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Experimental and Numerical Investigation for Simulation of Thermophysical Properties for Polypropylene 575 Polymer Melts in Single Screw Extruder

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Abstract

A numerical model for Polypropylene 575 polymer melts flow along the solid conveying screw of a single screw extruder under constant heat flux using ANSYS-FLUENT 17.2 software ha sbeen conducted. The model uses the thermophysical properties such as Viscosity, thermal conductivity, Specific heat and density of polypropylene 575 that measured as a function of temperature, and residence time data for process simulation. The numerical simulation using CFD models for single screw extruder and the polymer extrusion was analysed for parameters such as (thermal conductivity, specific heat, density and viscosity) reveals a high degree of similarity to experimental data measured. The most important outcome of this study is that geometrical, parameter and conditions have been obtained from the simulation used to minimize the size, cost and time of operation for extruder.

Keywords: *Ansys Fluent, CFD, Single Screw Extruder, Numerical Simulation, Polymer melt, Polypropylene575, Solid Works, Thermophysical properties.*

1. Introduction

The production procedure of polymer slides begins in an extruder, where extrusion is a process of production long products of Constant cross-section (sheets, rods, pipes, wire insulation, coating films). Identifying of rheological behaviour for polymers is necessary for finding the best or most favourable situation of melt processing, like temperature, rate of flow, and for estimating the desirable machine capacity [1]. Many different laws have been used to describe the flow of these complex material such as power law, Bingham law, Bird-Carreau law and Carreau-Yasuda law [2]. Simulation software is applied to enhance the turnaround times, productivity, quality, and resource employment in polymer processing. However, the feasibility of a simulation software is extremely dependent on the reliability of the material data and models in its database, the skilfulness of the employer, and on the understanding of the material behaviour [1]. This study deals with the single screw extruder design for polymeric processing using (CFD) software ANSYS FLUENT 17.2, while the geometrical creation by using SOLID WORKS 2016 [2]. Fig. (1) Show the commercial single screw extruder and Fig. (2a) Show the schematic diagram of single screw extruder.

Fig. 1. Single screw extruder equipment (SJ30 / 28).

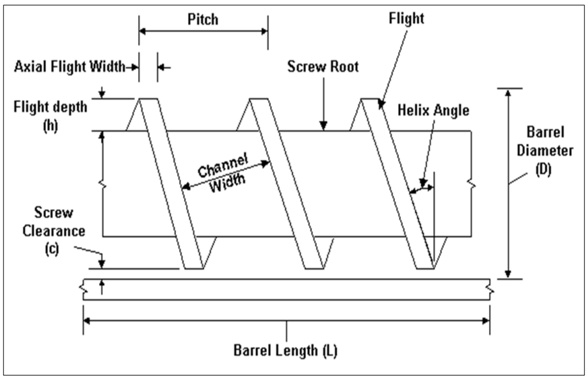


Fig. 2a. Schematic diagram of the extruder.

2. a Experimental Setup

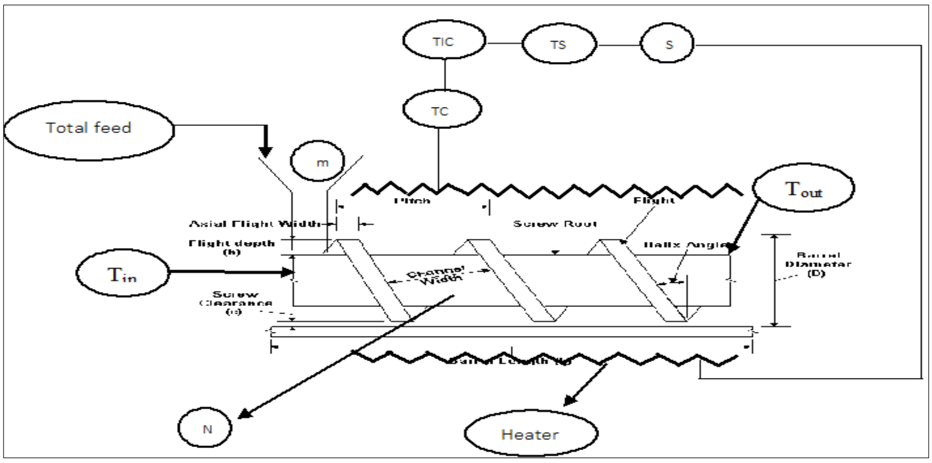


Fig. 2b. Schematic diagram of the extruder with setup details.

