Die swell of Polypropylene flow through a slit die: experiment and 3D simulation

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ABSTRACT: Extrusion as one of the most important processing method is widely applied in industrial applications. Die swell or extrudate swell results in difficulty in obtaining a final manufacturing product with the corresponding profiles. This study aims at investigating the extrudate swell behavior of neat Polypropylene (PP) flow through a slit die. A real-time measurement method is used to investigate the effect of processing conditions on die swell both in height direction and width direction. In addition, a 3D full numerical simulation based on two types of constitutive models, cross law model and 4-mode differential Phan-Thien Tanner (PTT) model are conducted to predict the flow behavior. Compared with the measurement results, it is found that both models could predict well the pressure values of flow in the die channel. A good agreement between the modelling swell behavior by PTT model and the experimentally measured results is achieved. In contrast, the cross law model obviously underestimated the swelling ratios and the difference increases with an increase in volumetric flow rate.

Keywords: extrusion, die swell, Polypropylene, simulation

1 INTRODUCTION

Extrusion as one of the most important processing method is widely applied in industrial applications. A quantitative understanding of the viscoelastic properties of polymer melts in actual processing is one of the most significant issues regarding the polymer processing science. The complicated extrudate deformation behavior through the die exit during the free surface flows, which is generally known as die swell or extrudate swell, results in difficulty in obtaining a final manufacturing product with the corresponding profiles [1]. Therefore, it is of great significance to figure out the extrudate behavior in die design and processing controls.

A general agreement has been achieved that extrudate swell is a viscoelastic problem dependent on the viscoelastic properties of the material and flow history related to the flow channel dimensions [2]. However, the flow behavior in the channel are typical 'black boxes' problems. Numerical modelling method is a good choice to have a sight into the flow patterns and investigate the swelling behavior. Since Luo and Tanner et al. [3, 4] simulated the viscoelastic flow behavior of IUPAC-LDPE melt for capillary dies using the realistic differential PTT constitutive model and K-BKZ integral constitutive model separately instead of the unrealistic differential Maxwell constitutive model based on a streamline element scheme, researchers' attention to the extrusion swelling problem in polymer processing has been moved to those realistic models away from those unstable model such as Maxwell model. During the last decades, a great progress has been made in that field [5-9]. In addition, Azaiez et. al. [10] studied several single-mode differential models and concluded that single-mode models instead of multi-mode models were normally unable to correctively predict both linear or nonlinear properties of polymer solutions.

In this paper, the main objective of the present work is to investigate the swelling behavior of the viscoelastic flow through a slit die. A real-time measurement method is used to investigate the effect of processing conditions on die swell both in height direction and width direction. In comparison with the experiment results, a full 3D numerical simulation study of flow behavior, especially the swell behavior of the fluid emerging the die exit in isothermal extrusion process is carried out, using two types of the constitutive models, namely the cross law model and multi-mode differential PTT model.

2 MATHEMATICAL MODELING

2.1 Constitutive model

2.1.1 Cross law model

For the viscous Cross law model, the viscosity, η could be written as:

$$\eta = \frac{\eta_0}{1+(\lambda\dot{\gamma})^{1-m}} \qquad (1)$$

Where η_0 is the viscosities for fluids at zero shear rate, λ is the relaxation time, m means the cross law factor, and $\dot{\gamma}$ the shear rate.

2.1.2 PTT constitutive model

For the differential viscoelastic constitutive model, the extra stress tensor, $\boldsymbol{\tau}$, could be split into a purely viscous part, $\boldsymbol{\tau_N}$, and a viscoelastic part, $\boldsymbol{\tau_p}$.

