

Article

Investigating Non-Newtonian Flow Characteristics of Polypropylene: A Computational Fluid Dynamics Study Utilizing COMSOL Multiphysics

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Abstract. Polypropylene, a plastic used across industries showcases intricate flow behaviors essential for refining manufacturing techniques. This study utilizes fluid dynamics (CFD) to simulate the flow of polypropylene through an extrusion die focusing on how its viscosity alters under varying stress levels. With the intricate design of the extrusion die in mind the research seeks to comprehend viscosity changes, velocity patterns and pressure drops as molten polypropylene moves through the mold. The analysis divides the mold into three segments for examination: the inlet radial side, outlet radial side and a narrow pathway known as the choke point within the extrusion die. By employing COMSOL Multiphysics and the Carreau model researchers explore how adjusting pressure influences flow behavior and characteristics at these zones. Results indicate that heightened pressure results in increased flow rates as polypropylene tends to thin when stressed, leading to smoother flow conditions. Moreover, it is observed that viscosity profiles become more uniform with rising pressure levels. These findings provide insights into polypropylene properties, for optimizing mold design and polymer processing methods effectively. This interdisciplinary study combines expertise with applications to offer actionable guidance for enhancing polymer processing systems in terms of both design and operation.

Keywords: Non-Newtonian flow, polypropylene, computational fluid dynamics (CFD), COMSOL Multiphysics, rheological behavior, fluid mechanics.

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1. Introduction

Polypropylene, a type of polymer, is widely utilized in industries due to its distinct characteristics and ease of processing. Its behavior under flow conditions has attracted attention in the realm of computational fluid dynamics (CFD) [1]. Polypropylene is part of the polyolefin group and is distinguished by its high strength-to-weight ratio, chemical resistance, and thermal stability. It is produced by polymerizing propylene monomers and finds applications in packaging, textiles, medical equipment, automobile parts, and more [2]. One of polypropylene's main advantages is its versatility in processing methods, such as blow molding, extrusion, and injection molding, making it suitable for a broad range of applications [3].

Polypropylene's resistance to chemicals, acids, and bases renders it ideal for environments that require interaction with various materials. Additionally, its lower density compared to other polymers makes it perfect for lightweight applications without compromising strength [4]. Its ability to withstand high temperatures makes it suitable for demanding conditions, and its flexibility and impact resistance contribute to its durability. Furthermore, polypropylene can be recycled, supporting sustainability efforts.

In engineering and scientific research, CFD is instrumental in simulating and studying flow movements, heat transfer, and associated phenomena. Researchers use CFD to explore polymer melts, flow behaviors, and heat exchange processes during polypropylene processing [5]. For instance, CFD helps model the packing and filling stages in injection molding processes, predicting the flow within the mold cavity to optimize mold design and minimize issues like sink marks and warping. It also aids in die design optimization during extrusion processes by analyzing flow through extrusion dies, as well as predicting the cooling and solidification of polypropylene after processing [6]. Additionally, CFD can be employed in 3D printing to study the extrusion process and forecast filament flow behavior, thereby improving print quality and reducing defects in polypropylene filaments [7], [8].

In this study, polypropylene flow through a jet-nozzle-like die is simulated using COMSOL Multiphysics®. The focus is on three critical sections of the die: the inlet radial side, the outlet radial side, and the choke point—a narrow passage within the extrusion mold. Using the Carreau model, the influence of pressure adjustments on polypropylene flow at these points is investigated. The non-Newtonian behavior of polypropylene is predicted with parameters from the literature [9], [10]. Viscosity, velocity, and pressure profiles at different die locations are analyzed. The aim of this computational study is to examine the rheological characteristics of polypropylene (PP), utilizing CFD simulations in COMSOL Multiphysics. By focusing on an axisymmetric extrusion die setup, the study seeks to provide an in-depth analysis of polypropylene's non-Newtonian flow properties. This approach not only

enhances our theoretical understanding of polymer fluid mechanics but also bridges the gap between academic research and practical applications in polymer processing. Although past studies have examined polypropylene characteristics, there is a lack of research combining CFD modeling with experimental data to optimize processing parameters specifically for extrusion dies [5], [11]–[13] behaves under real world processing conditions. While past studies have looked into the characteristics of polypropylene there is a lack of investigations that combine computational fluid dynamics (CFD) modeling, with actual data to optimize processing parameters specifically for extrusion dies [5], [11]–[13].

