NUMERICAL ANALYSIS OF POLYMER MELTS FLOW BEHAVIOUR IN GROOVED CHANNEL

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DECLARATION

This work has not previously been accepted in substance for any degree and is not being concurrently submitted in candidature for any degree.

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ABSTRAK

Kesan tekanan masuk, saiz pic dan saluran acuan yang berbeza-beza terhadap kebolehliran propylene dikaji dari segi halaju, kadar alir, isipadu propylene dalam acuan dan nisbah propylene kepada jumlah campuran. Kajian dijalankan dengan menggunakan perisian simulasi Computational Fluid Dynamic (CFD), ANSYS Fluent. Fokus utama projek ini adalah untuk membandingkan kebolehaliran propylene dalam saluran acuan yang berbeza. Berdasarkan simulasi, aliran propylene menunjukkan aliran yang baik apabila tekanan masuk ditetapkan pada 25kPa. Isipadu propylene dalam acuan adalah paling tinggi yang menunjukkan kurang rongga udara terbentuk semasa simulasi. Sementara itu, apabila saiz pic dinaikkan, isipadu propylene dalam acuan juga meningkat. Walau bagaimanapun, isipadu propylene menurun selepas saiz pic dinaikkan kepada 150mm disebabkan oleh penurunan tekanan semasa simulasi. Alur yang berbeza dalam saluran mempengaruhi kebolehaliran propylene. Sebagai contoh, saluran segi tiga membenarkan lebih banyak isipadu propylene untuk mengisi acuan berbanding saluran bulat dan segi empat tepat kerana halaju propylene adalah paling rendah dalam saluran segi tiga, dengan itu meningkatkan kebolehliran propylene.

ABSTRACT

The effect of inlet pressure, pitch size, and varied mould channel on the flowability of the propylene are studied in terms of the velocity, flow rate, volume of the propylene in the mould, and ratio of the propylene to the total mixture. The study was conducted by using the Computational Fluid Dynamic (CFD) simulation software, ANSYS Fluent. The main focus of this project is to compare the flowability of the propylene in the different mould channels. Based on the simulation, the flow of propylene exhibits a proper flow when the inlet pressure is set at 25kPa. The volume of the propylene in the mould was the highest which indicates less air cavity is formed during the simulation. Meanwhile, when the pitch size is increased, the volume of propylene in the mould increases too. However, the volume of propylene drops after the pitch size is increased to 150mm due to pressure drop during the simulation. The different grooves in the channel affect the flowability of the propylene. For an instance the triangular channel allows more volume of propylene to fill up the mould as compared with circular and rectangular grooved channels as the velocity of the propylene is lowest in the triangular grooved channel, thereby improving the flowability of the propylene.

CHAPTER 1 INTRODUCTION

1.1 Overview

Plastics manufacturing has grown to become an important manufacturing process in the industry. The widespread use of commercial plastics can be seen in almost every sector, such as packaging, construction, consumer, and medical products. Polypropylene (PP), one of the commercially distributed plastics, is a type of semi-crystalline non-Newtonian fluid. Unlike Newtonian fluids which viscosity remains constant regardless of its speed and pressure applied as it is pushed through an orifice, the viscosity of non-Newtonian fluids varies depending on the speed (shear rate) at an applied level of pressure **Error! Reference source not found.**.

Injection moulding is a manufacturing process used to produce parts made of plastics and elastomers in large volumes. The design of parts produced with injection moulding can be of complex shapes of various sizes and thin walls, as well as good dimensional accuracy. The injection moulding machine consists of several parts, which are hopper, screw barrel, and mold [1].

A clamping unit and an injection unit are the two parts of an injection moulding machine. The clamping unit's functions include opening and closing a die as well as product ejection. The toggle clamping method and the straight-hydraulic clamping method, in which a mould is directly opened and closed using a hydraulic cylinder, are the two types of clamping methods.

The purpose of the injection unit is to heat plastic until it melts, then to inject the molten plastic into a mould. Turning the screw causes the plastic in the hopper to melt, and the molten plastic is collected in front of the screw (a process known as metering). Once there is sufficient molten plastic gathered, the injection procedure may start.

The machine controls the injection speed of the screw while molten plastic flows through a mould. On the other hand, it controls dwell pressure after cavities have been filled with molten plastic. When either the screw position or the injection pressure reaches a set value, the control is switched from speed to pressure.

