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Flow Analysis of Profile Extrusion by a Modified Cross-sectional Numerical Method

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Abstract: Flow analysis of profile extrusion is essential for design and production of a profile extrusion die. Velocity, pressure, and temperature distribution in an extrusion die are predicted and compared with the experimental results. A two dimensional numerical method is proposed for three dimensional analysis of the flow field within the profile extrusion die by applying a modified cross-sectional numerical method. Since the cross-sectional shape of the die is varied gradually, it is assumed that the pressure is constant within a cross-sectional plane that is perpendicular to the flow direction. With this assumption, the velocity component in the cross-sectional direction is neglected. The exact cross-sectional shape at any position is calculated based on the geometry of standard cross-sections. The momentum and energy equations are solved with proper boundary conditions at a cross-section and then the same calculation is carried out for the next cross-section using the current calculated values. An L-shaped profile extrusion die is produced and employed for experimental investigation using a commercially available polypropylene. Numerical prediction for the varying cross-sectional shape provides better results than the previous studies and is in good agreement with the experimental results.

Keywords: Profile extrusion die, Modified cross model, Modified cross-sectional method, Finite element method, Die design

Introduction

Various products such as pipe, film, fiber, continuous profile, and coated wire are processed continuously by extrusion which is one of the most frequently used polymer processing methods. The required cross-sectional shape is formed when the molten polymer flows through an extrusion die after it exits the barrel. Generally, the extrusion die consists of delivery channel, transition zone, and land[1]. The polymer melt generated in the extruder is transported to the transition zone through the delivery channel. The transition zone is needed to make the desired dimensions of the extrudate. In the land, normal stresses developed in the melt through the melting and delivery processes are allowed to relax. To design an extrusion die, the three zones must be studied and constructed effectively for production of a high quality extrudate. In engineering, the goal of the die design is to obtain the dimensional accuracy and achieve the highest possible productivity during extrusion of the desired shape. Semi-empirical methods are currently used for design of the extrusion die. Analytic solutions for cylindrical or thin rectangular channels are obtained and applied to the die design by trial and error.

Pressure and velocity fields should be known with the temperature distribution within the die to design the extrusion die successfully. Since the polymer melt shows non-newtonian behavior and the cross-sectional shape is complicated, numerical methods are generally used to obtain velocity and temperature distribution. In profile extrusion, the cross-sectional shape is complex and changing continuously. For the flow field analysis of the profile extrusion, three dimensional numerical methods are widely used[2]. However, two dimensional numerical methods are also used frequently because the three dimensional analysis usually requires long calculation time and difficulties are encountered in mesh generation. Hurez *et al.*[3,4] used the cross-sectional method for isothermal numerical analysis of the fluid flow within a profile extrusion die by assuming that the flow of a highly viscous polymer melt through a gradually changing cross-section is a fully developed flow parallel to the axis direction.

In this study, a non-isothermal numerical analysis is carried out by assuming a fully developed laminar flow perpendicular to the cross-section. Instead of the fictitious domain adopted by Hurez *et al.*[3], a precise geometrical shape is calculated and employed for the flow analysis within the transition zone. Temperature boundary conditions for the non-isothermal calculation are determined by considering conduction and convection heat transfer around the head and die by assuming that the head and die have a circular cylindrical shape. An L-shape profile extrusion die is prepared and used for experimental investigation. A commercially available polypropylene is fed to the extruder at three different die temperature with three different screw speeds.

Theoretical Modelling

Flow field within the die

Some assumptions are made to model the fluid flow in the die during profile extrusion of polymeric materials. The polymer melt is assumed to be incompressible and show the behavior of a generalized newtonian fluid. Gravity is neglected and a creeping flow is assumed because the inertia force is small. A steady state flow perpendicular to the cross-section

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is evaluated and pressure is assumed to be uniform in each cross-section because the rate of change in the cross-sectional shape is not significant. Momentum and energy equations are given with the above assumptions[5].

$$-\frac{\partial}{\partial x}\left(\eta\frac{\partial v_z}{\partial x}\right)-\frac{\partial}{\partial y}\left(\eta\frac{\partial v_z}{\partial y}\right) = -\frac{\partial P}{\partial z} \quad (1)$$

$$\rho C_p v_z\frac{\partial T}{\partial z}-\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)-\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) = \eta\left(\frac{\partial v_z}{\partial x}\right)^2+\eta\left(\frac{\partial v_z}{\partial y}\right)^2 \quad (2)$$

where x and y are coordinates in the cross-sectional plane, z is the coordinate axis perpendicular to the cross-section, v_z is the velocity in z-direction, p is the pressure, T is temperature, η is the viscosity, ρ is the density of the fluid, C_p is the specific heat, and k is the thermal conductivity. At boundaries of the cross-section, the fluid velocity is zero and the wall temperature is fixed as determined by the heat transfer analysis.