This study contributes by conducting an examination of how pressure and temperature impact the viscosity of polypropylene during extrusion. By merging CFD simulations with the Carreau model we present a framework for predicting flow behavior that can be directly utilized to enhance manufacturing processes.

This research fills a gap in the field where theoretical modeling meets implementation. Previous studies have. Focused on theory without real world validation or presented empirical findings without a solid theoretical foundation. Our interdisciplinary approach bridges this divide by offering both a model supported by evidence and practical recommendations for industry applications. This dual emphasis not only advances our knowledge of polymer flow but also provides valuable insights, for engineers and manufacturers.

2. Methodology

In this study, computational fluid dynamics (CFD) is employed to simulate the flow behavior of polypropylene within an extrusion die, with a focus on capturing the material's non-Newtonian characteristics. The objective is to model the shear-dependent viscosity of polypropylene, which plays a critical role in its processing under varying conditions. By analyzing the effects of different inlet pressures and temperatures, this research aims to gain insights into the flow dynamics that govern industrial extrusion processes. The study seeks to optimize processing parameters by providing a detailed understanding of how these variables influence the material's flow behavior, which can directly impact the quality and efficiency of extrusion operations. The aim of this study is to apply computational fluid dynamics (CFD) techniques to simulate the flow behavior of a polypropylene through an extrusion die, utilizing non-Newtonian fluid mechanics to accurately represent the material's shear-dependent viscosity [14]. This investigation focuses on understanding how varying levels of inlet pressure and temperature affect the flow dynamics of polypropylene, which are crucial factors in industrial extrusion processes.

2.1. Model Setup

The simulation was conducted using COMSOL Multiphysics, following the framework provided by the "Non-Newtonian Flow in a Die" example. This example typically illustrates the flow dynamics of a linear polystyrene solution and employs the Carreau model to describe the non-Newtonian behavior of the fluid. For our study, this model is adapted to simulate polypropylene (PP).

2.2. Analytical Derivation of Carreau Model Parameters

In this CFD modeling, we need to specify certain properties of the fluid under study, which is polypropylene (PP). These properties were sourced from the literature. The properties of the polypropylene used in this CFD simulation is summarized in Table 1.

Table 1. Properties of fluid under study (polypropylene).

Property	Values
1 Molecular weight	164 kg/mol
2 Density	905 kg/m ³
3 Melt-flow index (MFI)	3.0
4 Tensile strength	34 (MN/m ²)
5 Elongation at break (%)	350
6 Flexural modulus	190,000 (lb in ⁻²)
7 Brittleness temperature (°C)	+15
8 Vicat softening point (°C)	145–150
9 Rockwell hardness	95
10 Impact strength (ft-lb)	10

In this CFD study, COMSOL Multiphysics® carries out simulations based on the Carreau model which has the following equation:

$$\mu_{app}(\dot{\gamma}) = \mu_{\infty} + (\mu_0 - \mu_{\infty})[1 + (\lambda \dot{\gamma})^2]^{(n+1)/2}$$

The variables of Carreau equation is summarized in Table 2.

The Yasuda-Carreau model was selected for this simulation due to its proven ability to accurately describe the non-Newtonian behavior of polymer melts, including polypropylene, under various shear conditions. This model accounts for the complex shear-thinning behavior that is characteristic of many polymers, making it particularly suitable for capturing the viscosity variations experienced during the extrusion process. Unlike simpler models, the Yasuda-Carreau formulation incorporates a broader range of parameters, allowing for the fine-tuning of the transition between Newtonian and non-Newtonian flow regimes.

In the context of polypropylene processing, where the material experiences both low and high shear rates, the Yasuda-Carreau model provides the necessary flexibility to simulate viscosity variations over a wide range of

conditions. It is especially valuable in capturing the gradual shear-thinning effect, which is essential for accurate modeling of extrusion processes, where flow behavior significantly influences die design, flow uniformity, and product quality. Furthermore, the model's parameters can be adjusted to reflect experimental data, ensuring that the simulation closely mirrors real-world processing conditions. By employing the Yasuda-Carreau model, this study ensures a comprehensive understanding of polypropylene's flow characteristics, leading to more precise predictions and optimizations in polymer processing

Table 2. Carreau model parameters and its symbols with units.

