Problem Background and Mathematical Model of Polymer Movement and Melting

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Abstract: This paper offers a new theory of polymer melting in screw channels of plasticating extruders. The proposed approach is based on the solution of complete equations of mass, momentum and energy conservation. The variation of the longitudinal velocity in the flow channel direction is approximated by a piecewise constant function, which allows us to reduce the solution of 3D stationary problem considering polymer movement and heat transfer in a screw channel to 2D non-stationary problem. Qualitatively new characteristics of polymer melting, namely, the rate of melting at the interface, the shape of a solid polymer bed, the distribution of velocities and temperatures over the cross-section of the channel and along the screw, etc. are determined.

Key words: Plasticize extruder · Screw · Polymer · Mathematical model

INTRODUCTION

Nowadays, more than 60% of world manufactured plastics, about 50% of polyamide fibers and 40% of polyester fibers are processed by melting the polymer granulate in plasticating extruders. Most of the machines used for melting granulates are single screw plasticating extruders with Archimedean screws as working parts. Although these machines have found wide application, up to now there has been no rigorous theory of polymer melting in screw channels (for instance, analogous to the theory of viscous material extrusion) [1-4]. The lack of the appropriate approach can be explained by different causes and first of all by the difficulties associated with the mathematical treatment of the process.

Our aim in this section is to convince the reader that the proposed mathematical model for polymer movement and melting is not “out of thin air”. The problems of polymer processing have long been the topic of intensive research by many investigators whose pioneering studies paved the way toward understanding the physical processes encountered in plasticating extruders. The knowledge was gathered in crumbs. The proposed theories were refined mainly by reducing the number of assumptions and only a rapid growth of computing technique has enabled scientists to gain a more sophisticated insight into the problem leaving to computers the trivial round of tiresome computations.

Most of plastic or rubber extruders are single-screw machines, which have three distinct sections. In the first section, known as the feed zone, the polymer is always in a solid state. On the first 1.5-2 turns the polymer is compressed and conveyed through the channel in the form of a solid plug (the so-called solid bed) at a constant velocity [4, 5]. The movement of undeformed solid bed in the feed screw zone has been subjected to intensive experimental investigation since 1960 [6-10]. It was established that the pressure in the feed zone of the extruder increases along the screw axis and reaches considerable values. Tadmore et al [11] investigated the influence of the barrel temperature and the basic parameters of the granulate movement on the length of the feed zone. They arrived at the conclusion that the length of the feed zone is not confined to the section, in which the barrel temperature reaches the melting point- the effective length of the feed zone is much longer. To define pressure the authors [11] used the balance equation for the moments of forces acting on the solid bed, in which the contribution of both components of the frictional force at the barrel surface was taken into account. The experimental work [12] dealing with the behavior of polymeric materials in compression enabled
the investigators to estimate quantitatively the anisotropy of pressure distribution (the normal to radial stress ratio) over the solid bed for a number of polymers. Further studies were conducted taking into account the obtained estimations [1].

It should be noted that most of the studies on the subject neglect the zone of melting delay. However it is quite obvious now that for an adequate mathematical modeling of this zone one should consider, in addition to heat transfer processes, the hydrodynamics of polymer flow in conditions of phase transition. The approach proposed by Tadmor and the models constructed on its basis cannot provide an appropriate description of this zone [1]. The notion of melting delay zone was first introduced by Tadmor. This is the section of the screw channel that extends from the end of the feed zone to the point where the screw flights begin to scrape the melt off the barrel surface. In this zone, melting of the polymer pellets occurs simultaneously with their deformation. The distinguishing features of this process are that melting of the solid polymer takes place at the melt film–solid polymer interface due to heat generation by a viscous dissipation in the melt film and that melt circulation is absent.

A mathematical model of the flow and heat transfer in the melting delay zone was proposed in [13]. Here it was pointed out that for a granulated polymer, the 0.2mm. thickness of the melt film suffices to fill the spaces between the pellets. However, the formation of the melt pool begins when the film thickness is 3-4 times greater than the size of a clearance between the screw flight and the barrel.

A systematic investigation of melting processes in the screw extruders traces back to the study by B.H. Maddock [14], which has long acknowledged as the classical work in this field. His merit lies in the fact that he first attempted to describe melting mechanisms operating in the extruder channels relying on visual observations. To ensure the generality of conclusions the tests were run for a variety of polymers and extruders. In this work, Maddock also gave a general outline of the mathematical model for calculation of plasticating extruders.