2. b Experimental Work

The experiments were carried out to study the effects of thermophysical properties such as (viscosity, thermal conductivity, specific heat and density) for Polypropylene 575 through single screw extruder at a different flow rate, variable rpm and constant heat flux (7803.571 w/m^2), to see more details show Fig. (2b). The physical and thermophysical properties of the polymer were measured as a function of temperature by (AR-G2) rotational rheometer, (plate-plate) geometry [3, 4] (TCi thermal conductivity analysers), and DSC equipment [5]. The data obtained from this equipment was used as polynomial equation then employed as input data for simulation process as illustrated in the equations (A-D) below. Fig. (3) Shows the experimental behaviour of thermophysical properties for polypropylene 575 at different temperature.

$$\mu = 0.2905T^2 - 294.5T + 76012 \quad \text{... (a)}$$

$$K = 8E\text{-}06T^2 - 0.0081T + 2.2014 \quad \text{... (b)}$$

$$Cp = -0.1036T^2 + 102.73T - 22458 \quad \text{... (c)}$$

$$\rho = -0.0184T^2 + 17.98T - 3491.1 \quad \text{... (d)}$$

In addition, the laboratory experiments were carried out on the laboratory extruder as illustrated in Fig. (1). The experiments were conducted using Chinese extruder in Babil governorate, this part of the work involves conducting the practical experiments on the polypropylene 575 and simulating these experiments, then validates the results with the experimental work, table (1) Shows the overall data of single screw extruder.

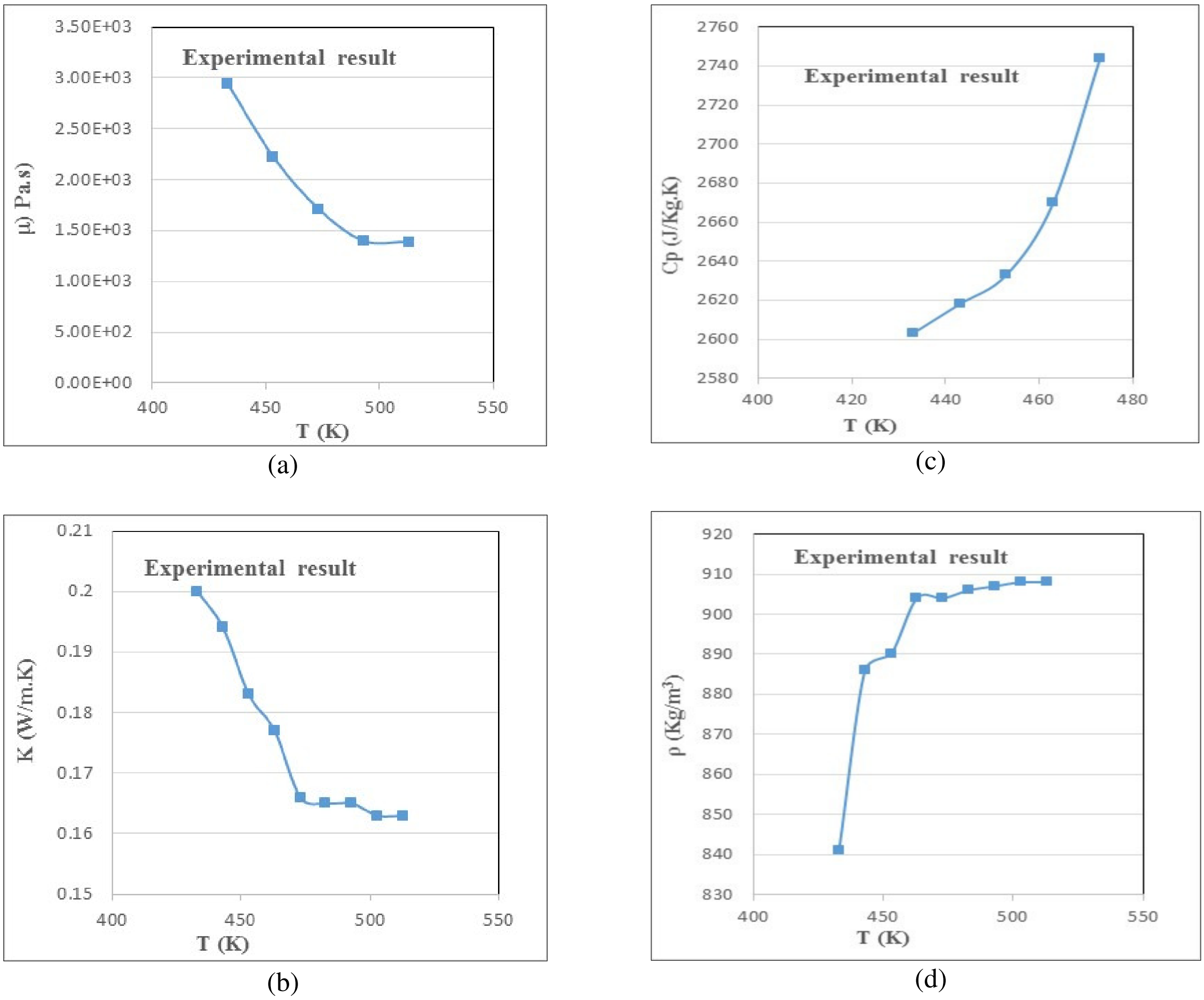


Fig. 3. The thermophysical properties of polypropylene 575 at different temperature. **(a)Viscosity. (b) thermal conductivity. (c) Specific heat. (d) Density.**

Table 1,
Overall data for the practical part of single screw Extruder.