Name	Symbol	SI Unit
Dynamic viscosity	μ_{app}	Pa · s
Shear rate	$\dot{\gamma}$	s ⁻¹
Zero shear rate viscosity	μ_0	Pa · s
Infinite shear rate viscosity	μ_{∞}	Pa · s
Power index	n	Dimensionless
Relaxation time	λ	s

The flow of polypropylene through an extrusion die was studied using the Yasuda-Carreau model at 200 °C . The parameters for the Carreau-Yasuda model for polypropylene at 200 °C are provided in Table 3.

Table 3. Carreau model parameter values for propylene.

Parameter	200°C
μ_{∞} (Pa·s)	0
μ_0 (Pa·s)	476
n	0.3254
λ (s)	0.0254
R^2	0.99

In COMSOL, the geometry for the extrusion die was developed with the following parameters: an inlet radius of 9 mm, a height of 40 mm, and an outlet outer radius of 6 mm. The first step was mesh generation. In computational modeling, after constructing the geometry as described above, meshing is a crucial step. As shown in Fig. 1, a mesh divides the model into small elements of uniform or irregular shapes [14]. These elements are the fundamental building blocks used in the calculations to obtain the solution.

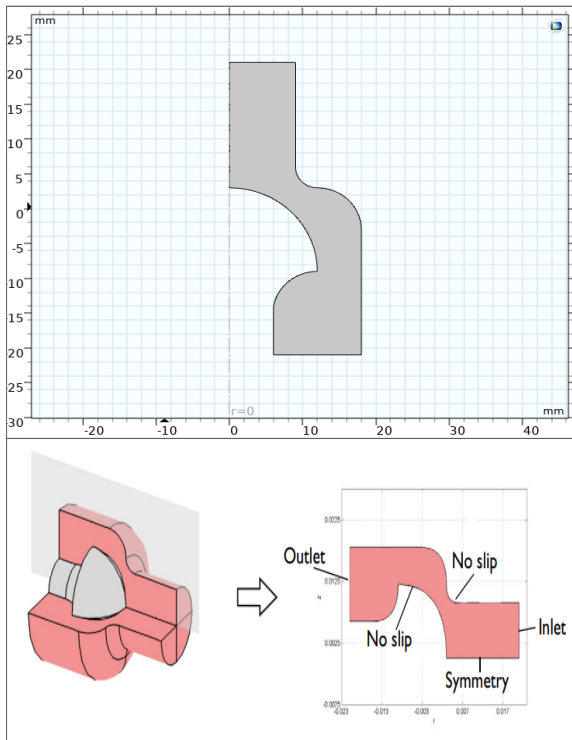


Fig 1. 3D and 2D geometry of extraction Die polypropylene (PP) flow path.

2.3. Boundary Conditions

Inlet: The inlet boundary condition will involve varying the inlet pressure and temperature to study their impacts on the flow dynamics.

$$P=P_{in}=100 \text{ KPa}$$

Outlet: A standard atmospheric pressure will be set at the outlet.

$$P=0$$

Walls: No-slip boundary conditions will be applied to the walls of the die.

$$U=0$$

A steady-state solver will be used initially to gain insights into the flow patterns. In addition to study the effect of viscosity at different inlet pressures, parametric solver is used to vary p_{in} from 100 kPa to 2100 kPa.

3. Results and Discussion

The extrusion process of polypropylene involves melting the polymer and forcing it through a shaped die to create products like films, pipes, or sheets [15]. Accurately estimating the flow velocity profile through the extrusion die is crucial, as it impacts the quality and consistency of the final product. Understanding the velocity profile helps in optimizing the die design and processing conditions, ensuring uniform flow, reducing defects, and enhancing the mechanical properties of the extruded material. The

velocity field at the outlet experiences a significantly lower average velocity compared to the inlet, primarily due to the presence of rotational symmetry [16], [17]. Figure 2 indicates that the area with the most substantial velocity gradient is within the contraction region, indicating the highest shear rate occurs at that point,

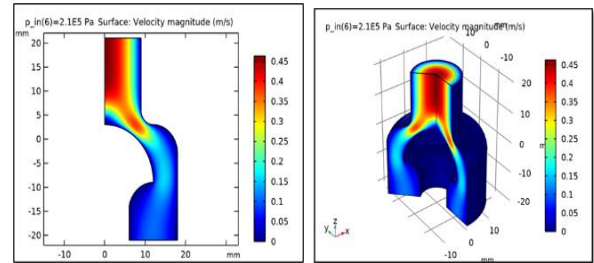


Fig. 2. Velocity profile for melted polypropylene flow through the extrusion die.