Two years later L. Street published the results of experimental investigation of the melting processes [15]. The experimental technique used in this study was similar to that of Maddock. The data obtained by Street for a number of polymers served as experimental verification of the melting mechanisms proposed by Maddock.

An essential contribution to the theory of polymer melting in plasticating extruders was made by Tadmor. Most of his calculations were based on the conclusions of Maddock and Street about melting mechanism. In search for solution to the polymer melting mechanism Tadmor was forced to introduce a large number of simplifying assumptions [16].

These assumptions allowed Tadmor to reduce the problem of polymer melting to one-dimensional problem of heat and mass transfer. However with this formulation it was impossible to correctly take into account convective and diffusion heat transfer, energy dissipation, etc, which led to obvious contradictions between the theoretical and experimental results [16].

The further studies of the melting zone were mostly based on the Tadmor's model and the authors excluded one or another assumption. In [17] the channel of variable height was examined. Unlike Tadmor's approach Rauwendaal [18] took into account the dependence of polymer viscosity on shear rate and temperature. Authors in [19] considered a finite height of the solid phase in the melting zone and predetermined constant temperature on the surface of the screw. In [20-22] other mathematical models of the melting process were used and one-dimensional setting was being kept. In [23] quasi-3D approach for describing movement and melting of polymers in a long rectangular channel was proposed. Fields of velocity, temperature and pressure in the cross section and along the length of the screw were obtained.

A number of experimental works reported in [19, 24-31] pursued dual purpose: to verify the fitness of the mathematical models for real processes and the validity of the adopted assumptions and to establish new relationships governing the melting processes in plasticating extruders. Experimental studies have shown that the agreement between the experimental and theoretical data obtained with using one-dimensional mathematical models in most cases is unsatisfactory. In case of quasi-3D models the divergence at pressure does not exceed 20 % and at temperature 1 %.

A great number of papers is devoted to the study of flow and heat transfer in the metering extruder. Authors [32-34] considered the Couette flow between two infinite plates. In [35-37] a 2D mathematical formulation taking into account the longitudinal circulation of the polymer melt is presented. Using the 3D mathematical models [23, 38, 39] allowed to take into account the effect of the side walls of the channel (propeller) and consequently the transverse circulation of the polymer melt.
In [40] the experimental investigation of temperature fields in the channels of the extruder and forming tool is given. It is noted that with the increasing flow rate the maximum temperature in the center portion of the extruder increases too, which substantially exceeds the maintained temperature of the extruder housing.

Mathematical Model of Polymer Movement in the Feed Zone: A schematic diagram of the plasticating extruder, its functional zones, geometrical dimensions and the direction of coordinate axes are given in Fig. 1. The x-axis is directed along the length of the channel, y- and z-axes have the cross channel and the channel depth directions, respectively. The lead of a screw and the channel width S are constant whereas the channel depth H may vary. If the screw root of the examined extruder is not fitted with a tapered section, then $H=\text{const.}$, otherwise in the feed zone the channel depth $H$ is greater than the channel depth $H_s$ in the metering zone. In the case where the polymer flow in the screw channel is considered without taking into account the radial clearances $h=0$ and vice versa, when calculations are made with allowance for radial clearances, $h$ is assumed constant throughout the length of the channel.

In plasticating extruders the initial solid polymer in the form of pellets is supplied through the hopper to the feed zone where it is entrapped by the screw flights and conveyed along the channel. The movement of the solid polymer is caused by friction of the polymer at the inner surface of the barrel. Approximately at the first 1.5 – 2 unheated turns the polymer pellets are compressed forming a solid bed or “plug”, which moves down the screw channel with a constant velocity [6, 22].

To construct a mathematical model of motion and heat transfer in the feed section of the extruder we introduced the following assumptions:

- The process is stationary;
- The velocity of the solid bed is constant (the first turn of the screw providing compression of solid polymer is ignored);
- The screw channel is developed on a plane and the principle of rotation reversal is used which means that the screw rotation is arrested while the barrel continues to rotate with the same speed as the screw but in the opposite sense;
- Diffusion of heat along the channel is neglected.

Thus, the movement of the polymer in the screw channel is modeled by a steady-state nonisothermal movement of the solid bed in a rectangular channel with two side walls. The upper plane surface of the channel moves with a constant velocity $V_0$ at a helix angle $\varphi$ of the screw lead to the channel axis, as shown in Fig. 2.

