calculated as:

$$S_a = \frac{A_B \delta + A_C \delta}{A_B + A_C}, \quad A_B = A_C \quad (3.7)$$

where, A_B and A_C are areas of region B and C respectively.

As a result, for the square column profile, the effective roughness height (δ) in terms of the average roughness is $\delta = S_a$. The volume fraction (θ) is 0.5 in the roughness layer.

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Figure 3.6 Three-dimensional homogeneous square column roughness profile

For the three-dimensional homogeneous pyramid roughness profile as shown in Figure 3.7, the average roughness (S_a) can be calculated as:

$$S_a = \frac{\frac{1}{3} A_B \delta + \frac{1}{3} A_C \delta}{A_B + A_C}, \quad A_B = A_C \quad (3.8)$$

As a result, for the homogeneous pyramid roughness profile, the effective roughness height (δ) in terms of the average roughness is $\delta = 3S_a$. Moreover, for the homogeneous pyramid roughness profile, the area/volume occupied by mold material at any cross-sectional plane, D, can be calculated as:

$$A_D = \left(\frac{\delta - y}{\delta}\right)^2 A_B, \quad A_B = A_C \quad (3.9)$$

Thus, the volume fraction (θ) can be obtained as

$$\theta = \begin{cases} 1 - \frac{1}{2} \left(\frac{\delta - y}{\delta}\right)^2 & 0 \leq y \leq \delta \\ \frac{1}{2} \left(\frac{\delta + y}{\delta}\right)^2 & -\delta \leq y < 0 \end{cases} \quad (3.10)$$

Figure 3.7 Three-dimensional homogeneous pyramid roughness profile

3.2 Justification of the roughness model

The proposed roughness model is based on the assumption that the roughness will change the overall thermal conductivity and heat capacity of the roughness region, and thus heat transfer between the polymer melt and the mold. To justify this assumption, steady-state heat conduction in a channel with the two dimensional homogeneous rectangle roughness profile on its bottom wall (see Figure 3.8) was analyzed. The analytical result of the temperature distribution obtained using the proposed roughness model was compared with the numerical result obtained directly using the software COMSOL FEMLab.

Figure 3.8 Schematic diagram of the steady-state heat conduction problem

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For the analytical result, the governing equation of the steady-state heat conduction problem is given as

$$\frac{\partial}{\partial y}(\kappa(y) \frac{\partial T}{\partial y}) = 0 \quad (3.11)$$

According to the roughness model, the thermal conductivity of the roughness layer (i.e., $0 < y < \sigma$) is

$$\kappa(y) = \frac{(\kappa_1 + \kappa_2)}{2} \quad (3.12)$$

As a result, the analytical temperature distribution along the y-direction can be obtained as

$$T(y) = \begin{cases} T_0 + \frac{T_1 - T_0}{H - \delta} \cdot (y - \delta) & y \geq \delta \\ T_2 + \frac{T_0 - T_2}{\delta} \cdot y & y < \delta \end{cases} \quad (3.13)$$

where,

$$T_0 = \frac{T_1 \kappa_1 \delta + T_2 \kappa_2 (H - \delta)}{\kappa_1 \delta + \kappa_2 (H - \delta)} \quad (3.14)$$

For the numerical result, the software COMSOL FEMLab was used to analyze the steady-state heat conduction problem. Table 3.2 gives the input data and the boundary conditions used in the numerical analysis.

Table 3.2 Input data and boundary conditions for the steady-state heat conduction problem

H (mm)	δ (mm)	κ_{melt} (W/m.K)	κ_{mold} (W/m.K)	On the top wall	On the bottom wall	On the left and right walls
0.8	0.2	29	0.14	T =490K	T=330K	$\partial T / \partial x = 0$

Figure 3.9 shows the analytical and numerically predicted results of the temperature distribution along the y-direction. It can be observed that the analytical result obtained

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using the proposed model agrees well with the numerically predicted result. This justifies the proposed roughness model. In this problem, the temperature within the roughness layer is close to the boundary temperature (T_2). This is because the thermal conductivity ratio between the mold material and the polymer material is very large (i.e., larger than 200), whereas, the volume occupied by the polymer material and the mold material are the same, which leads to a much higher thermal conductivity of the roughness layer than that of the polymer material, and thus a much lower temperature gradient in the roughness layer than outside it. However, with an increase in the ratio between the volume occupied by the polymer material and that occupied by the mold material, the temperature gradient in the roughness layer will increase, which will be demonstrated in Chapter 7.

Figure 3.9 Analytical and numerically predicted results of the temperature distribution

3.3 Concluding remarks

In this chapter, the roughness effects were mathematically modeled. Firstly, to take into account the roughness effect on cavity volume, the roughness mean plane was

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proposed to represent the effective mold wall such that the cavities with the same thickness but different roughness will have the same cavity volume. Secondly, several two and three dimensional homogeneous roughness profiles were proposed to represent the physical roughness. The effective roughness heights (δ) of these roughness profiles can be expressed in terms of the experimentally measurable average roughness (R_a or S_a). Thirdly, to account for the roughness effect on heat transfer, the thermal conductivity and heat capacity of the homogenous roughness layer were modeled in terms of the effective roughness height (δ) and the ratio (θ) between the volume occupied by the polymer melt and that occupied by the mold material. Finally, the proposed roughness model was validated by comparing the analytical result of the temperature distribution obtained using this model with the numerical result obtained directly using the commercial software for a steady-state heat conduction problem.

Chapter 4 Experimental investigations into roughness effects

In this chapter, filling of polymer melt into a disk-shaped micro-thickness cavity mold are experimentally investigated. The roughness effects on the filling of the cavity are demonstrated by using four round core inserts, where each insert consists of two semicircular halves of different roughness. Experimental setup, fabrication of the core inserts, measurement of surface roughness, approach to determine the irregular flow area of the molded part and experimental procedure are outlined. The roughness effects are analyzed based on statistical analysis of the experimental results. The factors that contribute to the significance of roughness effects, such as the mold and melt temperatures, roughness magnitude and cavity thickness are studied.

4.1 Experimental setup

Injection molding of a thin disk with polyoxymethylene (POM) was performed on an injection molding machine (JMW-015S-5t) to investigate the effects of cavity surface roughness. Figure 4.1 shows the design of the part to be molded, together with its dimensions. The diameters of the part and the pinpoint gate are 8mm and 0.4mm respectively. The thickness of the cavity can be varied. The top of the part has uniform surface roughness, whereas, the bottom has different surface roughness on its two semicircular halves. Correspondingly, the cavity wall has uniform surface roughness and the core wall has different roughness on its two semicircular halves.

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Figure 4.1 The design of the molded part

The core insert was mounted onto an ejector pin to form the core wall of the cavity. Figure 4.2 shows the installation of the core insert. The thickness of the mold cavity was controlled using the same mechanism as described in (Ong & Koh, 2005), i.e., thin stainless steel shims were placed in between the height gauge and the ejector pin head to control the thickness of the cavity, while the thickness of the ejector washer was reduced to accommodate the dimensional increase. Moreover, the separating line between the two semicircular halves of the core insert was adjusted vertically in the mold such that the gravity has the same effect on the filling of the two semicircular halves of the cavity. Therefore, it is reasonable to assume that the two semicircular halves of the cavity are filled under the same processing conditions (e.g., the same filling pressure, melt and mold temperatures, etc.) and the difference in the filling flow areas between the two halves is predominantly caused by the difference in the roughness between them.

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Figure 4.2 Installation of the core insert

Figure 4.3 shows the layout of the mold plates for molding the part. Polymer melt is injected from the inlet, flows through the runner cavity and then enters the mold cavity. At the end of the molding cycle, the molded part is ejected by the ejector pin, on which the core insert was mounted. Figures 4.4 to 4.5 show the pictures of the cavity plate with the cavity insert and the core plate with the core insert, respectively. Figure 4.6 shows the molded part together with its connected runners.

Figure 4.3 The layout of the mold plates for molding the part

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Figure 4.4 The cavity plate with the cavity insert

Figure 4.5 The core plate with the core insert

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Figure 4.6 The molded micro disk together with its connected runners

The temperatures of the cavity plate and the core plate were controlled using an external heating controller. The temperature of the heater plate was controlled directly by the molding machine. The connection of the mold temperature control system is shown in Figure 4.7 (Ong et al., 2006).

Figure 4.7 Connection of the mold temperature control system

Figure 4.8 shows the picture of the mold in the open position in an injection molding machine. Figure 4.9 shows the external mold temperature controller, i.e.,

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HASCO Z122/1/2/16. The digits shown on the top indicate the actual mold temperature. The lower digits show the preset temperature.

Figure 4.8 Mold in the open position

Figure 4.9 External mold temperature controller

4.2 Machining of the core inserts

Four core inserts were machined using the Electro-Discharge-Machine (EDM). Their surface roughness was measured using a Talyscan 150 dual gauge system as shown in Figure 4.10.

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Figure 4.10 Talyscan 150 dual gauge system

To ensure that the two semicircular halves of the core insert have different surface roughness but the same roughness mean planes, the machining procedure as shown in Figure 4.11 was used. One half was first machined using a specific cut depth (i.e. ΔH) and a high surface roughness level as described in the specification of the machine, which is identified by $R_{\max}$ and R_a . Subsequently, the second half was machined using a low roughness level, which is identified by $R'_{\max}$ and R'_a . The cut depth is set as $(\Delta H + R_{\max} - R'_{\max})$. After that, the surface profile of the machined insert was measured using the Talyscan 150 dual gauge system to check if the roughness mean planes of the two semicircular halves are at the same level within an acceptable tolerance. If not, the process was repeated until the roughness mean planes of the two halves can be considered to be at the same level.

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(b)

Figure 4.11 Machining procedure for the core insert: (a) rougher half, (b) smoother half

Four core inserts were machined and used as the core walls to obtain reliable experimental results. For convenience of discussion, they were numbered as I, II, III and IV. Figure 4.12 shows the microscopic images of the surfaces of the four core inserts.

Figure 4.12 Microscopic images of the surface of core inserts: (a) I, (b) II, (c) III, (d) IV

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To precisely measure surface roughness of the core inserts, three-dimensional roughness measurement was performed. For each half of the core insert, surface roughness was measured on three different square regions (2mm x 2mm) as illustrated in Figure 4.13. Tables 4.1–4.4 give the measurement results of surface roughness of the four core inserts, respectively. Table 4.5 gives the measurement results of surface roughness of the cavity insert. The definitions of the measured roughness parameters (e.g., S_a , S_q , etc.) were given in Appendix A.

Figure 4.13 Measurement regions on the surface of the core insert

Table 4.1 Roughness measurement results of core insert I (μm)

	Repeat	S_a	S_q	S_{sk}	S_{ku}	S_p	S_v	S_t	S_z
Rougher half	1	14.70	18.37	-0.06	2.76	58.35	56.95	115.30	101.83
	2	14.72	18.57	0.13	3.07	67.08	62.24	129.32	96.36
	3	13.60	17.08	-0.10	2.88	53.92	54.29	108.20	96.93
	Ave.	14.34	18.01	-0.01	2.90	59.78	57.83	117.61	98.37
	Std. Div.	0.64	0.81	0.13	0.16	6.70	4.05	10.75	3.01
Smoother half	1	0.31	0.39	0.25	5.14	4.82	1.60	6.42	3.77
	2	0.30	0.38	0.33	5.52	4.36	1.68	6.04	3.57
	3	0.30	0.38	0.36	6.22	4.27	1.70	5.97	3.44
	Ave.	0.30	0.38	0.31	5.63	4.48	1.66	6.14	3.59
	Std. Div.	0.01	0.01	0.06	0.55	0.30	0.05	0.24	0.17

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Table 4.2 Roughness measurement results of core insert II (μm)

	Repeat	S_a	S_q	S_{sk}	S_{ku}	S_p	S_v	S_t	S_z
Rougher half	1	16.64	20.41	0.40	2.70	68.89	47.24	116.12	103.00
	2	17.22	21.07	0.39	2.75	69.40	51.53	120.93	112.18
	3	16.28	19.96	0.26	2.62	65.91	47.71	113.62	103.47
	Ave.	16.71	20.48	0.35	2.69	68.07	48.83	116.89	106.22
	Std. Div.	0.47	0.56	0.08	0.07	1.89	2.35	3.72	5.17
Smoother half	1	0.38	0.48	0.09	2.96	1.86	1.78	3.65	3.29
	2	0.36	0.46	0.11	3.13	2.06	1.69	3.75	3.34
	3	0.37	0.46	0.02	3.49	2.76	3.54	6.30	4.21
	Ave.	0.37	0.47	0.07	3.19	2.23	2.34	4.57	3.61
	Std. Div.	0.01	0.01	0.05	0.27	0.47	1.04	1.50	0.52

Table 4.3 Roughness measurement results of core insert III (μm)

	Repeat	S_a	S_q	S_{sk}	S_{ku}	S_p	S_v	S_t	S_z
Rougher half	1	8.11	10.30	0.46	3.66	47.84	30.60	78.44	55.91
	2	7.03	8.70	0.13	2.80	33.72	30.16	63.88	54.77
	3	10.85	13.89	0.79	3.82	58.47	36.81	95.28	74.48
	Ave.	8.66	10.96	0.46	3.43	46.68	32.52	79.20	61.72
	Std. Div.	1.97	2.66	0.33	0.55	12.42	3.72	15.71	11.07
Smoother half	1	0.41	0.51	0.17	3.42	2.87	1.91	4.78	4.05
	2	0.35	0.45	-0.02	5.23	2.07	4.85	6.91	4.09
	3	0.46	0.57	0.13	4.09	2.97	4.31	7.28	3.30
	Ave.	0.41	0.51	0.09	4.25	2.64	3.69	6.32	3.81
	Std. Div.	0.06	0.06	0.10	0.92	0.49	1.56	1.35	0.45

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Table 4.4 Roughness measurement results of core insert IV (μm)

	Repeat	S_a	S_q	S_{sk}	S_{ku}	S_p	S_v	S_t	S_z
Rougher half	1	14.03	17.06	0.09	2.40	38.41	46.64	85.06	80.42
	2	14.85	18.13	0.10	2.37	40.03	50.94	90.97	80.21
	3	14.79	17.94	0.09	2.34	39.77	47.19	86.97	78.78
	Ave.	14.56	17.71	0.09	2.37	39.40	48.26	87.67	79.80
	Std. Div.	0.46	0.57	0.01	0.03	0.87	2.34	3.02	0.89
Smoother half	1	4.17	5.80	-2.04	6.87	8.07	31.59	39.66	33.17
	2	3.03	4.57	-2.44	9.30	5.66	28.93	34.59	29.60
	3	2.94	4.46	-2.45	9.50	5.56	28.32	33.87	29.64
	Ave.	3.38	4.94	-2.31	8.56	6.43	29.61	36.04	30.80
	Std. Div.	0.69	0.74	0.23	1.46	1.42	1.74	3.16	2.05

Table 4.5 Roughness measurement results of the cavity insert (μm)

Repeat	S_a	S_q	S_{sk}	S_{ku}	S_p	S_v	S_t	S_z
1	0.20	0.36	3.18	49.70	6.05	4.06	10.11	7.53
2	0.24	0.46	-2.44	56.88	6.35	6.54	12.89	8.65
3	0.18	0.26	0.29	14.72	1.79	3.14	4.93	3.80
Ave.	0.21	0.36	-1.08	35.80	4.07	4.84	8.91	6.23
Std. Div.	0.04	0.14	1.93	29.81	3.22	2.40	5.63	3.43

It is important to ensure that the two semicircular halves of the core insert have the same roughness mean plane, as the difference in the mean plane will influence the volume of the cavity, and thus the flow on the two halves, which will have an effect on the experimental results. To evaluate the difference in the mean planes between the two semicircular halves, the procedure as described in the following was used.

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Figure 4.14 shows a schematic diagram of a two-dimensional surface profile of the core insert. The vertical distance from the roughness mean line/plane of the rougher half (i.e., line l_1) to that of the smoother half (i.e., line l_2) can be expressed as

$$\Delta d = H_r - (H_1 - H_2) \quad (4.1)$$

where, H_1 is the distance from a peak point P_1 to the mean line of the rougher half (i.e., l_1), H_2 is the distance from a peak point P_2 to the mean line of the smoother half (i.e., l_2), and H_r is the vertical distance from point P_1 to point P_2 . Thus, $\Delta d = 0$ means the mean lines of the two halves are at the same level, $\Delta d > 0$ means the mean line of the rougher half is higher than that of the smoother half, and $\Delta d < 0$ means that mean line of the rougher half is lower than that of the smoother half.

Figure 4.14 Schematic diagram of the surface profile of the cavity insert

For each core insert, five two-dimensional roughness profiles were measured to determine the Δd value. For each roughness profile, measurements were performed at three different locations. Figure 4.15 illustrates the five measurement positions. Table 4.6 gives the measurement results of the Δd values for the four core inserts. To avoid

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significant error caused by $\Delta d \neq 0$, the cavity thicknesses ranging from 200 μm to 300 μm were used, which limit $\Delta d/H$ in the order of 1%.