Pellets or granules are fed into the hopper, where it is melted into molten plastic in the heated cylinder. The screw barrel is then rotated to force the molten plastic across the barrel and accumulate in front of the screw. The pressures developed are usually in the range of 70 – 200 MPa [4]. When the required amount of molten plastic is accumulated, the screw stops rotating and it is pushed forward hydraulically, consequently injecting molten plastic into the mould. The moving speed of the screw, or injection speed can be controlled by the machine moulding process due to small variations of PP viscosity at temperature 185-195°C [1].

Similar to a single-screw extruder, a barrel is used to feed raw materials that are then spun into a polymer melt by external heating. Once the viscosity of the polymer has been reduced to a particular point, intense pressure is applied to the melt to force it to flow into a closed mould until the cavity is filled. The pressure is preserved for a certain amount of time by keeping the screw in place after injection. In order to account for the contraction caused by the polymer shrinking after it enters the relatively cold mould, additional ingredients are injected during packing. The screw then retracts, and material is fed into its front end for the following shot. The mould opens to release the finished object when the moulded polymer has sufficiently cooled and hardened. A fresh dosage of polymer is injected to start a new cycle when the mould is shut once again [13].

The time required to cool the component dominates the entire cycle time. Although quick cooling can save cycle time, high-quality goods are often produced in moulds that are rather hot. The control system optimises the cycle time and the quality of the mouldings. Injection moulding enables the high-yield creation of complicated goods with exact dimensions, where three-dimensional structures are created by combining numerous cavities. The resultant pieces can be made of flexible rubbers or stiff polymers, with highly repeatable surface details. High pressure is the main restriction of injection moulding. Furthermore, the stock temperature must be higher than the polymer's glass transition temperature to ensure flow, which may result in material deterioration due to heat exposure. To counteract the high viscosity of the polymers, large injection pressures are utilised, therefore all sections of the mould are composed of strong materials, often tool steels. A runner system made of spruce, runners, and gates is used to push the melt into the cavity of the mould. The flow travels through the spruce and the channels of the runners when the machine nozzle makes contact with the mould, spreading ingredients into different cavities via tiny holes called as gates. To lessen mechanical stress on the material, the operating system's design should minimise flow resistance, which is dictated by cavity diameter, material properties, and processing conditions. The material in the spruce and runners is separated from the product and fed back into the injection unit after each ejection of the product. The mould cavity is the most important component in ensuring the final part's dimensions, although it should be remembered that shrinking of the polymers after cooling always results in smaller mouldings than cavities. The voids must be polished, hardened, and typically chrome-plated to ensure the product's surface quality **Error! Reference source not found.**.

The cooling system is an important part of mould design. Constant cooling enhances product quality by removing internal tensions, voids, differential shrinkage, and challenges with mould release, while quick cooling can reduce the moulding cycle and increase productivity. The mechanical properties and performance of the finished product are significantly influenced by the manufacturing process and a range of factors, including product design, injection mould configuration, process conditions, and machine operations. The viscoelastic parameters of polymer melts and mould design, for example, influence melt distribution in the mould; packing, polymer crystallisation, mould geometry, and cooling speed influence material shrinkage throughout the cavity; and the material's microstructure and morphology are determined by the thermomechanical history of the polymer experienced during processing. Computer modelling is an effective approach for assessing the interrelated architectural parts [16].

1.2 Project Background

Injection moulding is widely used in manufacturing due to its advantages. As compared with subtractive manufacturing processes like CNC machining, injection moulding produces lower scrap rates. It is also capable of high production rates due to its repeatability. Typical parts that can be produced using injection moulding are joints, brackets, or housings. Changes in the temperature and pressure of the mould affects the flow characteristics of the injected molten plastic.

Factor that should be taken into consideration is the decrease in viscosity of molten plastic due to the loss of heat to the surface of the mould. When the viscosity falls below a certain limit, the leading edge of molten plastic will solidify due to cooling, consequently making melt flow to be impossible thereafter [4].

Therefore, design considerations should always be emphasized to minimize defects in parts during production. However, the equipment and tooling cost for injection moulding is high, and conventional experiments to determine the optimum mould design is consuming in several aspects: time, cost, and materials, especially when physical modification of the mould is involved. In order to prevent wastage that is caused due to injection moulding, pre-moulding analysis is advantageous to the engineers so that they are able to cut down the wastage cost.

Computational simulation with mould flow software for simulation of the injection moulding process with various parameters is more efficient to determine the optimum design of mould. Research shows that computational simulation such as ANSYS software for injection moulding process will visualize the behaviour of the shape and type of material with their size to be larger than 200 μm. By using the analysis of the simulation together with the experimental results, the unique characteristic of the mould filling in the injection moulding can be shown. In an existing work by Stickel and Powell [4], it also stated that the moulding parameters such as temperature and velocity together with the choice of thermal conductivity will affect the results of mould filling in injection moulding.

