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FLOW REGIMES OF A HIGH-VISCOSITY POLYMER MASS BOUNDED BY THE FREE SURFACE IN THE REGION OF DRASTIC EXPANSION OF A CHANNEL

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Flow regimes of the polymer mass filling cylindrical variable-section molds are studied by means of the numerical solution of the problem of a nonlinear viscoplastic fluid flow with a free surface in cylindrical channels of geometrically complicated shapes. A mathematical formulation of the problem is given, and factors affecting the molding process are analyzed. Numerical experiments performed in a wide range of problem parameters make it possible not only to elucidate the specific features of the hydrodynamic behavior of the free surface of the moving polymer mass, but also to establish the existence of two flow regimes depending on the ratio of the generalized Reynolds number to the Froude number.

Key words: *non-Newtonian fluid, mold, free surface, motion regimes, mathematical modeling, numerical solution.*

Introduction. High-quality and defect-free production of large-scale articles from polymer materials by injection molding is mainly ensured by structural and mechanical (rheological) properties of polymer materials, technological regime of their processing, and structural features of the processing equipment used. Therefore, scientifically grounded requirements to parameters of the technological process can only be formulated after in-depth studies of both rheological characteristics of polymer compositions and the most important features of the process proper.

Filling of cylindrical molds by the polymer mass by the method of injection molding (as well as by the method of cast molding) is characterized by an important hydrodynamic feature, namely, the presence of the free surface of the moving mass. From this viewpoint, mold filling by the polymer mass is the process of formation and evolution of the free surface of the moving mass and its disappearance by the end of the cycle. Transformation of the surface during its interaction with structural elements of the press equipment is the main reason for formation of defects in the form of voids filled by air. The emergence of air-filled voids is most probable at those stages of molding where the front of the moving mass experiences significant and rapid changes. Thus, the study of possible formation of air-filled voids mainly reduces to studying how the shape of the moving mass surface behaves at different stages of molding.

Experimental studies [1–3] show that the character of the polymer material flow in the elements of the press equipment is determined by several factors that may be classified into three groups.

1. Hydrodynamic and rheological factors: mass flow in the mold determined by the productive capacity of the processing equipment, mold geometry, physical and mechanical properties of the mass (density, viscosity, rheological characteristics, etc.), and mass forces.

2. Thermophysical factors: temperature regime of molding (temperature of the incoming polymer mass, temperature and insulation properties of the mold walls, and ambient temperature) and thermophysical properties of the polymer material.

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3. Physical and chemical factors: features associated with the process of solidification, which are eventually responsible for the time and character of the action of the first two groups of factors.

The direct study of the influence of various factors on polymer material molding under the production conditions is economically inefficient. Therefore, it is necessary to use methods of physical and mathematical modeling with subsequent verification and application of the results obtained in actual production. It is difficult to take into account all factors simultaneously in mathematical modeling; hence, it seems reasonable to simplify the problem, based on available experimental data, and to consider the effect of the most important factors only. The research performed shows that the shape of the free surface of the moving mass in elements of the press equipment is mainly determined by hydrodynamic and rheological parameters of the technological regime of molding articles from polymer materials [3–9].

1. Mathematical Formulation of the Problem. The flow is assumed to be laminar, isothermal, and axisymmetric. In this case, the system of equations that describe the process of filling of vertically aligned molds by a rheologically complex fluid in the cylindrical coordinate system (z, r, φ) with the use of dimensionless variables is presented in the following form [5]:

$$\mathrm{Re}\Big(\frac{\partial v_r}{\partial t}+\frac{1}{r}\,\frac{\partial(rv_r^2)}{\partial r}+\frac{\partial(v_r v_z)}{\partial z}\Big)=-\frac{\partial p}{\partial r}+B\Big(\Delta v_r-\frac{v_r}{r^2}\Big)+2\,\frac{\partial B}{\partial r}\,\frac{\partial v_r}{\partial r}+\frac{\partial B}{\partial z}\Big(\frac{\partial v_r}{\partial z}+\frac{\partial v_z}{\partial r}\Big),$$