Since the above two equations are coupled, they should be solved simultaneously. If it is assumed that the material and rheological properties of the fluid are determined by fluid properties of the previous location in z-direction, the two equations can be treated separately[6]. Because only z-directional velocities are taken into consideration, governing equations at $z = z_{i+1}$ are expressed by using material properties and velocities at $z = z_i$.

$$-\frac{\partial}{\partial x}\left(\eta_i\frac{\partial v_z}{\partial x}\right)-\frac{\partial}{\partial y}\left(\eta_i\frac{\partial v_z}{\partial y}\right) = -\frac{\partial P}{\partial z} \quad (3)$$

$$\rho C_p v_{zi}\frac{\partial T}{\partial z}-\frac{\partial}{\partial x}\left(k_i\frac{\partial T}{\partial x}\right)-\frac{\partial}{\partial y}\left(k_i\frac{\partial T}{\partial y}\right) = \eta_i\left(\frac{\partial v_z}{\partial x}\right)_i^2+\eta_i\left(\frac{\partial v_z}{\partial y}\right)_i^2 \quad (4)$$

where the subscript i represents the i^{th} cross-section. Once the temperature and velocity fields on the i^{th} cross-section are obtained, viscosity, thermal conductivity, and velocity gradients are calculated on the i^{th} cross-section and used to determine the velocity and temperature fields on the $(i+1)^{th}$ cross-section. A Finite Element Method(FEM) is employed to solve the equations (3) and (4) for a given cross-section.

Temperature distribution in the solid die

Temperature distribution in the solid die should be identified to provide proper boundary conditions for equation (2). Instead of the three dimensional heat transfer analysis, two dimensional numerical solutions are obtained by assuming that the head and die have the hollow circular cylindrical shape. Because temperature inside the solid die is influenced by the temperature of the head, temperature distribution in the head and solid die is calculated at the same time. The steady state heat conduction equation for cylindrical coordinate system is expressed as below[7].

$$\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) = 0 \quad (5)$$

where T is temperature and k is thermal conductivity of the solid material used for the construction.

Adiabatic conditions are assumed at the center along the axis and at the exit of the die. Temperature is fixed at the entrance of the head and at the joint interface between the barrel and the head. It is also assumed that the temperature at each sensor location is maintained constant without fluctuations. Convection boundary conditions are used for other surfaces of the head and die with proper convection heat transfer coefficients.

Viscosity model

Among many Generalized Newtonian Fluid(GNF) models, the 5-constant modified Cross model[8] is selected as the constitutive equation. The five constants are determined by measuring the viscosity of the polypropylene at different shear rate and temperature.

$$\eta = \frac{\eta_0(T,p)}{1+(\eta_0\dot{\gamma}/\tau^*)^{1-n}} \quad (6)$$

$$\eta_0(T,p) = B\exp\left(\frac{T_b}{T}\right)\exp(\beta p)$$

where η_0 is the zero shear rate viscosity and $\dot{\gamma}$ is the shear rate.

$$\dot{\gamma} = \sqrt{(\dot{\gamma}_{ij}\dot{\gamma}_{ij})/2} \quad (7)$$

$$\dot{\gamma}_{ij} = v_{i,j}+v_{j,i}$$

Numerical Analysis

A numerical analysis is conducted to obtain the velocity and temperature distribution of the polymer melt in the die. A modified cross-sectional method is developed by using a finite element method. Geometric data of the varying cross-sectional shape is needed for the numerical analysis to be carried out. The exact shape of each cross-section can be evaluated with the geometric data. The governing equations (3) and (4) are solved numerically for a given flow rate at the current cross-section. The same calculation is carried out for a cross-section at the next position using the current evaluated results.