By using computational simulation, the effects of system pressure and operating temperature during the filling process can be determined. It is revealed that the system pressure is dominant to filling time, flow front advancement and velocity profile but the operating temperature will slightly affect the injection moulding process due to small variations of PP viscosity at temperature in the range between 185-195℃ [1].

1.3 Problem Statement

Injection moulding is a manufacturing process which is carried out by injecting molten material into a mould in order to create parts. The flowability of polymer is affected by pressure. Hence, the input pressure at the inlet should be at the ideal level in order for the polymer to completely fill up the mould. As higher pressure in the inlet of the mould will cause the polymer not to fill up the mould completely and lower pressure will cause the polymer to harden before it completely fills up the mould. In this case, the pressure difference and shape of the mould would be varied in order to study the flowability of the polymer.

1.4 Objective

To study the influence of the temperature and pressure on the polymer melts behaviour

1. To study the influence of the pressure on the polymer melts behaviour
2. To investigate the flowability of the polymer by varying the inlet pressure
3. To evaluate and compare the flow of the polymer in different shapes of grooved channel and pitch size

1.5 Scope of Work

The project will be focusing on the numerical study on the polymer melting flow behaviour with the use of ANSYS Fluent 2022 software. To evaluate the polymer flow behaviour in different pressures. In addition to that the polymer melting behaviour will be studied by manipulating the pressure which is set at the inlet of the mould. The ratio of the polymer to the total mixture in the mould will be evaluated. Moreover, the changes to input velocity due to different pressures will also be observed. The simulation will be carried out using a VOF model in order to study the flowability of the polymers. Various input parameters such as the temperature at the inlet (463.15 K) and surface condition of the wall (no slip wall condition) will be plugged into the simulation to study the flow of the polymer in the mould. Besides that, other parameters such as the shape of the mould and the pitch size will also be investigated.

CHAPTER 2 LITERATURE REVIEW

2.1 Polymer

A polymer can be defined as a long-chain molecule composed of several chemically connected repeating components known as monomers. The term polymer derives from Greek, with the term "poly" means many and "mer" means part **Error! Reference source not found.**. In other words, many of the same component are linked together to produce a polymer, which is a lengthy chain.

Natural polymers are compounds found in nature that originate from either plants or animals. Nature developed them for a specific purpose, namely the preservation of life [1], [3]. They come into one of three categories: polysaccharides, nucleic acids, or proteins. Sugar molecules are covalently bound together by polysaccharides, which are low molecular weight polymer chains (comprised of numerous hydroxyl groups). The most significant polysaccharides are those that are made of glucose or its by-products. Glucose is necessary for both polysaccharides that build up plant structure, starch and cellulose. Natural cellulose is very strong and highly crystalline due to the many hydroxyl groups found along the polymer chains, which enable strong intermolecular connections via hydrogen bonding.

As a result, they have superior textile properties than their synthetic equivalents. Proteins, on the other hand, are polypeptides formed by the polymerization of amino acids that serve as the building blocks of animals. Each type of protein has a unique amino acid sequence and structure that determines its unique function or purpose. They can be made up of long-chain molecules or cross-linked chains. The proteins haemoglobin, albumin, collagen, and actin are all crucial. DNA and RNA are two additional natural polymers found in living things. They are linear polymers made mostly of sugar molecules, phosphates, and bases that are responsible for storing and reading genetic information.

In a laboratory, synthetic polymers are generated using controlled polymerization conditions that allow the polymers' properties to be customised to specific purposes. The majority of the materials that make up our environment are synthetic polymers, with nylon and polyolefins like polyethylene and polypropylene serving as examples of materials that are mass-produced all over the world. Natural polymers are chemically changed in some cases to increase their properties and economic worth. Semi-synthetic polymers include vulcanised rubber, which is created by chemically cross-linking the chains of natural rubber with sulphur [3].

Polymers are classified into three types depending on their structure: linear, branching, and cross-linked. The most significant and widely used polymers frequently have a basic linear structure. The backbone of this kind of polymer is made up of lengthy, continuous chains of monomers joined by covalent bonds [1]. Having viscoelastic and non-Newtonian properties, polymer melts and solutions are viscous liquids. Engineering procedures increasingly depend on the flow characteristics of molten polymers or liquids.