Figure 4.15 Measurement positions for determination of Δd values of the core inserts

Table 4.6 Measurement results of Δd for the four core inserts (μm)

Position	Insert I	Insert II	Insert III	Insert IV
1	-1.4	0.3	-1.9	0.2
2	-1.9	0.4	-1.8	0.3
3	-1.9	0.3	-1.7	0.1
4	-1.6	0.4	-1.9	0.2
5	-2.1	0.5	-2.5	0.2
Ave.	-1.8	0.4	-1.9	0.2
Std. Div.	0.2	0.1	0.3	0.1

4.3 Approach of flow area measurement

The difference in roughness between the two semicircular halves will result in a difference in the filling volume between the two cavity halves. Considering that the two halves of the cavity have the same thickness, the flow areas of the two halves can be used to represent the flow volumes. As a result, the roughness effects can be investigated by comparing the flow areas in the two semicircular cavity halves. It

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should be noted that the effect of $\Delta d \neq 0$ could be accounted for in the proposed numerical model. However, for a large value of Δd , the effects of roughness might not be highlighted easily.

The determination of the flow area of the partially filled part is not an easy task considering the fact that the geometry of the part is not exactly regular. To accurately measure the flow area, a graph digitization software kit, GetData, together with AutoCAD was employed. The molded part was first scanned using a scanner and saved as an image of .tif format. Subsequently, the image was imported into GetData and the edge of the part was discretized by a set of points. These points were then exported to an AutoCAD recognized .dxf file. Finally, the AutoCAD was used to import the .dxf file and its area calculation function was used to obtain the area of the region surrounded by the set of points. Figure 4.16 summarizes the procedure for the determination of the flow area and Figure 4.17 illustrates the procedures. For each molded part, the measurement of flow area was performed three times by selecting different discretizing positions on the edge of the part in GetData.

Figure 4.16 The procedure for determination of the flow area of the molded part

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(a)

(b)

(c)

Figure 4.17 The illustration for determination of flow area of the molded part: (a) the scanned image with the reference scale, (b) the outline discretized by a set of points and the coordinates of these points in GetData, (c) the obtained area of the region surrounded by the points exported from GetData

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4.4 Experimental procedure

The cavity wall has a uniform surface roughness and its roughness is small (i.e., $S_a=0.21\pm0.04\text{ }\mu\text{m}$). For each core insert, the separating line between its smoother and rougher halves was adjusted vertically in the mold such that gravity has the same effect on filling of the two semicircular cavity halves. Therefore, it is reasonable to assume that the two semicircular halves of the cavity are filled under the same process conditions (e.g., the same mold and melt temperatures, filling pressure, etc.) and the difference in the flow areas between the two halves of the molded part is predominantly caused by the difference in surface roughness between the two semicircular halves of the core insert.

The material used in the experiment was polyoxymethylene (POM), Ultraform W2320 003. Partially filled parts of different sizes were obtained by varying the injection rates within a small range. Two mold temperature levels of 323K and 383K, and two melt temperature levels of 453K and 473K, were used to investigate the significance of the roughness effects. For every change in the processing parameter setting, five specimens were collected only after 10 injection cycles. This was to stabilize the parameter setting and to obtain consistent plastic parts.

4.5 Experimental results and discussion

4.5.1 Flow patterns

Figure 4.18 shows the parts of different sizes molded using injection rates ranging from $2.3\text{cm}^3/\text{s}$ to $3.4\text{cm}^3/\text{s}$ for core insert I. Mold temperatures were 323K and 383K, and melt temperatures were 453K and 473K. It can be observed that the flow area on the smoother half (i.e., upper half) is obviously larger than the flow area on the rougher half (i.e., lower half), indicating that surface roughness does resist the flow of polymer melt. Similarly, Figures 4.19 – 4.21 show the molded parts for the other three

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core inserts. The same observations can be made, i.e., the flow area on the smoother half is obviously larger than the flow area on the rougher half.

(a)

(b)

(c)

(d)

Figure 4.18 Molded parts for core insert I with: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

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(a)

(b)

(c)

(d)

Figure 4.19 Molded parts for core insert II with: (a) $T_{\text{melt}} = 453\text{K}$, $T_{\text{mold}} = 323\text{K}$, (b) $T_{\text{melt}} = 453\text{K}$, $T_{\text{mold}} = 383\text{K}$, (c) $T_{\text{melt}} = 473\text{K}$, $T_{\text{mold}} = 323\text{K}$, (d) $T_{\text{melt}} = 473\text{K}$, $T_{\text{mold}} = 383\text{K}$

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(a)

(b)

(c)

(d)

Figure 4.20 Molded parts for core insert III with: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

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(a)

(b)

(c)

(d)

Figure 4.21 Molded parts for core insert IV with: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

4.5.2 Evolution of the flow areas of the two halves

The evolution of the flow areas on the two halves with increasing total flow area for the four core inserts were shown in Figure 4.22. The mold and melt temperatures were 323K and 453K respectively. At the early stage of cavity filling, polymer melt advances simultaneously on the two semicircular halves of the cavity, with higher speed on the smoother half and lower speed on the rougher half. However, once the smoother half is almost completely filled (i.e., the flow area on the smoother half is close to 25.1mm^2), the melt on the rougher half will flow faster than it does on the smoother half (e.g., see Figure 4.22b). This is because the cavity boundary will prevent polymer melt to flow further on the smoother half and push the melt to flow on the rougher half. It indicates that the cavity boundary will influence the difference in filling flow area on the two halves once the polymer melt touches the cavity boundary. To avoid the influence of the cavity boundary and to make the roughness difference between the two semicircular halves of the core insert a unique predominant factor affecting flow front advancement (i.e., represented by flow area development) in the two semicircular cavity halves, only the parts with flow area on the smoother half less than 23mm^2 were investigated. The measurement results and error analysis of the flow areas of molded parts for the four core inserts were given in Appendix B.

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(a)

(b)

(c)

(d)

Figure 4.22 Evolution of the flow areas on each half with increasing total flow areas with $T_{\text{melt}}=453\text{K}$ and $T_{\text{mold}}=323\text{K}$ for core insert: (a) I, (b) II, (c) III, (d) IV

4.5.3 Regression analysis of roughness effects

The scatter diagrams shown in Figure 4.22 suggested that a straight line could be used to express the relationship between the flow area on each half and the entire flow area

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of the molded part. Furthermore, considering the fact that the flow area on each half should be zero when the entire flow area is zero, the zero intercept regression model seems intuitively reasonable (Montgomery et al., 2006). As the flow areas on the two halves are strictly correlated, i.e., their sum equals to the total flow area of the part, only flow area on the rougher half are investigated. Therefore, the relationship between the flow area on the rougher half and the entire flow area is modeled by the zero intercept regression model, which is written as

$$A_r = kA_t \quad (4.2)$$

where, A_r stands for the flow area of the rougher half, A_t the entire flow area of the part and k is the slope, which identifies the significance of the roughness effect. As the slope (k) is defined using the rougher half, it is expected that the k value is bounded between 0 and 0.5. There will be negligible roughness effect if $k = 0.5$, indicating the same flow area on the two halves. The larger the difference in k value from 0.5, the more significant is the roughness effects.

Figure 4.23 shows the regression results of 95% confidence interval of k value for core insert I when melt and mold temperatures were 453K and 323K respectively. The t statistic for testing $H_0: k = 0$, $H_1: k \neq 0$ is $t_0 = 539.48$, for which the P value is 0.000 (rounded), indicating that the regression is statistically significant. Meanwhile, the non-zero intercept model, i.e., $A_r = kA_t + \beta_0$, was also used to fit the experimental data for comparative purposes. This results in $A_r = (0.449 \pm 0.005)A_t - (0.026 \pm 0.141)$. The t statistic for testing $H_0: \beta_0 = 0$, $H_1: \beta_0 \neq 0$ is $t_0 = -0.38$, for which the P value is 0.707, indicating that β_0 is not statistically significant and can be neglected. Therefore, the zero intercept model can describe accurately the relationship between the flow area on the rougher half and the entire flow area, which is consistent with the physical reasoning of a zero intercept.

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Similarly, Figures 4.24 – 4.26 give the 95% confidence intervals of k value for other combinations of the melt and mold temperature levels. Table 4.7 summarizes the regression and significance test results for core insert I. For the other three core inserts, the 95% confidence intervals of the k value, together with the standard error, t-value and the p-value were given in Tables 4.8 – 4.10.

Figure 4.23 The regression line and 95% confidence interval of k value for insert I ($T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$)

Figure 4.24 The regression line and 95% confidence interval of k value for insert I ($T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$)

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Figure 4.25 The regression line and 95% confidence interval of k value for insert I ($T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$)

Figure 4.26 The regression line and 95% confidence interval of k value for insert I ($T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$)

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Table 4.7 Regression results for core insert I

Temperatures	95% CI* of k value	SE*	t-value	Prob (t)
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=323\text{K}$	0.448 ± 0.002	0.001	539.48	0.000
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=383\text{K}$	0.477 ± 0.004	0.002	274.97	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=323\text{K}$	0.474 ± 0.003	0.001	318.24	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=383\text{K}$	0.485 ± 0.003	0.001	368.20	0.000

* CI stands for the confidence interval and SE stands for the standard error.

Table 4.8 Regression results for core insert II

Temperatures	95% CI of k value	SE	t-value	Prob (t)
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=323\text{K}$	0.386 ± 0.002	0.001	478.70	0.000
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=383\text{K}$	0.414 ± 0.003	0.001	292.00	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=323\text{K}$	0.416 ± 0.005	0.002	181.51	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=383\text{K}$	0.423 ± 0.004	0.002	238.27	0.000

Table 4.9 Regression results for core insert III

Temperatures	95% CI of k value	SE	t-value	Prob (t)
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=323\text{K}$	0.368 ± 0.005	0.002	149.96	0.000
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=383\text{K}$	0.410 ± 0.004	0.002	219.14	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=323\text{K}$	0.425 ± 0.005	0.002	176.96	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=383\text{K}$	0.433 ± 0.004	0.001	319.35	0.000

Table 4.10 Regression results for core insert IV

Temperatures	95% CI of k value	SE	t-value	Prob (t)
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=323\text{K}$	0.443 ± 0.005	0.002	208.75	0.000
$T_{\text{melt}}=453\text{K}, T_{\text{mold}}=383\text{K}$	0.450 ± 0.005	0.002	180.04	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=323\text{K}$	0.451 ± 0.005	0.002	247.21	0.000
$T_{\text{melt}}=473\text{K}, T_{\text{mold}}=383\text{K}$	0.463 ± 0.005	0.002	226.89	0.000

Figures 4.27 - 4.30 summarize the 95% confidence intervals of the k value for the four core inserts for different melt and mold temperature levels. It can be observed that the k values varied with the melt and mold temperatures even using the same core

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insert. This indicates that the roughness effects (i.e., the k value) may be dependent on the melt and mold temperatures. Therefore, in the following, the influences of the melt and mold temperatures on the significance of roughness effects (i.e., the k value) will be addressed.

Figure 4.27 k values for core insert I

Figure 4.28 k values for core insert II

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Figure 4.29 k values for core insert III

Figure 4.30 k values for core insert IV

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4.5.4 Dependence of roughness effects on mold temperature

To investigate the dependence of roughness effects on the mold temperature, the k values of the molded parts at two mold temperature levels were compared by employing the two-sample t test.

When the melt temperature was kept constant at 453K, for the four core inserts, the results for testing the hypothesis $H_0: k_{323} = k_{383}$ versus $H_1: k_{323} < k_{383}$ are given in Table 4.11, where k_{323} and k_{383} are the population means of the k values at the mold temperature of 323K and 383K, respectively. Similarly, when the melt temperature was kept constant at 473K, the two-sample t tests for testing $H_0: k_{323} = k_{383}$ versus $H_1: k_{323} < k_{383}$ are given in Table 4.12.

Table 4.11 Two-sample t tests for the melt temperature of 453K

Two-sample t test for: $H_0: k_{323} = k_{383}$ versus $H_1: k_{323} < k_{383}$		
Insert No.	t-value	p-value
I	-16.78	0.000
II	-16.12	0.000
III	-14.37	0.000
IV	-2.57	0.009

Table 4.12 Two-sample t tests for the melt temperature of 473K

Two-sample t test for: $H_0: k_{323} = k_{383}$ versus $H_1: k_{323} < k_{383}$		
Insert No.	t-value	p-value
I	-3.08	0.003
II	-2.03	0.028
III	-3.83	0.001
IV	-4.86	0.000

From the test results shown in the above tables, the null hypothesis can be rejected with 95% confidence for all the four core inserts. Therefore, it can be safely

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concluded that when the melt temperature was kept constant, the roughness effect is more significant at the lower mold temperature level (i.e., 323K).

4.5.5 Dependence of roughness effects on melt temperature

To investigate the dependence of roughness effects on the melt temperature, the k values of the molded parts at two melt temperature levels were compared by employing the two-sample t test.

When the mold temperature was kept constant at 323K, for the four core inserts, the results for testing the hypothesis $H_0: k_{453} = k_{473}$ versus $H_1: k_{453} < k_{473}$ are given in Table 4.13, where k_{453} and k_{473} are the population means of the k values at the melt temperature of 453K and 473K, respectively. Similarly, when the mold temperature was kept constant at 383K, the two-sample t tests for testing $H_0: k_{453} = k_{473}$ versus $H_1: k_{453} < k_{473}$ are given in Table 4.14.

Table 4.13 Two-sample t tests for the mold temperature of 323K

Two-sample t test for: $H_0: k_{453} = k_{473}$ versus $H_1: k_{453} < k_{473}$		
Insert No.	t -value	p -value
I	-14.28	0.000
II	-12.21	0.000
III	-14.35	0.000
IV	-2.28	0.016

Table 4.14 Two-sample t tests for the mold temperature of 383K

Two-sample t test for: $H_0: k_{453} = k_{473}$ versus $H_1: k_{453} < k_{473}$		
Insert No.	t -value	p -value
I	-2.86	0.005
II	-3.58	0.001
III	-10.17	0.000
IV	-3.24	0.002

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From the test results shown in the above tables, the null hypothesis can be rejected with 95% confidence for all the four core inserts. Therefore, it can be safely concluded that when the mold temperature was kept constant, the roughness effect is more significant at the lower melt temperature level (i.e., 453K).

4.5.6 Dependence of roughness effects on roughness magnitude

Figure 4.31 shows the k values for core inserts I and II, with the same cavity thickness (i.e., $0.30\mu\text{m}$). It can be observed that for each combination of the melt and mold temperature levels the k value for core insert I was higher than that for core insert II. This is because the roughness on the rougher half of insert I (i.e., $S_a=14.3\pm0.6\mu\text{m}$) is smaller than that of insert II (i.e., $S_a=16.7\pm0.5\mu\text{m}$) and the smoother halves of the two inserts have comparable roughness (i.e., $S_a=0.30\pm0.01\mu\text{m}$ and $0.37\pm0.01\mu\text{m}$, respectively). This demonstrates that the higher the surface roughness, the more significant is the roughness effect.

Figure 4.31 k values for core inserts I and II

4.5.7 Dependence of roughness effects on cavity thickness

Figure 4.32 shows the k values for inserts I and III. For each combination of the melt and mold temperature levels, although the roughness of the rougher half of core insert I (i.e., $S_a=14.3\pm0.6\mu\text{m}$) is larger than that of core insert III (i.e., $S_a=9\pm2\mu\text{m}$) and the roughness of the smoother halves of the two inserts are comparable (i.e., $S_a=0.30\pm0.01\mu\text{m}$ and $0.41\pm0.06\mu\text{m}$, respectively), the k value for insert III is obviously smaller than that for insert I. This is mainly due to the difference in cavity thicknesses for the two inserts (0.30mm and 0.20mm, respectively), i.e., the smaller the cavity thickness, the more significant is the roughness effect.

Figure 4.32 k values for core inserts I and III

4.6 Concluding remarks

In this chapter, the filling of polymer melt into a disk-shaped micro-thickness cavity mold was investigated through experiment. The roughness effects on the filling of the cavity were conclusively demonstrated by having different roughness on the two

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semicircular halves of the round core insert. Based on regression analysis, the ratio between the flow area of the rougher half and the entire flow area of the molded part (i.e., the k value) was defined to quantify the significance of the roughness effects.

The experimental results of the k values revealed that the significance of the roughness effects is dependent on the melt and mold temperatures. With the aid of the two-sample t test, it was observed that the roughness effect is more significant at the lower mold temperature when the melt temperature was kept constant. Similarly, it is more significant at the lower melt temperature when the mold temperature was kept constant. Moreover, the larger the magnitude of the roughness, the more significant is the roughness effect. The smaller the cavity thickness, the more significant is the roughness effect.