$$\mathrm{Re}\Big(\frac{\partial v_z}{\partial t}+\frac{1}{r}\,\frac{\partial(rv_r v_z)}{\partial r}+\frac{\partial v_z^2}{\partial z}\Big)=-\frac{\partial p}{\partial z}+B\,\Delta v_z+\frac{\partial B}{\partial r}\Big(\frac{\partial v_r}{\partial z}+\frac{\partial v_z}{\partial r}\Big)+2\,\frac{\partial B}{\partial z}\,\frac{\partial v_z}{\partial z}-\frac{\mathrm{Re}}{\mathrm{Fr}}; \qquad (1)$$

$$\Delta p=-\,\mathrm{Re}\Big(\frac{1}{r}\,\frac{\partial^2(rv_r^2)}{\partial r^2}+\frac{2}{r}\,\frac{\partial^2(rv_r v_z)}{\partial r\,\partial z}+\frac{\partial^2 v_z^2}{\partial z^2}\Big)+2\,\frac{\partial B}{\partial r}\,\Delta v_r+2\,\frac{\partial B}{\partial z}\,\Delta v_z$$

$$+\,2\,\frac{\partial^2 B}{\partial r^2}\,\frac{\partial v_r}{\partial r}+2\,\frac{\partial^2 B}{\partial r\,\partial z}\Big(\frac{\partial v_r}{\partial z}+\frac{\partial v_z}{\partial r}\Big)+2\,\frac{\partial^2 B}{\partial z^2}\,\frac{\partial v_z}{\partial z}. \qquad (2)$$

The dimensionless variables are the parameters $\bar r = r/L$, $\bar z = z/L$, $\bar v_z = v_z/U$, $\bar v_r = v_r/U$, $\bar t = tU/L$, and $\bar p = (p - p_0)(L/(\mu U))^{n/m}$ (the bar over the dimensionless quantities is omitted). In Eqs. (1) and (2), $L = R$ (R is the radius of the input channel), $U = Q/(\pi R^2)$ is the flow-rate-averaged velocity, Q is the volume flow rate of the fluid, p_0 is the atmospheric pressure, μ is the dynamic viscosity of the fluid at a zero shear rate, n and m are constants in the rheological model [10], $\mathrm{Re} = \rho L^{n/m}U^{2-n/m}/\mu^{n/m}$ is the generalized Reynolds number, $\mathrm{Fr} = U^2/(gL)$ is the Froude number, and g is the acceleration due to gravity. The variable B is the effective viscosity of the fluid, which is described by the following formula, as is mentioned in [10]:

$$B = (\mathrm{Se}^{1/n} + I_2^{1/m})^n/(I_2 + \varepsilon_0). \qquad (3)$$

Here $\mathrm{Se} = \tau_0 L^{n/m}/(U^{n/m}\mu^{n/m})$ is the dimensionless parameter of nonlinear viscoplasticity and τ_0 is the yield stress of the fluid. The expression for the strain-rate intensity I_2 in Eq. (3) is written as

$$I_2=\Big[2\Big(\frac{\partial v_r}{\partial r}\Big)^2+2\Big(\frac{v_r}{r}\Big)^2+\Big(\frac{\partial v_z}{\partial z}\Big)^2+\Big(\frac{\partial v_r}{\partial z}+\frac{\partial v_z}{\partial r}\Big)^2\Big]^{1/2}.$$

To perform continuous computations of viscoplastic fluid flows, we introduce a small parameter ε_0 into Eq. (3); the value of this parameter is chosen for the effective viscosity in the viscous flow region to be $\approx 10^{-4}$ of the viscosity in the flow core (in problems of the dynamics of nonlinearly viscous fluids, $\varepsilon_0 = 0$).

The initial and boundary conditions are also imposed in dimensionless form.