Through Newton's postulate, the flow curve of an ideal liquid (curve ① in **Figure 2.1**) should be a straight line and the shear viscosity (η), which is obtained via dividing the shear stress (τ) by shear rate (γ), remains constant and independent of shear rate [4]. All liquids exhibiting these behaviours are called "Newtonian liquids", such as water, glycerine, alcohol, molasses, mineral oils, bitumen, etc.

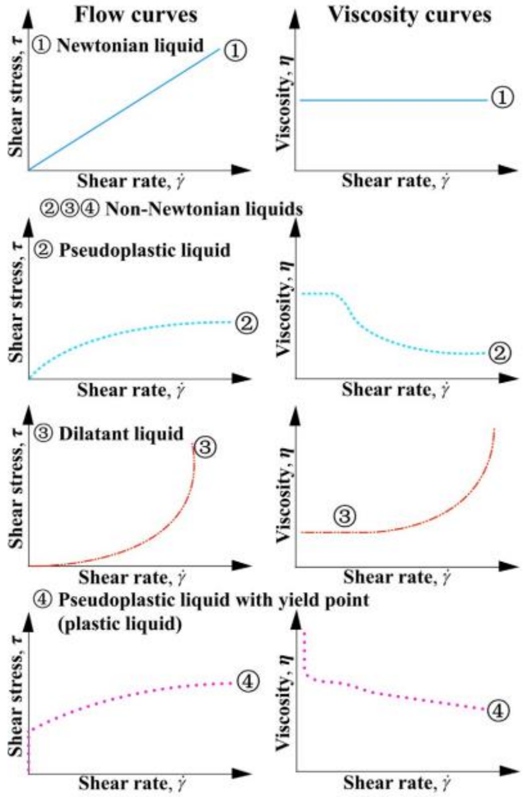

Figure 2.1 Typical flow behaviours of Newtonian and non-Newtonian liquids

2.2 Polymer rheology

Polymer rheology is the investigation of the deformation and flow of polymers [5]Error! Reference source not found.. A strong understanding of polymer rheology is required for effective material design and processing techniques. In practise, the majority of polymers exhibit "viscoelastic" behaviour during flow, which means they exhibit both viscous and elastic behaviour. Most polymer melts and suspensions may have their shear flow behaviour modified by modifying polymer parameters (such as molecular weight, molecular weight distribution, chain branching, and so on) and rheological factors such as temperature, shear, and pressure.

2.3 Viscosity of polymer melts

The variable viscosity of polymers as shear rate changes is recognised as a significant property in many industrial operations [6]. Because shear rate dominates most polymer operations, the viscosity of polymer melts/solutions is typically evaluated with shear-deformed devices. **Figure 2.2** shows the simple shear flow characteristics produced by a sliding plate rheometer equipped with a shear stress transducer [8].

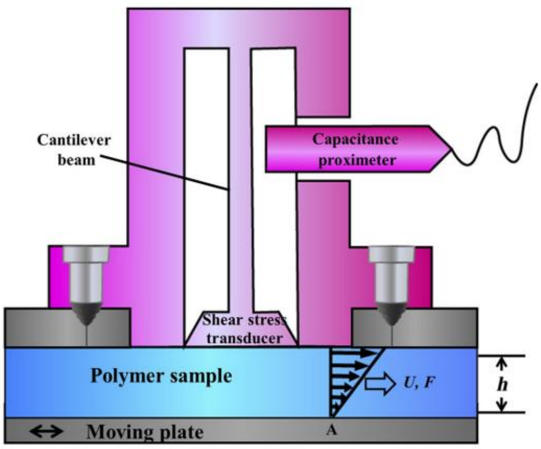

Figure 2.2 Configuration of a sliding plate rheometer coupled with shear stress transducer.

Giacomin et al. [9] created this type of sliding plate rheometer at McGill University in 1987, and Interlaken Technology Corporation commercialised it [9], [10]. The shear stress created in the flow as the polymer melts are pressed between the parallel plates is described by

$$\tau = \eta\gamma, \tag{2.1}$$

where τ is the shear stress (the force F per unit area A necessary to move the plate, F/A), which is connected to the velocity gradient (i.e., shear rate) γ indicated by U/h, and η is the viscosity.

The suggested **Eq. (1)** shows the behaviour of a basic Newtonian fluid with an inherent viscosity. Molten polymers and solutions have more intricate flow properties than Newtonian liquids because they are highly viscous, non-Newtonian, and viscoelastic. They also have certain elastic solid-like properties. Shear-thinning fluids characterise the majority of polymer melts and suspensions. The shear-thinning effect, as previously noted, is the decline in viscosity with increasing shear rate, also known as pseudoplasticity. Temperature, polymer melts and entanglements, molecular weight distribution, chain branching, additive action, and pressure all impact the non-Newtonian behaviour of polymer melts and suspensions [11], [12].