Let us consider dynamic and heat balance of the solid bed element as it moves along the channel. As the polymer moves down the channel, its temperature increases due to heat generated and conducted by dry friction. The energetic balance in the plug is defined by the equation, which takes into account the variation of temperature in three directions.

$$c_p \rho u \frac{dT}{dx} = k_1 \left( \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)$$

1
where \( c_v, \rho, k_v, u \) are the heat capacity, density and heat conductivity of the solid polymer, respectively, velocity of the solid bed.

Depending on the initial processing conditions the boundary conditions of the problem may vary. In the case when the barrel of the extruder is kept at fixed temperature the temperature of the upper boundary is assumed to be that of the isothermal wall (note that in the general case the barrel temperature \( T_b \) varies lengthwise)

\[
T|_{z=H} = T_b(x). \tag{2}
\]

If the barrel temperature is not prescribed, then with a given heat flux from the external heat source, it is necessary to take into account the heat flux to the solid bed as a result of dry friction dissipation

\[
k_b \frac{\partial T}{\partial z} \bigg|_{z=H} = q, \tag{3}
\]

where \( A \) is the coefficient allowing for the amount of heat conducted to the polymer; \( q_b \) is the heat flux from the external sources (the extruder barrel); \( k, \rho, c_v \) are heat conductivity, density and heat capacity of the barrel.

The screw surface is assumed to satisfy the following isothermal or adiabatic conditions:

\[
T|_{z=0} = T|_{y=0} = T|_{y=S} = T_s, \tag{4}
\]

\[
\frac{\partial T}{\partial z} \bigg|_{z=0} = \frac{\partial T}{\partial y} \bigg|_{y=0} = \frac{\partial T}{\partial z} \bigg|_{y=S} = 0. \tag{5}
\]

The initial condition for polymer temperature is given by

\[
T|_{t=0} = T_0. \tag{6}
\]

where \( T_0 \) is the temperature of the solid polymer fed into the hopper.

Equation (1) was solved by the finite difference method. The values of pressure and temperature were calculated up to the time of formation of a thin melt layer (the first layer on the finite difference grid at the temperature equal to a melting point of the polymer). This moment of time corresponds to the end of the feed zone and the beginning of the melting delay zone.

**Mathematical Model of Polymer Movement and Heat And Mass Transfer in the Zone of Melting Delay:**

The zone of polymer melting delay is defined as a portion of the screw, in which the polymer exists in two states - the phase of a solid polymer bed and that of a liquid polymer in the form of a thin melt film. The differential characteristics of this zone are the substitution of dry friction at the barrel surface for a viscous friction (compared to the feed section) and the absence of circulatory motion of the liquid polymer across the screw channel. As the polymer moves forward along the zone of melting delay it is continuously heated up not only by the external source but also by internal heat generated by viscous dissipation. The thickness of the melt film is constantly growing. When its thickness becomes greater than the flight clearance, the excess of melted polymer is collected in the pool of melt in front of the pushing flight
where a circulatory motion of the melt takes place. This is considered to be the point where the process passes in the melting zone.

The analysis of processes occurring in the zone of melting delay should consider both the equation of energy and the equations of hydrodynamics. Since a polymer flow in this zone is assumed to be confined between two infinite plates, which in the real extruder are the inner barrel surface and the interface of two phases (Fig. 3), the system of constitutive equations for a liquid phase is essentially simplified

\[
\frac{\partial}{\partial z} \left( \eta \frac{\partial v_y}{\partial z} \right) = \frac{\partial p}{\partial y};
\]

\[
\frac{\partial}{\partial z} \left( \eta \frac{\partial v_x}{\partial z} \right) = \frac{\partial p}{\partial x};
\]

\[
\rho \int_0^H v_x dz = G;
\]

\[
\int_0^H v_y dz = 0;
\]

\[
c p \frac{\partial T}{\partial x} = k \frac{\partial^2 T}{\partial z^2} + \eta \left[ \left( \frac{\partial v_x}{\partial z} \right)^2 + \left( \frac{\partial v_y}{\partial z} \right)^2 \right]
\]

where \( \eta \) is the consistency index, \( [\beta] \) is the temperature coefficient of viscosity (pre-exponential), \( I_2 \) is the square invariant of the strain rate tensor and \( n \) is the viscosity anomaly.