Generation of the geometric data of the cross-section

Although the shape of the cross-section alters continuously in profile extrusion, some cross-sections can be selected as the 'standard cross-section'. Standard cross-section is used as the basis for calculation of the cross-sectional shape in the die. For example, the cross-section S_1 and S_2 are standard cross-sections as shown in Figure 1(a). Selection of the standard cross-section can be different depending upon the varying cross-sectional shape. The standard cross-sections and distances between them are essential for identification of

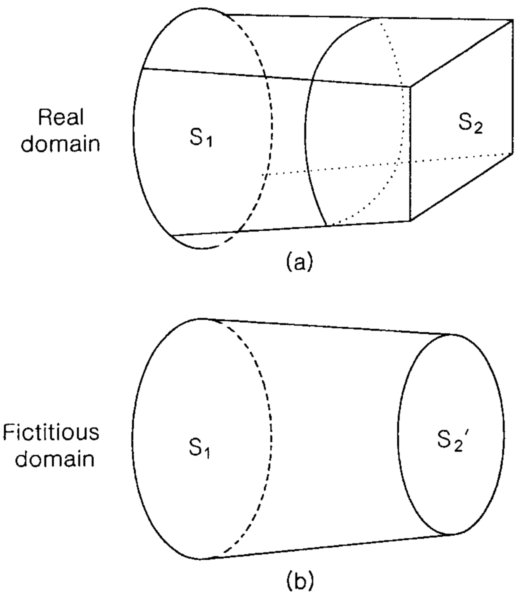

Figure 1. Real and fictitious domains for modeling of the die channel.

the die.

Determination of the cross-sectional shape based on the standard cross-section

For the real flow domain shown in Figure 1(a), Hurez *et al.*[3] approximated the flow domain by applying the concept of material conservation. They assumed the fictitious domain as shown in Figure 1(b), where a cross-sectional shape(S_2') has the same shape as S_1 and the same area as S_2. They performed an isothermal numerical analysis for the cross-section S_1. The results were applied to all cross-sections within the fictitious domain by assuming that if the cross-sectional shape is the same, similar velocity distribution will developed due to the constant flow rate. The advantage of the fictitious domain method is that the calculation time is reduced and implementation is simple. But if the shape of the cross-section is varied with complexity, it is hard to obtain good results.

In order to improve the numerical calculation, a modified cross-sectional method is proposed in this study. The cross-sectional shapes between two standard cross-sections are calculated directly, based on the fact that the cross-sectional shape changes linearly between two standard cross-sections in the profile extrusion die. A simple mapping technique is employed to evaluate the exact shape of the cross-section using the geometric data of the standard cross-sections.

Calculation of the velocity distribution

Mathematical FEM formulation is used to solve the equation (3) at any cross-section[9]. The final formulated equation becomes

$$\sum_{j=1}^{n} K_{ij}^{(e)} a_j = F_i^{(e)} \tag{8}$$

where

$$K_{ij}^{(e)} = \iint_{(e)} \frac{\partial \phi_i^{(e)}}{\partial x} \eta \frac{\partial \phi_j^{(e)}}{\partial x} dxdy + \iint_{(e)} \frac{\partial \phi_i^{(e)}}{\partial y} \eta \frac{\partial \phi_j^{(e)}}{\partial y} dxdy \tag{9}$$

$$F_i^{(e)} = -\iint_{(e)} \frac{\partial P}{\partial z} \phi_i^{(e)} dxdy + \oint_{(e)} \tilde{\tau}_{-n}^{(e)} \phi_i^{(e)} ds \tag{10}$$

where superscript (e) means element, ϕ_i is the shape function in each element, and $\tilde{\tau}_{-n}$ is the inward flux component.

An iteration method is used to solve the equation (8) because the flow rate is known instead of the pressure gradient in the polymer fluid. A pressure gradient is assumed at a cross-section to obtain the velocity distribution and the flow rate. By comparing the predicted flow rate with the given flow rate, the pressure gradient is adjusted for iteration. The Secant method is used for the numerical iteration[10].