Chapter 5 Numerical modeling of mold filling

In this chapter, a numerical procedure, which implements the finite volume method and the level set method and incorporates the proposed roughness model, was presented for the simulation of the axisymmetric flow of polymer melt. Subsequently, using a newly proposed inlet-velocity iteration approach, the numerical procedure was extended to simulate the pseudo-axisymmetric filling flow encountered in the experiment for a cavity with different roughness at the two halves. Finally, the accuracy of numerical solution was assessed, including the effects of fictitious fluid viscosity, number of grids and time step.

5.1 Numerical model for axisymmetric flow

In this section, the mold filling of polymer melt into an axisymmetric geometry was numerically modeled. Figure 5.1 shows the schematic diagram of the axisymmetric filling flow. The polymer melt enters the cavity with a uniform and constant velocity and temperature, pushing the air out of the cavity.

Figure 5.1 Schematic diagrams of the axisymmetric filling flow

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5.1.1 Governing equations

The filling polymer melt flow is governed by three conservation equations of mass, momentum and energy, which are also called the governing equations. The effects of gravity can be neglected considering the fact that the gravitation forces are very small as compared with the viscous force for the melt (Haagh & Vosse, 1998). Surface tension can also be neglected for the molded parts with dimensions much larger than $1\mu\text{m}$ (Yao & Kim, 2002). Although wall-slip may occur when the channel size decreases below ten of micrometers (Yao & Kim, 2002; Young, 2007), it can be neglected as the channel size was limited to a range above $100\mu\text{m}$ in this investigation. Furthermore, the roughness may prevent the occurrence of wall-slip. As a result, the governing equations for the filling flow in the cavity are written as:

Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (5.1)$$

Momentum equation

$$\left(\frac{\partial \rho \vec{v}}{\partial t} + \vec{v} \cdot \nabla \rho \vec{v} \right) = -\nabla p + \nabla \cdot (\eta \dot{\underline{\underline{\gamma}}}), \quad \dot{\underline{\underline{\gamma}}} = \nabla \vec{v} + (\nabla \vec{v})^T \quad (5.2)$$

Energy equation

$$\left(\frac{\partial \rho C_p T}{\partial t} + \vec{v} \cdot \nabla \rho C_p T \right) = \nabla \cdot (\kappa \nabla T) + \eta \dot{\underline{\underline{\gamma}}}^2, \quad \dot{\underline{\underline{\gamma}}} = \sqrt{\frac{1}{2} \dot{\underline{\underline{\gamma}}} : \dot{\underline{\underline{\gamma}}}} \quad (5.3)$$

where, ρ , η , C_p and κ are the density, viscosity, specific heat and conductivity of the fluid flow respectively. The detailed governing equations in the Cartesian and axisymmetric coordinate systems are given in Appendix C.

The proposed roughness model can be easily included in the energy equation (Eq.(5.3)), i.e., in the roughness layer occupied by the polymer melt, κ and ρC_p are

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determined using the proposed roughness model. Otherwise, ρ , C_p and κ are the density, specific heat and conductivity of the fluid respectively.

5.1.2 Viscosity model

The polymer melt is a non-Newtonian fluid, the viscosity of which is dependent on the temperature, shear rate and cavity pressure. The widely-used Cross-WLF model is used to calculate the viscosity of the polymer melt, which can be expressed as

$$\eta(T, \dot{\gamma}, P) = \frac{\eta_0(T, P)}{1 + (\eta_0(T, P) \cdot \dot{\gamma} / \tau^*)^{1-n}} \quad (5.4)$$

$$\eta_0(T, P) = D_1 \cdot \exp\left\{-\frac{A_1 \cdot (T - T^*)}{A_2 + (T - T^*)}\right\}$$

where,

$$T^*(P) = D_2 + D_3 P$$

$$A_2 = \tilde{A}_2 + D_3 P$$

$n, \tau^*, D_1, D_2, D_3, A_1, \tilde{A}_2$ are constants.

5.1.3 PVT model

To account for the variation in the polymer density with temperature, the modified two-domain Tait PVT model was used (Xu Chen et al., 2004), which is written as

$$V(T, P) = V_0(T) [1 - C \ln(1 + P/B(T))] + V_t(T, P) \quad (5.5)$$

where, $V(T, P)$ is the specific volume at temperature T and pressure P , V_0 is the specific volume at zero pressure, C is a constant, 0.0894 and B accounts for the pressure sensitivity of the material. When the material temperature is higher than its transition temperature,

$$V_0 = b_{1m} + b_{2m}(T - b_5) \quad (5.6)$$

$$B(T) = b_{3m} \exp[-b_{4m}(T - b_5)] \quad (5.7)$$

When the material temperature is lower than its transition temperature,

$$V_0 = b_{1s} + b_{2s}(T - b_5) \quad (5.8)$$

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$$B(T) = b_{3s} \exp[-b_{4s}(T - b_5)] \quad (5.9)$$

where, b_5 is the transition temperature at zero pressure and b_6 the linear increase in transition temperature with pressure, which is

$$T_{trans}(P) = b_5 + b_6 P \quad (5.10)$$

For non-amorphous (crystalline) materials, an additional transition function is required:

$$V_t(T, P) = b_7 \exp(b_8(T - b_5) - b_9 P) \quad (5.11)$$

The unknown constants can be determined by curve fitting to the polymer material data.

5.1.4 Capturing of flow front

The flow front of polymer melt is captured using the level set method (Osher & Sethian, 1988). A scalar variable φ is used to identify the interface between the melt and air, i.e. the zero-level set of φ indicates the polymer-air interface, $\varphi < 0$ indicates polymer occupied region and $\varphi > 0$ indicates air occupied region. φ is transported by the fluid motion. The transport equation of the level set function, φ , is written as

$$\frac{\partial \varphi}{\partial t} + \vec{v} \cdot \nabla \varphi = 0 \quad (5.12)$$

where, φ is the normal distance from the melt/air interface, which satisfies

$$|\nabla \varphi| = 1 \quad (5.13)$$

To maintain φ as a distance function at all time steps, a re-distancing (or re-initializing) equation is defined:

$$\frac{\partial \xi}{\partial t} = \text{sign}(\varphi)(1 - |\nabla \xi|), \quad \xi(\vec{x}, 0) = \varphi(\vec{x}, t + \Delta t) \quad (5.14)$$

The steady-state solution of ξ are the values of φ at time $t + \Delta t$.

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One common problem encountered in the level set method is mass loss or mass addition during the simulation. To solve this, a mass conservation term M_{cor} is introduced to Eq. (5.14) to ensure global mass conservation (Yap et al., 2006), which is expressed as

$$\frac{\partial \xi}{\partial t'} = \text{sign}(\varphi)(1 - |\nabla \xi|) + M_{cor} \quad (5.15)$$

When mass is conserved at “steady-state”, M_{cor} is zero, the M_{cor} is written as

$$M_{cor} = \text{Sign}(\varphi_{ref}) \frac{M_o - M_c}{M_o} \quad (5.16)$$

where, M_o and M_c are the original mass and the most current mass of the reference phase (ie., polymer melt), respectively.

The mass conservation (Eq.(5.15)) and re-distancing operations (Eq.(5.14)) can be divided into two separate steps: (1) At the end of the transport equation given by Eq.(5.12), the re-distancing equation given by Eq.(5.14) can be solved to ensure that φ remains as the distance function which satisfies Eq.(5.13); (2) In case mass is not conserved at the end of the solution of Eq.(5.14), a step which ensures mass conservation is performed. This mass preservation step can be written as

$$\frac{\partial \xi}{\partial t''} = M_{cor} \quad (5.17)$$

where, t'' and M_{cor} are pseudo-time and mass conservation term, respectively. Once “steady state” is reached, the ξ in Eq. (5.17) ensures mass conservation of the reference phase. However, ξ might not be a distance function. The re-distancing equation is then solved to ensure that ξ and thus φ , remain as distance function and thus satisfies Eq.(5.13).

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5.1.5 Fictitious fluid approach

The high ratio of the properties, such as fluid density, viscosity, thermal conductivity, etc., between the polymer melt and the air, is a challenge to the stability and convergence of the numerical solution. To enhance the stability and convergence without sacrificing significant accuracy, the fictitious fluid approach, which is similar to the pseudo-concentration method, was employed. In this approach, a fictitious fluid is introduced to represent the air downstream of the polymer flow front. The main consideration of this fictitious fluid is that its viscosity is to be set to a value at least 10^{-3} times smaller than that of polymer melt, exceeding the real value of air viscosity by several orders of magnitude. The other properties of the fictitious fluid are the same as those of air.

5.1.6 Properties near flow front

The sudden change in the properties at the interface between the melt and the fictitious fluid, such as fluid density, viscosity and thermal conductivity, may lead to instability and divergence of the numerical solution. To avoid such a problem, a Heaviside function is used to define a smeared interface, i.e., the property α near the interface is calculated using

$$\alpha = (1-h)\alpha_1 + h\alpha_2 \quad (5.18)$$

where, α_1 and α_2 stand for the properties of polymer melt and the fictitious fluid, respectively, such as density, viscosity, specific heat and thermal conductivity. The Heaviside function h is written as (Y. C. Chang et al., 1996)

$$h = \begin{cases} 0 & \varphi < -\varepsilon \\ \frac{\varphi + \varepsilon}{2\varepsilon} + \frac{1}{2\pi} \sin\left(\frac{\pi\varphi}{\varepsilon}\right) & |\varphi| \leq \varepsilon \\ 1 & \varphi > \varepsilon \end{cases} \quad (5.19)$$

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where, ε is related to the grid size and is usually taken as a factor of the grid spacing. A thickness of 2ε is recommended (Sussman & Puckett, 2000; Sussman et al., 1994).

5.1.7 Initial and boundary conditions

Initially, the melt is assumed to rest somewhere in the cavity. At the inlet, the velocity and the temperature of polymer melt are kept constant. At the outlet, the outflow boundary condition is imposed. The temperature of the melt/mold interface is assumed to be equal to the wall temperature, namely, the heat transfer coefficient between the mold and the melt is assumed to be very high. To allow occurrence of the fountain effect and advancement of the melt flow front, the boundary conditions of the flow field change dynamically, i.e., the no-slip boundary condition is imposed on the melt filled domain, and free-slip boundary condition on the unfilled domain (R. Y. Chang & Yang, 2001; Haagh & Vosse, 1998).

In summary, the initial and boundary conditions are given as

$$u = U_{in}, T = T_{melt} \text{ at the inlet ; } T = T_{mold} \text{ on the effective wall} \quad (5.20)$$

where, U_{in} , T_{melt} and T_{mold} are the inlet velocity, inlet melt temperature and mold temperature, which are assumed to be constant.

$$\varphi = \phi_{ini} \text{ at } t = 0 \quad (5.21)$$

where, Φ_{ini} is the initial level set values in the domain.

$$u = 0 \text{ on the melt-wetted wall; } \frac{\partial u}{\partial y} = 0 \text{ on the unwetted wall} \quad (5.22)$$

$$\frac{\partial u}{\partial x} = 0; \frac{\partial T}{\partial x} = 0 \text{ at the axisymmetric axis} \quad (5.23)$$

5.1.8 Summary of the solution procedure

The solution procedure for capturing the flow front of polymer melt can be summarized as:

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1. Specify the locations of the flow front at time $t=0$.
2. Calculate the normal distances for all nodes from the interface.
3. Specify the properties for all nodes using Eq. (5.18).
4. Solve the governing equations given by Eqs. (5.1)- (5.3) at $t+\Delta t$.
5. Solve for ϕ (Eq. (5.12)) using the velocities obtained in step 4.
6. Solve for the “steady-state” ζ (Eq.(5.15)) using the values of ϕ from step 5 as the initial values.
7. Set $\phi(x, t+\Delta t) = \zeta(x)$.
8. Repeat steps 3 through 7 for all time steps.

5.2 Numerical solution method

The governing equations and the level set equations may be expressed in the general form:

$$\frac{\partial}{\partial t}(\bar{\rho}\phi) + \frac{\partial}{\partial x_j}(\bar{\rho}u_j\phi) = \frac{\partial}{\partial x_j}(\Gamma \frac{\partial \phi}{\partial x_j}) + S \quad (5.24)$$

For the continuity equation (Eq. (5.1)), $\bar{\rho}=1$, $\phi=1$, $\Gamma=0$ and $S=0$; for the momentum equation (Eq. (5.2)), $\bar{\rho}=1$, $\phi=u_i$, $\Gamma=\eta/\rho$ and

$S=-\frac{1}{\rho}\nabla p + \frac{\partial u_j}{\partial x_i} \frac{\partial}{\partial x_j}(\frac{\eta}{\rho})$; for the energy equation (Eq. (5.3)), $\bar{\rho}=\rho C_p$, $\phi=T$, $\Gamma=\kappa$

and $S=\eta\dot{\gamma}^2$; for the level set equation (Eq.(5.12)), they correspond to 1, ϕ , 0, and 0;

for the re-distancing equation (Eq.(5.14)), $\bar{\rho}=1$, $u_i=0$, $\Gamma=0$, and $S= \text{sign}(\phi)(1-|\nabla \xi|)$;

for the mass correction equation (Eq.(5.17)), $\bar{\rho}=1$, $u_i=0$, $\Gamma=0$, and $S=M_{\text{cor}}$.

The finite volume method of Partankar (1980) was used to solve the general equation (Eq.(5.24)). A fixed and staggered grid was used, with the scalar variables stored in the centers of the control volumes, while the velocities were located at the control volume faces (see Figure 5.2). The coupling between velocity and pressure

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was handled by the SIMPLER algorithm, and the diffusion-convection effect in the momentum equations was modeled by the power-law scheme. The fully implicit scheme was used to discretize the transient term. The upwind scheme was used to model the convection of the level set equations. The resulting algebraic equations were solved using the TriDiagonal Maxtrix Algorithm.

Figure 5.2 Schematic diagram of the staggered grid

5.3 Numerical model for pseudo-axisymmetric flow

In this investigation, the flow of polymer melt is not strictly axisymmetric during cavity filling due to the difference in surface roughness between the two semicircular halves of the core insert as illustrated in Figure 5.3. To simulate such a non-axisymmetric (or pseudo-axisymmetric) filling flow, the numerical procedure for simulating the axisymmetric filling flow was extended by using a newly proposed inlet-velocity iteration approach.

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Figure 5.3 Schematic diagram of the cavity filling encountered in the experiment

During the cavity filling, the polymer melt is assumed to enter the cavity with a uniform and constant velocity, pushing the air out of the cavity. Due to the difference in surface roughness between the two semicircular halves of the core insert, the speed of the melt flow will be different on the two halves, thus leading to different filling volumes (areas) on the two halves. However, the pressure on the separating line shared by the two semicircular halves will be the same. Following this physical reasoning, an inlet-velocity iterative approach was proposed and developed based on the procedure used for simulating the axisymmetric flow. For each individual half, axisymmetric flow is assumed, but each half has different velocity. For every time step, the inlet velocities on the two semicircular halves change simultaneously through iterations until the pressure at the center of the core insert for the two halves can be considered the same within a pre-defined tolerance. More details are given in the following.

At the beginning of the first time step, it is assumed that the inlet velocities on the two halves are the same, i.e.,

$$V_1 = V_2 = U_{in} \quad (5.25)$$

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where, V_1 and V_2 are inlet velocities for the smoother half and rougher half respectively, U_{in} is the physical inlet velocity.

As the surface roughness values used in the simulation for the two semicircular halves are different, the same inlet velocities for the two halves (i.e., V_1 and V_2) will result in different pressures at the center of the core insert, namely P_1 and P_2 . The difference between P_1 and P_2 is written as

$$\Delta P = P_1 - P_2 \quad (5.26)$$

To enforce the same pressure at the center of the core insert on the two halves, i.e., $\Delta P=0$, the inlet velocities for the two halves need to be adjusted simultaneously satisfying

$$V_1 + V_2 = 2U_{in} \quad (5.27)$$

The adjusted inlet velocities for the two halves can be written as

$$V_1 = V_1 - \Delta U \times \text{Sign}(1.0, \Delta P) \quad (5.28)$$

$$V_2 = 2U_{in} - V_1$$

where, ΔU is the change in the inlet velocities for the two halves for each iteration, which can be determined using

$$\Delta U = \beta U_{in} \quad (5.29)$$

where, β is the percentage of U_{in} , which typically ranges from 1% to 5%.

From Eq. (5.28), if $\Delta P > 0$, V_1 will be reduced in the next iteration in order to obtain a lower P_1 and a higher P_2 , and thus smaller ΔP . Similarly, if $\Delta P < 0$, V_1 will be increased in the next iteration in order to obtain a higher P_1 and a lower P_2 , and thus smaller ΔP .