Multi-mode PTT model with a relaxation time spectrum is selected, which is expressed as:

$$\boldsymbol{\tau_p} = \sum_{i=1}^{N} \boldsymbol{\tau_{pi}},$$

$$\boldsymbol{exp}\left[\frac{\varepsilon_i\ \lambda_i}{\eta_i}\boldsymbol{tr}(\boldsymbol{\tau_{pi}})\right]\tau^{(i)} + \boldsymbol{\lambda_i}\left[(\mathbf{1}-\frac{\xi_i}{2})\check{\boldsymbol{\tau}}_{\boldsymbol{p\imath}} + \frac{\xi_i}{2}\widehat{\boldsymbol{\tau}}_{\boldsymbol{p\imath}}\ \right] = \mathbf{2}\boldsymbol{\eta}_i\boldsymbol{D} \quad (2)$$

Where ε_i and ξ_i control extensional and shear behavior of polymer fluid, respectively. λ_i means the relaxation time of the polymer melt in each mode.

2.2 Geometry and mesh

A 3D flow domain including the slit die and the upstream part is developed in Fig. 1. A half of the extrusion flow domain is computed in order to reduce the computational cost. The boundary conditions are described like [2]:

Inlet: flow rate of the flow (mm^3/s);

Die wall: a non-slip condition is assumed: $v_n=v_t=0$;

symmetry plane: $v_n = 0$, $f_t = 0$;

Free surface: $\mathbf{v}\cdot\mathbf{n}=0$;

Outlet: $f_t = f_n = 0$;

Where **v** and f mean the velocity and force applied at flow.

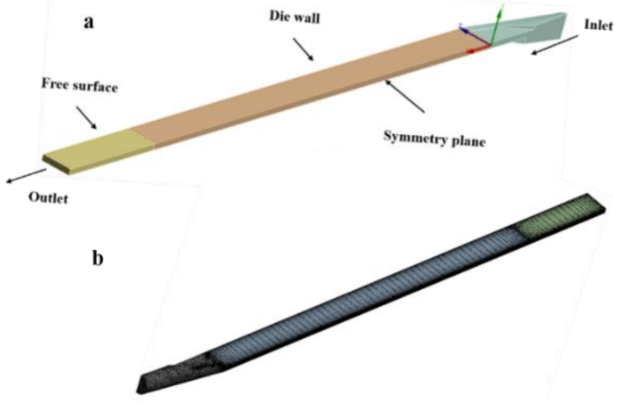

Fig. 1. Schematic diagram of 3D flow domain of slit die profile (a), mesh profile for slit die (b).

3 EXPERIMENT AND CHARACTERIZATION

3.1 Rheology measurement

The commercial Polypropylene (PP 575P) investigated in this study was purchased from the SABIC company in Germany, whose density and melt flow rate were 905 kg/m^3 and 10.5 g/10 min at 2.16 kg at 230 °C measured according to ISO 1133 method.

Measurements in dynamic oscillatory mode and steady shear mode were performed on a strain-controlled rotational rheometer (ARES, TA Instruments, USA) separately at 200 °C. The disk samples with a diameter of 25 mm and a thickness of 2 mm were prepared using a standard compressing processing. The frequency sweep was conducted in an angular velocity range of 0.1-500 rad/s with a gap value of 1.7 mm. A relaxation time spectrum of 4 mode was used to fit the linear viscoelastic parameters in Fig. 2. The nonlinear parameters of PTT model could be obtained by fitting the shear viscosity and normal stress difference data. The parameters for PTT model and cross law model are shown in Table 1.

3.2 Measurement of pressure and die swell

Neat PP flow was extruded from a single screw extruder (P. Brabebder 19 with a diameter of 19 mm, L/D ratio of 25) with a slit die (length: 160 mm, height: 2 mm, and width: 20 mm) with a processing temperature profile (185, 190, 195 °C for the three zones of the extruder and 200 °C for the die separately) to investigate the flow behavior. A volumetric flow rate range of 196.4–869.32 mm^3/s, was selected in this study. The pressures were measured by two pressure sensors mounted at the positions 40 mm and 140 mm in front of the die exit respectively. The online measurements for extrudate swell were performed using two HD cameras connected with the computers. The cameras used in the measurement are webcams, more specifically the 'LOGITECH WEBCAM Brio 4K Stream Edition'. Pictures taken with the HD cameras were analyzed by image analysis. It should be noted that in our experiment, due to the difficulty in measuring the middle height of the extrudate, the edge height of the extrudate was measured instead. The reported die swells for each flow rate are the average of analyzing at least 4 different pictures. More details could be found in Fig.3a. Fig. 3b and c show the extrudate profile from the cameras from bottom view and edge view, respectively.