Calculation of the temperature distribution

Finite element formulation[9] of the equation (4) gives the following equation;

$$[C(z)]^{(e)} \left\{ \frac{da(z)}{dz} \right\} + [K(z)]^{(e)} \{a(z)\} = \{F(z)\}^{(e)} \tag{11}$$

where

$$C_{ij}^{(e)} = \iint_{(e)} \rho C_p v_z(x,y) \phi_i^{(e)} dxdy \tag{12}$$

$$K_{ij}^{(e)} = \iint_{(e)} \frac{\partial \phi_i^{(e)}}{\partial x} k \frac{\partial \phi_j^{(e)}}{\partial x} dxdy + \iint_{(e)} \frac{\partial \phi_i^{(e)}}{\partial y} k \frac{\partial \phi_j^{(e)}}{\partial y} dxdy \tag{13}$$

$$F_i^{(e)} = \iint_{(e)} \eta \left\{ \left(\frac{\partial v_z}{\partial x} \right)^2 + \left(\frac{\partial v_z}{\partial y} \right)^2 \right\} \phi_i^{(e)} dxdy + \oint_{(e)} \tilde{\tau}_{-n}^{(e)} \phi_i^{(e)} ds \tag{14}$$

Various methods have been used to solve the initial boundary value problem given by the equation (11). The Euler explicit method is used in this study because it has two advantages; one is that the temperature distribution of a given cross-section is affected by the velocity and temperature distribution of the very previous cross-section and the other is that the equations are decoupled and then solved without iteration.

When Euler explicit method is applied at z_{n-1}, equation (11) becomes

$$[C]_{n-1} \left\{ \frac{da}{dz} \right\}_{n-1} + [K]_{n-1} \{a\}_{n-1} = \{F\}_{n-1} \tag{15}$$

By assuming that

$$\left\{ \frac{da}{dz} \right\}_{n-1} \cong \frac{\{a\}_n - \{a\}_{n-1}}{\Delta z_n} \tag{16}$$

equation (15) then becomes

$$\frac{1}{\Delta z_n}[C]_{n-1}\{a\}_n=\{F\}_{n-1}+\left(\frac{1}{\Delta z_n}[C]_{n-1}-[K]_{n-1}\right)\{a\}_{n-1} \tag{17}$$

The final finite element equation is derived.

$$[K_{eff}]\{a\}_n = \{F_{eff}\} \tag{18}$$

where

$$[K_{eff}] = \frac{1}{\Delta z_n}[C]_{n-1} \tag{19}$$

$$[F_{eff}] = \{F\}_{n-1}+\left(\frac{1}{\Delta z_n}[C]_{n-1}-[K]_{n-1}\right)\{a\}_{n-1} \tag{20}$$

Repetition of the iteration for each cross-section

Velocity and temperature distribution is calculated for the current cross-section with the above numerical methods and the viscosity and viscous heat generation are predicted based on the results. The same calculation is conducted for the next cross-section by utilizing the numerical data of the previous cross-section because the cross-section that is perpendicular to the flow direction is shifted to the z direction by the prescribed interval Δz. This numerical procedure is continued through the entire die.

Verification of numerical analysis program

In order to validate the proposed method and verify the numerical analysis code, a numerical analysis was carried out for the same condition that was employed by Hurez *et al.* [3]. The temperature distribution was not calculated because isothermal condition was assumed by Hurez *et al.* The die channel changes from a circular cross-section to a square cross-section and the maximum approach angle was 26.5° in the transition zone. Because of the symmetry, one quarter of the flow domain was considered for numerical analysis as shown Figure 2. The entire flow domain was used in this study because the computer code was constructed to solve the problem that has boundary conditions of zero velocity in the cross-section.

The Pressure drop was calculated between the die entry and the exit for both Newtonian and power law($n = 0.4$) fluids. Table 1 shows that the pressure drop given by the modified cross-sectional method is in better agreement with the numerical solution obtained by the three dimensional analysis than that of Hurez *et al.*[3].

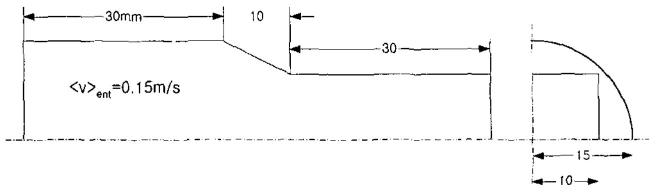

Figure 2. Die geometry used for validation of the numerical analysis.

Table 1. Comparison of the pressure drop for different numerical methods

$m = 10^5$ Pa·s^n	$n = 1.0$ ΔP (Pa)	$n = 0.4$ ΔP (Pa)
Fictitious domain method[a)]	8.2260×10^7	6.8947×10^6
Proposed method	8.5591×10^7	7.1040×10^6
3-D numerical result[a)] (1920 elements)	8.6649×10^7	7.3463×10^6

a) Hurez *et al.*[3].