As it is difficult or even impossible to make $\Delta P=0$ through the inlet-velocity iterations, a tolerance range of ΔP (i.e., PL) is defined in order to control the number of iterations of the inlet velocities for the two halves, which is written as

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$$\frac{|P_1 - P_2|}{0.5(P_1 + P_2)} < PL \quad (5.30)$$

where, PL is a percentage value typically taken as 1%, which can be varied depending on the required accuracy in ΔP between the two halves.

During the iteration of the inlet velocity, if Eq. (5.30) is not satisfied, the iteration will continue based on Eq. (5.28). Else, the iteration stops, and the simulation of the next time step starts. The inlet velocity iteration procedure repeats in the next time step. Figure 5.4 gives the flow chart of the inlet-velocity iteration procedure.

Figure 5.4 Flow chart of the inlet-velocity iteration procedure for simulation of the pseudo-axisymmetric flow

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5.4 Material properties of POM

Throughout this thesis, the material used in the simulation was POM (i.e., the same as the material used in the experiment) unless explicitly stated otherwise. The material data of POM, such as its density, viscosity, thermal conductivity and specific heat were obtained from the widely accepted Moldflow MPI 5.0 material database (Bhagavatula & Castro, 2007; Koh et al., 2004; H. L. Zhang et al., 2007a).

For POM, the coefficients in the modified two-domain Tait PVT model are given in Table 5.1. Figure 5.5 shows the predicted PVT data together with the material data of POM. The coefficients in the Cross-WLF model for POM are given in Table 5.2. Figure 5.6 shows the predicted viscosity together with the material data.

Table 5.1 Coefficients in the modified two-domain Tait PVT model for POM

b_{1m}	b_{2m}	b_{3m}	b_{4m}
0.000838 m ³ /kg	5.404e-7 m ³ /(kg.K)	1.51158e8 Pa	0.003952 1/K
b_{1s}	b_{2s}	b_{3s}	b_{4s}
0.0007642 m ³ /kg	4.506e-7 m ³ /(kg.K)	2.2726e8 Pa	0.004413 1/K
b₅	b₆	b₇	b₈
419.85 K	1.6e-7 K/Pa	7.45e-5 m ³ /kg	0.1091 1/K
b₉			
1.962e-8 1/Pa			

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Figure 5.5 Predicted PVT data using the modified two-domain Tait model and the material data of POM

Table 5.2 Coefficients in the Cross-WLF model for POM

Material	n	τ^* (Pa)	D_1 (Pa.s)	D_2 (K)	D_3	A_1	$\tilde{A}_2$ (K)
POM	0.382	2.29×10^5	7.54×10^{12}	223	0	28.5	51.6

Figure 5.6 Predicted viscosity using the Cross-WLF model and the material data of POM

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To take into account the variation in specific heat of POM (C_p) with temperature, a piecewise linear regression model against the material data was used (see Eq. (5.31)). Figure 5.7 shows the predicted data using the regression model together with the material data of POM. Other properties used in the simulation are given in Table 5.3.

$$C_p = \begin{cases} 10.8T - 1847 & 296K \leq T < 400K \\ 915T - 363056 & 400K \leq T < 413.8K \\ -1761T + 743796 & 413.8K < T < 421.6K \\ 1.65T + 1307 & T \geq 421.6K \end{cases} \quad (5.31)$$

Figure 5.7 Predicted specific heat using the regression model and the material data of POM

Table 5.3 Density, thermal conductivity and specific heat of POM melt, fictitious fluid and mold material used in the simulation

Material	ρ (kg/m ³)	κ (W/m.K)	C_p (J/kg.K)
POM melt	-	0.14	-
Fictitious fluid (air)	1.0	0.037	1.0
Mold (steel)	7800	29	460

5.5 Assessment of numerical accuracy

The developed numerical procedure was firstly applied to simulate the filling of a thin circular cavity with POM, without consideration of cavity surface roughness to evaluate the factors that influence numerical accuracy. In the simulation, the diameters of the inlet and the cavity are 0.4mm and 8mm respectively. The cavity thickness is 0.30mm and the inlet velocity is 19.6m/s. The melt and mold temperatures are 453K and 323K, respectively.

5.5.1 Effect of fictitious fluid viscosity

A fictitious fluid with viscosity of 1.0Pa.s, instead of air (where viscosity is in the order of 10^{-5} Pa.s), was used in the simulation throughout this thesis to enhance the stability and convergence of the numerical solution. To evaluate its effect on the numerical accuracy, Figure 5.8 shows the predicted pressure distribution along the radial direction in the cavity at different times. Point (0,0) denotes the position of the inlet where polymer melt enters and point (4,0), the position of the cavity boundary. The small circles indicate the flow front positions at different times, with polymer melt on the left and the fictitious fluid on the right side. It can be observed that the pressure drop caused by the fictitious fluid (from the flow front to the cavity boundary) is much smaller than the pressure drop caused by the polymer melt (from inlet to the flow front). This indicates that the use of the fictitious fluid with viscosity of 1.0Pa.s, instead of air, will not significantly influence the numerical accuracy.

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Figure 5.8 Predicted pressure distribution along the radial direction in the mold cavity

For further justification of the use of the fictitious fluid, the development of the cavity pressure at the center of the cavity was simulated by using different fictitious fluid viscosities (see Figure 5.9). Figure 5.10 gives the relative simulation differences for the different fictitious fluid viscosities, by comparing to the simulation result obtained using the viscosity of 0.01 Pa.s. The relative differences is defined as

$$Diff. = \frac{1}{n} \sum_{i=1}^n \left| \frac{P_i - P'_i}{P'_i} \right| \quad (5.32)$$

where, P_i is the predicted pressure at the i th time step by using a specific fictitious fluid viscosity, P'_i is the predicted pressure by using the viscosity of 0.01 Pa.s and n is total number of time steps. It can be observed that the simulation accuracy does not increase much by using a fictitious fluid viscosity smaller than 1.0 Pa.s (i.e., 0.1 Pa.s). Therefore, it is reasonable to use the fictitious fluid viscosity of 1.0 Pa.s in the simulation.

Figure 5.9 Predicted pressure development for different fictitious fluid viscosities at the center of cavity

Figure 5.10 Relative simulation differences for different fictitious fluid viscosities at a filling time of 5×10^{-3} s

5.5.2 Effect of number of grids

The number of grids used to discretize the computing domain has influence on the simulation accuracy. In general, the higher the number of grids used, the more accurate is the solution, but at the expense of computing time. Figure 5.11 shows the

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predicted pressure development at the center of the cavity for different number of grids. Figure 5.12 gives the relative differences of predicted pressure for the different numbers of grids, by comparing to the simulation result obtained using 30x300 grids. It can be observed that the simulation accuracy cannot be significantly improved by using grids more than 20x200. Therefore, in most cases, 20x200 grids are acceptable to save computing time without sacrificing significant accuracy.

Figure 5.11 Predicted pressure development for different number of grids

Figure 5.12 Relative simulation differences for different number of grids at a filling time of 3×10^{-3} s

5.5.3 Effect of time step

Although the value of time step used in the simulation will not cause divergence of the solution due to the implicit scheme used, it does influence the simulation accuracy. In general, using smaller time steps will result in more accurate simulation results but will require more computing time. Figure 5.13 shows the predicted pressure development at the center of the core insert for different time step values. Obvious differences in the predicted pressures for different time steps can be observed at the early filling stage (e.g., when filling time is less than 20×10^{-4} s). Such differences decrease with filling times. Figure 5.14 gives the relative differences of the predicted pressure for the different time step values, by comparing the simulation result obtained by using the time step of 0.625×10^{-4} s. It can be observed that the relative difference is significantly dependent on the time step. Therefore, a larger time step (e.g., 5×10^{-4} s) can only be used in cases where the effect of the initial filling stage is not of interest, whereas, a smaller time step should be used where the simulation results are to provide information on the initial filling stage.

Figure 5.13 Predicted pressure for different time step values

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Figure 5.14 Relative simulation differences for different time step values at a filling time of 5×10^{-3} s

5.6 Concluding remarks

In this chapter, a numerical procedure, which implements the finite volume method and the level set method and incorporates the proposed roughness model, was firstly presented for simulating the axisymmetric flow of the polymer melt. Subsequently, by using a newly proposed inlet-velocity iteration approach, the numerical procedure was extended to simulate the pseudo-axisymmetric flow encountered in the experiments. Finally, the simulation accuracy for different fictitious fluid viscosities, number of grids and time steps were evaluated.

In the numerical procedure, the level set method was used to capture the polymer flow front. The Cross-WLF model was used to model polymer melt viscosity. The modified two-domain Tait PVT model was employed to account for the variation in polymer density with temperature and pressure. The variation in specific heat of polymer with temperature was also taken into consideration. The fictitious fluid with viscosity of 1.0 Pa.s was introduced to replace the air downstream of the polymer flow

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front to enhance numerical convergence without sacrificing significantly simulation accuracy.

The finite volume method was used to solve the partial differential equations. A fixed and staggered grid, with the scalar variables stored in the centers of the control volumes, while the velocities were located at the control volume faces, were used for discretizing the computing domain. The coupling between velocity and pressure in the governing equations was handled by the SIMPLER algorithm. The diffusion-convection effect in the momentum equations was modeled by the power-law scheme. The fully implicit scheme was used to discretize the temporal term. The upwind scheme was used to model the convection terms in the level set equations. The resulting algebraic equations were solved using the TriDiagonal Maxtrix Algorithm.

The effect of the use of the fictitious fluid on the simulation accuracy was evaluated. It was justified that the use of the fictitious fluid with a viscosity of 1.0Pa.s, instead of air, will not lead to significant loss of simulation accuracy. Moreover, the simulation accuracy for different number of grids and time steps was investigated.

Chapter 6 Validations of roughness and numerical models

In this chapter, the numerical procedure for simulating the axisymmetric polymer flow was firstly validated by comparing its numerically predicted results of cavity pressure versus time with the experimentally measured data. Subsequently, the numerically predicted results of average filling flow length versus time were compared with both experimental and analytical data. For further validation, the numerical results of fully developed Newtonian and non-Newtonian modified power law flow were compared with the analytical results.

To validate the proposed roughness model and the proposed numerical procedure for simulating the pseudo-axisymmetric polymer flow encountered in the experiment, for each core insert, the numerically predicted results of flow area development on the rougher half versus the increasing total flow area of the molded part were compared with the experimental data. Moreover, the numerically predicted k values were compared with those obtained from the experiment.

6.1 Validations of the numerical model for axisymmetric filling flow

6.1.1 Experimental setup

The numerical procedure for simulating the axisymmetric polymer flow was validated by comparing its numerically predicted cavity pressure development with the experimentally measured data. A new core insert with a smooth surface (i.e., average roughness, $S_a=1.1\pm0.1\mu\text{m}$) was machined and used in the experiment. To measure cavity pressure, one piezoelectronic sensor of 1mm diameter is mounted inside the

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core insert as shown in Figure 6.1. The head of the sensor is located in the center of the core insert.

Figure 6.1 Pressure sensor and core insert assembly

A data acquisition system was designed to acquire the measured pressure data. Figure 6.2 shows the schematic connection diagram of the pressure acquisition system. Table 6.1 lists the parts used in the data acquisition system. The measured pressure is converted into electric charge, then amplified and converted into a voltage signal, and finally, registered by the computer through the NI-A/D card and visualized by DaisyLab software.

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Figure 6.2 Schematic connection diagram of the cavity pressure acquisition system.

Table 6.1 Part list of the cavity pressure acquisition system

No.	Description	Model	Qty
1	NI-A/D card	National Instruments PCI-6023E	1
2	Connecting block	National Instruments CB-68LP	1
3	Junction box		1
4	Miniature charge amplifier	Kistler 5039A232	1
5	Quartz miniature force sensor	Kistler 9211	1
6	Cavity pressure sensor	Kistler 6183AE	1

6.1.2 Cavity pressure versus filling time

As the cavity pressure sensor measures the average pressure over an area of 1mm diameter as illustrated in Figure 6.3, in the simulation, the corresponding average pressure (P_{ave}) was calculated according to the following expression:

$$P_{ave} = \frac{\int_0^A p dA}{\int_0^A dA} = \frac{\int_0^{0.5} p 2\pi r dr}{\int_0^{0.5} 2\pi r dr} = \frac{\int_0^{0.5} p 2\pi r dr}{[\pi r^2]_0^{0.5}} \quad (6.1)$$

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Figure 6.3 Pressure distribution over the cavity pressure sensor

Figures 6.4 – 6.7 show the numerically predicted and experimentally measured cavity pressures versus filling time for different melt and mold temperatures. The cavity thickness was 0.36mm. The injection rate was $2.8\text{cm}^3/\text{s}$. For each combination of the melt and mold temperatures, three cavity pressure curves were experimentally obtained. Reasonable agreement was observed, with the numerically predicted pressure curves lying within or close to the band formed by the experimental curves.

Figure 6.4 Numerically predicted and experimentally measured cavity pressure curves for $T_{\text{melt}}=453\text{K}$ and $T_{\text{mold}}=323\text{K}$

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Figure 6.5 Numerically predicted and experimentally measured cavity pressure curves for $T_{\text{melt}}=453\text{K}$ and $T_{\text{mold}}=383\text{K}$

Figure 6.6 Numerically predicted and experimentally measured cavity pressure curves for $T_{\text{melt}}=473\text{K}$ and $T_{\text{mold}}=323\text{K}$

Figure 6.7 Numerically predicted and experimentally measured cavity pressure curves for $T_{\text{melt}}=473\text{K}$ and $T_{\text{mold}}=383\text{K}$

6.1.3 Average flow front position versus filling time

To achieve different flow front positions during cavity filling, short shot experiments were performed through varying injection pressure and dosage while keeping the injection rate constant at $3.0\text{cm}^3/\text{s}$. Figure 6.8 shows the molded parts with different filling flow length.

Figure 6.8 Molded parts with different filling flow length

The average filling flow length, represented by the equivalent radius of the molded part, can be derived from the measured flow area of the molded part as:

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$$R_f = \sqrt{\frac{A_f}{\pi}} \quad (6.2)$$

where, R_f is the equivalent filling flow length and A_f the measured flow area. The corresponding filling time can be obtained as:

$$t_f = \frac{A_f H_{cav}}{R_{inj}} \quad (6.3)$$

where, t_f is filling time, H_{cav} cavity thickness and R_{inj} injection rate.

For each change in the processing parameters (i.e., injection pressure or dosage), three molded samples were collected for the determination of the average filling flow length (i.e., R_f). On the other hand, the average filling flow length can be analytically obtained by using the mass conservation principle through the following procedure.

The volume of the melt entering the cavity during time t can be expressed as

$$Vol_{in} = \frac{U_{in} \pi d_1^2}{4} \quad (6.4)$$

where, U_{in} is the velocity at the inlet and d_1 is the diameter of the inlet.

For flow with its filling flow length of r , the volume of melt in the cavity can be written as

$$Vol_{ca} = \pi r^2 H_{eff} \quad (6.5)$$

where, H_{eff} is the effective cavity thickness.

For the initial flow front position of $r = d_{ini}/2$, the initial volume of the melt in the cavity is

$$Vol_{ini} = \frac{\pi d_{ini}^2 H_{eff}}{4} \quad (6.6)$$

According to the mass conservation principle, the melt volume in the cavity at time t equals to the sum of its initial volume in the cavity and the volume entering the cavity, i.e.,

$$\text{Vol}_{\text{ca}} = \text{Vol}_{\text{ini}} + \text{Vol}_{\text{in}} \quad (6.7)$$

Therefore, the average position of the melt front in the radial direction at time t can be obtained analytically as:

$$r(t) = \sqrt{\frac{d_{\text{ini}}^2 H_{\text{eff}} + d_1^2 U_{\text{in}} t}{4H_{\text{eff}}}} \quad (6.8)$$

Figure 6.9 shows the experimental, analytical and simulation results of the average flow front position versus filling time, as well as the relative simulation errors to the experimental and analytical data. It can be observed that the simulation result is in good agreement with both the experimental and the analytical results.

Figure 6.9 Experimental, analytical and simulation results of average flow front position versus filling time

6.1.4 Fully developed flow

For further validation of the numerical procedure, simulations of fully developed flow of Newtonian and non-Newtonian modified power law (MPL) fluids in an

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axisymmetric geometry were performed. The simulation results were compared to the theoretical results.

For a fully developed laminar flow of Newtonian fluid in an axisymmetric geometry, the Poiseuille number, i.e., the product of the friction factor (f) and the Reynolds number (Re), is a constant and equals to 64, i.e.,

$$fRe=64, \quad Re = \frac{\rho \bar{U} D_h}{\eta} \quad (6.9)$$

where, D_h is the hydraulic diameter.

Moreover, the velocity profile can be expressed as

$$u = 2\bar{U} \left[1 - \left(\frac{r}{R} \right)^2 \right] \quad (6.10)$$

The numerically predicted Poiseuille number for the Newtonian fluid flow is 63.96, which is very close to the theoretical result (i.e., 64). Figure 6.10 shows the good agreement between the simulation and theoretical results for the velocity profile.

