MATHEMATICAL MODEL AND NUMERICAL ANALYSIS OF HEAT-TRANSFER PROCESSES ASSOCIATED WITH THE MELTING OF POLYMERS IN PLASTICATING EXTRUDERS

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A model of polymer melting in an extruder, based on the solution of the two-dimensional nonstationary conservation equations, is proposed.

Specialists estimate that over 40% of world plastics production is processed by extrusion, which generally involves the use of plasticating screw extruders. Despite the widespread utilization of these machines, we still lack a rigorous and correct theory of the melting of polymeric materials in the screw channels similar, for example, to the theory of extrusion of materials characterized by viscous flow [1, 2]. There are many reasons for this, in particular difficulties of a mathematical nature.

Numerous and convincing experiments, carried out by various investigators (only the latest work in this area has been cited [3-5]), confirm the melting model proposed by Maddock [6]. In their turn, practically all the known mathematical melting models merely refine, to some extent, the Tadmor model, on which the latter's theory of the motion and melting of polymeric materials is based [7, 8].

In [4, 5] it is pointed out that the Tadmor theory, which is based on a set of simplifying assumptions (in some respects unfounded and arbitrary), does not correspond to reality and does not make it possible to describe those characteristics of extrusion which are of most practical importance. The weaknesses of this theory include, in particular, the assumption that the phase interface is rectangular and that the plug melts only on one side, the disregarding of the circulation of the melt, and the incorrect allowance for viscous energy dissipation and convective heat transfer.

Thus, there is a clear need to construct a new, improved theory of melting in extruders. The development of such a theory, based on the solution of the fundamental conservation equations, is the subject of this article.

Let us consider the motion and heat transfer of a polymer in a plasticating extruder with a rectangular screw channel section and a ratio of the channel depth H to the inside diameter of the barrel D that is much less than unity. This assumption, valid for most extruders, makes it possible to neglect the channel curvature. If we now develop the channel and invert the motion, i.e., make the barrel rotate and stop the screw, then the heat and mass transfer in the extruder can be simulated by the motion and heat exchange of a polymeric material in a long rectangular channel, as illustrated in Fig. 1. The upper surface of this channel moves at a certain velocity W directed at a certain angle φ to the longitudinal z_1 axis of the channel. The angle φ is equal to the helix angle. It is assumed that deformation processes in the solid plug, which is treated as homogeneous and isotropic, and elastic effects in the polymer melt can be neglected.

Polymer in the form of a solid plug, consisting of granules or powder, enters the screw channel, which is at the perfectly definite temperature T_0. As experiments have shown [5, 9] the velocity W_2 of this plug, which determines the material throughput Q, is constant over the entire length of the channel, except for the entrance zone. Under the action of the heat from the hot barrel, the plug is heated as it moves along the channel. At a certain distance from the inlet a thin polymer melt is formed on the hot moving surface. When the thickness of the melt exceeds the gap between the screw edge and the barrel, the plug begins to melt at the wall of the screw, against which the flow of melt impinges [6].

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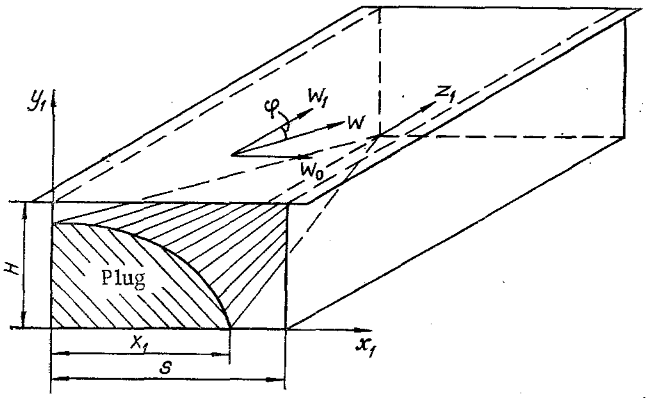

Fig. 1. Diagram of the process of polymer melting in a rectangular channel.

From this brief description of the machine and the process it follows that the problem of the motion and melting of a polymer in an extruder and its simulation reduces to the integration of the three-dimensional stationary transport equations. However, the solution of three-dimensional problems is associated with a number of computational difficulties associated with the limited speed and storage capacity of the computer.