Figure 3 presents a contour plot illustrating the pressure distribution experienced by melted polypropylene as it flows through the extrusion die. The pressure is highest at the inlet of the die (approximately $94.9 \times 10^3 \text{ Pa}$ or 100 kPa) and decreases as the material progresses through the die. This pressure drop is attributed to the shear-thinning properties of polypropylene, where the viscosity of the material decreases as the shear rate increases. As pressure forces the polypropylene through the die, the increasing shear rate results in a reduction in viscosity, thereby lowering the resistance to flow and consequently reducing the pressure [10].

The pressure reaches a minimum value of approximately $-3.5 \times 10^3 \text{ Pa}$ at the outlet of the die. The negative pressure values suggest that the pressure in these regions is lower than the reference pressure used in the simulation.

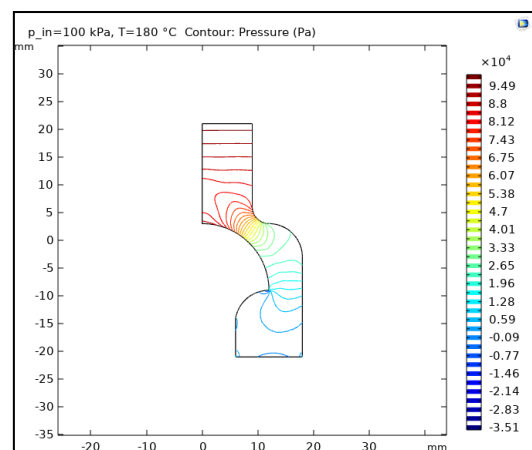


Fig. 3. Pressure distribution for melted polypropylene flow through the extrusion die.

Figure 4 illustrates the simulated viscosity (in $\text{Pa}\cdot\text{s}$) across the width (mm) of the extrusion die. Consistent with the shear-thinning nature of polypropylene, the viscosity is highest (approximately $2.5 \text{ Pa}\cdot\text{s}$) near the walls

(around -20 mm and 20 mm), where the shear rate is close to zero. Moving towards the center of the die (around 0 mm), the shear rate increases due to the narrowing channel, resulting in a decrease in viscosity (approximately 0.5 Pa·s). This trend confirms that the shear rate experienced by the fluid significantly influences its viscosity [18]. This simulation represents a specific set of conditions for polypropylene flow and die geometry. For instance, the inlet pressure (p_{in}) is set to 100 kPa, and the temperature (T) is set to 200 °C .

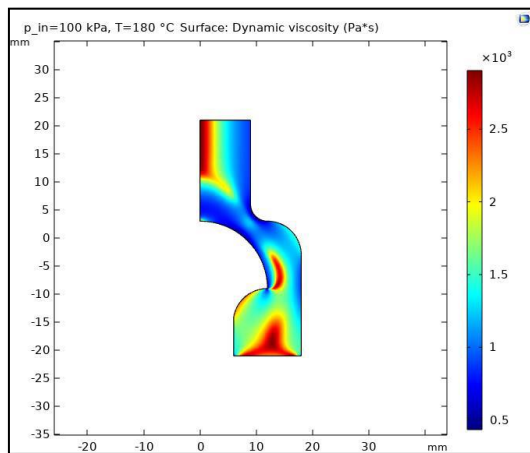


Fig. 4. Viscosity profile for melted polypropylene flow through the extrusion.

3.1. Sampling Sides for Viscosity, Velocity, and Pressure Profiles

To better understand the melt flow of polypropylene within the complex structure of an extrusion die mold, we studied velocity, viscosity, and pressure profiles at 200°C, using COMSOL Multiphysics. Figure 5 illustrates the choke point, the inlet radial side of the die, and the outlet radial side of the die, where we examined these properties.

3.2. Viscosity, velocity, and pressure profiles at the choke point at 200 ° C.

Figure 6 shows that the viscosity of the polypropylene melt at the choke point decreases as the temperature increases. This is due to the polymer chains becoming more mobile at higher temperatures, allowing them to slide past each other more easily and contributing less to the overall viscosity. Additionally, applying more pressure results in a wider range of viscosity profiles. For instance, in Fig. 6, at the lowest pressure, viscosity does not vary much across the choke point. However, at the highest pressure, it ranges between 380 Pa·s and 720 Pa·s. This is because higher pressure generates regions with high shear rates. Since polypropylene melt exhibits shear-thinning behavior, its viscosity decreases at higher shear rates and pressures.