Figure 6.10 Simulation and theoretical results of the velocity profile for a fully developed Newtonian flow in an axisymmetric geometry

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For fully developed non-Newtonian modified power law (MPL) flow in an axisymmetric geometry, Poiseuille number (i.e., fR_e) is a constant depending on the flow index, n , and the shear rate parameter, β , which can be generally expressed as (Kreith, 2000)

$$f \cdot Re = \frac{1 + \beta}{\frac{1}{64} + \frac{\beta}{2^{3n+3} \left(\frac{3n+1}{4n}\right)^n}} \quad (6.11)$$

$$f = \frac{2 \frac{\Delta p}{L} D_h}{\rho \bar{U}^2}, \quad Re = \frac{\rho \bar{U} D_h}{\eta^*}, \quad \eta^* = \frac{\eta_0}{1 + \beta}, \quad \beta = \frac{\eta_0}{m} \left(\frac{\bar{U}}{D_h} \right)^{1-n} \quad (6.12)$$

where, η_0 , m and n are constants in the MPL viscosity model.

Table 6.2 gives the theoretical and numerical results of fR_e for different η_0 , m and n values in the MPL model. Good agreement was achieved, i.e., the maximum relative simulation error is 1.3%.

Table 6.2 The analytical and simulation results of fR_e for non-Newtonian MPL fluid flow in an axisymmetric geometry

η_0	m	n	Analytical fR_e (V_a)	Predicted fR_e (V_b)	Simulation error $\left \frac{V_b - V_a}{V_a} \right \times 100\%$
486.33	17795.55	0.41	44.9	45.5	1.3%
381.63	15895.24	0.42	46.5	46.9	0.9%
302.87	15103.00	0.42	47.8	48.2	0.8%

6.1.5 Concluding remarks

The numerical procedure for simulating the axisymmetric filling flow was validated from several aspects. Firstly, the numerically predicted cavity pressures at different melt and mold temperatures were compared with the experimentally measured cavity pressures. Reasonable agreement between the numerical and the experimental results

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was achieved. Subsequently, the numerically predicted result of flow front positions versus time was compared to both experimental and analytical results. The numerical results were in good agreement with the experimental and analytical data. For further validation of the numerical procedure, simulations of fully developed Newtonian and non-Newtonian MPL fluid flow were performed. The simulation results were also in good agreement with the analytical results. Therefore, the developed numerical procedure for simulating the axisymmetric flow is effective and accurate for numerical investigations of mold filling in micro injection molding.

6.2 Validations of the roughness model and the numerical model for the pseudo-axisymmetric filling flow

6.2.1 Description of simulation cases

To validate the proposed roughness model and the numerical model for simulating the pseudo-axisymmetric filling flow encountered in the experiment, for each of the four core inserts, the numerically predicted flow area development on the rougher half versus the increasing total flow area were compared with the experimentally measured data. The numerically predicted k values were also compared with the experimental data.

In the simulation, the three-dimensional homogeneous pyramid roughness profile was used to represent the physical roughness of the core inserts. To justify this, the measured roughness profiles of the core inserts were compared with the homogeneous pyramid roughness profile. Figure 6.11 gives five typical two-dimensional roughness profiles of the rougher half of core insert II. The measured volume fraction (θ) on the roughness mean plane for these profiles is $\theta=0.49\pm0.03$, which is close to 0.5 of the homogenous pyramid profile. Moreover, from its appearance in Figure 6.12, the

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measured three-dimensional roughness profile is similar to the homogeneous pyramid roughness profile.

Figure 6.11 Two-dimensional roughness profiles of the rougher half of core insert II

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Figure 6.12 Three-dimensional roughness profiles of the rougher half of core insert II

To check whether the roughness effect is isotropic in different directions, the two-dimensional average roughness (R_a) was measured in four different directions as illustrated in Figure 6.13. For each core insert, three square regions were measured. Table 6.3 gives the measured R_a values in the four directions for the four core inserts. It can be observed that for each core insert, the measured R_a values in the different directions are comparable. This indicates that the roughness effects in different directions can be considered isotropic.

Figure 6.13 Schematic diagram of roughness measurement in different directions

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Table 6.3 Measurement results of R_a in different directions for the four core inserts (μm)

Insert	Measurement direction	Measurement Region			Average	Standard deviation
		1	2	3		
I	1	9	9	7	8	1
	2	8	11	8	9	2
	3	10	9	9	9	1
	4	7	7	7	7	0
II	1	10	6	6	7	2
	2	10	7	8	8	2
	3	8	9	7	8	1
	4	9	10	11	10	1
III	1	5	6	4	5	1
	2	5	4	4	4	1
	3	5	5	5	5	0
	4	5	6	4	5	1
IV	1	6	13	9	9	3
	2	10	9	9	9	0
	3	10	6	10	9	2
	4	13	9	10	11	2

In the simulation, the thickness of the molded part was used to represent the cavity thickness (The measurement results of the thickness for the four core inserts were given in Appendix D). For the three-dimensional pyramid roughness profile, the effective roughness height (δ) is three times of the measured average roughness (S_a). The height difference between the mean planes of the two semicircular halves of the core insert (Δd) was also taken into consideration. Table 6.4 gives the cavity thickness, effective roughness height (δ) and Δd values used in the simulation for the four core inserts.

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Table 6.4 Cavity thickness, effective roughness height and Δd values used in the simulation

Insert	Cavity thickness (mm)	Effective roughness height on rougher half (μm)	Effective roughness height on smoother half (μm)	Δd (μm)
I	0.30	43	1	-2
II	0.30	50	1	0
III	0.20	26	1	-2
IV	0.24	44	10	0

The diameters of the inlet and the cavity, and the melt and mold temperatures used in the simulation were the same as those used in the experiment. The injection rate was $2.5\text{cm}^3/\text{s}$, which is in the same order as used in the experiment.

6.2.2 Comparison of flow area development

For core insert I, Figure 6.14 shows the experimentally measured and numerically predicted flow area of the rougher half versus the increasing total flow area for different melt and mold temperatures. The absolute and relative simulation errors were also given. It can be observed that the relative simulation errors are close to 10%. Figure 6.15 gives the k values obtained by linear fitting to the experimental and numerical data. Also, the relative simulation errors are less than 10%. Thus, the simulation results are in good agreement with the experimental data for core insert I.

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(a)

(b)

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(c)

(d)

Figure 6.14 Experimentally measured and numerically predicted flow area of the rougher half for core insert I for: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

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Figure 6.15 Experimental and numerically predicted k values for core insert I

For core insert II, Figure 6.16 shows the experimentally measured and numerically predicted flow area of the rougher half versus the increasing total flow area for different melt and mold temperatures. The relative simulation errors are less than 10%. Figure 6.17 gives the k values obtained by linear fitting to the experimental and numerical data. The maximum relative simulation error is 6%. The simulation results are in good agreement with the experimental data for core insert II.

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(a)

(b)

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(c)

(d)

Figure 6.16 Experimentally measured and numerically predicted flow area of the rougher half for core insert II for: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

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Figure 6.17 Experimental and numerically predicted k values for core insert II

For core insert III, Figure 6.18 shows the experimentally measured and numerically predicted flow area of the rougher half versus the increasing total flow area for different melt and mold temperatures. The relative simulation errors are less than 20%. Figure 6.19 gives the k values obtained by linear fitting to the experimental and numerical data. The relative simulation errors are less than 15%. The simulation results are in an acceptable agreement with the experimental data for core insert III.

Chapter 6: Validations of Roughness and Numerical Models

(a)

(b)

Chapter 6: Validations of Roughness and Numerical Models

(c)

(d)

Figure 6.18 Experimentally measured and numerically predicted flow area of the rougher half for core insert III for: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

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Figure 6.19 Experimental and numerically predicted k values for core insert III

For core insert IV, Figure 6.20 shows the experimentally measured and numerically predicted flow area of the rougher half versus the increasing total flow area for different melt and mold temperatures. The relative simulation errors are less than 10%. Figure 6.21 gives the k values obtained by linear fitting to the experimental and numerical data. The maximum relative simulation error is 7%. The simulation results are in good agreement with the experimental data for core insert IV.

Chapter 6: Validations of Roughness and Numerical Models

(a)

(b)

Chapter 6: Validations of Roughness and Numerical Models

(c)

(d)

Figure 6.20 Experimentally measured and numerically predicted flow area of the rougher half for core insert IV for: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

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Figure 6.21 Experimental and numerically predicted k values for core insert IV

6.2.3 Concluding remarks

Among the sixteen simulation cases, the relative simulation errors are close or less than 10% for fifteen cases, and 20% for one case. Therefore, the simulation results are in good agreement with the experimental data. Moreover, for the four core inserts, the simulation results reveal that the roughness effects are more significant at the lower mold temperature level when the melt temperature was kept constant, and more significant at the lower melt temperature level when the mold temperature was kept constant. This also agrees with the observations obtained from the experiments. Therefore, the proposed roughness model and the numerical model for simulating the pseudo-axisymmetric polymer flow encountered in the experiments are valid and effective for numerical investigation of the roughness effects in micro injection molding.

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Besides the experimental errors, the factors that may contribute to the differences between the experimental and simulation results include: (1) the effect of the separating line between the two semicircular halves of the core insert used in the experiment was not taken into consideration in the simulation; (2) the limitation of the roughness model, which uses three-dimensional homogeneous pyramid roughness profile to represent the physical roughness profile of the core insert; (3) the limitation of simulation accuracy, which assumes pseudo-axisymmetry, i.e., axisymmetry exists individually for each half.

Chapter 7 Further explorations of roughness effects

In this chapter, the roughness effects on the quantities that are not easily measured experimentally were further explored through numerical simulation. Firstly, filling of the cavity that has different roughness on its two semicircular halves of the core insert was investigated, including the inlet-velocity development on the two cavity halves during mold filling, the roughness effect (i.e., the k value) for different cavity thicknesses and for different injection velocities. The filling of the cavity having uniform roughness was then discussed. The fluid flow profiles of temperature, velocity, viscosity and shear rate for different roughness values and different melt and mold temperatures, were investigated. Furthermore, for different roughness profiles, the roughness effect on the cavity pressure was investigated.

7.1 Filling of the cavity having different roughness on its two semicircular halves

7.1.1 Inlet-velocity development on the two cavity halves

Under the roughness effects, the equivalent inlet-velocities on the two semicircular cavity halves are different, i.e., the inlet-velocity on the smoother half is larger than that on the rougher half. Figure 7.1 shows the numerically predicted development of the inlet velocities on the two cavity halves for different mold and melt temperatures. The injection velocity was 19.6m/s and cavity thickness 0.30mm. The three-dimensional homogeneous pyramid roughness profile was used. The effective roughness heights (δ) on the two halves were 50 μ m and 0 μ m respectively. It can be observed that the change in the inlet-velocities on the two halves is fast at the initial filling stage, e.g. earlier than 1×10^{-3} s as shown in Figure 7.1a. After that, the change in the inlet-velocities on the two halves is slow. Moreover, the development of the

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inlet-velocities on the two halves is obviously affected by the mold and melt temperatures. When the melt temperature is kept constant, the overall difference in the inlet-velocities between the two halves is bigger at the lower mold temperature. Similarly, when the mold temperature is kept constant, the overall difference in the inlet-velocities between the two halves is bigger at the lower melt temperature.

(a)

(b)

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(c)

(d)

Figure 7.1 Development of the inlet-velocities on the two cavity halves for: (a) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=323\text{K}$, (b) $T_{\text{melt}}=453\text{K}$, $T_{\text{mold}}=383\text{K}$, (c) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=323\text{K}$, (d) $T_{\text{melt}}=473\text{K}$, $T_{\text{mold}}=383\text{K}$

7.1.2 Roughness effects for different cavity thicknesses

Figure 7.2 shows the numerically predicted k values together with the regression fitting curve against the k values for the cavity thicknesses of 50 μm , 100 μm , 200 μm , 400 μm and 800 μm . The mold and melt temperatures were 323K and 453K respectively. The effective roughness height (δ) was 40 μm , the inlet velocity 19.6m/s and the time step 1×10^{-5} s. In general, the roughness effects (i.e., referring to the k value) decrease with an increase in cavity thickness (a k value of 0.5 indicates that the roughness effect is negligible). The logarithm function can be used to approximate the relationship between the k value and the cavity thickness. When the cavity thickness is less than 400 μm , i.e., the ratio between the effective roughness height (δ) and cavity thickness is 10%, a decrease in cavity thickness will result in an obvious increase in the roughness effects. However, when the cavity thickness is greater than 400 μm , the change in the k value is less obvious.

Figure 7.2 k values for different cavity thicknesses with $T_{\text{melt}}=453\text{K}$ and $T_{\text{mold}}=323\text{K}$

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7.1.3 Roughness effects for different injection velocities

Figure 7.3 shows the numerically predicted k values for the injection velocities of 0.1m/s, 1m/s, 10m/s and 100m/s. The mold and melt temperatures were 323K and 453K respectively. The effective roughness height (δ), the cavity thickness and the time step were 40 μ m, 0.10mm and 1×10^{-5} s respectively. In general, the roughness effects (i.e., referring to the k value) decrease with an increase in the injection velocity. For injection velocities less than 1m/s, a change in injection velocity will result in a great change in the roughness effects (i.e., the higher the injection velocity, the less significant the roughness effects). However, when the injection velocity is greater than 1m/s, a change in the velocity will only result in a small change in k value. This justifies the assumption made in the experiment that a small variation of injection rate will not lead to a significant change in the k value as the injection velocity used in the experiment is typically greater than 19.6m/s.

Figure 7.3 k values for different injection velocities with $T_{\text{melt}}=453\text{K}$ and $T_{\text{mold}}=323\text{K}$

7.2 Filling into the cavity of uniform roughness

In this section, the roughness effects were investigated through numerical simulation of filling polymer melt (i.e., POM) into a thin disk-shaped mold cavity, which has a smooth cavity wall (i.e., no roughness) and a rough core wall. The cross-sectional flow profiles of velocity, temperature, viscosity, shear rate, as well as cavity pressure, different roughness values, various mold and melt temperatures and different roughness profiles were investigated.

7.2.1 Problem description

Figure 7.4 shows the schematic diagram of the problem considered. The diameters of the inlet and the cavity are 0.4mm and 8mm respectively. The cavity thickness (H) is 0.30mm. The cavity wall is assumed to have no surface roughness and the core wall is assumed to have a three-dimensional homogenous pyramid roughness profile unless explicitly stated otherwise. The polymer melt enters the cavity with a constant and uniform velocity (i.e., 19.6m/s), pushing the air out. It is reasonable to assume that the polymer flow is axisymmetric during cavity filling, therefore, only two-dimensional axisymmetric analysis was performed.

Figure 7.4 Schematic diagram of the problem

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7.2.2 Roughness effect on the temperature profile

According to the proposed roughness model, surface roughness influences the temperature profile of the filling polymer. Figure 7.5 shows the predicted thermal patterns of the polymer flow in the cavity with no roughness on its core wall at different time. The melt and mold temperatures were 453K and 323K respectively. It can be observed that the thermal boundary layer near the core wall is very thin (the thickness of thermal boundary layer is defined as the distance from the wall to the position where the melt temperature is 99% of the inlet melt temperature (i.e., 453K)). The thickness of the thermal boundary layer increases with time due to heat transfer between the polymer melt and the mold.

Figure 7.5 Thermal patterns at different time in the smooth cavity

Figure 7.6 shows the predicted temperature patterns in the cavity with roughness ($\delta = 40\mu\text{m}$) on its core wall at different time. Compared with Figure 7.5, the thermal boundary layer at the core wall is thicker. This is because the thermal conductivity of the roughness layer increases due to roughness effects, which enhances heat transfer between the polymer flow and the mold.

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Figure 7.6 Thermal patterns at different time in the cavity with roughness

Figure 7.7 shows the temperature profiles of the polymer at the filling time of 0.005s and at the cross-section of $r=2.0\text{mm}$ for the cavity with roughness values of $\delta=0$, $40\mu\text{m}$ and $80\mu\text{m}$. As expected, the higher the roughness, the thicker is the thermal boundary layer. This can be explained by the high thermal conductivity ratio between the mold material (i.e., 29W/m.k) and the polymer melt (i.e., 0.14W/m.k), which results in high thermal conductivity of the roughness layer, and thus, smaller temperature gradient in the roughness layer. It should also be pointed out that the maximum flow temperature near the roughness layer is lower for higher roughness.

Figure 7.8 shows the cross-sectional temperature profiles of the polymer for different mold temperatures (i.e., 323K , 383K and 453K). The melt temperature was kept constant at 453K . The effective roughness height was $40\mu\text{m}$. With an increase in mold temperature, the thickness of thermal boundary layer near the core wall decreased, and vanished when the mold temperature was the same as the inlet melt temperature (i.e., 453K). This indicates that the significance of roughness effects decreases with an increase in the mold temperature when the melt temperature is kept constant.