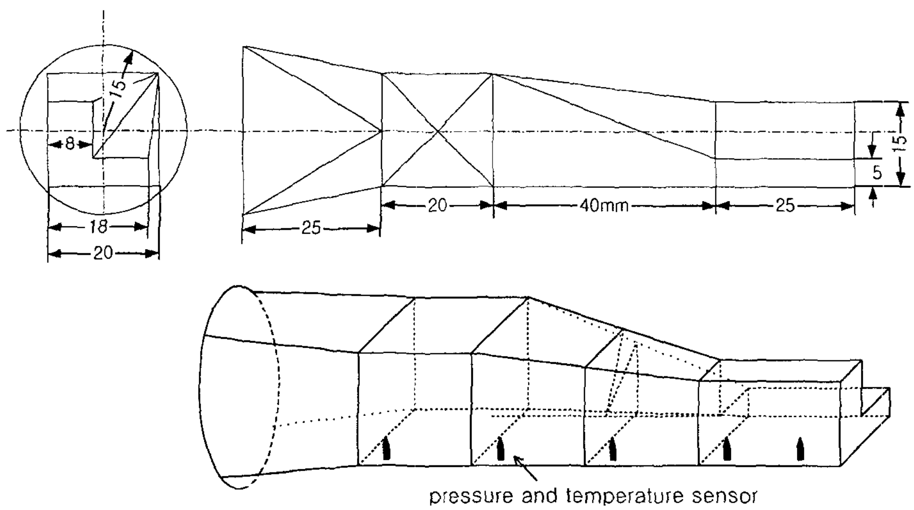

Figure 3. Geometry of the L-shape profile extrusion die used for numerical and experimental investigation.

Experiments

L-shaped profile extrusion die

L-shaped profile extrusion die used in the experiment is shown in Figure 3. A commercially available polypropylene (Hopelen, Honam Petrochemical Corp.) is used for the experiment. Temperature of the cylinder in the extruder was maintained at 190°C in feeding section and at 200°C in metering section through the experiment. The head of the extruder was heated to keep the temperature at 200°C. Temperature of the die was set at 180, 200, or 220°C and the rotational speed of the screw was fixed at 30, 60, or 90 rpm.

In order to measure the flow rate of the polymer melt which was extruded at each processing condition, the extrudate was collected for 30 seconds and its weight was measured. The flow rate was not affected by the different temperature conditions of the die and it was observed that the flow rate increased linearly with respect to the screw speed. The screw speed may be considered as the same as the flow rate in this study. Pressure and temperature transducers were used to determine the pressure and temperature of the polymer melt in the flow channel. Data were acquired at five different points placed in the die as shown in Figure 3.

Measurement of viscosity

Viscosity of the polypropylene was obtained with cone and plate rheometer, because the shear rate in the experiment was small. Viscosity was measured at different temperature, 180, 195, and 210°C as the shear rate was varied. Experimental results were obtained and then fitted to the 5-constant modified Cross model[8]. The five constants obtained for polypropylene listed in Table 2, which also contains constants for different polymers[11] for comparison.

Results and Discussion

Temperature distribution in the solid die

The governing equation (5) was solved numerically by the finite element method to determine the temperature field in the extruder head and die. The boundary conditions were selected such that they represented the operating conditions. Figure 4 shows the temperature variation of the die along the boundary of the channel. Heat convection outside the die lowered the temperature of the die. Numerical and experimental results are in good agreement with each other. However, the numerical results have lager variation than the experimental results because the thermocouples are actually located in the polymer melt. The numerical results represent the temperature of the solid die wall instead of that of the

Table 2. Five constants of the viscosity model determined from the measurement

	PP (Profax 6323)[a]	PS (Styron 678D)[a]	PP (Hopelen)
n	0.315	0.274	0.342
τ^*(Pa)	1.07E + 4	2.31E + 4	7.52E + 3
B(Pa·s)	5.71E − 2	3.04E − 9	2.36E − 2
T_b(K)	5.210E + 3	1.33E + 4	5.236E + 3
β(Pa^{-1})	1.5E − 8	3.5E − 8	1.5E − 8

a) Heiber *et al.*[11].