Another two processing temperature profiles are also used in the study, namely (170, 175, 180 and 185 °C) and (200, 205, 210 and 215 °C), to investigate the effect of processing temperature on swelling behaviors. The schematic of cross section of slit die is shown in Fig. 3d. Swelling ratio (B) is defined as the ratio between dimension of extrudate and die exit. To investigate the swelling anisotropy of the extrudate due to the die with a large width/height ratio width of die

(10:1), we define several swelling ratios, B_1 and B_2 separately, which denotes the swelling in width and the edge height of extrudate. They are written as follows:

$$B_1 = \frac{L_{\mathrm{extrudate}}}{L_{\mathrm{die}}};\quad B_2 = \frac{D_{\mathrm{extrudate}}}{D_{\mathrm{die}}}$$

Where $L_{\mathrm{extrudate}}$ and L_{die} are the width of extrudate and die, while $D_{\mathrm{extrudate}}$ and D_{die} are the edge height of extrudate and die separately.

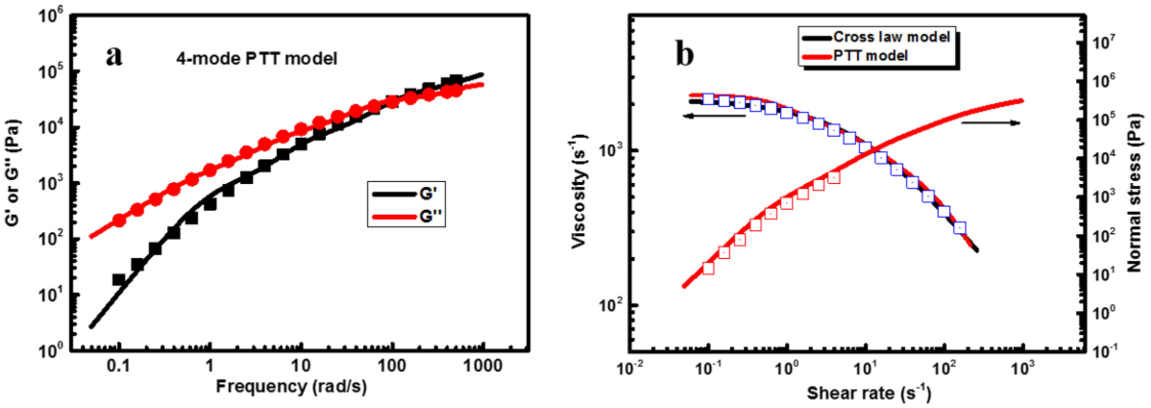

Fig. 2. Rheology data of neat PP from experiment (symbols) and fitted by cross law model and 4-mode PTT model (solid lines) at 200 °C.