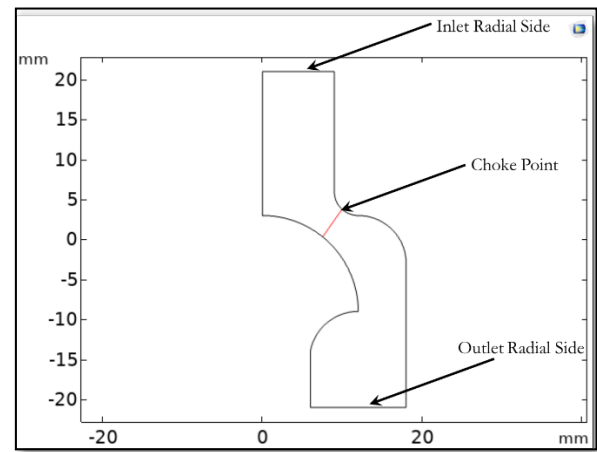


Fig. 5. 2D cutlines at different point in extrusion die. (a) choke point.(b) inlet radial side (c) outlet radial side.

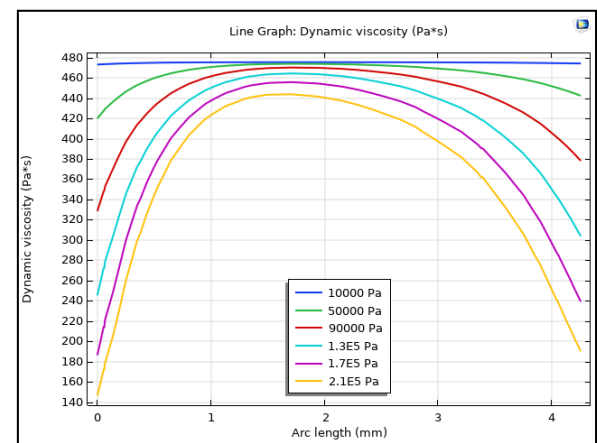


Fig. 6. Viscosity profiles at the choke point at 200 °C.

Similarly, higher pressures force the melt through the extrusion die more rapidly, further boosting the flow velocity. From Fig. 7, it can be observe that the polypropylene melt exhibits higher velocities at increased pressures and higher temperatures. This indicates that, overall, increasing both the temperature and pressure results in higher flow velocities of the polymer melt. At higher temperatures, the polymer chains become more mobile, reducing resistance to flow and thereby increasing velocity [19].

The pressure experienced at the choke point increases as the temperature rises. This phenomenon occurs because, at higher temperatures, the polymer melt becomes more fluid and the polymer chains can slide past each other more easily. As a result, the melt flow encounters less resistance, allowing it to move more freely through the choke point without a significant reduction in pressure [16]. Consequently, higher temperatures facilitate easier flow, maintaining or even increasing the pressure at the choke point. Figure 8 represents a pressure drop profile at choke point in die mold at 200 °C.

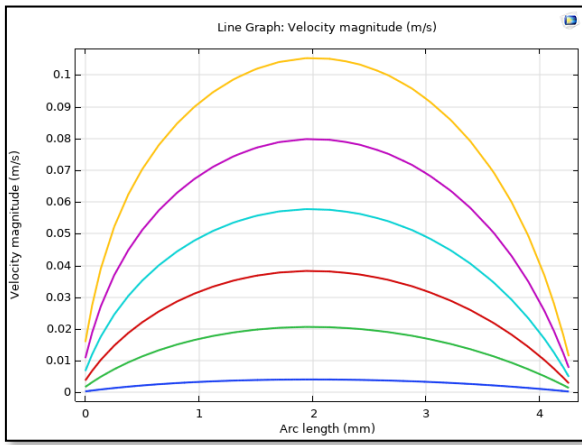


Fig. 7. Velocity profiles at the choke point at 200 °C.

3.3. Viscosity, Velocity, and Pressure Profiles at the Inlet Radial side at 200 ° C.

From Fig. 9, it is evident that the viscosity of the polypropylene melt at the inlet radial side decreases as the temperature increases. This reduction in viscosity with higher temperatures is due to the increased mobility of the polymer chains, which allows them to slide past each other more easily, reducing internal friction and resistance to flow.