The solution of the problem can be much simplified by making just one assumption, based on the fact that the velocity and temperature fields vary along the z_1 axis much less than with respect to the other two coordinates. Then the velocity w_z can be approximated by a piecewise-constant function. In other words, it is assumed that over relatively small sections of the channel the velocity and temperature fields are constant and change only on the next section. Obviously, for any point of the section considered the relation between the z_1 coordinate and time t takes the form

$$z_1 = w_z t. \tag{1}$$

This assumption makes it possible to reduce the solution of the three-dimensional stationary problem to that of the two-dimensional nonstationary problem. In fact, if we neglect the second derivatives with respect to z_1 in view of their smallness, and take into account Eq. (1), then convective terms of the type $w_z \partial K/\partial z_1$ may be transformed as follows:

$$w_z \frac{\partial K}{\partial z_1} = w_z \frac{\partial K}{\partial t} \frac{\partial t}{\partial z_1} = \frac{\partial K}{\partial t}.$$

Here, by K we understand w_x, w_y, and T.

In the part of the channel where there is still no melt, all the points of the plug move at the same speed $w_z = W_2$, and the heat transfer is described by the nonstationary heat conduction equation

$$\frac{\partial \theta}{\partial t} = \frac{1}{\mathrm{Pe}} \Delta\theta. \tag{2}$$

When the polymer melt develops, it is necessary to consider the equations of hydrodynamics as well as the energy equation.

Thus, the system of differential equations describing the motion and melting of the polymer, written in terms of the stream function ψ and the vorticity ω, takes the form

$$\frac{\partial \theta}{\partial t} = \frac{1}{\mathrm{Pe}} \Delta\theta - \frac{\partial \psi}{\partial x} \frac{\partial \theta}{\partial y} + \frac{\partial \psi}{\partial y} \frac{\partial \theta}{\partial x} + \frac{\mathrm{Ek}}{\mathrm{Re}} \Phi, \tag{3}$$

$$\frac{\partial \omega}{\partial t} = \frac{1}{\mathrm{Re}} \Delta\omega - \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} + \frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial x}, \tag{4}$$

$$\Delta\psi = \omega, \tag{5}$$

$$\frac{1}{\mathrm{Re}} \Delta v_z - \frac{\partial \psi}{\partial x} \frac{\partial v_z}{\partial y} + \frac{\partial \psi}{\partial y} \frac{\partial v_z}{\partial x} + \mathrm{Eu} = 0. \tag{6}$$

Equations (2)-(6) have been written in dimensionless form: all the geometric dimensions have been divided by the channel depth H, the dynamic variables by the velocity of the upper

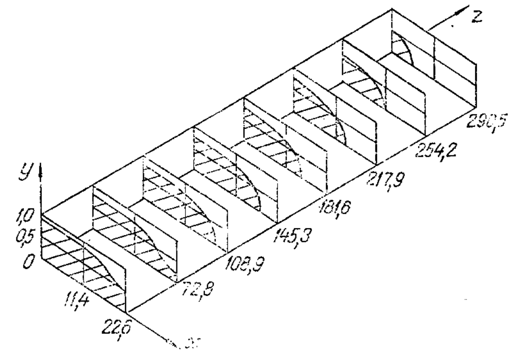

Fig. 2. Variation of plug dimensions along length of screw.

plate W_0, and temperature by the melting point T_*. Re, Ek, and Eu denote the Reynolds, Eckert, and Euler numbers respectively. The dissipation function Φ in Eq. (3) is a heat source and for the given problem

$$\Phi = \eta(\theta)\left[4\left(\frac{\partial^2\psi}{\partial x\partial y}\right)^2 + \left(\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi}{\partial y^2}\right)^2 + \left(\frac{\partial v_z}{\partial x}\right)^2 + \left(\frac{\partial v_z}{\partial y}\right)^2\right]. \tag{7}$$

Since the Euler number Eu, which contains the unknown pressure gradient $\partial P/\partial z_1$, enters into Eq. (6), to system of Eqs. (3)-(6) it is necessary to add the condition of constancy of the mass throughput Q in any cross section of the channel

$$Q = \int_0^S \int_0^H w_z \rho\, dx_1 dy_1 = \text{const}. \tag{8}$$

The boundary conditions for the variables ψ, ω, and v_z were determined from the assumption of no slippage at hard impermeable surfaces, i.e., the channel walls and the phase interface. It was assumed that the stationary walls of the screw are adiabatic surfaces and the extruder barrel, whose thermal resistance is neglected, an isothermal surface. As initial conditions we used the equations

$$\psi(x,\ y,\ 0) = \omega(x,\ y,\ 0) = 0,$$
$$v_z(x,\ y,\ 0) = W_2/W_0,\ \theta(x,\ y,\ 0) = T_0/T_*.$$

System of differential equations (3)-(6), closed by the initial and boundary conditions, together with the additional relations for the physicomechanical parameters of the polymer and condition (8), was solved by the method of nets. In this case, for solving the heat conduction (2) and energy (3) equations we used a two-layer explicit difference scheme with the convective terms written "against the flow" [10].