Total feed in Kg	m Total feed rate Kg/s	N Screw Speed rpm	Heat flux inlet W/m²	Heat flux outlet W/m²	Temperature of inlet polymer °C	Temperature of polymer outlet °C	Setting Temperature °C
0.25	$1.812*10^{-4}$	10	7803.571	7203.57	23	157	160
0.25	$2.193*10^{-4}$	20	7803.571	7626.1	23	153	160
0.25	$3.472*10^{-4}$	30	7803.571	7633.48	23	148	160
0.25	$5.952*10^{-4}$	40	7803.571	7750	23	143	160
0.5	$2.6*10^{-4}$	10	7803.571	7201.72	23	178	180
0.5	$3.33*10^{-4}$	20	7803.571	7310.335	23	175	180
0.5	$4.39*10^{-4}$	30	7803.571	7540.455	23	171	180
0.5	$5.56*10^{-4}$	40	7803.571	7575.45	23	168	180

3. Polymer Used

In this research, polypropylene 575 was used because it has a good mechanical and physical properties, such as an excellent insulator, therefore, it was used in an electrical industry, melting point ranging between (157-171) °C, and in clinical filed due to low moisture absorption [6]. As well as polypropylene 575 is strongly influenced by the length and size of chain likewise increasing the length of chain which leads to enhancing melting point temperature because of increasing the joint between the chains [7,8].

4. Simulation Process

Based on practical experiments, it is know that the increasing usage of (CFD) packages Computational Fluid Dynamics to study the flow of complex melting polymer in different processing and complex devices need some usable material modelling technique. For this purpose, it is necessary to study the model describing the behaviour of polymer melting specifically. As well as, the commercial CFD packages supply only some liner model such as (the model of the linear viscous body for viscous fluids) [9, 10]. For incompressible fluids, all CFD packages simulation started from the governing equations for continuity and momentum [11]. The arithmetical models using the commercial CFD software's (SOLID WORKS 2016) for model creation, table (2) shows the dimensions of single screw extruder and (ANSYS FLUENT 17.2) used and evaluated against the experimental findings to validate the observed results. Three steps of the CFD Simulation Process including pre-processing, solving and post-processing steps are followed to analyse the fluid flow and heat transfer model. Pre-processing is the first stage in analysing and building a CFD model which taking place before the numerical solution process. In this step, the model geometries of single screw extruder were created and identified based on the boundary types, then the domain of benefits was divided into smaller segments which known as a grid (mesh) generation. This stage is the most important and the most time-consuming step in the CFD process. ANSYS FLUENT meshing has been used as a result of its simplicity and flexibility in application [12]. While in the solver step, the definition of material, operating conditions and boundary condition at an inlet, outlet, and across the whole fluid flow were selected. Pressure-based solver (PBCS) was selected to solve the governing equations for heat transfer and flow. The PBCS solver can be used for a broad range of flow regimes from low-speed incompressible flow to high-speed compressible flow and hence was selected. The precise identification of the properties, parameters, the appropriate models for the solution methods, accuracy and convergence are very important factor to get a realistic solution [13]. As well as post-processing is the last step of the CFD process where the results with their parameters can be extracted and analysed using meaningful graphics, vector plots, contour plots, animations and reports. Numerous of commercial post-processing packages are available to view results for analysis [14].

Table 2,
Dimension of screw.

Extruder length(mm)	L/D Ratio	Shaft diameter(mm)	Screw diameter(mm)	Cylinder diameter(mm)	Pitch (mm)	Screw speed(rpm)	Weight capacity(Kg)
1000	28	14	30	35.7	25	10-40	1-8

5. Assumption for Simplification of Model

The assumptions which were considered for simulation the model are as following: (i) The polymer fluid was assumed as Non-Newtonian having a pseudo plastic characteristic and incompressible fluid, (ii) The fluid flow was assumed as a laminar flow due to the rpm of screw was very low and there is no slippage between fluids and the cylinder wall, (iii) The heat flux was assumed constant with negligible radiation effects, (iv) The particles were presumed to be spherical and single phase model was used, and (v) The thermos-physical properties of fluids were variable with temperatures [15]. The following governing equations for cylindrical coordinates have been used for simulation [16].