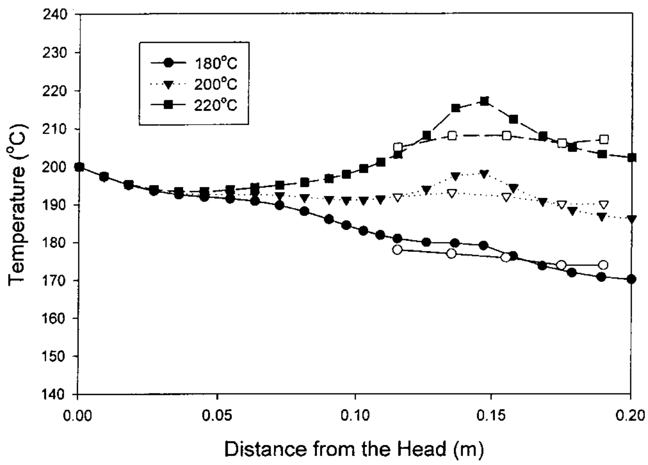

Figure 4. Temperature variation of the die along the boundary of the channel for head temperature of 200°C and for three different die temperature at the sensor; filled symbols are numerical and hollow experimental.

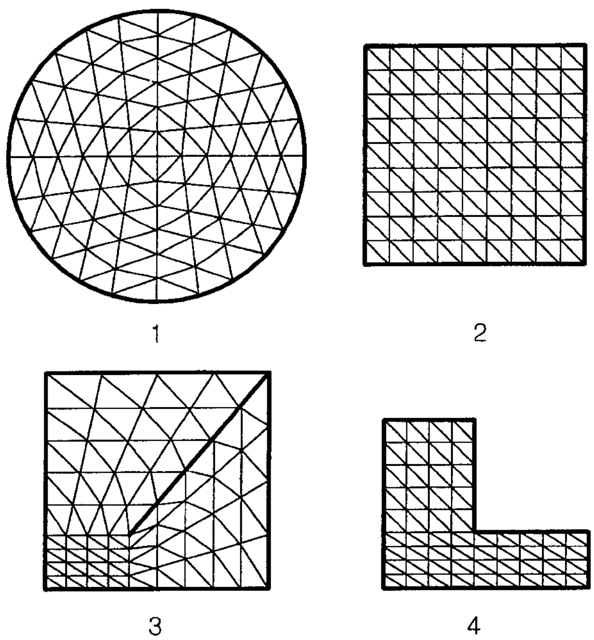

Figure 5. Finite element mesh of the standard cross-sections used for the numerical analysis of the L-shape profile extrusion die.

melt at the wall.

The numerical results could not predict the exact temperature distribution in the head and die because of the assumptions which are made in the numerical analysis. For simplicity, a two dimensional numerical method was selected for head conduction problem. A three dimensional numerical analysis including the head and die will give reliable temperature distribution and boundary conditions.

Velocity and pressure distribution in the die

In order to represent the flow domain in the extruder head and the L-shaped profile extrusion die mathematically, finite element meshes are generated for the four standard cross-sections as shown in Figure 5. Flow of the polymer melt entering the head is assumed to be a plug flow where all fluid elements move at the same velocity and at constant

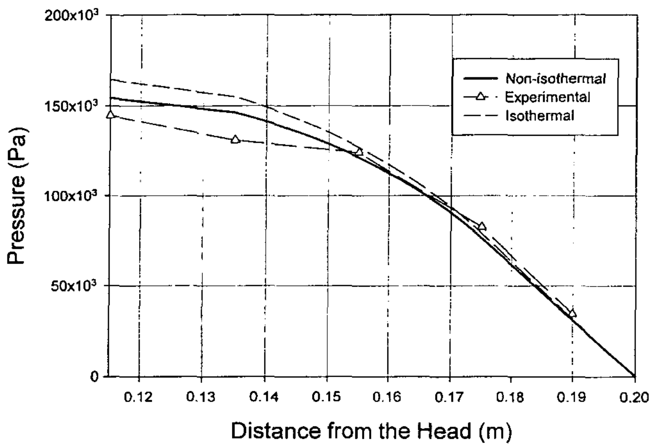

Figure 6. Pressure variation of the polymer melt along the boundary of the channel for die temperature of 180°C and screw speed of 60 rpm.

temperature of 200°C. The step size Δz_n in the flow direction is 0.1 mm, which turns out to be the best interval for both accuracy and efficiency. The numerical calculation needs about five minutes when the program was run in the Microsoft Windows NT system with the Intel Pentium Pro 200 MHz.