2.4 Injection moulding

Injection moulding is a main method for mass producing complicated structures out of plastic materials. Most thermoplastics with customised rheology and some thermosets with adequate shear flow can benefit from it. Injection moulding machines are made up of two basic components: an injection unit and a clamp unit. The injection unit is usually a single-screw reciprocating extruder that prepares the polymer melt and transfers it into the mould. The mould is held securely against the injection pressure in the clamp unit, opened for demoulding, then closed for the next shot. The equipment is primarily powered by hydraulic energy, which is provided by an electric motor and a hydraulic pump. Hydraulic systems allow hydraulic oil to flow through pipes, creating a maximum pressure of roughly 14 MPa in the absence of sophisticated mechanical transfer mechanisms **Error! Reference source not found.**.

2.5 Analysis on Polymer Flow

Various studies have been performed in order to analyse the polymer flow behaviour when the injection moulding process is conducted. Fernandes et al. [17] researched-on optimization of the injection-moulding (IM) process. These optimization techniques include design of experiments, artificial neural networks, and evolutionary algorithms. The strengths and weaknesses of each approach were discussed. He also discussed on the optimization research performed in the IM process regarding some of the specific features associated with the processes such as runner system and cooling channel configurations, process conditions, gate location, and cavity pressure balancing. He also mentioned that the numerical simulation has the advantage of providing helpful information for part design, mould design, and IM process design. A variety of processing settings can be used. Simulation packages can be used to obtain results. However, this method necessitates the creation of a finite element model and the execution of a simulation. To get suitable moulding parameters, a large number of simulations has to be performed [17].

The transient finite element approach may be used to analyse the mechanism of the flow markings, according Grillet et al. [18]. The base state streamlines and polymer stresses are determined by steady finite element computations of a model injection moulding flow employing a single mode, exponential Phan-Thien-Tanner constitutive equation. Simulators were utilised to create and evaluate the numerical strategy for this intricate flow. Investigated was the impact of extensional rheology on steady flow and stability behaviour. In steady flows of strain hardening materials, it was shown that large polymer stresses might accumulate along the free surface and extend some distance downstream into the channel flow [18].

Moreover, a study was also done by analysing the fill time of injection moulding in order to reduce the defects that are usually found on the plastics such as poor weld line. The parameters used for this investigation are the melting temperature, the mould temperature, the injection duration, and the number of gate locations on the moulding machine. The Response Surface Method (RSM) was utilised to find the most important and optimal factors affecting the fill time on the reservoir. In the examination of the results, it was discovered that the injection time was the most important parameter that had an impact on the fill time, accounting for 99 percent of the variance. The outcome demonstrates that there is no interaction between process parameters and fill time, with the injection duration being the sole significant factor influencing fill time. Mould temperature at 60°C, injection duration at 4s, and the number of gates with two gates in each place are the most optimal parameters for increasing the injection time. For this reason, it is possible to eliminate defects in moulded parts by increasing the injection duration during the injection moulding process [19].

Rusdi et al. [20] studied on the pressure distribution and velocity drop during injection moulding. The melt front pressure in the mould cavity demonstrates that it was influenced by the form of the mould cavity and the filling stage during the moulding operation. The melt front pressure will drop as the flow progresses farther away from the sprue, but it will dramatically rise when the mould is ready to be completely filled with the melt. When the molten flow contacts the rib of the tray, a tiny pressure reduction was noted. The cause of this pressure drop is yet to be known.

Higher injection pressure resulted in a faster injection rate than lower injection pressure, although the speed of the melt front reduced quickly after it had completely filled the cavity. Besides that, study on the effect of pressure and temperature on the melt filling during injection moulding process by using the ANSYS Fluent 14 was also conducted. In this study, the pressure and operating temperature were the manipulating variables. The influence of these two parameters were observed in terms of filing time, flow front advancement, and velocity profile. In this result, it is revealed that the system pressure is dominant to filling time, flow front advancement, and velocity profile. Meanwhile, operating temperature only has small effect on the current injection moulding process [20].