The free surface of the polymer mass at the time $t = 0$ is assumed to be located at the bottom level and to be flat. The no-slip condition $v_z = v_r = 0$ is set on all motionless rigid boundaries Γ_1, Γ_2, and Γ_3 (Fig. 1). The condition imposed on the input boundary A is the velocity profile of a stabilized flow of this polymer composition in the channel considered:

$$v_z = f(r), \qquad v_r = 0. \qquad (4)$$

The form of the function $f(r)$ in Eq. (4) depends on the rheological properties of the fluid and on the geometry of the mold to be filled. Numerical experiments show that setting the velocity profile on the input boundary in the form corresponding to the flow of the chosen fluid in the channel considered does not produce any more significant influence on the flow pattern than the Newtonian velocity profile. This effect can be attributed to the fact that the

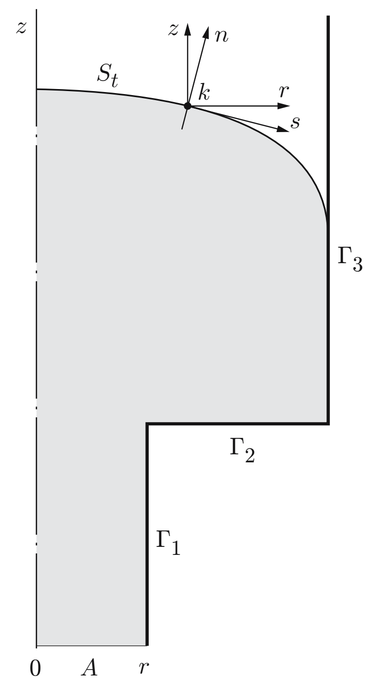


Fig. 1. Boundaries of the computational domain.

distance between the input boundary and the original position of the free surface is greater than the length of the hydrodynamic segment. Therefore, the conditions for the velocity-vector components at the input boundary are set in the form

$$v_z = 2(1 - r^2), \qquad v_r = 0.$$

The conditions on the axis of symmetry are

$$\frac{\partial v_z}{\partial r} = 0, \qquad \frac{\partial p}{\partial r} = 0, \qquad v_r = 0, \qquad \frac{\partial B}{\partial r} = 0.$$

Two boundary conditions are set on the free surface S_t: identical values of the normal stress and the pressure in the medium bordering the fluid and the absence of shear stress. These conditions are written in the local coordinate system fitted to each point of the free surface (see Fig. 1) and have the form

$$p = 2B\,\frac{\partial u_n}{\partial n}, \qquad \frac{\partial u_s}{\partial n} + \frac{\partial u_n}{\partial s} - \frac{u_s}{R_s} = 0, \tag{5}$$

where R_s is the curvature of the coordinate line in the direction s.

The magnitude of the effective viscosity B in the first equation of (5) is determined by Eq. (3). The strain-rate tensor deviator I_2 present in the expression for B can be written in the following form [9] in the local orthogonal curvilinear coordinate system fitted to each kth point of the free surface, in which Eqs. (5) are also written:

$$I_2 = \Big[2\Big(\frac{\partial u_n}{\partial n}\Big)^2 + 2\Big(\frac{v_r}{r}\Big)^2 + 2\Big(\frac{\partial u_s}{\partial s} + \frac{u_n}{R_s}\Big)^2\Big]^{1/2}.$$

In addition, the free surface should obey the kinematic condition

$$\frac{dz}{dt} = v_z, \qquad \frac{dr}{dt} = v_r.$$

Thus, the problem posed is solved by using a system consisting of two equations of motion in the directions r and z, Poisson's equations for pressure, and equations that relate the effective viscosity to the field of velocities.

The problem is solved numerically by the finite-difference method. For this purpose, the computational domain is covered by an Eulerian grid of cells. The cell sizes are h_1 and h_2 in the axial and radial directions, respectively. The method of solving difference analogs of the original system of differential equations with the use of Libman-type iterative schemes was described in detail in [4, 5]. An original technique of implementation of the boundary conditions on the free surface in the precise statement is also described in those papers.