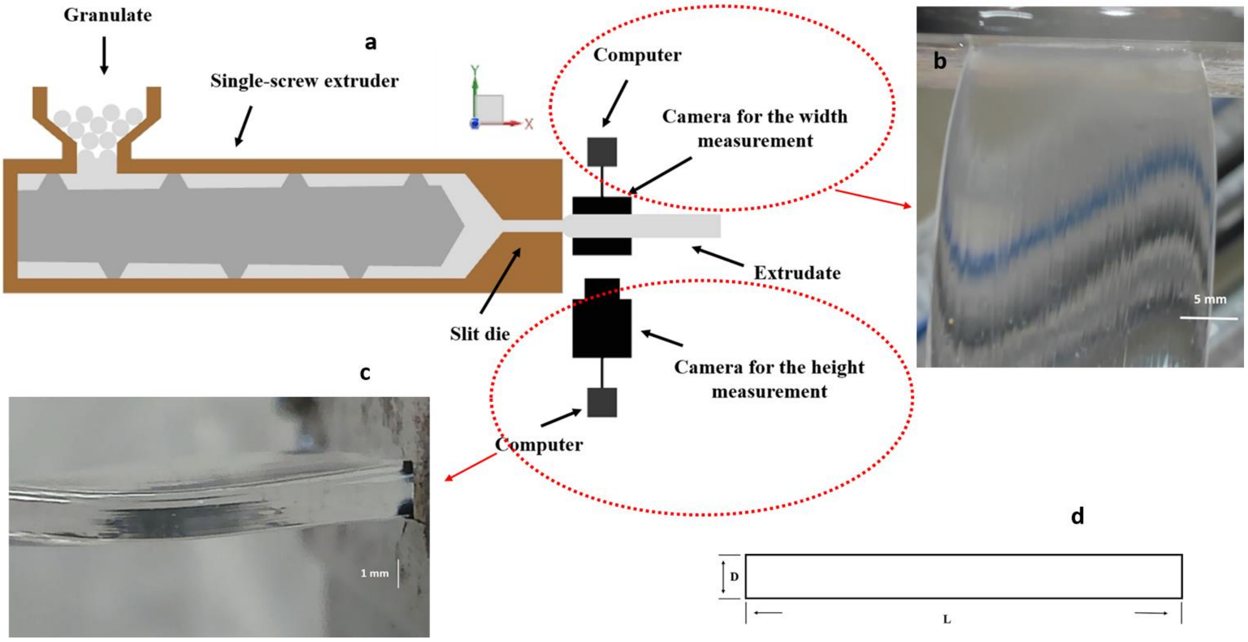

Fig. 3. schematic of experimental setup to measure die swell (a); the extrudate profile from bottom view (b); the extrudate profile from side view (c) and the cross section of the slit die (d).

Table 1. Materials parameters for PTT model and cross law model at 200 °C

			PTT model						
Materials	Mode	λ_i (s)		η_i (pa.s)		ε_i		ξ_i	
	1	λ_1	0.001	η_1	96.12	ε_1	0.12	ξ_1	0.4
	2	λ_2	0.01	η_2	400	ε_2	0.15	ξ_2	0.2
Neat PP	3	λ_3	0.1	η_3	706.1	ε_3	0.14	ξ_3	0.12
	4	λ_4	1	η_4	1022.3	ε_4	0.4	ξ_4	0.15
				Cross law					
		η_0		λ	m				
		2248.3		0.096	0.6723				

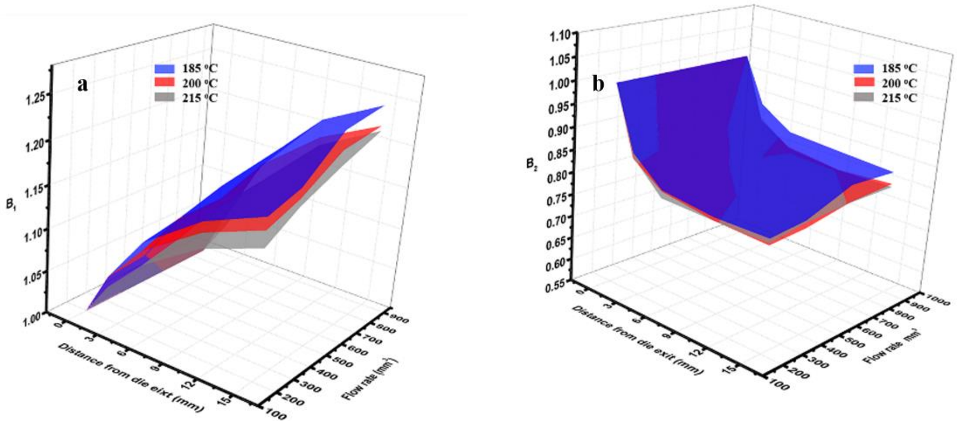

Fig. 4. The evolution of extrudate swell B_1 and B_2 away from die exit with different processing temperatures and flow rates.