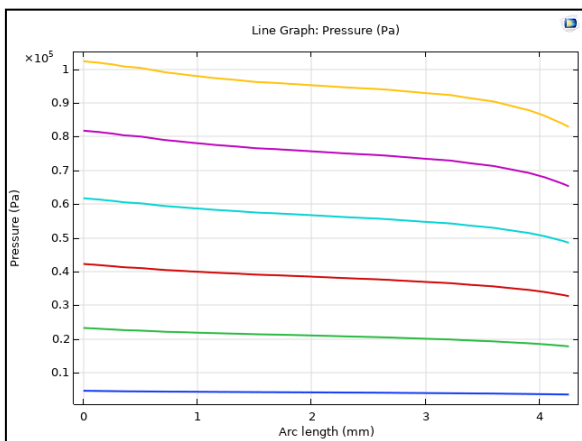


Fig. 8. Pressure drop profiles at the choke point at 200 °C.

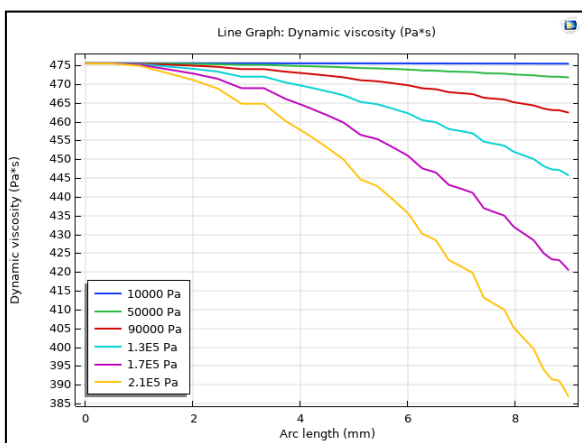


Fig. 9. Viscosity profiles at the inlet radial side at 200 °C.

Additionally, applying higher pressure results in a wider range of viscosity profiles. At increased pressures, the polymer melt is forced through the inlet radial region with greater force, generating regions with higher shear rates. Given the shear-thinning nature of polypropylene, the viscosity decreases more significantly in areas experiencing high shear rates, thus broadening the overall viscosity range. This behavior indicates that both temperature and pressure play critical roles in modulating the flow characteristics of the polymer melt, which is crucial for optimizing the design and operation of extrusion processes.

From Fig. 10, it is evident that the polypropylene melt exhibits higher velocities at elevated pressures and temperatures. This means that, overall, increasing the temperature and pressure leads to an increase in the velocity of the polymer melt [20].

At higher temperatures, the polymer chains gain more kinetic energy and become more mobile, reducing the internal friction and viscosity of the melt. This enhanced mobility allows the melt to flow more rapidly through the extrusion die. Additionally, higher pressures push the melt through the die more forcefully, further accelerating its flow. In the inlet radial region, the velocity profile of the polymer melt is also influenced by these factors.

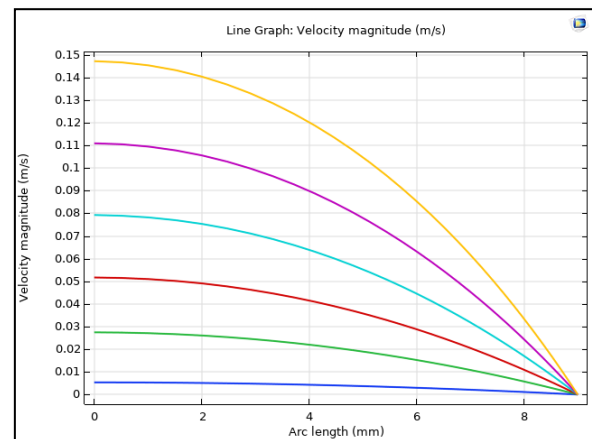


Fig. 10. Velocity profiles at the inlet radial side at 200 °C.

As the melt enters the die, it encounters initial resistance that is overcome more efficiently at higher temperatures and pressures. The increased pressure drives the melt into the die with greater force, while the reduced viscosity at higher temperatures allows for smoother and faster flow. This combination results in a more uniform and higher velocity profile at the inlet radial region, facilitating better filling and reduced cycle times in the extrusion process.

Figure 11 shows that the pressure profile at the inlet radial side remains relatively constant across different temperatures. This constancy is observed because the inlet is at the very beginning of the extrusion process, where the initial conditions are set and external factors, such as temperature, have not yet had a significant impact on the melt flow. At this early stage, the polymer melt is just

entering the die, so the pressure is primarily influenced by the feed rate and the initial push from the extruder rather than the temperature-dependent flow characteristics that develop later in the process. Additionally, the inlet region is typically designed to ensure a steady and uniform entry of the melt into the die. This design consideration further stabilizes the pressure at the inlet, making it less susceptible to variations in temperature. As the polymer melt progresses through the die and encounters varying geometries and shear rates, the influence of temperature becomes more pronounced, leading to the pressure variations observed in downstream regions such as the choke point and outlet.