Continuity equation:

$$\frac{\partial \rho}{\partial t}+\frac{1}{r}\frac{\partial\left(\rho r v r\right)}{\partial r}+\frac{1}{r}\frac{\partial\left(\rho v\,\theta\right)}{\partial \theta}+\frac{\partial\left(\rho v\,z\right)}{\partial z}=0 \quad \dots (1)$$

Momentum equation:

$$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\cdot\frac{\partial v_r}{\partial \theta}+v_z\frac{\partial v_r}{\partial z}-\frac{v^2{}_\theta}{r}\right)= -\frac{\partial p}{\partial r}+\mu\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\cdot\frac{\partial}{\partial r}(r v_r)\right) +\frac{1}{r^2}\cdot\frac{\partial^2 vr}{\partial \theta^2}+\frac{\partial^2 v_r}{\partial z^2}-\frac{2}{r^2}\cdot\frac{\partial v_\theta}{\partial \theta}\right]+\rho g_r \quad \dots (2)$$

$$\rho(\frac{\partial vz}{\partial t}+vr\,\frac{\partial vz}{\partial r}+\frac{v\theta}{r}\cdot\frac{\partial v_z}{\partial \theta}+vz\,\frac{\partial v_z}{\partial z})=$$
$$-\frac{\partial p}{\partial z}+\mu[\frac{1}{r}\cdot\frac{\partial}{\partial r}(r\cdot\frac{\partial v_z}{\partial r})+ \qquad \dots (3)$$
$$\frac{1}{r^2}\cdot\frac{\partial^2 v_z}{\partial \theta^2}+\frac{\partial^2 v_z}{\partial z^2}]+\rho g_z$$

Energy equation:

$$\rho Cp\;\frac{\partial T}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right)+ \qquad \dots (4)$$
$$\frac{1}{r^2}\frac{\partial}{\partial \varphi}\left(k\;\frac{\partial T}{\partial \varphi}\right)+\frac{\partial}{\partial z}\left(k\;\frac{\partial T}{\partial z}\right)+g$$

6. Results

Temperature Contour planes were displayed illustrated in the following figuers. Fig. (4) A-D at heat flux of 7803.571 W/m^2 and 250 gm as a weight and Fig. (8) A-D but at 500 gm as a weight, represents Contour planes of the temperature distribution along the extruder with revolution per minute ranging between (10-40) rpm. Increase rpm led to reduction in residance time, which affects the heating of polypropelene 575 material within the extruder.It can also be observed that the temperature of the material increased to a certain extent inside the extruder and then decreased very slightly in few degrees before the material started to exit out of extruder .This is can be seen clearly, especially when the rpm increased, where the loss in temperature increased. Also it can be inferred that temperature of polymer near the screw surface and near the barrel wall is the highest. The polymer material in the middle has lower temperature [15].
Fig. (5) A-D at a heat flux of 7803.571 W/m^2 and 250 gm as a weight and Fig. (10) A-D with 500 gm as a weight, represent Contour planes of the density behavior along the extruder at rpm ranging between (10-40). Where increasing temperature led to increase density to a certain extent, this is observed especially when increasing the rpm. Because of the interstitial materials that contain air between their granules, it is known that by increasing the temperature leads to an increase in the density of these materials, because when the temperature increases these grains begin to melt, which leads to reducing the volume with the mass constant, thus led to increase density [17]. Fig. (6) A-D at heat flux 7803.571 W/m^2 and 250 gm as a weight and, Fig. (11) A-D but with 500 gm as a weight, represent Contour planes of the viscosity behavior along the extruder at rpm ranging between (10-40). Where Increase temperature led to decreasing the viscosity and this is clearly observed in the practical results when the viscosity decreased by increasing the temperature. Fig. (7) A-D at heat flux 7803.571 W/m^2 and 250 gm as a weight, and Fig. (12) with 500 gm as a weight, represent Contour planes of the thermal conductivity behavior along the extruder at rpm ranging between (10-40). Where increasing the temperature led to slightly decreasing in thermal conductivity because of polymeric materials used as an insulator. The phonon transport is the main mechanism for interaction of heat energy with each other and with subatomic particles [18]. Drag Phonon is the increase in effective mass of electrons conduction or valence holes due to interactions with crystal lattice in moving the electron. As an electron moves the past atoms in the lattice, its polarizes or charge distorts the nearby lattice. This effect leads to an electron decrease (as may be the case, hole) mobility, which results in a thermal conductivity decreased [19]. Fig. (8) A-D at heat flux 7803.571 W/m^2 and 250 gm as a weight, and Fig. (13) A-D with 500 gm as a weight, represent Contour planes of the specific heat behavior along the extruder at rpm ranging between (10-40). Where increasing the temperature led to increase in specific heat. Specific heat capacity is a measuring of substance ability to absorb heat. The heat first goes to increase the kinetic energy of the molecules. These molecules also can store energy in rotation and vibration. As heats up the substance, the average kinetic energy of molecules increases. The collisions impart energy enough to allow rotation occur. Then rotation contributes to internal energy and raises the specific heat capacity of material [20]. It is clearly shawn in Fig. (14 & 15) a, b, c, & d that a significant matching between the experimental results and the results of process simulations with a slight difference. This difference resulting from the degree of complexity of the form "Single screw extruder" and the process of mesh generation.