Yang et al. [21] conducted research on the polypropylene-filled glass beads' melt flow behaviour. Melt flow rate (MFR), capillary rheometer, and torque rheometer studies were used to determine how the composition, size, and production method of the glass beads affected the melt flow properties of the composites. A TSSL-25 co-rotating twin extruder (Chengguang Chemical Institute, Chengdu, PRC) was used to combine polypropylene and glass beads in the molten state with a temperature profile between 160 and 230 °C after easy mixing. After extrusion, the extrudate was pelletized. After drying the sample to eliminate any moisture that could have remained during extrusion, the pellets were used to examine the rheological parameters of the sample. The MFR of glass bead filled polypropylene composites was more affected by glass bead content and preparation methods than by bead size. Although did not substantially change with the tested bead sizes, the apparent viscosity (η) of the materials first rose with the addition of glass beads and then decreased with increasing glass bead concentration. In comparison to composites generated by twin screw extruders, single screw composites have a higher viscosity.

When Liang et al. [22] looked into how pressure and temperature affected the melt density and melt flow rate of LDPE and glass bead-filled LDPE composite, they found that the Arrhenius equation predicted that the MFR of the melts increased exponentially with temperature and quadratically with pressure. Additionally, when the pressure is not too high, the MFR values for LDPE/GB are a little bit lower than those for unfilled LDPE at the same temperature.

In addition, designing the gating system is a crucial step in the creation of an injection mould because the gate serves as a vital conduit connecting the runner and cavity. The gate's design influences both the costs and advantages of production by influencing not only the melt filling process but also the demoulding process and the separation of products and waste **Error! Reference source not found.**. Gate size, being a crucial feature of gate design, has a significant impact on part quality. A proper gate should be able to ensure quick and liquid plastic filling. Tor et al. [23] investigated the effects of gate size on the quality of powder injection moulding using five rectangular gates with varied width and depth ratios. They assessed the influence of different gate sizes by analysing the weight and density of the samples moulded for each of the five gates. The results show that increasing the width or depth of the gate produces varied effects even when the overall cross-sectional area of the gate remains constant. Samples moulded with deeper gates have a higher weight and density.

Xie and Ziegmann [25] studied the influence of gate dimension on micro injection moulded weld line strength with polypropylene (PP) and high-density polyethylene (HDPE) and discovered a relationship between gate size and micro-moulded component quality. Each cavity responds to different gate dimensions, which are labelled as Gate Nr.1(1.5×0.1×0.5mm), Nr.2(1.0×0.1×0.5mm), Nr.3(1.0×0.05×0.5mm), and Nr.4(0.5×0.1×0.5mm). The results for polypropylene demonstrate that when injection pressure and mould temperature are changed, Gate Nr.3 corresponds to the strongest weld strength; Gate Nr.2 is next; and Gates Nr.4 and Nr.1 are at the end. The distinction between them is not evident. According to the simulation research, stick materials and dirt are obstructing Gate Nr.1 for high-density polyethylene, preventing it from being completely filled. The investigation was restricted to the other three gate sizes; the results demonstrate that, independent of the processing parameters, Gate Nr.3 consistently offers the strongest weld line strength, followed by Gate Nr.4, and finally Gate Nr.2.

Mehdi et al. [26] investigated the behaviour of bubbles in foam injection moulding. The melt injection temperature was set at 290°C, while the mould wall temperature was fixed at 15°C. A full shot totally filled the mould cavity. Holding pressure was used to pack the gas-charged molten polymer in order to analyse the collapse behaviour of bubbles. Bubble formation, expansion, and collapse were then captured using a high-speed camera with a recording speed of 30 frames per second. Photographs taken with the prepared setup revealed that bubbles formed by lowering the pressure below the solubility pressure moved with the flow front. When the system pressure is raised, the bubbles tend to collapse (holding pressure). The classical nucleation theory helps explain this behaviour. The amount of holding pressure has a significant impact on the rate of bubble collapse.

Residual stress is the primary source of dimensional and form errors in moulded components, as well as environmental stress cracking [27], [28]. The size of the gate effects polymer molecule orientation, fibre orientation, and the mechanical and physical characteristics of moulded components **Error! Reference source not found.**, [29]. As a result, evaluating the residual stress of the goods can offer a foundation for selecting the gate size. Residual birefringence may be used to measure polymer molecular orientation and residual stress [31], but it can also reveal the microscopic morphological structure of polymer products [32]. According to Friedl [33], the refractive index effectively provides all of the information needed to characterise the status features of transparent injection products.