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Figure 7.9 shows the cross-sectional temperature profiles of the polymer flow for different inlet melt temperatures (i.e., 453K, 473K and 493K). The mold temperature was kept constant at 453K. The effective roughness height was $40\mu\text{m}$. It can be observed that an increase in the melt temperature does not result in an obvious difference in the temperature distribution within the roughness layer, although the temperature profiles outside the roughness layer are quite different. This is also due to the high thermal conductivity ratio between the mold and the polymer melt.

Figure 7.7 Temperature profiles at the cross-section of $r=2.0\text{mm}$ for different roughness values

Figure 7.8 Temperature profiles for different mold temperatures

Figure 7.9 Temperature profiles for different melt temperatures

7.2.3 Roughness effect on the velocity profile

Figure 7.10 shows the velocity profiles at the cross-section of $r=2.0\text{mm}$ for different roughness values. The melt and mold temperatures were 453K and 323K respectively. Similar to the roughness effect on the flow temperature profile, the thickness of the velocity boundary layer near the core wall increases with an increase in the roughness (the thickness of velocity boundary layer is defined as the distance from the wall to the position where the velocity is 99% of the cross-sectional average velocity). Moreover, it can be observed that the higher the roughness value, the larger is the maximum velocity at the vicinity of the center of the cross section.

Figure 7.11 shows the flow velocity profiles at the cross-section of $r=2.0\text{mm}$ for different mold temperatures. The melt temperature was kept constant at 453K . It can be observed that the velocity gradient within the roughness layer increases with an increase in mold temperature. As a result, the flow velocity profile is more blunted for a high mold temperature, which indicates that the significance of roughness effect on the flow velocity profile decreases with an increase in the mold temperature.

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Figure 7.12 shows the flow velocity profiles at the cross-section of $r=2.0\text{mm}$ for different melt temperatures. The mold temperature was kept constant at 323K . It can be observed that there is only a slight difference in the flow velocity profiles within the roughness layer for the different melt temperatures. This is because the flow temperature within the roughness layer is less dependent on its inlet melt temperature, which results in almost the same melt viscosity within the roughness layer for the different melt temperatures, and thus almost the same velocity gradient.

Figure 7.10 Radial velocity profiles at the cross-section of $r=2.0\text{mm}$ for different roughness values

Figure 7.11 Radial velocity profiles for different mold temperatures

Figure 7.12 Radial velocity profiles for different melt temperatures

7.2.4 Roughness effect on the viscosity profile

Roughness influences the flow viscosity through its effect on the melt flow temperature. Figure 7.13 shows the flow viscosity profiles at the cross-section of $r=2\text{mm}$ for different roughness values. The melt and mold temperatures were 453K and 323K respectively. As expected, the flow viscosity within the roughness layer increases with an increase in the roughness value.

Figure 7.14 shows the flow viscosity profiles for different mold temperatures. The melt temperature was kept constant at 453K. The flow viscosity within the roughness layer decreases with an increase in mold temperature.

Figure 7.15 shows the flow viscosity profiles for different melt temperatures. The mold temperature was kept constant at 323K. Within the roughness layer, no obvious difference in the flow viscosity is observed. However, there is a difference in the viscosity outside the roughness layer between the melt temperatures of 453K and 473K.

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Figure 7.13 Viscosity profiles at the cross-section of $r=2.0\text{mm}$ for different roughness values

Figure 7.14 Viscosity profiles for different mold temperatures

Figure 7.15 Viscosity profiles for different melt temperatures

7.2.5 Roughness effect on the shear rate profile

Figure 7.16 shows the flow shear rate profiles at the cross-section of $r=2\text{mm}$ for different roughness values. The melt and mold temperatures were 453K and 323K respectively. It can be observed that the locations of the maximum shear rate near the core wall are different for different roughness. The maximum shear rate occurs in the vicinity of the top of the roughness layer.

Figure 7.17 shows the flow shear rate profiles for different mold temperatures. The melt temperature was kept constant at 453K. Within the roughness layer, the shear rate decreases with an increase in the mold temperature.

Figure 7.18 shows the flow shear rate profiles for different melt temperatures. The mold temperature was kept constant at 323K. Within the roughness layer, no obvious difference in the flow shear rate is observed. However, the difference outside the roughness layer is observed between the melt temperatures of 453K and 473K.

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Figure 7.16 Shear rate profiles at the cross-section of $r=2\text{mm}$ for different roughness values

Figure 7.17 Shear rate profiles for different mold temperatures

Figure 7.18 Shear rate profiles for different melt temperatures

7.2.6 Roughness effect on the cavity pressure

Figure 7.19 shows the pressure development at the center of the core insert for different roughness values. The melt and mold temperatures were 453K and 323K, respectively. As expected, for the same filling time, a higher pressure is required for a surface of higher roughness.

Figure 7.20 shows the pressure development for different mold temperatures. The melt temperature was kept constant at 453K. For the same filling time, a lower pressure is required for filling of a mold of higher temperature, e.g., for the same filling time of 0.004s, the pressure required is 40MPa, 37MPa and 33MPa for a mold temperature of 323K, 383K and 453K respectively.

Figure 7.21 shows the pressure development for different melt temperatures. The mold temperature was kept constant at 323K. Similarly, for the same filling time, a lower pressure is required for a melt of higher temperature, e.g., for the same filling time of 0.004s, the pressure required is 40.0MPa, 29.1MPa and 29.0MPa for a melt

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temperature of 453K, 473K and 493K respectively. However, it should be noted that there is only a slight difference in the pressures between the melt temperatures of 473K and 493K.

Figure 7.19 Pressure development for different roughness values

Figure 7.20 Pressure development for different mold temperatures

Figure 7.21 Pressure development for different melt temperatures

To investigate whether different roughness profiles with the same effective height (δ) have similar effects, the cavity pressures for filling the mold cavity with a homogenous square column profile and pyramid profile were investigated. The effective roughness heights (δ) of the two roughness profiles are the same, i.e., $\delta=40\mu\text{m}$. The melt and mold temperatures were 323K and 453K respectively. Figure 7.22 shows the predicted pressure development for the two different roughness profiles. For the same filling time, the pressure for the square column profile is higher than that for the pyramid profile. This is because the thermal conductivity of the roughness layer for the square column profile is higher than that of the pyramid profile, which results in lower flow temperature and thus higher overall flow viscosity within the roughness layer.

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Figure 7.22 Pressure development for different roughness profiles with the same effective roughness height

As the average roughness (i.e., S_a) is widely used in engineering practice, it is necessary to investigate whether different roughness profiles with the same S_a have similar effects. Figure 7.23 shows the pressure development for filling the cavity with the homogenous square column profile and pyramid profile. The two roughness profiles have the same S_a (i.e., $40\mu\text{m}$). The melt and mold temperatures were 323K and 453K, respectively. It can be observed that the pressure development curves for the two roughness profiles are quite different, i.e., for the same filling time, the pressure for the pyramid profile is obviously higher than that for the square column profile. This is because, for the same S_a (i.e., $40\mu\text{m}$), the corresponding effective roughness height (δ) is $120\mu\text{m}$ for the pyramid profile and $40\mu\text{m}$ for the square column profile. Therefore, the effective roughness height (δ), instead of the average roughness (S_a), is a determining factor for the roughness effects.

Figure 7.23 Pressure development for different roughness profiles with the same S_a

7.2.7 Concluding remarks

In this chapter, further explorations of the roughness effects on the quantities not easily measured experimentally were performed through numerical simulation. Firstly, filling of the cavity with different roughness on the two semicircular halves of the core wall was numerically investigated. Subsequently, filling of the cavity having uniform roughness on its core wall was discussed.

For the filling of the cavity having different roughness on the two semicircular halves of the core wall, it was observed that:

- Under the roughness effect, the equivalent inlet-velocity on the smoother cavity half was higher than that on the rougher half. The overall difference in the inlet-velocity between the two halves is dependent on the melt and mold temperatures, i.e., the higher the mold temperature, the smaller is the difference. Similarly, the higher the melt temperature, the smaller is the difference.

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- The significance of roughness effects (i.e., the k value) is dependent on the mold cavity thickness. The larger the thickness, the less significant is the roughness effect. The relationship between the k value and the cavity thickness can be approximated by a logarithm function.
- The significance of roughness effects (i.e., the k value) is dependent on the injection velocity. The higher the injection velocity, the less significant is the roughness effect. However, in the high injection velocity range (e.g., greater than 10m/s), a change in the injection velocity will not result in a significant change in the k value.

For the filling of the cavity having uniform roughness on its core wall, it was observed that:

- The significance of roughness effects on the temperature profile and on the velocity profile is mainly dependent on the effective roughness height and mold temperature, but less dependent on the melt temperature. This can be explained by the high thermal conductivity ratio between the mold material and the polymer melt. When the mold temperature is lower than the inlet melt temperature, the presence of roughness will increase the thickness of thermal boundary layer of the polymer flow, as well as the thickness of the velocity boundary layer.
- The roughness will increase the polymer flow viscosity within the roughness layer when the mold temperature is lower than the melt temperature. With an increase in the mold temperature, the roughness effect decreases and vanishes when the mold temperature is the same as the inlet melt temperature.
- The roughness will change the location of the maximum shear rate near the roughness layer when the mold temperature is lower than the melt temperature.

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In general, the maximum shear rate occurs in the vicinity of the top of roughness layer. With an increase in the mold temperature, the roughness effect decreases.

- When the mold temperature is lower than the melt temperature, higher pressure is required for filling the cavity with higher roughness. With an increase in mold temperature, the required pressure decreases. Similarly, with an increase in melt temperature, the required pressure decreases, although such decrease is not quite obvious in some situations.
- For the two different roughness profiles with the same effective roughness height, the pressure required for filling the cavity with the square column profile is higher than that for filling the cavity with the pyramid profile.
- For the two different roughness profiles with the same average roughness, the pressure required for filling the cavity with the pyramid profile is obviously higher than that for filling the cavity with the square column profile.
- The effective roughness height (δ), instead of the average roughness (S_a), is a determining factor for the roughness effects.

Chapter 8 Conclusions and recommendations

In this thesis, the roughness effects on cavity filling in micro injection molding process were for the first time mathematically modeled and systematically investigated through experiments and numerical simulations.

Firstly, the surface roughness was mathematically modeled. Secondly, experimental investigations of polymer filling into a disk-shaped micro-thickness cavity mold were carried out. The effects of roughness on the filling of the cavity were conclusively demonstrated by using four round core inserts, where each insert consists of two semicircular halves of different roughness. Thirdly, a numerical procedure for axisymmetric filling of polymer flow was presented. This numerical procedure was then extended to simulate the pseudo-axisymmetric flow filling encountered in the experiments by using a newly proposed inlet-velocity iteration approach. Fourthly, the proposed numerical procedures and the roughness model were validated by comparing the numerically predicted results with the experimentally measured or analytical data. Finally, the roughness effects on the quantities not easily measured experimentally were further explored through numerical simulations.

A simple but effective formulation was proposed to model the roughness effects. Effective dimensions were proposed to represent the geometry of mold cavity in the analysis of micro injection molding as opposed to the dimensions used in a conventional analysis. The physical surface roughness is represented by the proposed homogenous roughness profile, which is characterized by the effective roughness height (δ) and the volume fraction parameter (θ). The thermal properties of the roughness layer, such as thermal conductivity and heat capacity, are determined by combining those of polymer melt and of mold material, depending on the effective roughness height and the volume fraction parameter (θ).

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In the experiments, the effects of roughness on the filling of the cavity were demonstrated by having different roughness on the two semicircular halves of the round core insert. Four round core inserts were machined and used respectively to form the core wall of the cavity while keeping the cavity wall fixed. The significance of the roughness effects was quantitatively represented by the ratio of the flow area of the rougher half to the total flow area of the molded part. The significance of roughness effects (i.e., the k value) for different mold and melt temperatures were investigated with the aid of the two-sample t test. The dependence of roughness effects on roughness magnitude and cavity thickness was also demonstrated.

In the numerical procedures, the level set method was employed to capture the polymer flow front. The fictitious fluid approach, which is similar to the pseudo-concentration method, was adopted to enhance the stability and convergence of the numerical solution. The variation in polymer density with temperature and pressure was taken into account by using the modified two-domain Tait model. The variation in specific heat of polymer with temperature was also considered. The Cross-WLF law was used to model the non-Newtonian viscosity of polymer melt.

The numerical procedure for axisymmetric filling of polymer was first validated by comparing its numerically predicted results of cavity pressure versus time with the experimentally measured data. Subsequently, the numerically predicted results of the average filling flow length versus time were compared with both experimental and analytical data. For further validation, the numerical results of fully developed Newtonian and non-Newtonian modified power law flows were compared with the analytical results. To validate the proposed roughness model and the proposed numerical procedure for the pseudo-axisymmetric filling of polymer encountered in the experiments, for each core insert, the numerically predicted results of flow area

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development on the rougher half versus the increasing total flow area of the molded part were compared with the experimental data. Moreover, the numerically predicted k values were compared with those obtained from the experiments.

The roughness effects on the quantities not easily measured experimentally were further explored by using the proposed numerical procedures. For filling of the mold cavity having different roughness on its two halves, the roughness effects on the inlet-velocity development on the two halves were investigated. Subsequently, the roughness effects for different cavity thicknesses and injection velocities were discussed. For filling of the mold cavity of uniform roughness, the roughness effects on the flow profiles of temperature, velocity, viscosity, shear rate, as well as cavity pressure, were studied.

8.1 Conclusions

1. The proposed roughness model is effective for taking into account the roughness effects in plastic micro injection molding. By using this roughness model, the numerically predicted results of roughness effects (i.e., the k value) at different mold and melt temperatures were in good agreement with the experimental data.
2. The proposed numerical procedure for the axisymmetric polymer flow is effective. The numerically predicted results were in good agreement with the experimental data.
3. The proposed numerical procedure for the pseudo-axisymmetric polymer flow encountered in the experiments is effective. The numerically predicted results of flow area development on the rougher half with the increasing total flow area of the molded part and the k values were in good agreement with the experimental data.

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4. For roughness effects on the filling flow area, both experimental and numerical results revealed that the roughness effects are dependent on mold and melt temperatures. The roughness effects are more significant at the lower mold temperature level. Similarly, the roughness effects are more significant at the lower melt temperature level.
5. The significance of roughness effects (i.e., the k value) is dependent on cavity thickness and injection velocity. The smaller the cavity thickness, the more significant is the roughness effect. The relationship between the k value and the cavity thickness can be approximated by a logarithm function. The smaller the injection velocity, the more significant is the roughness effect. However, in the range of high injection velocities as used in the experiments, a small change in the injection velocity will not lead to a significant difference in the roughness effects.
6. During mold filling, the surface roughness influences the flow profiles of temperature, velocity, viscosity, shear rate, as well as the cavity pressure. The significance of the roughness effects on these profiles is dependent on the roughness magnitude, mold temperature and melt temperature. In general, when the mold temperature is lower than the melt temperature, the higher the roughness, the more significant is the roughness effect. With an increase in the mold temperature, the roughness effects decrease. However, the melt temperature has little effect on the flow profiles within the roughness layer.
7. For different roughness profiles with the same effective roughness height (δ), the roughness effects may be different. Similarly, for different roughness profiles with the same average roughness (S_a), the roughness effects may also be different.

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8. The effective roughness height (δ), instead of the average roughness (S_a), is a determining factor for the roughness effects in micro injection molding.

8.2 Recommendations

This thesis built the foundation for future research on roughness effects in micro injection molding. For future research work, some recommendations are suggested below:

1. Improvement of the proposed roughness model.

The current model only uses two parameters to represent the physical roughness, i.e., the effective roughness height (δ) and the volume fraction parameter (θ). In future, other parameters can be considered to represent the physical surface roughness more precisely.

2. Carrying out three-dimensional numerical investigation.

In this research, only two-dimensional numerical simulation was carried out. Due to its limitation, some three-dimensional features were not considered. For example, the effect of the separating line between the two semicircular halves of the core insert cannot be simulated using the current code. Therefore, in future, three-dimensional codes can be used to improve the simulation results.

3. Investigation of filling the cavities with other geometries

In this research, only polymer filling into a thin-thickness disk-shaped cavity was investigated. In future work, filling of cavities with other geometries can be investigated, for example, filling polymer melt into curves or twisted flow channels.

4. Fabrication of inserts using different processes.

Chapter 8: Conclusions and Recommendations

In this research, the inserts used in the mold were fabricated using EDM. As different machining processes may result in different surface roughness profiles, the inserts fabricated using other machining processes can be investigated.

5. Use of different polymer materials.

In this research, only POM was used in the investigation. As different material may have significantly different responses to the mold and melt temperatures and shear rate, it is necessary to use different materials in the experiments and simulations to improve or correct the observations made in this current research.