Figures 6 to 8 show pressure variation of the polymer melt along the boundary of the channel for screw speed of 60 rpm and die temperature of 180, 200, and 220°C, respectively. In isothermal numerical analysis, temperature of the fluid was assumed to be maintained at given die temperature and the viscosity used in the analysis was therefore calculated at that temperature. In non-isothermal analysis, data shown in Figure 4 were used as the temperature boundary conditions. In the figures, experimental results are compared with those of both isothermal and non-isothermal numerical analyses. The pressure increases with increasing screw speed of the extruder and decreasing temperature of the die as expected. Experimental results are in better agreement with the non-isothermal case than the isothermal case. But a considerable deviation is observed between the non-isothermal numerical results and the experimental results. This discrepancy may be explained by the temperature boundary condition in the channel given by the two dimensional numerical analysis of the heat transfer in the solid die and the assumption that the head and die have the hollow circular cylindrical shape.

In Figure 9, velocity contour plots are shown in four different cross-sections in the die under the non-isothermal condition. Temperature contours in the cross-section can be also obtained readily by the modified cross-sectional method. Maximum velocity in the last channel is located at the larger branch of the L-shape as shown in Figure 9. As the velocity contour plot shows, the L-shape die is not balanced as an profile extrusion die.

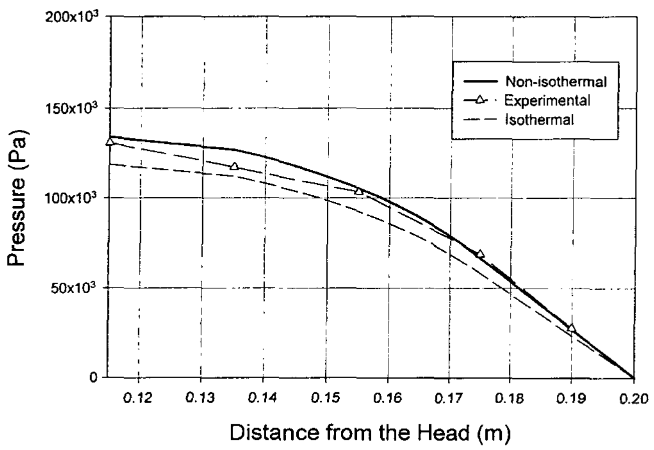

Figure 7. Pressure variation of the polymer melt along the boundary of the channel for die temperature of 200°C and screw speed of 60 rpm.

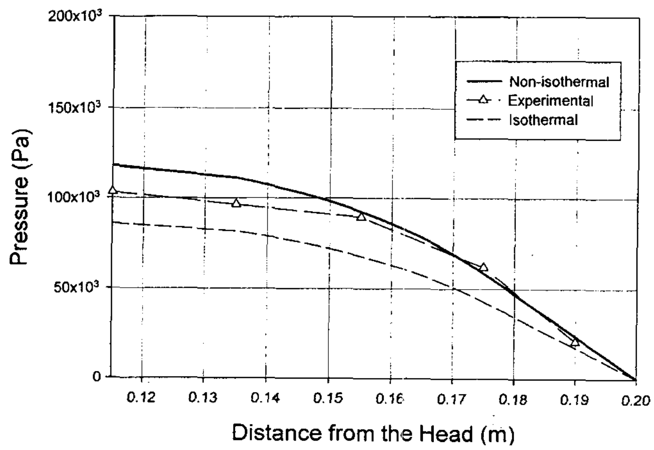

Figure 8. Pressure variation of the polymer melt along the boundary of the channel for die temperature of 220°C and screw speed of 60 rpm.