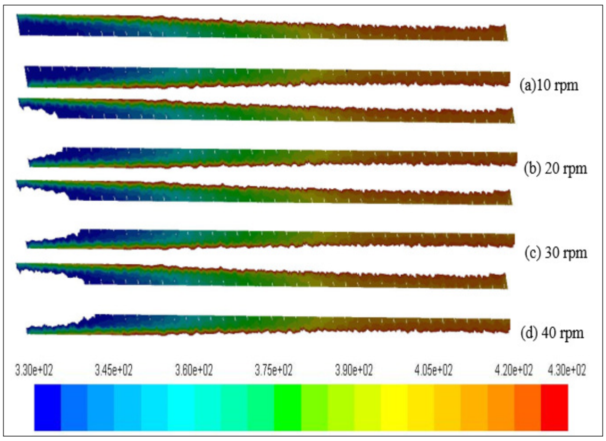


Fig. 4. Temperature Contour plane at 250 gm.

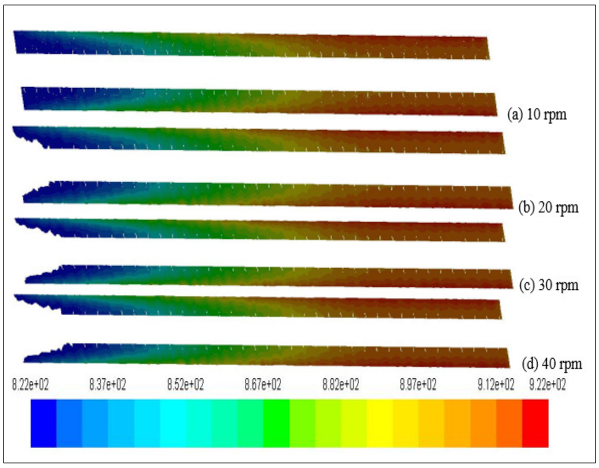


Fig. 5. Density Contour plane at 250 gm.

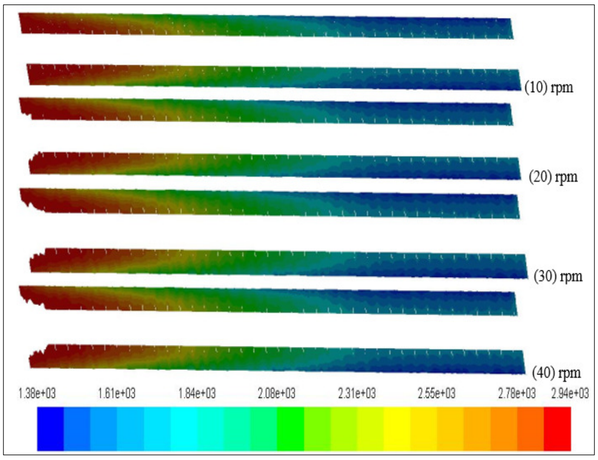


Fig. 6. Viscosity Contour plane at 250 gm.

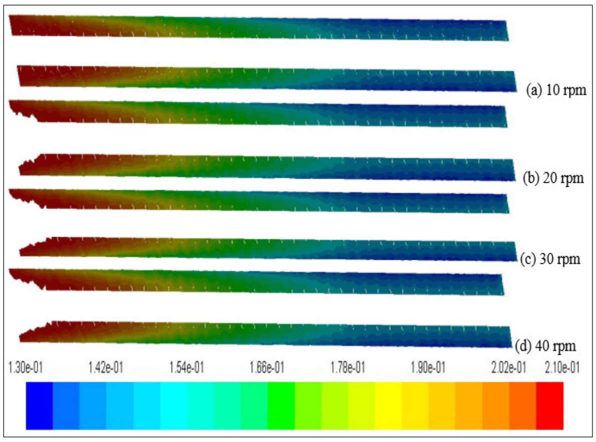


Fig. 7. Thermal conductivity Contour plane at 250 gm.

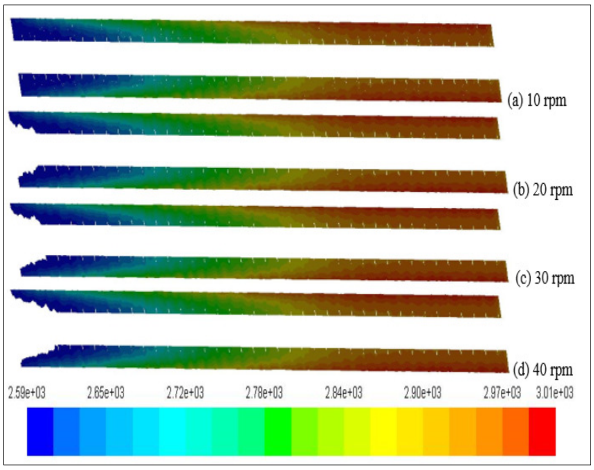


Fig. 8. Specific heat Contour plane at 250 gm.