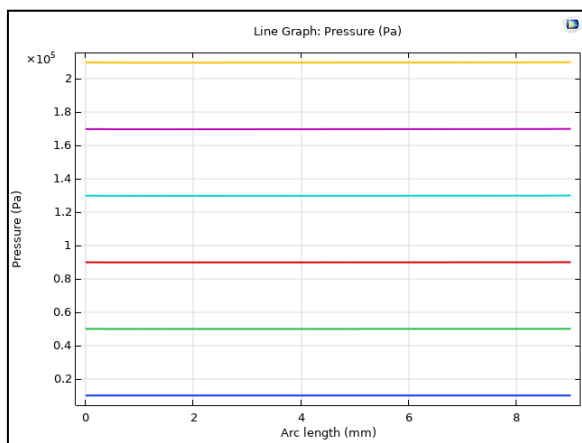


Fig. 11. Pressure drop profiles at the inlet radial side at 200 °C.

3.4. Viscosity, Velocity, and Pressure Profiles at the Outlet Radial Side at 200 °C.

Figure 12 illustrates that the viscosity of the polypropylene melt at the outlet radial side decreases as the temperature increases. This reduction in viscosity with rising temperature is due to the increased thermal energy, which enhances the mobility of the polymer chains, allowing them to slide past each other more easily and thus reducing the overall resistance to flow.

Additionally, the application of higher pressure results in a broader range of viscosity profiles. Under increased pressure, the melt experiences higher shear rates, especially at the outlet radial region where the flow expands and slows down. Since polypropylene is a shear-thinning material, its viscosity decreases with increasing shear rate. Therefore, at higher pressures, the viscosity profile exhibits more significant variation across the outlet radial side, reflecting the complex interplay between pressure, shear rate, and temperature in determining the flow characteristics of the polymer melt.

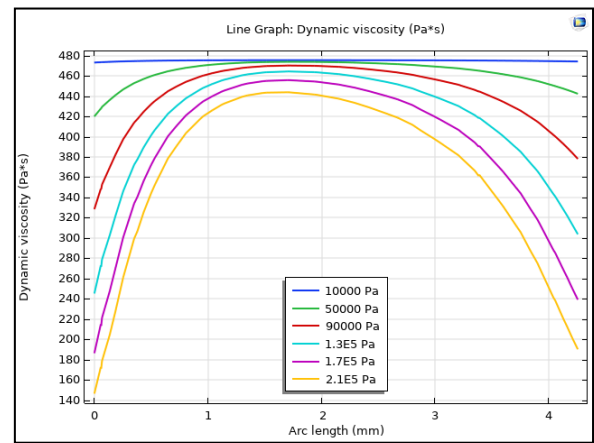


Fig. 12. Viscosity profiles at the Outlet radial side at 200 °C.

Figure 13 showed that the polypropylene melt exhibits higher average velocities at increased pressures and higher temperatures. This trend indicates that, overall, increasing both the temperature and pressure enhances the velocity of the polymer melt. At higher temperatures, the polymer chains gain increased mobility, reducing intermolecular friction and allowing the melt to flow more easily. This reduced resistance translates into higher flow velocities. Similarly, higher pressures exert a greater driving force on the melt, pushing it through the extrusion die more rapidly and further increasing the velocity.

In the outlet radial region, the velocity profile of the polymer melt is particularly influenced by these factors. At elevated temperatures, the melt's viscosity decreases, promoting a smoother and faster flow. When higher pressure is applied, the driving force behind the flow intensifies, resulting in higher velocities as the melt exits the die. This combination of higher temperature and pressure ensures that the polymer melt achieves a more uniform and accelerated flow at the outlet, optimizing the overall extrusion process [8].

