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 has been 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 skillfulness 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.
2. a Experimental Setup

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.

\[ \mu = 0.2905T^2 - 294.5T + 76012 \]  \hspace{1cm} \text{... (a)}

\[ K = 8 \times 10^{-6}T^2 - 0.0081T + 2.2014 \]  \hspace{1cm} \text{... (b)}

\[ C_p = -0.1036T^2 + 102.73T - 22458 \]  \hspace{1cm} \text{... (c)}

\[ \rho = -0.0184T^2 + 17.98T - 3491.1 \]  \hspace{1cm} \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.

<table>
<thead>
<tr>
<th>Total feed in Kg</th>
<th>m (Total feed rate Kg/s)</th>
<th>N (Screw Speed rpm)</th>
<th>Heat flux inlet W/m²</th>
<th>Heat flux outlet W/m²</th>
<th>Temperature of inlet polymer °C</th>
<th>Temperature of polymer outlet °C</th>
<th>Setting Temperature °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>1.812*10^{-4}</td>
<td>10</td>
<td>7803.57</td>
<td>7203.57</td>
<td>23</td>
<td>157</td>
<td>160</td>
</tr>
<tr>
<td>0.25</td>
<td>2.193*10^{-4}</td>
<td>20</td>
<td>7803.57</td>
<td>7626.1</td>
<td>23</td>
<td>153</td>
<td>160</td>
</tr>
<tr>
<td>0.25</td>
<td>3.472*10^{-4}</td>
<td>30</td>
<td>7803.57</td>
<td>7633.48</td>
<td>23</td>
<td>148</td>
<td>160</td>
</tr>
<tr>
<td>0.25</td>
<td>5.952*10^{-4}</td>
<td>40</td>
<td>7803.57</td>
<td>7750</td>
<td>23</td>
<td>143</td>
<td>160</td>
</tr>
<tr>
<td>0.5</td>
<td>2.6*10^{-4}</td>
<td>10</td>
<td>7803.57</td>
<td>7201.72</td>
<td>23</td>
<td>178</td>
<td>180</td>
</tr>
<tr>
<td>0.5</td>
<td>3.33*10^{-4}</td>
<td>20</td>
<td>7803.57</td>
<td>7310.335</td>
<td>23</td>
<td>175</td>
<td>180</td>
</tr>
<tr>
<td>0.5</td>
<td>4.39*10^{-4}</td>
<td>30</td>
<td>7803.57</td>
<td>7540.455</td>
<td>23</td>
<td>171</td>
<td>180</td>
</tr>
<tr>
<td>0.5</td>
<td>5.56*10^{-4}</td>
<td>40</td>
<td>7803.57</td>
<td>7575.45</td>
<td>23</td>
<td>168</td>
<td>180</td>
</tr>
</tbody>
</table>

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 known 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 linear 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].

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].

Table 2, Dimension of screw.

<table>
<thead>
<tr>
<th>Extruder length(mm)</th>
<th>L/D Ratio</th>
<th>Shaft diameter(mm)</th>
<th>Screw diameter(mm)</th>
<th>Cylinder diameter(mm)</th>
<th>Pitch (mm)</th>
<th>Screw speed(rpm)</th>
<th>Weight capacity(Kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>28</td>
<td>14</td>
<td>30</td>
<td>35.7</td>
<td>25</td>
<td>10-40</td>
<td>1-8</td>
</tr>
</tbody>
</table>

Continuity equation:

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho \nu \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \rho \nu \theta \right) = 0 \quad \ldots (1)
\]

Momentum equation:

\[
\rho \left( \frac{\partial \nu}{\partial t} + \nu \frac{\partial \nu}{\partial r} + \frac{\nu \theta}{r} \frac{\partial \nu}{\partial \theta} + \frac{\nu}{r} \frac{\partial \nu}{\partial z} - \frac{\nu^2}{r} \right) =
\]

\[
\frac{\partial p}{\partial r} + \mu \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \nu}{\partial r} \right) \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( r \nu r \right) \right) \quad \ldots (2)
\]

\[
+ \frac{2}{r^2} \frac{\partial}{\partial \theta} \left( r \nu r \right) + \rho g,
\]
\[
\rho (\frac{\partial \nu_z}{\partial t} + \nu_r \frac{\partial \nu_z}{\partial r} + \nu \frac{\partial \nu_z}{\partial \theta} + \nu_z \frac{\partial \nu_z}{\partial z}) = \\
-\frac{\partial p}{\partial z} + \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \nu_z}{\partial r} \right) + \frac{\partial \nu_z}{\partial z} \right] + \rho g_z
\] ...

\[
\rho C_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( kr \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( k \frac{\partial T}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + g
\] ...

6. Results

Temperature Contour planes were displayed illustrated in the following figures. Fig. (4) A-D at heat flux of 7803.571 W/m² 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 residence time, which affects the heating of polypropylene 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 the extruder. This 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/m² 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 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/m² and 250 gm as a weight, and Fig. (12) with 500 gm as a weight, represent Contour planes of the viscosity behavior along the extruder at rpm ranging between (10-40). Where increasing the 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/m² and 250 gm as a weight, and Fig. (11) A-D but 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. 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 shown 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)
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.

Acknowledgments

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8. References


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التخليص التجريبي والعددي لمحاكاة الخصائص الحرارية الحرارية للبوليمير الذائب بوليبروبيلين 575 في الطارد ذي البرغي الواسع

الخلاصة

النموذج العددي للبوليمير الذائب بولي بروبلين 575 يتيح من خلال مسار مفرد تحت كمية حرارة معلومة، معدل تدفق متغير. وكذلك مسألة الدقة مختلفة حيث تم إجراءه باستخدام برنامج TNEULF-SYSLA. يستخدم النموذج الخاص بالرزمية للبوليمير الذي يطغي على نماذج الهيكلية محاكاة العمليات التجريبية. حيث تم تصنيف النماذج المعادلة باستخدام نموذج (DFC) لمعالجة مثل درجة الحرارة وال든지وة والكثافة النوعية والتوصيلية الحرارية وكذلك الكثافة حيث تم درجات عالية من التشابه مع البيانات التجريبية المقدمة. وفقاً للنتائج المهمة لهذا البحث تم الحصول على الشكل الهندسي وتحديد ظروف العمل لتنقية الكتلة ووقت التشغيل.