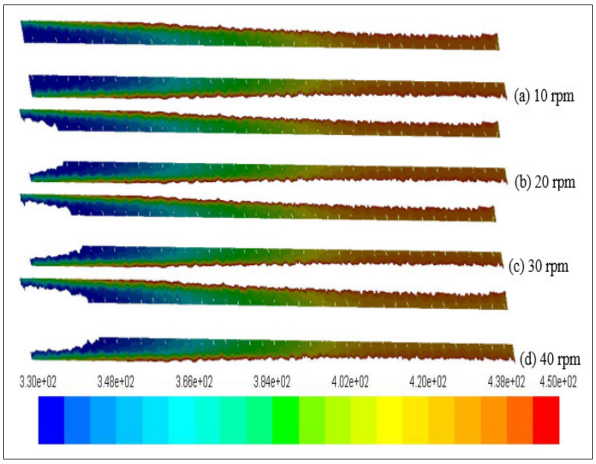


Fig. 9. Temperature Contour plane at 500 gm.

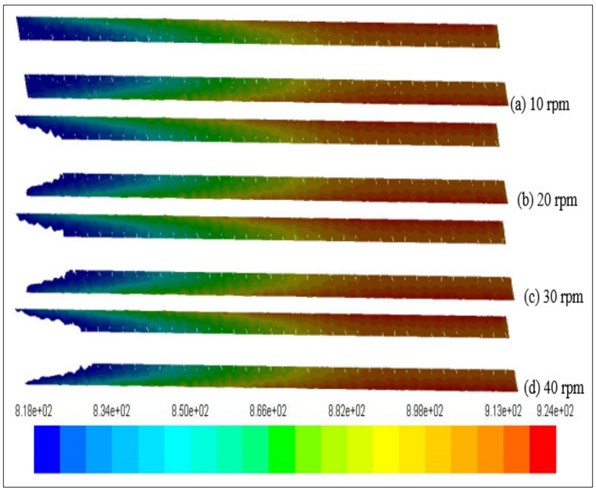


Fig. 10. Density Contour plane at 500 gm.

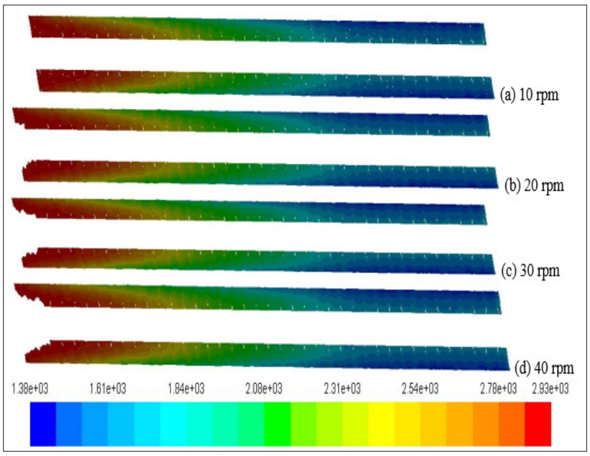


Fig. 11. Viscosity Contour plane at 500 gm.

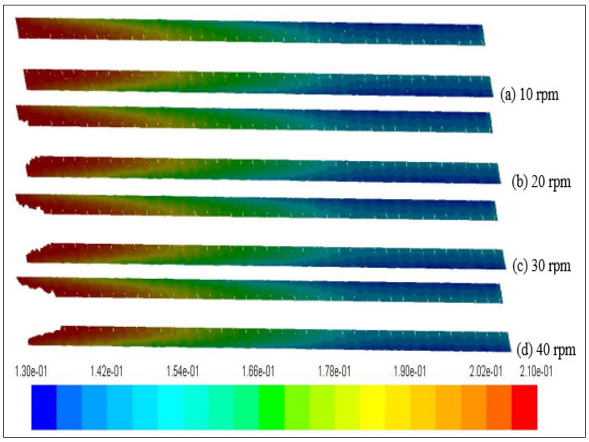


Fig. 12. Thermal conductivity Contour plane at 500 gm.