For the solution of the boundary-value problem described by system (1)–(3) with the corresponding initial and boundary conditions to be equivalent to the solution of the boundary-value problem described by the system consisting of the continuity equation

$$\frac{\partial v_z}{\partial z} + \frac{1}{r}\frac{\partial (r v_r)}{\partial r} = 0$$

and Eqs. (1) and (3), we impose the condition that the equation of continuity is satisfied on all boundaries of the computational domain.

2. Calculation Results. We consider the process of filling of a vertical cylindrical channel with a variable section by the polymer mass supplied through the input pipe (see Fig. 1).

An analysis of numerous experiments performed under both laboratory and production conditions shows that defects may arise directly as the mold is being filled by the polymer mass. One of the most probable reasons for formation of defects is the hydrodynamic features of the flow in the region of the input orifice, which are formed as the first portions of the polymer mass enter the chamber. Indeed, it follows from the results of model experiments [1] that, though the front of the moving polymer mass acquires a smooth form with time, the initial stage of molding may be different, depending on parameters characterizing this hydrodynamic process. At least two variants of front formation are possible:

1. Emergence of a high cylindrical column above the input orifice. The column experiences an extremely irregular transformation into a smooth front (collapse, swirl, and agglutination of individual coils), which can lead to formation of defects in the form of air-filled voids in the resultant article.

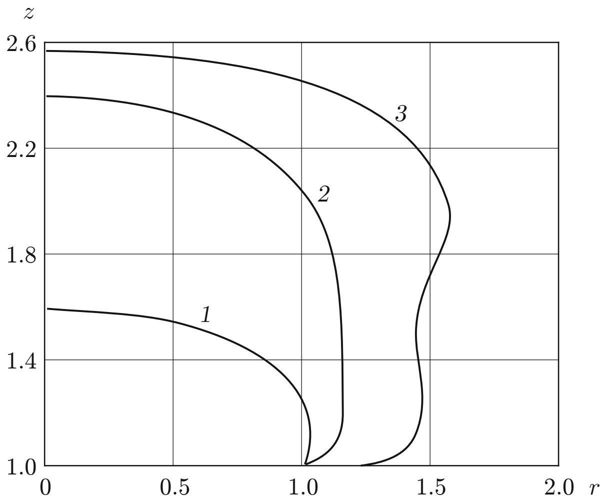
2. Emergence of a mushroom-shaped "cap" uniformly spreading in the radial direction. The smooth shape of the free surface starts developing from the very beginning of the process, which prevents formation of air-filled voids.

Thus, to ensure the regime with the initially defect-free stage of article molding, it is necessary to find parameters that exert the major effect on spreading in the vicinity of the input orifice. Numerical experiments show that two regimes of the polymer mass flow in the vicinity of the input orifice may exist. These regimes may be conventionally called the favorable and the adverse regimes. The governing parameter was found to be $W = \mathrm{Re}\,/\,\mathrm{Fr}$. It seems impossible, however, to find the only value of the criterion W, which is the critical value separating the two flow regimes described above. The character of spreading in the vicinity of the input orifice is also affected by other flow parameters, such as the parameter of nonlinear viscoplasticity Se and the rheological parameters n and m. Thus, in processing the results of computations performed in a wide range of the values of the basic hydrodynamic parameters of the process ($\mathrm{Re} = 1$–10^{-8}, $\mathrm{Fr} = 10^{-3}$–10^{-11}, $\mathrm{Se} = 0$–150, $n = 0.2$–1.5, and $m = 0.7$–1.3), we managed to distinguish a certain range of the parameter W ($6 < W < 30$), where the flow regime is uncertain, i.e., it may be either favorable or adverse. A computational experiment showed that the flow regime outside this region is adverse for $W < 6$ and favorable for $W > 30$.

Figures 2 and 3 show the results computed for two flow regimes considered. It follows from Fig. 2 that the fluid escaping from the input pipe and bounded by the free surface rises in the form of a column at the initial time and retains this form practically without spreading. Then there occurs insignificant spreading, and the free surface of the polymer mass gradually acquires a wavy shape, which finally results in irregular motion of the free boundary. This behavior shows that the adverse flow regime occurs. In this case, $W = 5.68$.