6. Use of different mold materials

The thermal conductivity ratio between the mold material and polymer melt plays a critical role in the roughness effects. In this research, the mold material used was steel. Its conductivity is 29W/m.K. In future work, the mold of different materials can be used to investigate thoroughly the significance of the thermal conductivity ratio. For example, the core inserts made of pure copper can be used. Its thermal conductivity can be as high as 386W/m.K.

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APPENDICES

Appendix A: Definitions of roughness parameters

All these parameters are defined in comparison with a mean plane obtained through levelling of the mean square plane of the measured surface and then through centering of heights around the mean.

S_a : Arithmetic mean of the deviations from the mean.

$$S_a = \frac{1}{MN} \sum_{x=0}^{N-1} \sum_{y=0}^{M-1} |z_{x,y}|$$

This parameter is included in the EUR 15178 EN report.

S_q : Quadratic mean of the deviations from the mean.

$$S_q = \sqrt{\frac{1}{MN} \sum_{x=0}^{N-1} \sum_{y=0}^{M-1} z_{x,y}^2}$$

Computes the efficient value for the amplitudes of the surface (RMS). This parameter is included in the EUR 15178 EN report.

S_t : Total height of the surface.

Height between the highest peak and the deepest hole. This parameter is supplied in conformity with the 2D parameters.

S_p : Highest peak of the surface.

Height between the highest peak and the mean plane. This parameter is supplied in conformity with the 2D parameters.

Appendices

S_v : Deepest valley of the surface.

Depth between the mean plane and the deepest valley. This parameter is supplied in conformity with the 2D parameters.

S_z : Height of the 10 points of the surface. Mean of distance between the 5 highest peaks and the 5 deepest holes. A neighbourhood of 3X3 is taken into account to find out the peaks and the valleys. This parameter is included in the EUR 15178 EN report.

S_{sk} : Symmetry of the distribution curve of depths.

$$S_{sk} = \frac{1}{MNS_q^3} \sum_{x=0}^{N-1} \sum_{y=0}^{M-1} z_{x,y}^3$$

A negative S_{sk} indicates that the surface is composed with principally one plateau and deep and fine valleys. In this case, the distribution is sloping to the top. A positive S_{sk} indicates a surface with lots of peaks on a plane. The distribution is sloping to the bottom. Due to the big exponent used, this parameter is very sensitive to the sampling and to the noise of the measurement. This parameter is included in the EUR 15178 EN report.

S_{ku} : Flatness of the distribution curve of depths.

$$S_{ku} = \frac{1}{MNS_q^4} \sum_{x=0}^{N-1} \sum_{y=0}^{M-1} z_{x,y}^4$$

Due to the big exponent used, this parameter is very sensitive to the sampling and to the noise of the measurement. This parameter is included in the EUR 15178 EN report.

Appendix B: Measurement results of flow area of molded parts

Table B1. Flow area measurement for insert I ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	12.87	12.85	12.86	12.86	0.01	5.60	5.60	5.60	5.60	0.00
2	15.10	15.13	15.09	15.11	0.02	6.83	6.84	6.81	6.83	0.02
3	14.30	14.31	14.30	14.30	0.01	6.40	6.40	6.40	6.40	0.00
4	14.45	14.46	14.45	14.45	0.01	6.49	6.50	6.49	6.49	0.01
5	15.23	15.21	15.25	15.23	0.02	6.82	6.83	6.86	6.84	0.02
6	18.68	18.70	18.70	18.69	0.01	8.28	8.29	8.30	8.29	0.01
7	23.56	23.53	23.55	23.55	0.02	10.70	10.65	10.68	10.68	0.03
8	19.27	19.26	19.27	19.27	0.01	8.58	8.58	8.59	8.58	0.00
9	20.36	20.35	20.36	20.36	0.01	9.00	9.02	9.02	9.01	0.01
10	17.03	17.01	17.01	17.02	0.01	7.68	7.71	7.69	7.69	0.02
11	29.66	29.64	29.65	29.65	0.01	13.36	13.36	13.36	13.36	0.00
12	27.09	27.07	27.09	27.08	0.01	12.12	12.12	12.13	12.12	0.01
13	29.29	29.26	29.27	29.27	0.02	13.24	13.22	13.23	13.23	0.01
14	28.65	28.68	28.66	28.66	0.02	12.71	12.75	12.73	12.73	0.02
15	29.29	29.27	29.29	29.28	0.01	13.11	13.11	13.12	13.11	0.01
16	39.83	39.82	39.81	39.82	0.01	17.95	17.94	17.93	17.94	0.01
17	41.27	41.26	41.28	41.27	0.01	18.58	18.58	18.60	18.59	0.01
18	39.97	39.99	39.95	39.97	0.02	18.01	18.04	18.00	18.02	0.02
19	40.98	40.96	40.90	40.95	0.04	18.29	18.29	18.22	18.27	0.04
20	38.62	38.64	38.63	38.63	0.01	16.98	16.99	16.99	16.99	0.01
21	42.26	42.23	42.25	42.25	0.02	18.95	18.93	18.95	18.94	0.01
22	44.83	44.85	44.82	44.83	0.02	20.90	20.88	20.87	20.88	0.02
23	44.31	44.3	44.31	44.31	0.01	20.67	20.67	20.68	20.67	0.00
24	43.87	43.86	43.84	43.86	0.02	20.20	20.20	20.18	20.19	0.01
25	44.15	44.13	44.12	44.13	0.02	20.63	20.62	20.61	20.62	0.01

Appendices

Table B2. Flow area measurement for insert I ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	27.04	27.06	27.03	27.04	0.02	12.96	12.96	12.95	12.96	0.01
2	26.21	26.20	26.23	26.21	0.02	12.48	12.48	12.53	12.50	0.03
3	26.52	26.51	26.53	26.52	0.01	12.53	12.53	12.56	12.54	0.02
4	27.50	27.52	27.51	27.51	0.01	13.04	13.09	13.06	13.06	0.03
5	25.66	25.68	25.67	25.67	0.01	12.41	12.40	12.38	12.40	0.02
6	39.53	39.51	39.54	39.53	0.02	19.16	19.13	19.15	19.15	0.02
7	41.15	41.12	41.11	41.13	0.02	19.46	19.46	19.44	19.45	0.01
8	42.38	42.35	42.35	42.36	0.02	20.42	20.42	20.40	20.41	0.01
9	41.65	41.66	41.68	41.66	0.02	19.93	19.96	19.95	19.95	0.02
10	44.33	44.35	44.32	44.33	0.02	20.78	20.81	20.78	20.79	0.02
11	46.97	46.95	46.95	46.96	0.01	23.00	22.96	22.97	22.98	0.02
12	46.19	46.17	46.20	46.19	0.02	22.84	22.83	22.84	22.84	0.01
13	44.60	44.62	44.64	44.62	0.02	21.37	21.37	21.41	21.38	0.02
14	45.12	45.13	45.15	45.13	0.02	21.90	21.92	21.90	21.91	0.01
15	46.53	46.55	46.54	46.54	0.01	21.31	21.33	21.31	21.32	0.01

Appendices

Table B3. Flow area measurement for insert I ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	18.12	18.10	18.11	18.11	0.01	8.60	8.57	8.61	8.59	0.02
2	19.51	19.50	19.52	19.51	0.01	9.40	9.40	9.40	9.40	0.00
3	22.24	22.22	22.25	22.24	0.02	10.49	10.44	10.48	10.47	0.03
4	26.12	26.10	26.11	26.11	0.01	12.63	12.60	12.63	12.62	0.02
5	23.90	23.91	23.90	23.90	0.01	11.57	11.56	11.56	11.56	0.01
6	43.89	43.90	43.92	43.90	0.02	20.63	20.62	20.63	20.63	0.01
7	40.77	40.75	40.78	40.77	0.02	19.28	19.27	19.29	19.28	0.01
8	43.88	43.85	43.87	43.87	0.02	20.81	20.76	20.77	20.78	0.03
9	44.95	44.92	44.93	44.93	0.02	21.39	21.38	21.36	21.38	0.02
10	44.80	44.78	44.81	44.80	0.02	21.25	21.22	21.24	21.24	0.02

Appendices

Table B4. Flow area measurement for insert I ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	14.03	14.01	14.02	14.02	0.01	6.67	6.63	6.69	6.66	0.03
2	22.40	22.42	22.44	22.42	0.02	10.65	10.70	10.67	10.67	0.03
3	18.68	18.65	18.64	18.66	0.02	9.03	8.99	9.01	9.01	0.02
4	15.05	15.01	15.03	15.03	0.02	7.23	7.21	7.20	7.21	0.02
5	25.52	25.50	25.53	25.52	0.02	12.55	12.54	12.57	12.55	0.02
6	29.00	28.98	28.99	28.99	0.01	14.06	14.09	14.09	14.08	0.02
7	28.57	28.55	28.54	28.55	0.02	13.74	13.73	13.74	13.74	0.01
8	25.88	25.85	25.89	25.87	0.02	12.61	12.60	12.67	12.63	0.04
9	28.09	28.10	28.11	28.10	0.01	13.64	13.68	13.70	13.67	0.03
10	36.70	36.69	36.67	36.69	0.02	17.94	17.96	17.92	17.94	0.02
11	41.35	41.32	41.34	41.34	0.02	20.05	20.00	20.04	20.03	0.03
12	47.39	47.36	47.37	47.37	0.02	23.31	23.34	23.32	23.32	0.02
13	43.45	43.46	43.44	43.45	0.01	22.13	22.15	22.11	22.13	0.02
14	44.12	44.10	44.12	44.11	0.01	22.76	22.78	22.79	22.78	0.02
15	45.32	45.30	45.33	45.32	0.02	23.01	23.05	23.04	23.03	0.02

Appendices

Table B5. Flow area measurement for insert II ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	20.41	20.42	20.42	20.42	0.01	7.77	7.77	7.78	7.77	0.00
2	22.63	22.60	22.61	22.61	0.02	8.93	8.95	8.94	8.94	0.01
3	22.13	22.13	22.14	22.13	0.01	8.51	8.50	8.52	8.51	0.01
4	21.55	21.57	21.56	21.56	0.01	8.22	8.26	8.24	8.24	0.02
5	23.35	23.37	23.37	23.36	0.01	9.00	9.02	9.02	9.01	0.01
6	35.26	35.29	35.23	35.26	0.03	13.56	13.63	13.55	13.58	0.04
7	31.46	31.49	31.47	31.47	0.02	12.20	12.20	12.20	12.20	0.00
8	31.25	31.28	31.30	31.28	0.03	12.06	12.07	12.10	12.08	0.02
9	34.53	34.55	34.53	34.54	0.01	13.43	13.43	13.42	13.43	0.01
10	31.67	31.69	31.66	31.67	0.02	12.14	12.14	12.12	12.13	0.01
11	41.88	41.79	41.83	41.83	0.05	17.70	17.56	17.63	17.63	0.07
12	40.96	41.01	40.98	40.98	0.03	16.76	16.86	16.81	16.81	0.05
13	41.44	41.43	41.44	41.44	0.01	17.46	17.44	17.46	17.45	0.01
14	39.06	39.10	39.08	39.08	0.02	15.70	15.78	15.74	15.74	0.04
15	42.90	42.98	42.99	42.96	0.05	18.52	18.58	18.60	18.57	0.04
16	48.08	48.10	48.07	48.08	0.02	23.17	23.24	23.18	23.20	0.03
17	45.80	45.90	45.84	45.85	0.05	20.52	20.70	20.60	20.60	0.09
18	47.15	47.17	47.18	47.17	0.02	21.87	21.88	21.89	21.88	0.01
19	46.75	46.70	46.72	46.72	0.03	22.44	22.35	22.39	22.39	0.05
20	46.45	46.48	46.46	46.46	0.02	22.28	22.33	22.30	22.30	0.03

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Table B6. Flow area measurement for insert II ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm ²)					Flow area of the rougher half (mm ²)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	22.68	22.67	22.67	22.67	0.01	9.30	9.28	9.27	9.28	0.02
2	18.39	18.40	18.39	18.39	0.01	7.58	7.61	7.62	7.60	0.02
3	21.40	21.41	21.43	21.41	0.02	8.81	8.84	8.83	8.83	0.02
4	23.46	23.44	23.44	23.45	0.01	9.88	9.84	9.83	9.85	0.03
5	21.00	21.03	20.98	21.00	0.03	8.76	8.75	8.68	8.73	0.04
6	27.66	27.69	27.70	27.68	0.02	11.31	11.31	11.29	11.30	0.01
7	31.93	31.95	31.91	31.93	0.02	13.36	13.37	13.34	13.36	0.02
8	28.41	28.45	28.43	28.43	0.02	11.88	11.83	11.83	11.85	0.03
9	29.51	29.53	29.52	29.52	0.01	12.16	12.16	12.17	12.16	0.01
10	33.41	33.40	33.42	33.41	0.01	13.96	13.92	13.95	13.94	0.02
11	48.35	48.40	48.37	48.37	0.03	23.03	23.01	23.02	23.02	0.01
12	40.33	40.32	40.33	40.33	0.01	16.92	16.87	16.89	16.89	0.03
13	47.50	47.51	47.50	23.43	0.02	22.95	22.99	22.97	22.97	0.02
14	42.73	42.71	42.70	42.71	0.02	19.01	18.99	18.99	19.00	0.01
15	47.56	47.53	47.55	47.55	0.02	22.75	22.73	22.73	22.74	0.01

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Table B7. Flow area measurement for insert II ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	17.64	17.66	17.65	17.65	0.01	7.18	7.23	7.20	7.20	0.03
2	22.97	22.98	22.95	22.97	0.02	9.79	9.78	9.73	9.77	0.03
3	20.49	20.50	20.51	20.50	0.01	8.58	8.56	8.56	8.57	0.01
4	21.34	21.32	21.30	21.32	0.02	8.79	8.75	8.77	8.77	0.02
5	17.02	17.05	17.01	17.03	0.02	7.00	7.00	7.01	7.00	0.01
6	29.63	29.65	29.62	29.63	0.02	12.79	12.77	12.79	12.78	0.01
7	29.52	29.50	29.55	29.52	0.03	12.70	12.66	12.68	12.68	0.02
8	28.40	28.41	28.40	28.40	0.01	11.87	11.86	11.88	11.87	0.01
9	24.70	24.72	24.70	24.71	0.01	10.13	10.14	10.12	10.13	0.01
10	24.09	24.10	24.08	24.09	0.01	9.76	9.75	9.72	9.74	0.02
11	38.04	38.06	38.04	38.05	0.01	15.73	15.72	15.69	15.71	0.02
12	36.72	36.75	36.71	36.73	0.02	15.16	15.17	15.18	15.17	0.01
13	36.73	36.72	36.70	36.72	0.02	15.05	15.07	15.08	15.07	0.02
14	40.50	40.52	40.55	40.52	0.03	16.99	16.99	17.05	17.01	0.03
15	40.71	40.69	40.73	40.71	0.02	17.36	17.31	17.33	17.33	0.03
16	43.05	43.09	43.01	43.05	0.04	18.93	18.94	18.91	18.93	0.02
17	43.28	43.29	43.29	43.29	0.01	19.03	19.06	19.00	19.03	0.03
18	42.08	42.08	42.05	42.07	0.02	18.37	18.35	18.34	18.35	0.02
19	44.82	44.85	44.83	44.83	0.02	20.30	20.35	20.26	20.30	0.05
20	43.10	43.11	43.13	43.11	0.02	18.98	18.96	19.03	18.99	0.04
21	47.55	47.56	47.53	47.55	0.02	22.35	22.35	22.29	22.33	0.03
22	47.30	47.33	47.35	47.33	0.03	22.29	22.24	22.29	22.27	0.03
23	48.15	48.17	48.15	48.16	0.01	23.35	23.32	23.32	23.33	0.02
24	47.08	47.07	47.05	47.07	0.02	22.03	22.06	21.97	22.02	0.05
25	47.35	47.33	47.38	47.35	0.03	22.44	22.40	22.45	22.43	0.03

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Table B8. Flow area measurement for insert II ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	23.81	23.80	23.82	23.81	0.01	9.98	9.99	10.02	10.00	0.02
2	29.23	29.20	29.21	29.21	0.02	12.32	12.30	12.29	12.30	0.02
3	25.86	25.87	25.83	25.85	0.02	10.98	10.99	11.01	10.99	0.02
4	20.96	20.97	20.98	20.97	0.01	8.65	8.65	8.68	8.66	0.02
5	22.97	22.95	22.95	22.96	0.01	9.56	9.55	9.54	9.55	0.01
6	39.70	39.72	39.69	39.70	0.02	17.05	17.10	17.09	17.08	0.03
7	30.83	30.84	30.82	30.83	0.01	13.06	13.09	13.04	13.06	0.03
8	31.87	31.85	31.83	31.85	0.02	13.67	13.64	13.60	13.64	0.04
9	35.45	35.41	35.43	35.43	0.02	14.86	14.81	14.86	14.84	0.03
10	29.17	29.19	29.18	29.18	0.01	12.15	12.15	12.17	12.16	0.01
11	40.30	40.32	40.31	40.31	0.01	17.39	17.39	17.41	17.40	0.01
12	40.75	40.77	40.73	40.75	0.02	17.77	17.81	17.74	17.77	0.04
13	44.42	44.45	44.48	44.45	0.03	20.47	20.52	20.51	20.50	0.03
14	44.17	44.16	44.17	44.17	0.01	20.25	20.21	20.26	20.24	0.03
15	44.10	44.12	44.10	44.11	0.01	20.48	20.47	20.49	20.48	0.01