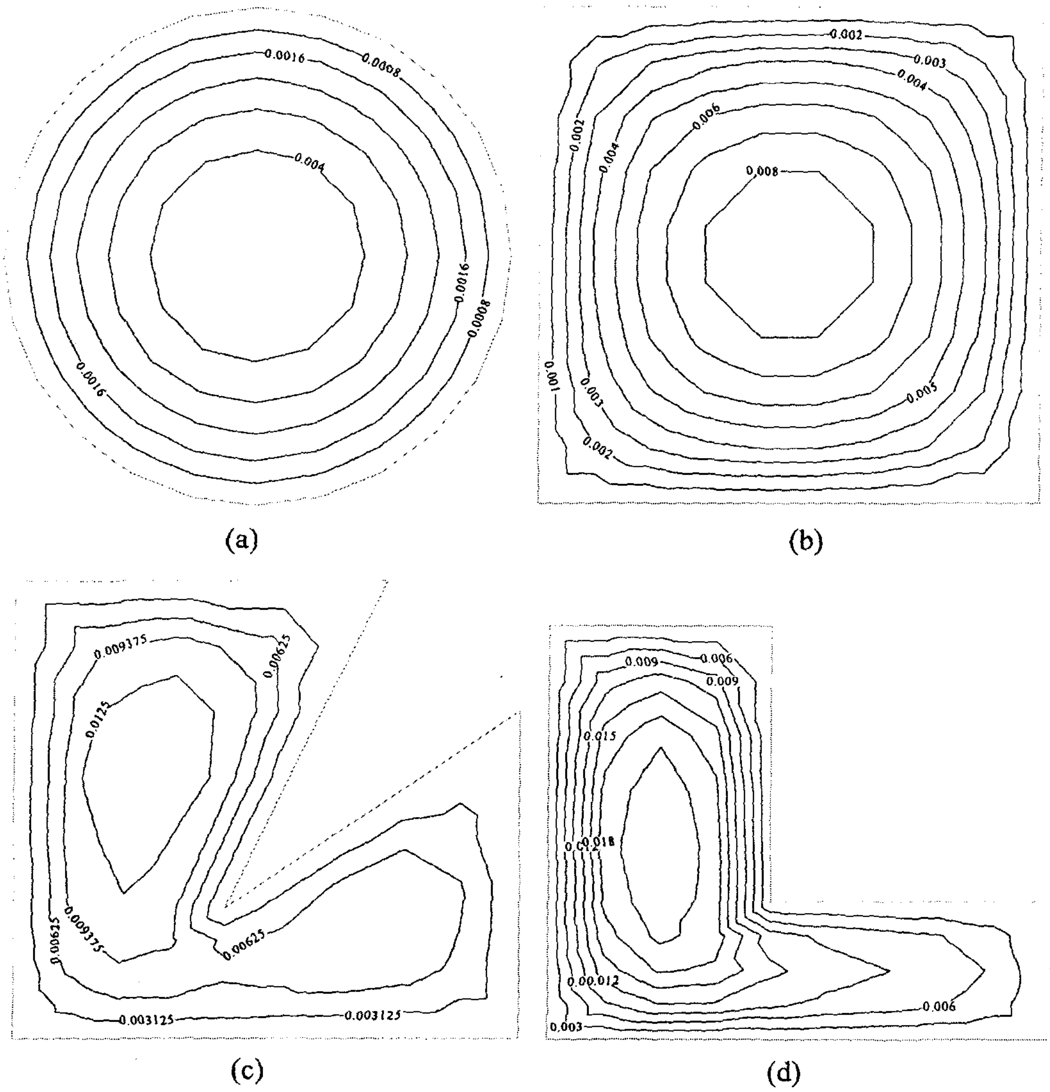

Figure 9. Velocity(m/s) contour plot for die temperature of 200°C and screw speed of 60 rpm (a) at z = 0.09 m, (b) at z = 0.135 m, (c) at z = 0.155 m, and (d) at z = 0.195 m from the head under non-isothermal conditions.

Conclusions

A modified cross-sectional numerical procedure is proposed to predict the velocity and temperature distribution in a profile extrusion die under the isothermal and non-isothermal conditions. The proposed method yields better solutions than the previous two dimensional method when compared with exact numerical solutions. In order to obtain the temperature boundary conditions of the flow channel, a numerical analysis is carried out by assuming that the head and die have the hollow circular cylindrical shape. Experimental results are compared with the numerical results for various conditions. The numerical results for the non-isothermal condition are more accurate than those for the isothermal case. A non-isothermal numerical analysis should be selected for modeling of a profile extrusion because temperature variation does exist in the die. This study may be applied to the analysis of die swell, spinning of non-circular cross-sectional fibers, and wire coating.

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