Most polymers, including those which formed the subject of our research, have a well-expressed temperature interval of phase transitions. Consequently, in the region of a phase transition the heat fluxes and heat capacities are continuous functions of temperature, and Eq. (3) is valid for both phases and the phase transition, the only difference being that for the solid phase it goes over into heat conduction equation (2). The phase interface was defined by the isotherm corresponding to a certain average melting point T_*.

To solve Eqs. (4)-(6) we used the method of variable (alternating) directions (MVD) [10, 11], which is equally suitable for solving stationary and nonstationary problems. For convenience, the solution of Eqs. (5) and (6) was found by the adjustment method. For Eqs. (4) and (6) we selected an implicit nonsymmetric MVD scheme, and for (5) an implicit symmetric MVD scheme [12]. The solution of the system of algebraic equations was obtained by the pivotal method.

An attempt to solve the problem using the algorithm proposed in [12] was unsuccessful, since it led to a divergent process for various accuracies and any combination of Δx, Δy, and $\Delta\tau$. Convergence of the method was achieved by joint integration of Eqs. (4) and (5) on a single time step.

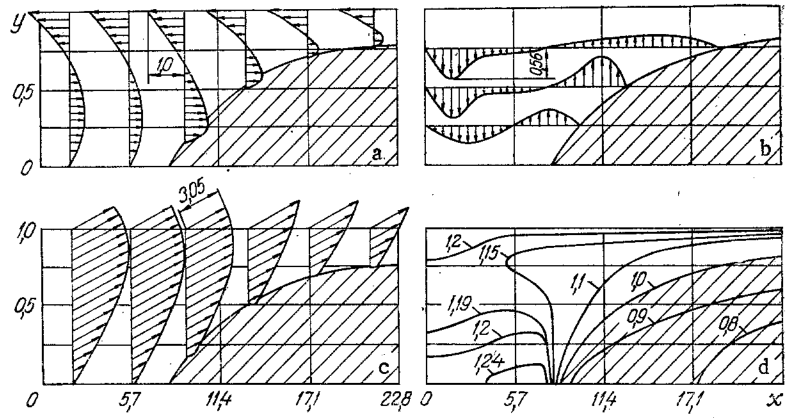

Fig. 3. Distribution of dimensionless variables over channel cross section: a) velocity v_x; b) velocity v_y; c) velocity v_z; d) temperature θ for $\theta_w = 1.24$.

In order to take into account the dependence of the viscosity on temperature and the state of shear (second invariant of shear rate tensor) we used the method of secant moduli [13]. The numerical investigation was carried out by means of a specially compiled FORTRAN program on BÉSM-6 and ES-1022 computers. The time required to solve one variant on a 17 × 17 net using the ES-1022 was about 2 h.

For investigation purposes we chose polycaprolactam, which has an average melting point of 220°C and up to a shear rate of 1000 sec^{-1} does not display any viscosity anomaly. The temperature dependence of its viscosity is quite well approximated by the exponential law $\eta(\theta) = 675 \exp(-5.94\ \theta)$, Pa·sec.

Calculations were made for the following values of the dimensionless quantities: $S/H = 22.8$; $Re = 1.2 \cdot 10^{-3}$; $Ek = 8.5 \cdot 10^{-9}$; $Pe = 1925$; $\theta_0 = 0.09$; $\theta_w = 1.24$.

A typical melting pattern for the polymeric material is shown in Fig. 2 (the shaded areas correspond to the solid phase) and convincingly confirms that the shape of the plug differs considerably from the rectangular shape on which the calculations in [7, 8] were based. Moreover, the melting process takes place not over the lateral surface but over the entire curved phase interface. This is assisted by the intense circulation and the associated convective heat transfer which, as an analysis shows, together with the energy dissipation plays a decisive part in the thermal processes associated with extrusion.

In Fig. 3, for the channel section located at a distance $z = 220$ from the beginning of the melting zone we have reproduced the distribution over the section of the dimensionless velocities v_x, v_y, and v_z and the temperature θ. The graphs clearly show that these variables vary considerably over the channel cross section.