Since the expression (7) involves the unknown pressure gradients \( \partial p/\partial y \) and \( \partial p/\partial x \), the flow rates are calculated numerically from the obtained velocity fields at each iteration step in the down channel direction and compared with the prescribed values. The flow rate discrepancy, for example, \( \Delta G \) at one iteration (at one and the same step along the channel length) was compared with the discrepancy at the previous iteration defined for the value of the pressure gradient from the previous iteration. With allowance for two errors in coordinates \( \partial p/\partial x \) the pressure gradient was then recalculated in such a way that the discrepancy in \( \Delta G \) vanishes. The iterative process accomplished in such a manner converges quickly and is completed at the value of the pressure gradient satisfying the flow rate equation.

In computation of the mass flow rate \( G \), the velocity component \( v_x \) for a solid phase is assumed to be equal to the velocity of the solid phase \( u \) and \( v_y \) is set equal to zero.

The dependence of melt viscosity on the shear rate and temperature is taken into account by the following expression:

\[
\eta = \mu_0 \exp[-\beta(T - T_m)] \left( \frac{I_2}{2} \right)^{n-1},
\]

where \( \mu_0 \) is the consistency index, \( [\beta] \) is the temperature coefficient of viscosity (pre-exponential), \( I_2 \) is the square invariant of the strain rate tensor and \( n \) is the viscosity anomaly.
The temperature field for the solid phase was evaluated from (1). The boundary conditions for the system of (1, 7) can be written as

\[
\begin{align*}
\frac{\partial v_x}{\partial z} |_{z=H} &= v_0 \cos \varphi, \\
\frac{\partial v_y}{\partial z} |_{z=H} &= v_0 \sin \varphi, \\
\frac{\partial T}{\partial z} |_{z=H} &= T_b, \\
\frac{\partial T}{\partial z} |_{z=0} &= 0, \\
\frac{\partial T}{\partial z} |_{z=H-h} &= T_m; \\
\end{align*}
\]

(9)

Here \( T_b \) and \( T_m \) are the temperature of the barrel and the melting point of the polymer, \( h \) is the thickness of the melt film (the flight clearance).

For amorphous polymers the melting point is assumed as the temperature averaged over the range of polymer softening temperatures.

The full system of (1,6-9) were solved by the finite difference method. The nonlinearity of viscosity and the dependence of thermophysical properties on temperature and variable thickness of the melt film were taken into account by using additional iteration procedures, which will be described below.

Mathematical Model of Polymer Flow and Heat Transfer in the Melting and Metering Zones: A mathematical description of polymer flow and heat transfer processes is based on the laws of conservation of mass, momentum and energy \([1, 2]\). These equations do not account for the relation between the stresses and corresponding strain rates. In order to characterize completely the behavior of the deforming polymer it is necessary to incorporate into the above system of equations the equations of state. These equations are combined with (14) into connected and essentially nonlinear system. At present searching for a solution to (12) the problem in the context of this formulation is a challenging task. Therefore in each specific case, theoretical developments should start from physically verified assumptions, which essentially simplify and modify the initial system of differential equations. Solution of theoretical problems is always based on certain assumptions whose number and significance could be reduced by refining the available mathematical models and up-dating computer facilities.

In the majority of cases a polymer flow in screw channels can be viewed as a circulation of a liquid with small volumetric flow rate towards the outlet or as a liquid motion, in which all parameters weakly depend on the longitudinal coordinate. Therefore, we may adopt the following assumptions. Let us divide the channel into a number of subsections and assume that within each section the velocity component \( \tau_x \) is constant in the down channel direction and changes its value jumpwise at the end of each section. Thus the function \( \tau_x \) of \( x \) (here and in the following the superimposed bar denotes the true value of a quantity) is approximated by a constant step function. Such an assumption is physically valid and not rigorous, since the ratio of the screw channel height \( L \) to its length \( R \) is 1:1000 and even less. Then, the flow at each point of the channel satisfies the following condition (\( v_x = \text{const} \)):

\[
\tau = \frac{\tau_x R}{v_x},
\]

(10)

where \( \tau \) is the true time.