Figure 3 illustrates the favorable flow regime ($W = 382$). It follows from Fig. 3 that the shape of the free surface changes with time, and significant spreading of the mass entering the mold occurs.

The study of the influence of the rheological parameters n and m for a fixed value of W and $\mathrm{Se} = 0$ shows that the values of n/m lower than $n/m = 1$ corresponding to the Newtonian fluid lead to an increase in velocity of the radial flow in the vicinity of the input orifice, i.e., spreading becomes more intense as the effective viscosity of the incoming mass decreases. The character of spreading is also affected by changes in the parameter of nonlinear viscoplasticity Se. As the parameter Se increases, the radial flow becomes decelerated. The main factor responsible for the flow character, however, is the parameter W, because the rheological characteristics of the polymer mass determined by the values of the parameters n, m, and Se normally change little in the course of production of articles from particular polymer materials.



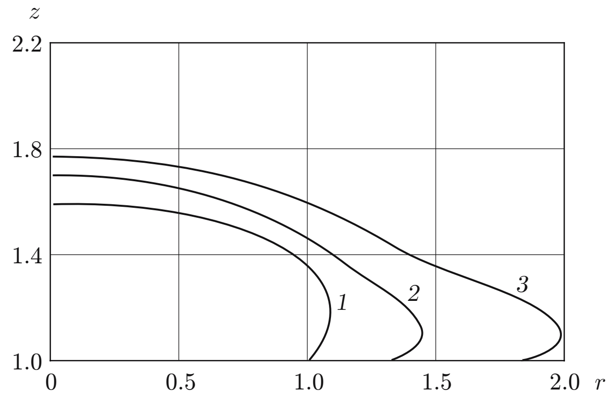
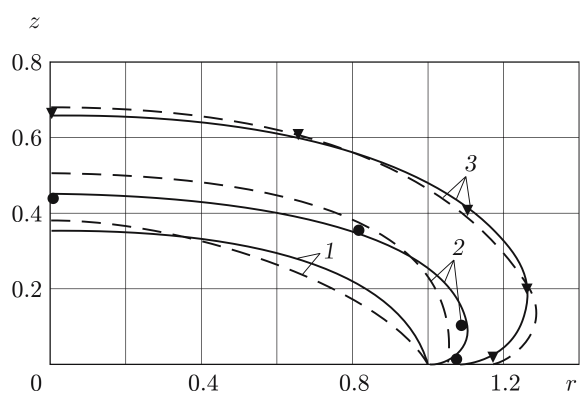


Fig. 2

Fig. 3

Fig. 2. Position and shape of the free surface for $W = 5.68$, Se = 0, $n/m = 0.7$, and $t = 0.56$ (1), 2.59 (2), and 9.35 (3).

Fig. 3. Position and shape of the free surface for $W = 382$, Se = 0, $n/m = 0.7$, and $t = 0.51$ (1), 1.32 (2), and 3.01 (3).



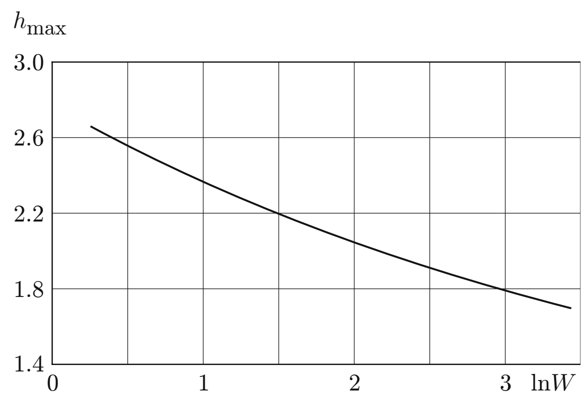


Fig. 4

Fig. 5

Fig. 4. Position and shape of the free surface for $W = 100$, Se = 0, $n/m = 1$, and $t = 0.25$ (1), 0.39 (2), and 0.78 (3); the solid curves are the results computed in the present work; the dashed curves show the numerical solution [3]; the points are the experimental data [3].