An injection mould was developed by Ozdemir et al. [34] that enables images to be retrieved from the plastic flow. At various injection pressures and velocities, the filling and flow properties of molten high-density polyethylene (HDPE) and polypropylene (PP) were measured. The computational forecasts of Moldflow 5.0 software were contrasted with the experimental results of flow front advancement. The experimental and computational simulations of the viscoplastic Carbopol gel's cavity filling time and filling flow pattern were assessed by Ruder and Schwarze [35]. Using a front and rear clear mould, the viscoplastic flow was observed. The numerical solution using FVM and VOF with shearthinning behaviour and yielding point effect of the gel was specified using the Herschel-Bulkley model. The OpenSource software OpenFOAM and FLUENT were used to solve the governing equations. They found that there was good agreement between simulation and experimental data for a cavity filling time and filling flow pattern.

In this project, the results from different articles and research will be studied to enhance our understanding on the polymer flow behaviour. By analysing the flow of polymer by varying the pressure and mould shape a better understanding on the polymer flow will be obtained. Also, the numerical simulation performed by other researchers focused more on strain rate of the polymer and flow of the polymer in a straight channel. Hence, this project is aimed to fill the gap that exists in order to gain insights on flowability of the polymer by varying the inlet pressure and having polymer flow in a grooved channel with the aid of simulation software ANSYS Fluent.

CHAPTER 3 METHODOLOGY

The simulation on polymer flow behaviour was conducted by using the simulation software ANSYS Fluent. It is computational fluid dynamics (CFD) software that could provide physical modelling of fluid flow for various application. It utilizes various numerical simulation method to compute for the solution either in steady or transient state. The governing equations of mass, momentum, and energy conservation may be used to explain the fluid motion of molten PP where it was injected into the mould cavity. ANSYS FLUENT solves the governing equations with Cartesian spatial coordinates and a velocity component. In the simulation model, the air, and molten PP are considered to be incompressible.

3.1 Governing Equation

The governing equations of mass, momentum, and energy conservation may explain the fluid motion of molten PP where it was injected into the mould cavity. ANSYS FLUENT solves the governing equations utilising Cartesian spatial coordinates and a velocity component to solve the governing equations.

3.1.1 Continuity equation

The conservation of mass or continuity equation is:

$$\frac{\partial \rho}{\partial \mathrm{t}} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{3.1}$$

where, ρ is the density of mixture and u_i is the velocity. The mass conservation equation in its general version, equation **(3.1)** is applicable to both compressible and incompressible flow.

3.1.2 Momentum equation

The momentum equation in *i* -th direction in an inertial (non-accelerating) reference frame is written as:

$$\frac{\partial \rho}{\partial \mathrm{t}}(\rho u_i) + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = \frac{\partial \mathrm{P}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho g_i + F_i \tag{3.2}$$

where, P represents the static pressure, τ_i as the viscous stress tensor, g_i and F_i is the gravitational acceleration and external body force in the i direction respectively.

3.1.3 Energy Equation

The energy equation expressed in terms of static enthalpy(h) may be expressed as follows.

$$\frac{\partial}{\partial \mathrm{t}}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_j}(k)\frac{\partial \mathrm{T}}{\partial x_i} + \eta\gamma \tag{3.3}$$

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

3.1.4 Volume of fluid (VOF) model's volume fraction equation

The VOF approach uses a scalar (f) to specify the percentage of the computational grid's cells that are occupied by liquid to find and develop the distribution of the liquid phase. As a result, when a cell exclusively contains molten PP, the factor f will equal 1 (f = 1), when a cell is devoid of molten PP (or air), the factor f will equal zero (f = 0), and when the factor f is between 0 and 1 ($0 < f < 1$), the cell is considered to be an "interface" cell or the molten PP front. The equation of the melt front with time was determined by the following transport equation.

$$\frac{\partial \mathrm{f}}{\partial \mathrm{t}} = \frac{\partial \mathrm{f}}{\partial \mathrm{t}} + \nabla.(u\mathrm{f}) = 0 \tag{3.4}$$

3.2 Geometry Modelling

The physical geometry of the model was built while referring to the geometry stated by Rusdi et al. [20], as illustrated in the **Figure 3.1**. The geometry was drawn in the Solidworks software and then was imported to ANSYS software. The **Figure 3.2** shows the model after it was imported to the ANSYS software.