In view of (10) the convective terms in the motion and energy equations are transformed to

\[
\frac{\partial \tau_x}{\partial \tau} = \frac{\partial \tau_x}{\partial t} - \tau_x \frac{\partial \tau_x}{\partial x} = \frac{1}{\tau_x} \frac{\partial M}{\partial \tau} = \frac{1}{\tau_x} \frac{\partial M}{\partial t},
\]

(11)

where \( M \) is taken to mean \( \tau_x \), \( \tau_x \) and \( \tau \). By virtue of assumption (10) such an expression for \( \tau_x \) within the limits of the integration domain goes to zero

\[
\frac{\partial \tau_x}{\partial \tau} = \frac{\partial \tau_x}{\partial t} = 0.
\]

(12)

The introduction of this assumption and substitution of the variable according to (11) allow us to change from a three-dimensional stationary problem to a two-dimensional quasi-stationary one. Hence the system of equations of continuity, motion and energy is written as

\[
\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho \tau_x}{\partial \tau} = 0;
\]

\[
\frac{\partial \rho \tau_x}{\partial \tau} + \frac{\partial \rho \tau_y}{\partial \tau} + \frac{\partial \rho \tau_z}{\partial \tau} = -\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho}{\partial \tau} (\eta \frac{\partial \tau_x}{\partial \tau} + \frac{\partial \tau_x}{\partial \tau}) + \frac{\partial \rho}{\partial \tau} (\eta \frac{\partial \tau_y}{\partial \tau} + \frac{\partial \tau_y}{\partial \tau});
\]

(13)

\[
\frac{\partial \rho \tau_x}{\partial \tau} + \frac{\partial \rho \tau_y}{\partial \tau} + \frac{\partial \rho \tau_z}{\partial \tau} = -\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho}{\partial \tau} (\eta \frac{\partial \tau_x}{\partial \tau} + \frac{\partial \tau_x}{\partial \tau}) + \frac{\partial \rho}{\partial \tau} (\eta \frac{\partial \tau_y}{\partial \tau} + \frac{\partial \tau_y}{\partial \tau});
\]

(14)

\[
\frac{\partial \rho \tau_x}{\partial \tau} + \frac{\partial \rho \tau_y}{\partial \tau} + \frac{\partial \rho \tau_z}{\partial \tau} = -\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho}{\partial \tau} (\eta \frac{\partial \tau_x}{\partial \tau} + \frac{\partial \tau_x}{\partial \tau}) + \frac{\partial \rho}{\partial \tau} (\eta \frac{\partial \tau_y}{\partial \tau} + \frac{\partial \tau_y}{\partial \tau});
\]

(15)
In (17) the quantity $F$ is the function of dissipation

$$F = 2 \left( \frac{\partial \nu_y}{\partial \nu} \right)^2 + 2 \left( \frac{\partial \nu_x}{\partial \nu} \right)^2 + \left( \frac{\partial \nu_x}{\partial \nu} + \frac{\partial \nu_y}{\partial \nu} \right)^2 + \left( \frac{\partial \nu_x}{\partial \nu} + \frac{\partial \nu_z}{\partial \nu} \right)^2 + \left( \frac{\partial \nu_y}{\partial \nu} + \frac{\partial \nu_z}{\partial \nu} \right)^2;$$

The quadratic invariant of the strain rate tensor $I$, and the mass flow rate of the polymer are expressed as

$$I = 2 \left[ \left( \frac{\partial \nu_y}{\partial \nu} \right)^2 + \left( \frac{\partial \nu_x}{\partial \nu} \right)^2 \right] + \left( \frac{\partial \nu_x}{\partial \nu} + \frac{\partial \nu_y}{\partial \nu} \right)^2 + \left( \frac{\partial \nu_x}{\partial \nu} + \frac{\partial \nu_z}{\partial \nu} \right)^2 + \left( \frac{\partial \nu_y}{\partial \nu} + \frac{\partial \nu_z}{\partial \nu} \right)^2;$$

$$G = \int_0^S \rho \left( \nu, \nu \right) d

In (14-16) the local time derivative plays the role of fictitious derivative, which will degenerate at each time step in the down channel direction. Since, in essence, the problem remains three-dimensional, the velocity of polymer movement is determined by the equation of flow rate constancy (20).

The system of (8,13-20) is written in terms of physical variables. The velocity and pressure fields can be readily obtained from the solution of this system. However, solution of equations of elliptical type presents a number of serious problems. First, it is rather difficult to impose and define boundary conditions for pressure, which at all boundaries are the Neumann conditions. The second problem is the instability of the obtained solution caused by nonlinearity of equations. In other words, the main difficulty with finding solutions to the non-Newtonian flow problems in terms of dynamic variable is to choose an appropriate method of solution, which could provide convergence and stability of the obtained solution [41]. The representation of equations in such a form reveals yet other imperfections associated with the iteration process involved in numerical realization of the problem. Therefore, in most cases (except in the problems with free surface) it proves to be more reasonable to write the system of equations in terms of the stream function $[\psi]$ and vorticity $[\omega]$ [41].