Fig. 5. Maximum height of the front versus the criterion W for Se = 0 and $n/m = 0.7$.

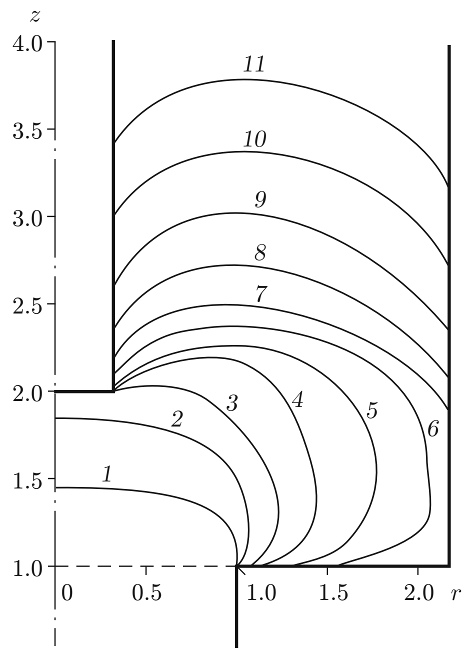


Fig. 6. Position and shape of the free surface in the case of filling a channel with a central body for Re $= 2.85 \cdot 10^{-3}$, Fr $= 1.02 \cdot 10^{-4}$, Se $= 0$, $n/m = 1$, and $t = 0.35$ (1), 0.78 (2), 1.23 (3), 2.52 (4), 3.21 (5), 4.85 (6), 6.04 (7), 6.98 (8), 8.37 (9), 10.19 (10), and 12.03 (11).

To verify the credibility of results computed by the present method, we compared them with the numerical solution of the model problem of filling a cylindrical cavity by a viscous fluid and with the experimental data [3] (Fig. 4). It is seen in Fig. 4 that there is some difference with the results obtained in [3] for the first two times ($t = 0.25$ and 0.39). The experimental data [3] are in better agreement with the results computed in the present work (solid curves), though there is a certain difference in the vicinity of the corner point. Thus, the method proposed here and the algorithm developed on the basis of this method allow obtaining reliable results.

Numerical experiments performed for the flow geometry considered show that the fluid front reaches a certain maximum height after a certain time in all cases. After that, the fluid flow in the axial direction ceases, and only the radial flow is observed. It seems of interest to determine the maximum height of the front as a function of the criterion W. This dependence is plotted in Fig. 5, which shows that the maximum height of the front decreases with increasing W.

After that, the front of the moving mass continues its upward motion only when the free surface reaches the outer wall of the mold. The study of the influence of the side wall on flow parameters is a separate problem, as well as the flow of the fluid with the free surface inside a corner formed by the bottom and side walls of the chamber.

Structural elements inserted into the mold in the vicinity of the input orifice can also substantially affect the hydrodynamic pattern of the flow and the shape of the free surface. Figure 6 shows the consecutive positions of the free surface formed during filling of a cylindrical mold with a cantilever-fixed central body in the form of a circular cylinder. In the course of filling, the free surface of the fluid experiences transformations, which are most significant after the fluid contacts the butt-end face of the central body. The upward motion of the front in the axial direction becomes slower, and an intense radial flow arises until the mass reaches the outer wall of the mold. After that, the shape of the free surface becomes stabilized rather rapidly, and the flow becomes similar to the motion of the mass in the gap between two coaxial cylinders.

Conclusions. An analysis of the present numerical studies of filling of cylindrical molds by the polymer mass shows that different flow regimes are possible, depending on the flow-rate characteristics, geometric features of the mold, and rheological parameters of the polymer mass. The values of the criterion W are determined, which ensure the optimal initial stage of mold filling without formation of air-filled voids in the resultant article.

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