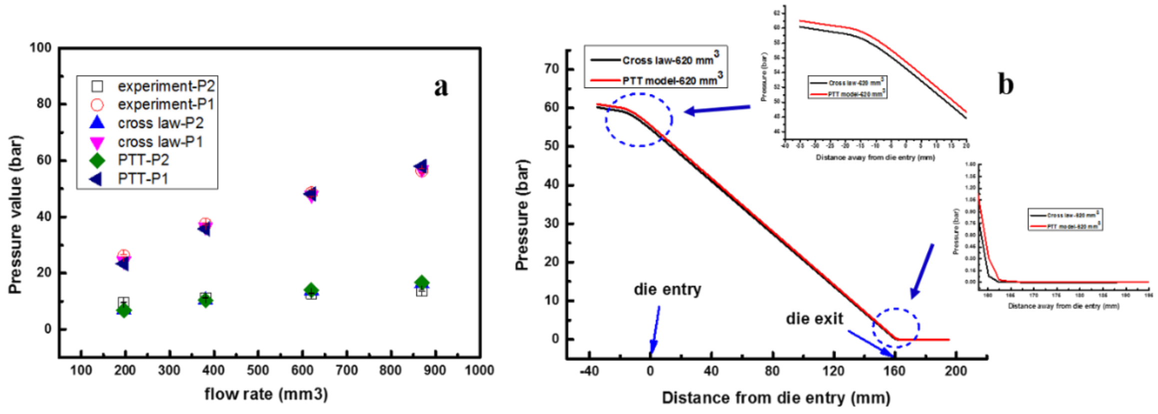

Fig. 5. A comparison of pressure values between experiment results and simulation predicted by PTT model and cross law model at several flow rates (a); pressure profiles of cross law flow and PTT flow at a flow rate of 620 mm^3/s.

4. RESULTS AND DISCUSSION

Fig.4 shows the evolution of extrudate swelling behavior after die exit by measurement at different processing temperatures. In Fig. 4a, it is found that the swelling ratio in width direction (B_1) increases quickly once the extrudate emerges from the die exit, then increases slowly after extrudate reaches to a distance of 10 mm after die exit. Fig.4b displayed the variations of the height of exturate edge with the distance away from die exit. In contrast with the swelling behavior in width direction of the extrudate, it shows a decrease instead of an increase in the edge height. In addition, processing conditions also have effects on the extrudate swell. It is noticed that in both Fig.4a and b, swelling ratio increases with the flow rate, while decreases with the processing temperature of die. Generally, higher flow rate could result in larger deformations of polymer molecules, which indicates more elastic relaxation, results in more expansion flows. In contrast, higher processing temperature increases the relaxation rate of the deformed polymer chains caused by shear or elongational force, decreasing extrudate swelling behavior.

A comparison of pressure values of PP flow at different flow rates between experiment results and simulations predicted by PTT flow and cross law is presented in Fig. 5. The pressure values increased with the flow rate. Both PTT model and cross law model could be used to simulate very well the pressure values in two different positions of slit die in Fig.5a (P1 is 20 mm downstream from the die entry, while P2 is 40 mm upstream from die exit. The distance between P1 and P2 is 100 mm). Fig. 5b shows the profile pattern of pressure value along the centerline direction of PP flow at a flow rate of 620 mm^3. In the slit die, the pressure profiles by PTT model and cross law model are almost the same. Near the die entry, it is found that pressure value by PTT model is a little higher than that from cross law model. It is due to the elastic properties of PTT flow. And this phenomenon is called the ‘entry effect’ of viscoelastic flows. When the flow leaves the die exit, it appears that the pressure value of PTT flow is still higher than cross law flow. The pressure difference after the die exit could lead to different extrudate behaviors, which would be discussed in next part.

Fig. 6 compares the evolution of the extrudate swelling behavior after the die exit by simulation and measurement at 200 °C. Fig.6a represents the evolution of width profile for four different flow rates. A good agreement between the experiment results and that predicted by PTT model is achieved in the present flow rate range. Cross law model underestimates