Before going to the system of equations represented in terms of the stream function and vorticity let us linearize the system of (13-27). This can be accomplished by the approximate methods of solution. The most-used methods are those, in which the initial nonlinear problem is reduced to a sequence of linear problems by employing procedures of successive approximations. Among these is the cross-module method, which is based on the method of variable elasticity parameters. A key point of the method is the way of constructing the relationship between the intensity of the shear stress tensor and the strain rate tensor, which is obtained from the flow curve of the polymer melt. At each iteration step it is assumed that this relation is linear.

Similarly, using the method of cross-modules we can readily linearize the energy equation with respect to the parameters $[\rho]$, $c$ and $k$, for which it will suffice to know the dependence of the given quantities on temperature.

Let us introduce the stream function $[\psi]$ and the function of vortex $[\omega]$ [41]

$$\bar{\omega} = \frac{\partial \nu_y}{\partial \nu} - \frac{\partial \nu_x}{\partial \nu}, \quad \bar{\psi}_y = -\frac{\partial \psi}{\partial \nu}, \quad \bar{\psi}_z = \frac{\partial \psi}{\partial \nu}. $$

(21)
Now after a little manipulation the initial system of equation can be rewritten in terms of the introduced functions. Before doing this, it is necessary to reduce the variables entering (13–20) to dimensionless form. To this end, all linear quantities should be assigned to the characteristic dimension $H$ (the depth of the screw channel) and all velocity quantities – to the characteristic velocity $V_c$ (barrel velocity) and temperature- to some melting point $T_m$

\[
y = \frac{y}{H}, \quad z = \frac{z}{H}, \quad v_y = \frac{v_y}{v_{oy}}, \quad v_z = \frac{v_z}{v_{oz} H}, \quad \psi = \frac{\psi}{v_{oy}}, \quad \omega = \frac{\partial H}{v_{oy}}, \quad T = \frac{T}{T_m}.
\] (22)

When choosing the way of converting the time to dimensionless form we must take into account the ratio of convective to diffusion terms in the equation of energy conservation. If the convective term is much larger than the diffusion term ($Re \gg 1$) the dimensionless time is defined as

\[
\tau = \frac{T}{H V_0}
\] (23)

Although the flow of polymeric materials in extruder is characterized by a small value of $Re$, heat transfer to a moving melt occurs mainly due to convection. This fact is of particular importance for nonisothermal problems of polymer melting and melt circulation. Therefore in the following we will use dimensionless “convective” time (23).

With account of (21-23) we obtain the following system of differential equations in dimensionless form:

\[
\frac{\partial \nu_x}{\partial \tau} = \frac{1}{Re} \Delta \nu_x + \frac{\partial \psi}{\partial y} \frac{\partial \nu_y}{\partial \tau} - \frac{\partial \psi}{\partial y} \frac{\partial \nu_x}{\partial \tau} - Eu;
\] (24)

\[
\frac{\partial \omega}{\partial \tau} = \frac{1}{Re} \Delta \omega + \frac{\partial \omega}{\partial y} \frac{\partial \psi}{\partial \tau} - \frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial \tau};
\] (25)

\[
\Delta \psi = \omega.
\] (26)

\[
\frac{\partial T}{\partial \tau} = \frac{1}{Pe} \Delta T + \frac{\partial \psi}{\partial y} \frac{\partial T}{\partial \tau} - \frac{\partial \psi}{\partial y} \frac{\partial T}{\partial \tau} + \frac{Ek}{Re} F;
\] (27)

\[
G = \int_0^S \int_0^H \nu_x dy = \text{const.}
\] (28)

Here $Re$, $Eu$, $Pe$, $Ek$ are the Reynolds, Euler, Peclet and Eckert numbers, $F$ is the dimensionless dissipation function, [delta] is the two-dimensional Laplace operator.

\[
Re = \frac{\rho H v_{oy}}{\mu_0}; \quad Eu = \frac{H}{\rho v_{oy} \partial x}; \quad Pe = \frac{c P H v_{oy}}{k}; \quad Eu = \frac{v_{oy}^2}{T_m c};
\]

\[
F = 4 \left( \frac{\partial^2 \psi}{\partial y^2} \right)^2 + \left( \frac{\partial^2 \psi}{\partial y^2} - \frac{\partial^2 \psi}{\partial z^2} \right)^2 + \left( \frac{\partial \psi}{\partial y} \right)^2 + \left( \frac{\partial \psi}{\partial z} \right)^2;
\] (29)

\[
\Delta = \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}
\]

After introduction of $Pe$, (27) for a solid phase is transformed in the process of calculation to the equation of heat conductivity
Thus, the solution to the initial nonlinear problem (13–20) is found by application of iterative procedure in the context of the cross-module method which means that at each iteration step we solve a linear (with respect to the coefficients involved) system of (24–28).