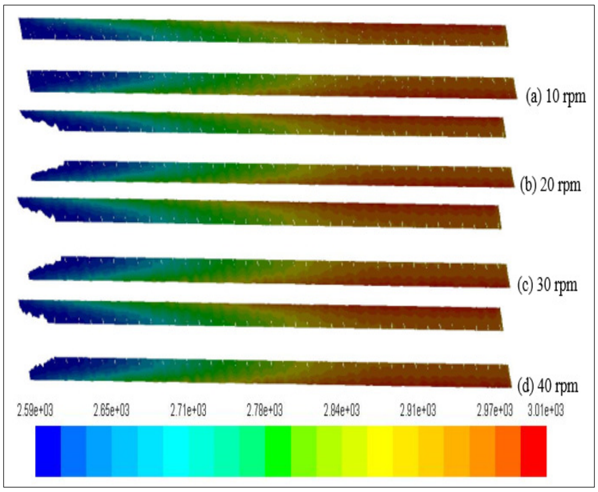
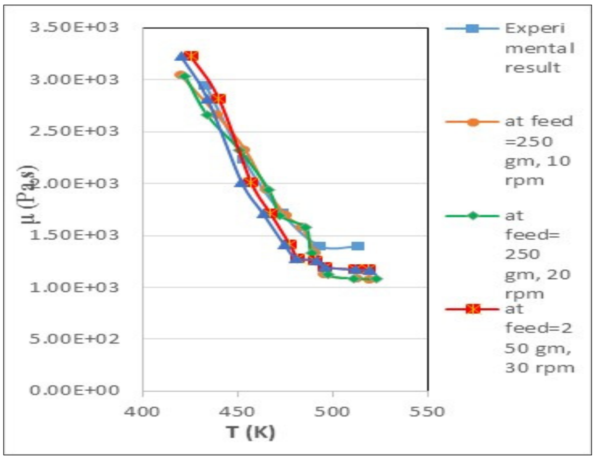
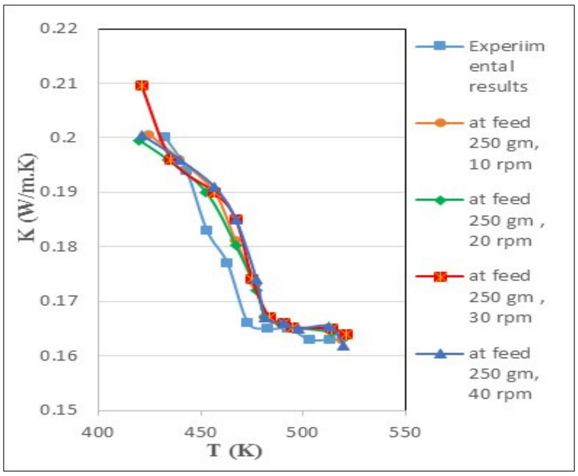


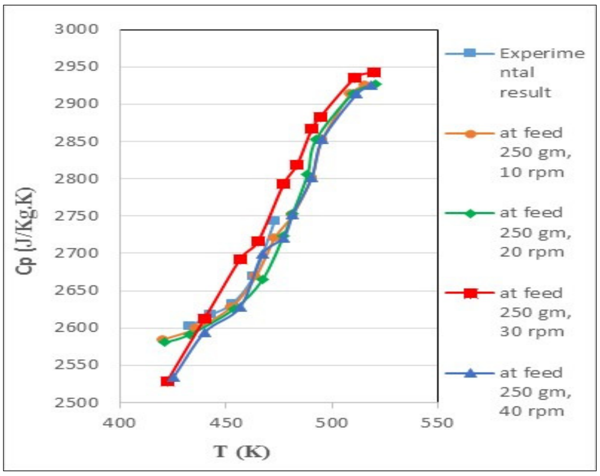
Fig. 13. Specific heat Contour plane at 500 gm.



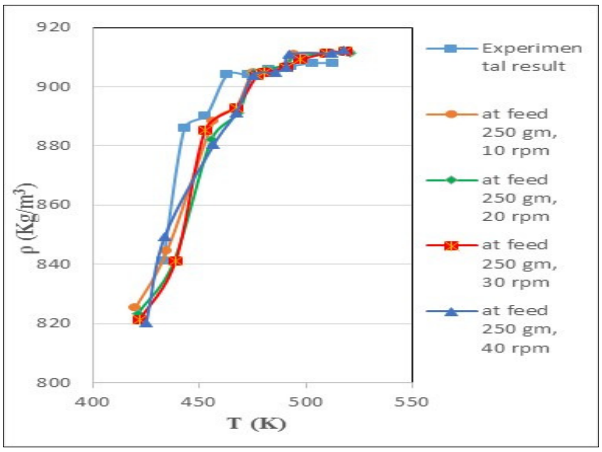
(a)



(b)

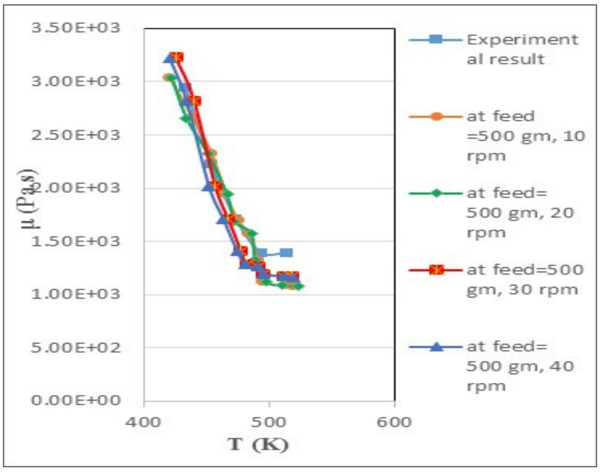


(c)