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Table B9. Flow area measurement for insert III ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	25.32	25.34	25.33	25.33	0.01	9.00	9.04	9.02	9.02	0.02
2	25.47	25.45	25.45	25.46	0.01	8.95	8.92	8.93	8.93	0.02
3	25.74	25.72	25.72	25.73	0.01	9.41	9.38	9.39	9.39	0.02
4	25.95	25.94	25.93	25.94	0.01	9.53	9.51	9.51	9.52	0.01
5	25.37	25.34	25.35	25.35	0.02	9.27	9.23	9.25	9.25	0.02
6	34.76	34.76	34.74	34.75	0.01	12.65	12.63	12.62	12.63	0.02
7	31.14	31.15	31.13	31.14	0.01	11.13	11.15	11.13	11.14	0.01
8	31.51	31.52	31.50	31.51	0.01	11.41	11.45	11.42	11.43	0.02
9	35.04	35.01	35.02	35.02	0.02	13.40	13.39	13.39	13.39	0.01
10	31.62	31.60	31.63	31.62	0.02	11.22	11.18	11.22	11.21	0.02
11	37.18	37.20	37.20	37.19	0.01	13.70	13.73	13.73	13.72	0.02
12	36.98	36.95	36.99	36.97	0.02	13.96	13.97	13.99	13.97	0.02
13	37.04	37.05	37.06	37.05	0.01	14.03	14.05	14.06	14.05	0.01
14	36.43	36.43	36.45	36.44	0.01	13.62	13.65	13.66	13.64	0.02
15	37.00	37.01	37.03	37.01	0.02	13.87	13.87	13.90	13.88	0.01
16	41.05	41.03	41.04	41.04	0.01	16.03	16.02	16.03	16.03	0.00
17	41.12	41.14	41.10	41.12	0.02	16.04	16.05	16.02	16.04	0.02
18	41.03	41.00	41.02	41.02	0.02	16.35	16.37	16.37	16.36	0.01
19	41.27	41.26	41.24	41.26	0.02	16.33	16.34	16.31	16.33	0.02
20	41.23	41.20	41.22	41.22	0.02	16.60	16.58	16.60	16.59	0.01

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Table B10. Flow area measurement for insert III ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	25.96	25.98	25.96	25.97	0.01	10.70	10.75	10.74	10.73	0.03
2	25.33	25.35	25.36	25.35	0.02	10.53	10.56	10.56	10.55	0.02
3	25.64	25.63	25.63	25.63	0.01	10.53	10.52	10.50	10.52	0.02
4	25.13	25.12	25.13	25.13	0.01	10.49	10.46	10.49	10.48	0.02
5	27.90	27.89	27.90	27.90	0.01	11.58	11.59	11.57	11.58	0.01
6	35.12	35.10	35.11	35.11	0.01	14.09	14.09	14.11	14.10	0.01
7	32.05	32.03	32.07	32.05	0.02	12.84	12.83	12.87	12.85	0.02
8	30.67	30.65	30.64	30.65	0.02	12.50	12.50	12.51	12.50	0.01
9	32.34	32.30	32.31	32.32	0.02	12.97	12.95	12.96	12.96	0.01
10	38.09	38.08	38.09	38.09	0.01	15.26	15.26	15.25	15.26	0.01
11	40.59	40.61	40.60	40.60	0.01	16.34	16.34	16.36	16.35	0.01
12	40.97	40.95	40.96	40.96	0.01	17.05	17.01	17.01	17.02	0.02
13	41.84	41.88	41.87	41.86	0.02	17.53	17.53	17.51	17.52	0.01
14	41.38	41.36	41.39	41.38	0.02	17.15	17.16	17.17	17.16	0.01
15	40.92	40.91	40.93	40.92	0.01	17.05	17.05	17.10	17.07	0.03

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Table B11. Flow area measurement for insert III ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	22.86	22.84	22.84	22.85	0.01	9.50	9.48	9.48	9.49	0.01
2	23.23	23.21	23.22	23.22	0.01	9.73	9.68	9.72	9.71	0.03
3	23.57	23.55	23.57	23.56	0.01	9.87	9.82	9.86	9.85	0.03
4	23.96	23.99	23.95	23.97	0.02	9.73	9.75	9.72	9.73	0.02
5	24.99	24.98	25.01	24.99	0.02	10.22	10.21	10.22	10.22	0.01
6	42.72	42.70	42.75	42.72	0.03	18.13	18.13	18.18	18.15	0.03
7	43.21	43.20	43.23	43.21	0.02	18.56	18.57	18.59	18.57	0.02
8	43.16	43.18	43.15	43.16	0.02	18.52	18.56	18.55	18.54	0.02
9	43.32	43.30	43.31	43.31	0.01	18.44	18.41	18.43	18.43	0.02
10	43.18	43.15	43.14	43.16	0.02	18.65	18.60	18.62	18.62	0.03

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Table B12. Flow area measurement for insert III ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	24.99	25.00	24.99	24.99	0.01	10.88	10.90	10.88	10.89	0.01
2	30.30	30.32	30.33	30.32	0.02	13.14	13.16	13.18	13.16	0.02
3	26.32	26.30	26.30	26.31	0.01	11.26	11.25	11.24	11.25	0.01
4	27.65	27.63	27.66	27.65	0.02	11.85	11.82	11.86	11.84	0.02
5	29.81	29.80	29.80	29.80	0.01	12.98	13.00	12.99	12.99	0.01
6	34.20	34.25	34.22	34.22	0.03	14.57	14.64	14.60	14.60	0.04
7	40.52	40.50	40.49	40.50	0.02	17.52	17.49	17.49	17.50	0.02
8	33.47	33.48	33.46	33.47	0.01	14.72	14.70	14.69	14.70	0.02
9	34.33	34.32	34.32	34.32	0.01	14.82	14.82	14.83	14.82	0.01
10	43.30	43.31	43.30	43.30	0.01	18.92	18.94	18.95	18.94	0.02
11	43.41	43.42	43.40	43.41	0.01	19.49	19.52	19.49	19.50	0.02
12	43.72	43.75	43.73	43.73	0.02	19.51	19.50	19.50	19.50	0.01
13	45.12	45.15	45.13	45.13	0.02	20.50	20.54	20.53	20.52	0.02
14	44.05	44.04	44.03	44.04	0.01	19.34	19.32	19.30	19.32	0.02
15	45.78	45.80	45.81	45.80	0.02	20.70	20.73	20.72	20.72	0.02

Table B13. Flow area measurement for insert IV ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	13.87	13.90	13.91	13.89	0.02	5.89	5.88	5.89	5.89	0.01
2	11.45	11.43	11.46	11.45	0.02	5.06	5.05	5.08	5.06	0.02
3	13.13	13.10	13.11	13.11	0.02	5.77	5.76	5.76	5.76	0.01
4	13.78	13.76	13.77	13.77	0.01	5.93	5.92	5.93	5.93	0.01
5	13.52	13.50	13.51	13.51	0.01	6.04	6.00	6.02	6.02	0.02
6	17.23	17.24	17.24	17.24	0.01	7.68	7.68	7.69	7.68	0.01
7	16.97	16.96	16.97	16.97	0.01	7.59	7.59	7.61	7.60	0.01
8	20.00	20.01	19.98	20.00	0.02	9.10	9.10	9.09	9.10	0.01
9	20.29	20.27	20.28	20.28	0.01	9.01	9.02	9.02	9.02	0.01
10	18.24	18.23	18.25	18.24	0.01	8.29	8.26	8.27	8.27	0.02
11	28.04	28.02	28.05	28.04	0.02	12.46	12.42	12.49	12.46	0.04
12	26.99	27.02	26.97	26.99	0.03	11.91	11.96	11.88	11.92	0.04
13	27.86	27.84	27.86	27.85	0.01	12.53	12.49	12.54	12.52	0.03
14	27.96	27.94	27.95	27.95	0.01	12.00	12.01	12.01	12.01	0.01
15	29.04	29.05	29.06	29.05	0.01	13.07	13.06	13.06	13.06	0.01
16	41.75	41.77	41.76	41.76	0.01	19.60	19.61	19.61	19.61	0.01
17	42.38	42.39	42.38	42.38	0.01	19.60	19.64	19.60	19.61	0.02
18	43.06	43.06	43.08	43.07	0.01	20.55	20.56	20.58	20.56	0.02
19	43.46	43.49	43.50	43.48	0.02	20.72	20.75	20.77	20.75	0.03
20	43.69	43.71	43.68	43.69	0.02	21.35	21.36	21.34	21.35	0.01

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Table B14. Flow area measurement for insert IV ($T_{\text{melt}} = 453\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	17.65	17.63	17.64	17.64	0.01	7.88	7.88	7.89	7.88	0.01
2	18.95	18.96	18.97	18.96	0.01	8.68	8.71	8.73	8.71	0.03
3	17.98	17.99	17.99	17.99	0.01	8.30	8.34	8.36	8.33	0.03
4	18.93	18.94	18.92	18.93	0.01	8.66	8.69	8.65	8.67	0.02
5	19.80	19.82	19.80	19.81	0.01	8.90	8.95	8.91	8.92	0.03
6	33.23	33.24	33.25	33.24	0.01	14.66	14.65	14.67	14.66	0.01
7	32.34	32.34	32.32	32.33	0.01	14.71	14.73	14.70	14.71	0.02
8	31.22	31.22	31.24	31.23	0.01	13.89	13.92	13.90	13.90	0.02
9	33.40	33.39	33.40	33.40	0.01	15.30	15.29	15.29	15.29	0.01
10	32.55	32.56	32.54	32.55	0.01	14.37	14.37	14.36	14.37	0.01

Table B15. Flow area measurement for insert IV ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 323\text{K}$)

Part	Flow area of the entire part (mm^2)					Flow area of the rougher half (mm^2)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	19.45	19.44	19.45	19.45	0.01	8.76	8.76	8.77	8.76	0.01
2	19.49	19.50	19.50	19.50	0.01	8.71	8.74	8.75	8.73	0.02
3	20.42	20.42	20.44	20.43	0.01	9.22	9.21	9.23	9.22	0.01
4	18.07	18.06	18.05	18.06	0.01	8.07	8.05	8.06	8.06	0.01
5	18.16	18.14	18.16	18.15	0.01	8.07	8.06	8.08	8.07	0.01
6	22.95	22.93	22.95	22.94	0.01	10.45	10.44	10.46	10.45	0.01
7	23.10	23.09	23.08	23.09	0.01	10.37	10.34	10.36	10.36	0.02
8	21.23	21.24	21.24	21.24	0.01	9.48	9.46	9.45	9.46	0.02
9	24.35	24.36	24.35	24.35	0.01	10.77	10.77	10.76	10.77	0.01
10	24.47	24.46	24.45	24.46	0.01	10.74	10.74	10.73	10.74	0.01
11	34.24	34.26	34.24	34.25	0.01	15.56	15.57	15.56	15.56	0.01
12	34.59	34.60	34.58	34.59	0.01	15.71	15.75	15.69	15.72	0.03
13	35.41	35.40	35.39	35.40	0.01	16.47	16.45	16.45	16.46	0.01
14	33.08	33.09	33.08	33.08	0.01	14.73	14.71	14.71	14.72	0.01
15	37.18	37.09	37.10	37.12	0.05	16.66	16.59	16.59	16.61	0.04

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Table B16. Flow area measurement for insert IV ($T_{\text{melt}} = 473\text{K}$ and $T_{\text{mold}} = 383\text{K}$)

Part	Flow area of the entire part (mm ²)					Flow area of the rougher half (mm ²)				
	Measurement repeat			Ave.	Std. Div.	Measurement repeat			Ave.	Std. Div.
	1	2	3			1	2	3		
1	36.22	36.20	36.21	36.21	0.01	16.66	16.62	16.66	16.65	0.02
2	27.75	27.73	27.76	27.75	0.02	12.72	12.70	12.75	12.72	0.03
3	30.41	30.40	30.40	30.40	0.01	14.29	14.30	14.27	14.29	0.02
4	29.92	29.90	29.93	29.92	0.02	14.01	14.00	14.03	14.01	0.02
5	23.65	23.63	23.64	23.64	0.01	10.69	10.67	10.70	10.69	0.02
6	43.81	43.84	43.83	43.83	0.02	20.03	20.07	20.04	20.05	0.02
7	39.04	39.06	39.03	39.04	0.02	18.41	18.46	18.42	18.43	0.03
8	41.79	41.82	41.78	41.80	0.02	19.10	19.12	19.09	19.10	0.02
9	42.58	42.60	42.59	42.59	0.01	19.97	20.00	19.98	19.98	0.02
10	41.33	41.35	41.30	41.33	0.03	19.02	19.05	19.01	19.03	0.02

Appendix C: Governing equations in Cartesian and axisymmetric coordinates

In Cartesian coordinate, the governing equations can be expressed as follows:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

Momentum equations:

x-component:

$$\left(\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho uv}{\partial y} \right) = \frac{\partial}{\partial x} (2\eta \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y} [\eta (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})]$$

y-component:

$$\left(\frac{\partial \rho v}{\partial t} + \frac{\partial \rho uv}{\partial x} + \frac{\partial \rho v^2}{\partial y} \right) = \frac{\partial}{\partial y} (2\eta \frac{\partial v}{\partial y}) + \frac{\partial}{\partial x} [\eta (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})]$$

Energy equation:

$$\left(\frac{\partial \rho C_p T}{\partial t} + \frac{\partial \rho C_p u T}{\partial x} + \frac{\partial \rho C_p v T}{\partial y} \right) = \frac{\partial}{\partial x} (\kappa \frac{\partial T}{\partial x}) + \eta \dot{\gamma}^2$$

$$\dot{\gamma} = \sqrt{2 \left(\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 \right) + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2}$$

In axisymmetric coordinate, the governing equations can be expressed as follows:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{1}{r} \frac{\partial (r \rho v)}{\partial r} = 0$$

The momentum equations:

Axial-component:

$$\left(\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho uv}{\partial r} \right) = \frac{\partial}{\partial x} (2\eta \frac{\partial u}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r} [r \eta (\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x})]$$

Radial-component:

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$$\left(\frac{\partial \rho v}{\partial t} + \frac{\partial \rho u v}{\partial x} + \frac{\partial \rho v^2}{\partial r}\right) = \frac{1}{r} \frac{\partial}{\partial r} \left(2\eta \frac{\partial v}{\partial r}\right) + \frac{\partial}{\partial x} \left[\eta \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x}\right)\right] - \frac{2\eta v}{r^2}$$

Energy equation:

$$\left(\frac{\partial \rho C_p T}{\partial t} + \frac{\partial \rho C_p u T}{\partial x} + \frac{\partial \rho C_p v T}{\partial y}\right) = \frac{1}{r} \frac{\partial}{\partial x} \left(\kappa r \frac{\partial T}{\partial x}\right) + \eta \dot{\gamma}^2$$

$$\dot{\gamma} = \sqrt{2 \left(\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial r} \right)^2 \right) + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial r} \right)^2 + 2 \left(\frac{v}{r} \right)^2}$$

Appendix D: Measurement results of thickness of molded parts

Sample No.	Thickness of molded parts (mm)			
	Insert I	Insert II	Insert III	Insert IV
1	0.285	0.287	0.185	0.240
2	0.289	0.295	0.178	0.241
3	0.285	0.286	0.185	0.230
4	0.288	0.289	0.179	0.248
5	0.289	0.285	0.178	0.239
6	0.309	0.305	0.205	0.248
7	0.310	0.300	0.205	0.245
8	0.300	0.302	0.200	0.245
9	0.309	0.300	0.215	0.239
10	0.305	0.300	0.206	0.247
11	0.310	0.300	0.205	0.241
12	0.315	0.295	0.204	0.240
13	0.310	0.297	0.205	0.249
14	0.311	0.301	0.204	0.247
15	0.308	0.300	0.205	0.241
16	0.298	0.305	0.201	0.250
17	0.298	0.307	0.200	0.249
18	0.299	0.304	0.205	0.247
19	0.295	0.308	0.203	0.250
20	0.290	0.303	0.206	0.245
Average	0.300	0.298	0.199	0.245
Standard deviation	0.010	0.007	0.011	0.005