Numerical solution to the problem was obtained by the finite difference method using as a starting point the finite difference approximation. Therefore, a necessary condition for combining the hydrodynamic equation with the energy equation (heat conductivity) is the requirement that the melt film must include at least three horizontal mesh lines. Unless the last condition is fulfilled we solve equation of conductivity (1).

The boundary conditions for temperature are defined based on the assumption that the fixed walls of the channel are adiabatic and the moving wall is isothermal according to (4, 5). Thus, part of the channel for which (1) is valid can be identified in the first approximation with the feed zone of the extruder. A key point to solving the problems of heat conductivity with phase transition is to select the most accurate approximation functions to describe temperature dependence of thermophysical material properties. It should be again noticed that the phase transition at fixed temperatures is typical for few polymers, only. For the most part, polymers have a certain temperature interval of phase transition, i.e. thermal flows and thermal capacity in the region of phase transition are also continuous functions of temperature and (1) holds for both phases and phase transition. In the numerical simulations of the Stephan problem, two equations of thermal conductivity for different phases and the condition of the forth kind on the phase interface are reduced to a similar equation. These equations are obtained by “smearing” thermal capacity in the region of phase transition over temperature.

The phase boundary is defined by isotherm corresponding to an average melting point of the polymer. When the thickness of the melt film reaches the preset value, the equation of energy for molten polymer is supplemented with the equation of hydrodynamics (24–26). Temperature distribution in the solid bed is obtained as before from the solution of heat conductivity (1).

The boundary conditions for variables [psi], [omega] and \( v \) are determined from the no-slip condition of the melt on the solid impermeable surface (channel walls and interface). The vortex is represented by the second order Woods formula. For initial conditions we assume zero value for [psi], [omega], \( v \), and \( T(y, z, 0) = T_o \).

The cross-section of the channel, at which the lowest polymer temperature approaches the melting point, is considered to be the end of the melting zone and the beginning of the metering zone. Calculations for metering zone were made only in terms of hydrodynamic (24–30).

**Method of Problem Solution:** At present the two most widespread computational methods used for solution of boundary value problems are the finite element and the finite difference methods [42]. The principal advantage of the finite element method is that it allows us to obtain highly accurate solutions to the problems with complex geometry of the examined region. However this method is computational costly. Relative to FEM the finite-difference method applies to the regions, whose boundaries coincide or parallel to coordinate axes. It requires much less memory and allows us to obtain solutions rather fast and with good accuracy. It is obvious that this method is best suited for our particular problem.

There are a lot of techniques for constructing difference schemes [42]. Application of one or another technique results in explicit or implicit schemes whose merits and drawbacks have been discussed in the literature. Nowadays a number of methods have been developed, which combine the best qualities of both schemes. Such schemes are called efficient and the method of alternating directions, adopted for our purpose, also falls into this category. With the method of alternating directions we can obtain a unified algorithm for solution of both stationary and nonstationary problems and employ the effective sweep method, although the latter has been devised for solution of linear equations (in our case the equations retain geometrical nonlinearity).

The central idea of the method is that transition from the time level \( m \) to the time level \( m+1 \) occurs in two steps with the mesh size in time 0,5\( \tau \). The initial equation is divided into two equations in such a way that their summation yields the initial implicit difference equation. First, on a half-time step we solve the first equation, which is implicit in the \( y \)-direction and explicit in the \( z \)-direction. Thus the solution of two-dimensional problem reduces to successive solution of one-dimensional problems along the rows and columns of the mesh. Vortex transfer equation is described by the following system of equations:

\[
\frac{\partial T}{\partial \tau} = \frac{1}{Pe} \left( \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)
\]
Here $\delta \zeta / \delta y$, $\delta \zeta / \delta z$, $\delta \zeta / \delta y^2$ and $\delta \zeta / \delta z^2$ denote typical three-point symmetric difference approximations of derivatives.