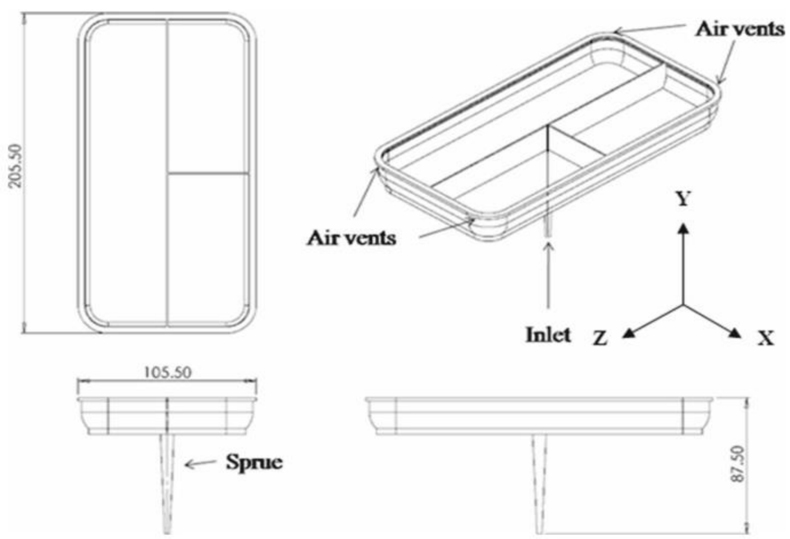

Figure 3.1 Physical geometry of mould

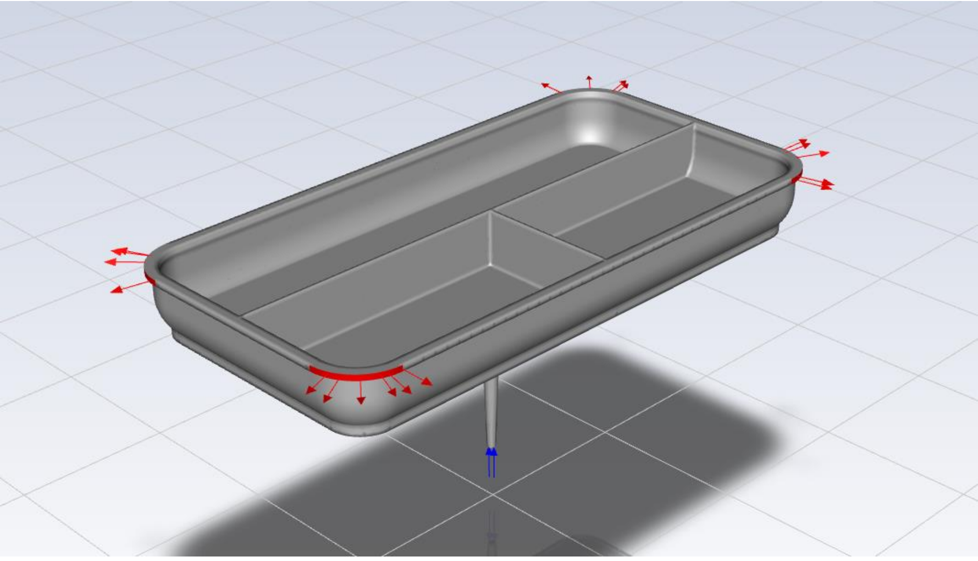

Figure 3.2 Mould shape in 'SOLUTION' before initialisation

3.3 Setting up the Simulation

3.3.1 Assumptions

The simulations are set up in Ansys Fluent 2022 R1. The following assumptions are made when setting up the simulation:

1. Both the air and propylene are considered to be laminar and incompressible.
2. All thermophysical properties of solid and fluid phases are shown as in **Table 3.1**, which is referenced from Rusdi et al. [20].
3. The pressure and the temperature of the inlet which is the sprue was set at 40 bar and 463.15 K respectively. The boundary conditions for the wall is set as '*stationary wall*' and '*no slip*', with the material of tool-steel and room temperature at 27 °C. The viscous model is set as '*Laminar Viscous Model'*.
4. The implicit body forces are considered and turned on.

Table 3.1 Thermophysical properties of solid and fluid phases

Parameter	**Air**	**Propylene**
Density (kg/m^3)	1.2	1.7
Viscosity (kg/ms)	1.78e-05	8.70e-06
Molecular Weight (kg/kmol)	28.966	42.081
Standard State Enthalpy (J/kg mol)	0	2.04e+07
Reference Temperature (K)	463.15	463.15

Air was assigned as the primary phase of the model as the Volume of Fluid (VOF) model in ANSYS Fluent would compute the solution based on the secondary phases. The propylene was assigned as the secondary phase. The viscosity of the propylene is assumed to remained constant for the simulation. For the walls of the model, the non-slip wall condition was selected and a zero specific shear was assumed for the walls in the boundary settings for the model. The corners of the model were set as the outlet. At the outlet, the gauge pressure was set to zero and the back flow volume fraction was set to zero for phase 2 to indicate that propylene that is injected to the mould will not exit the mould.