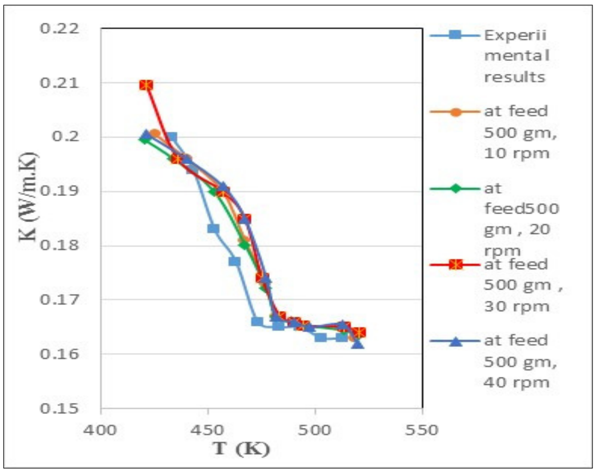


(d)

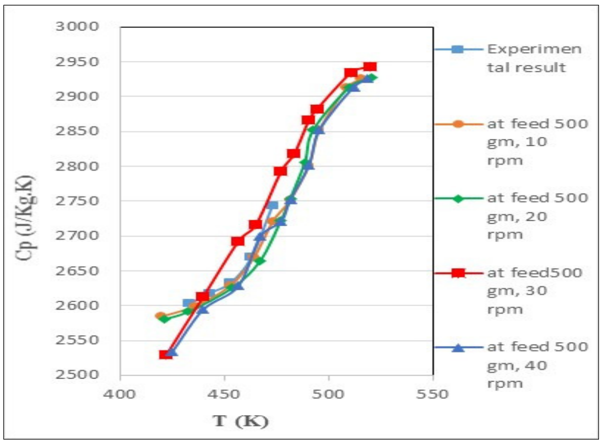
Fig. 14. Thermophysical properties of polypropylene 575 for experimental and simulation results at different temperature (a)Viscosity, (b) thermal conductivity, (c) Specific heat, (d) Density.



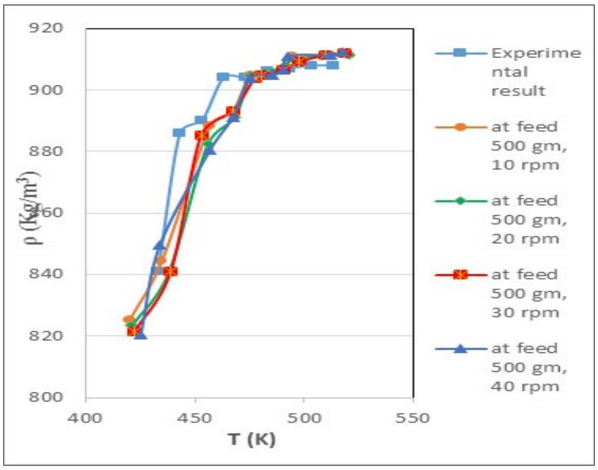
(a)



(b)



(c)



(d)

Fig. 14. Thermophysical properties of polypropylene 575 for experimental and simulation results at different temperature (a) Viscosity, (b) thermal conductivity, (c) Specific heat, (d) Density.

7. Conclusion

The numerical values showed closer fitting to the experimental values in the extruder. Where viscosity and thermal conductivity decreased with increasing temperature along the extruder. While the specific heat and density increased with temperature increased along the extruder. Consequently, this study was successfully validated by CFD simulation for single screw extruder.

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التحقيق التجريبي والعددي لمحاكاة الخصائص الحرارية للبوليمر الذائب بوليبروبيلين ٥٧٥ في الطارد ذي البرغي الوا□د

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الخلاصة

النموذج العددي للبوليمر الذائب بولي بروبلين ٥٧٥ الذي يتدفق على طول الطارد الذي يكون ذا مسمار مفرد تحت كمية حرارة معلومة ، معدل تدفق متغير، وكذلك دورة بالدقيقة مختلفة حيث تم اجراؤه بأستخدام برنامج (TNEULF-SYSNA ١٧,٢). يستخدم النموذج الخصائص الريولوجية للبوليمرالذي يقاس بوصفه دالة لدرجة الحرارة لمحاكاة العمليات التجريبية. حيث تم تحليل نتائج المحاكاة العددية بأستخدام نموذج (DFC) لمعاملات مثل درجة الحرارة و اللزوجة والكثافه النوعية والتوصيليه الحرارية وكذلك الكثافه حيث اثبتت درجة عالية من التشابه مع البيانات التجريبية المقاسة. وأحد النتائج المهمة لهذا البحث تم الحصول على الشكل الهندسي وتحديد ظروف العمل لتقليل التكلفة ووقت التشغيل.