By virtue of similarity of (24, 27) we present here only the system of two discretized equations obtained by applying the alternating direction method to equation

$$\frac{\nu_m^{m+0.5} - \nu_m^m}{0.5 \tau} = \frac{1}{Re} \left( \frac{\delta^2 \nu_m^{m+0.5}}{\delta y^2} + \frac{\delta \nu_m^{m+0.5}}{\delta y} \frac{\delta \nu_m^{m+0.5}}{\delta y} + \frac{\nu_m^{m+0.5}}{2} \right);$$

$$\frac{\nu_{m+1}^m - \nu_{m+1}^{m+0.5}}{0.5 \tau} = \frac{1}{Re} \left( \frac{\delta^2 \nu_{m+1}^{m+0.5}}{\delta z^2} + \frac{\delta \nu_{m+1}^{m+0.5}}{\delta y} \frac{\delta \nu_{m+1}^{m+0.5}}{\delta y} + \frac{\nu_{m+1}^{m+0.5}}{2} \right).$$

The equation for stream function is of elliptical type. In order that this equation can be solved by the same algorithm, it is necessary to introduce fictitious time derivative, which degenerates in the process of iteration

$$\frac{\partial \psi}{\partial t} = \Delta \psi - \omega.$$  

(33)

For (33) we adopt an implicit symmetrical scheme of the alternating direction method with fictitious time step $\psi$:

$$\frac{\psi^{n+0.5} - \psi^n}{0.5 \tau} = \frac{1}{2} \left( \frac{\delta^2 \psi^{n+0.5}}{\delta y^2} + \frac{\delta \psi^{n+0.5}}{\delta y} \frac{\delta \psi^{n+0.5}}{\delta y} - \omega^n \right);$$

$$\frac{\psi^{n+1} - \psi^{n+0.5}}{0.5 \tau} = \frac{1}{2} \left( \frac{\delta^2 \psi^{n+0.5}}{\delta z^2} + \frac{\delta \psi^{n+0.5}}{\delta y} \frac{\delta \psi^{n+0.5}}{\delta y} - \omega^n \right).$$

(34)

The equation of the energy balance is solved using the two-layer explicit difference scheme with convective terms written in counter-flow direction

$$\frac{T^{m+1} - T^m}{\tau} = \frac{1}{Eu} \left( \frac{\delta^2 T^m}{\delta y^2} + \frac{\delta^2 T^m}{\delta z^2} \right) - \frac{\delta \psi^m}{\delta y} \frac{\delta T^m}{\delta z} - \frac{\delta \psi^m}{\delta z} \frac{\delta T^m}{\delta y} + \eta E^n.$$  

(35)

The use of implicit schemes for the energy equation leads to diverging iterative process due to large values of the number $Pe$.

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<tr>
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<th>$\psi_{\text{analytical}}$</th>
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<th>$\psi_{\text{numerical}(17x25)}$</th>
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Table 1: Analytical and numerical solution to the slit flow problem

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Table 2: Analytical and numerical solutions of the energy equation for rectangular channel

Each of the obtained difference equation can be represented uniformly [41, 42]. The systems of (29, 30, 32) have specific coefficient matrices for the unknowns. The matrix of each system is categorized as a sparse matrix. A regular distribution of zero elements allows us to obtain simple computational schemes based on the sweep method [42]. In contrast to the other equations, (35) is solved in a straightforward manner without using auxiliary methods.

The results of numerical hydrodynamic calculations were compared with the analytical solution to the slit flow problem. The values of the stream function for different channel depths calculated numerically on 13x17 and 17x25 meshes and obtained analytically are found to agree fairly well (Table 1).

The results of analytical and numerical solutions of the energy equation for rectangular channel $S/H=50$ are also in good agreement, which clearly demonstrates that the assumptions and conclusions used in our treatment are justified (Table 2).

ACKNOWLEDGEMENTS

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Nomenclature:

|x, y, z| Coordinates
|S| Channel width
|H1, H2| Channel depth in feed and metering zones
|h| Radial clearance
|V0| Barrel velocity
|G| Flow rate
|ρ| Pressure
c, k, \[\rho\] = Capacity, heat conductivity, density
\[\mu\] = Viscosity
\(T\) = Temperature
\(v, v, v\) = Velocity components
\[\psi\] = Stream function
\[\omega\] = Vorticity
\(T_m\) = Melt temperature
\(T_b\) = Barrel temperature
\(I_2\) = Square invariant of the strain rate tensor

REFERENCES