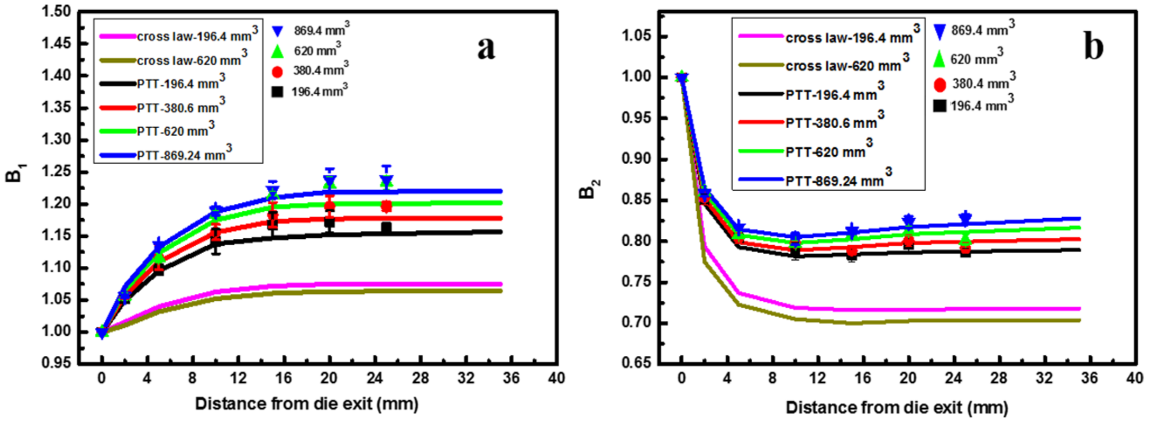

Fig. 6. A comparison of swelling ratio B_1 in width direction (a) and swelling ratio B_2 (b) in edge direction of extrudate between experiment (symbols) and simulations (solid lines) predicted by PTT model and cross law model between experiment results and simulation predicted by PTT model and cross law model in a flow rate range at temperature of 200 °C for die.

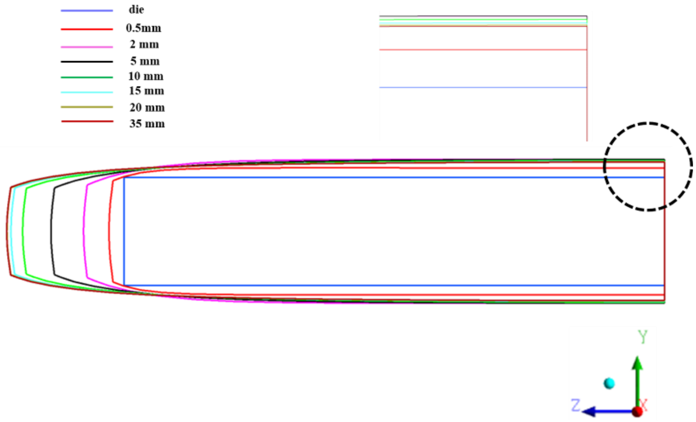

Fig. 7. The evolution of the cross section of extrudate after die exit with a flow rate of 620 mm^3/s at 200 °C

obviously the swelling ratio, in contrast, and the difference of the swelling ratio between cross law flow and PTT flow increases with the flow rate, which might be attributed to the more shear-thinning behaviors. Fig. 6b displays the variations of the height of exturate edge with the distance from die exit. It shows a decrease instead of an increase in the height of edge. Cross law model over-predicts the decrease.

Fig. 7 shows the evolution of the cross section of the extrudate after the die exit simulated by PTT model when the flow rate is at 620 mm^3/s. It appears that the width of the extrudate increased with the distance away from the die exit. The middle height of the extrudate shows a significant increase in comparison with that of the die, while the flow actually contracts at the corners (edge height). That corresponds well to the experimental measurement in Fig.4b.

5. CONCLUSION

In this study, the effect of processing parameters on die swell behavior of neat PP flow through a slit die is studied by experiment and numerical simulation separately. An increase in processing temperature results in a decrease in the swelling ratios of extrudate, while increasing flow rate leads to an increase in contrast. Two types of constitutive models, cross law model and PTT model, are selected to numerically simulate the flow behavior, especially the extrudate swell behavior of neat PP. Both models could predict the flow pressures very well. In comparison with cross law model which under-predicts the swelling ratios of extrudate, an agreement between swelling behavior predicted by PTT and the experiment measurements is good.

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