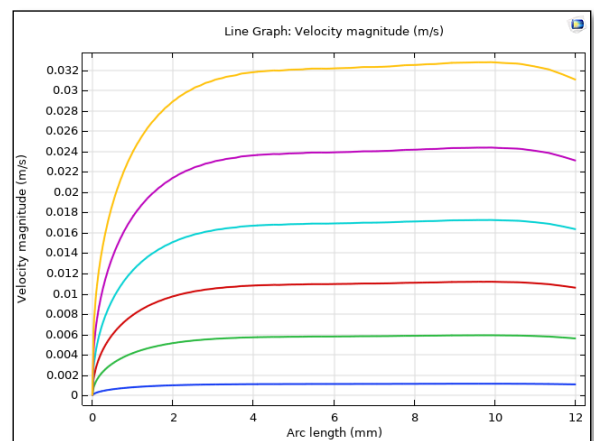


Fig. 13. Velocity profiles at the Outlet radial side at 200 °C.

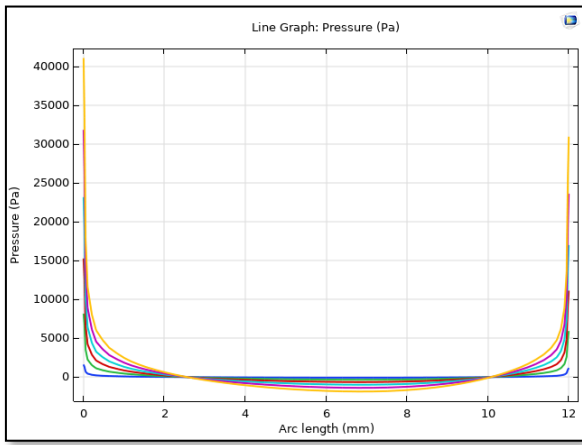


Fig. 14. Pressure drop profiles at the Outlet radial side at 200 °C.

Figure 14 showed that the pressure at the outlet radial side is generally higher at elevated temperatures compared to lower temperatures. This indicates that under more flowable conditions—achieved at higher temperatures—the polymer melt offers less resistance to pressure and transmits it more effectively [4].

At higher temperatures, the increased mobility of the polymer chains reduces internal friction within the melt. This enhanced flowability means that the melt can more easily conduct pressure throughout the extrusion die. Consequently, there is less pressure drop across the die, especially towards the outlet radial region. This reduced pressure drop is because the polymer melt, being less viscous at higher temperatures, encounters less resistance as it moves towards the exit. The ability of the melt to maintain higher pressure at the outlet radial side under these conditions is indicative of its improved flow characteristics at higher temperatures.

4. Conclusion

The simulation of polypropylene melt flow through an extrusion die has provided critical insights into the material's flow behavior, emphasizing the intricate relationship between processing conditions and the resulting product characteristics. The analysis revealed a consistent trend: increasing the inlet pressure directly correlated with higher flow rates. This phenomenon can be attributed to the shear-thinning nature of polypropylene, wherein viscosity decreases under stress, allowing the material to flow more freely. This behavior was consistently observed throughout all regions of the extrusion die, resulting in smoother and more uniform flow profiles at elevated pressures. A detailed examination of flow characteristics at three key sections—the inlet radial side, the outlet radial side, and the choke point—demonstrated that viscosity profiles became increasingly uniform with rising pressure. This uniformity indicates a more predictable and manageable flow behavior, which is crucial for maintaining consistent product quality in industrial applications. Additionally, higher pressures

resulted in increased velocities of the molten polypropylene, thereby enhancing overall flow dynamics and reducing the likelihood of defects such as voids or inconsistencies in the final product. By employing computational fluid dynamics (CFD) alongside the Carreau model, this research offers a nuanced understanding of how polypropylene behaves under varying stress conditions within the extrusion die. The findings underscore the importance of pressure as a critical parameter for optimizing the extrusion process. The clear correlation established between applied pressure and the rheological properties of polypropylene—specifically, viscosity and velocity—highlights the potential for fine-tuning extrusion processes to achieve desired outcomes.

These insights hold significant implications for the polymer processing industry. They enable engineers and manufacturers to make informed decisions regarding mold design and process optimization, ultimately leading to improved product quality and consistency. Moreover, the research suggests that effective pressure management can reduce material waste and enhance manufacturing efficiency, contributing to more sustainable production practices. The ability to predict how variations in pressure influence polypropylene flow behavior empowers industry professionals to refine extrusion and molding processes, resulting in more efficient and cost-effective production systems. Thus, the study not only advances theoretical knowledge but also provides practical guidance for optimizing polymer processing techniques in industrial settings.

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Credit Authorship Contribution Statement

Dr. Nagoor Basha Shaik: Supervision, Review and Editing; Qandeel Fatima Gillani: Simulation; Maria Shamim: Writing - review & editing; Bilal Siddiq: Methodology, Visualization, simulation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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