The temperature distribution, represented in the form of isotherms in Fig. 3, indicates that as it moves along the channel the plug is heated to very considerable temperatures, the highest temperature gradients being observed at the upper heated surface and on the channel bottom at the phase interface.

NOTATION

x_1, y_1, and z_1, Cartesian coordinates; x, y, and z, dimensionless Cartesian coordinates; H and S, depth and width of the screw channel, respectively; φ, helix angle; w_x, w_y, and w_z, velocity vector components; v_x, v_y, and v_z, dimensionless velocity vector components; W, velocity of the upper plate; W_0 and W_1, transverse and longitudinal components of the upper plate velocity; W_2, velocity of the solid plug; Q, extruder capacity; $\partial P/\partial z_1$, longitudinal pressure gradient; T, temperature of the material; T_*, melting point; T_0, plug temperature at the channel entrance; θ, dimensionless temperature; θ_w, dimensionless temperature of the barrel; t, physical time; Δ, Laplacian; Re, Reynolds number; Pe, Peclet number; Ek, Eckert number; Eu, Euler number; Φ, viscous energy dissipation function; ψ, dimensionless stream function; ω, dimensionless vorticity; ρ, density.

LITERATURE CITED

1. V. I. Boyarchenko, "Macrokinetic theory of extrusion of polymers and polymerizing materials," Author's Abstract of Doctoral Dissertation, Physicomechanical Sciences, Chernogolovka (1982).
2. W. P. Perwadtschuk (V. P. Pervadchuk) and W. I. Jankow (V. I. Yankov), "Zweidimensionale Strömung nicht-Newtonscher Medien in der Kanälen von Schneckmaschinen," Plaste Kautschuk, 28, No. 1, 36-44 (1982).
3. A. Z. Halmos, J. R. A. Pearson, and R. Trottnow, "Melting in single-screw extruders," Polymer, 19, 1199-1216 (1979).
4. E. M. Mount and C. I. Chung, "Melting behavior of solid polymers on a metal surface at processing conditions," Polym. Eng. Sci., 18, No. 9, 711-720 (1978).
5. H. Fukase, T. Kunio, S. Shinia, and A. A. Nomura, "A plasticating model for single-screw extruders," Polym. Eng. Sci., 22, No. 9, 578-586 (1982).
6. B. H. Maddock, "A visual analysis of flow and mixing in extruder screws," SPE J., 15, No. 5, 383-389 (1959).
7. Z. Tadmor, H. J. Divdevani, and I. Klein, "Melting in plasticating extruders. Theory and experiments," Polym. Eng. Sci., 7, No. 3, 198-217 (1967).
8. Z. Tadmor and I. Klein, Principles of Plasticating Extrusion, Van Nostrand Reinhold Co., New York (1970).
9. D. J. Marshall, I. Klein, and R. H. Uhl, "Measurement of screw and plastic temperature profiles in extruders," SPE J., 20, No. 4, 329-334 (1964).
10. P. J. Roache, Computational Fluid Dynamics, Hermosa (1976).
11. A. A. Samarskii, Theory of Difference Schemes [in Russian], Nauka, Moscow (1977).
12. T. V. Kuskova, "Difference methods of calculating viscous incompressible liquid flow," in: Computational Methods and Programming [in Russian], Moscow State Univ. (1967), No. VII, pp. 16-27.
13. N. N. Malinin, Applied Theory of Plasticity and Creep [in Russian], Mashinostroenie, Moscow (1975).

UTILIZATION OF THE THERMAL STRAIN OF SOLIDS FOR DETERMINING THE CONSTANTS OF INTERNAL HEAT TRANSFER OF SOLID-PHASE POLYMERS

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The article describes a rapid dilatometric method, absolute in instrumental provisions, of determining the heat-transfer coefficients, thermal diffusivity, coefficients of thermal expansion and of volumetric heat capacity of polymers.

The rapid dilatometric method of determining the thermal diffusivity of solid-phase materials of polycrystalline structure, described by a number of authors [1, 2], can be used successfully for the quantitative determination of the constants of thermal conductivity λ and of thermal diffusivity a, and also for studying the temperature dependence of the coefficient of thermal expansion β and of the volumetric heat capacity c_V correlated with the heat transfer constants by the known identity [3]:

$$\lambda = ac_V. \tag{1}$$

For this purpose it is expedient to make use of the special features of the kinetics of thermal expansion of cylindrical specimens (whose radius R is one and a half to two orders of magnitude smaller than their length L) in the regime of heating of the third kind and subsequent cooling from the lateral surface by a stream of coolant with constant temperature of the core of the stream [1].

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