Mathematical simulation of nonisothermal filling of plane channel with non-Newtonian fluid

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Abstract. In this paper, the fountain flow of a non-Newtonian fluid during the filling of a plane vertical channel with due account of dissipative heating is investigated. The rheological features of the medium are defined by Ostwald de Waele power-law with exponential temperature dependence of viscosity. The numerical solution of the problem is obtained using a finite-difference method, based on the SIMPLE algorithm, and the method of invariants for compliance with the natural boundary conditions on free surface. It was shown that the flow separates into a two-dimensional flow zone in the vicinity of the free surface and a one-dimensional flow zone away from it. The parametrical investigations of kinematic and thermophysical properties of the flow and the dependence of the free surface behavior on the basic criteria and rheological parameters are implemented.

1. Introduction

During the processing of polymeric materials the injection molding, based on the mold filling with a liquid medium, is a widespread technology. The flow of processed composition is characterized by a complicated rheological behavior and, generally, under nonisothermal conditions. The forecasting of quantity of the products requires the prior investigations of the technological process, which can be implemented by the physical and mathematical simulation methods. The mathematical simulation method is preferable as it is more efficient and informative than the physical simulation, which is used for verification of the theoretical results on the last investigation stage. The process of filling is accompanied by an existence of the free surface, nonisothermicity, which is connected with dissipative heating, chemical conversion, heat-exchange boundary conditions, and dependence of the rheological characteristics of the medium on the temperature. The results of researches of nonisothermal complicated rheological media flow in the channels without considering the free surface are introduced in [1, 2]. There are articles [3-6], which contain the description of computational technologies and the results of filling process investigations with taking into account the free surface. The aim of this work is to investigate the influence of the medium rheological parameters on the shape of free surface, and the kinematic of a fountain flow during the filling of the plane channel on the base of rheological Ostwald-de Waele equation.

2. Formulation of the problem

The nonisothermal filling of a planar vertical channel with a fluid of the complicated rheology in a gravity field is considered. The fluid flow direction is opposite to the gravity force. The flow area is shown in Fig. 1. The mathematical basis of the flow is formed by motion, heat-transfer, and continuity equations written in dimensionless variables as follows:

\[ \text{Re} \frac{d \mathbf{V}}{dt} = -\nabla p + \nabla \cdot (2B \mathbf{E}) + \mathbf{W}, \quad \text{Pe} \frac{dT}{dt} = \Delta T + BrB \mathbf{A}^2, \quad \nabla \cdot \mathbf{V} = 0. \]
Here, $\mathbf{V}$ is the dimensionless velocity vector; $p$ is the dimensionless pressure; $T$ is the dimensionless temperature; $t$ is the dimensionless time; $\mathbf{W} = \{W, 0\}$ is a dimensionless vector; $\mathbf{A}$ is the dimensionless intensity of a strain-rate tensor $\mathbf{E}$. The system of equations is completed by a rheological power-law, which defines the apparent viscosity as follows [6]:

$$B = \exp[-CT] A^{m-1},$$

where $m$ is the nonlinearity degree.

![Figure 1. Calculation domain](image)

The dimensionless similarity criteria are given by formulas

$$Re = \frac{\rho L^u U \bar{u}_0}{\mu_0}, \quad Pe = \frac{c \rho U L}{\lambda}, \quad W = \frac{\rho L^{m+1} g \bar{u}_0}{\mu_0 U^m L^0}, \quad Br = \frac{\mu_0 U^m L^0}{\lambda T_0}, \quad C = k T_0.$$

Here, $\rho$ is the fluid density; $L$ is the half-width of the channel; $U_0$ is the average velocity in the inlet section; $\mu_0$ is the power-law rheological parameter; $k$ is the parameter of nonisothermicity; $c$ is the heat capacity; $\lambda$ is the heat conductivity coefficient; $g$ is the gravity acceleration; $T_0$ is the dimensional wall temperature.

At the inlet boundary $\Gamma_2$ the velocity and the temperature profiles, which correspond to a one-dimensional nonisothermal fluid flow with a specified constant flow rate in the infinite channel, are assigned. The typical longitudinal velocity and temperature distributions at the inlet boundary are illustrated in Fig. 2. On the rigid walls $\Gamma_3$ the no-slip boundary conditions are realized, and the dimensionless temperature is set to zero. On the free surface $\Gamma_1$ the boundary conditions are the equality of the shear stress to zero, the equality of normal stress to the external pressure, and the absence of the heat flux. At the initial time moment, the free surface is plane and it is located in a distance from the inlet boundary, and the temperature of fluid is equal to the temperature of the wall in the area of initial filling. Moreover, the free boundary moves in compliance with the kinematic condition. The surface tension forces are not considered. The problem formulation is dimensionless. The values of dimensionless criteria are assigned so that the stationary solution for the nonisothermal flow in the plane infinite channel could exist [7].

Consequently, the boundary conditions are written as follows:

$$\Gamma_1: \frac{\partial u_x}{\partial s} + \frac{\partial u_x}{\partial n} = 0, \quad p = 2B \frac{\partial u_x}{\partial n}, \quad \frac{\partial T}{\partial n} = 0;$$

$$\Gamma_2: u = 0, \quad \nu = f_1(x), \quad T = f_2(x);$$

$$\Gamma_3: u = 0, \quad \nu = 0, \quad T = 0;$$

(1)
\[ \Gamma_4: u = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \frac{\partial T}{\partial x} = 0. \]

The conditions (1) are written in a local Cartesian coordinate system \((n, s)\), which is normally related with the free surface. The free boundary \(\Gamma_1\) moves in compliance with the kinematic condition written in the Lagrangian representation as follows:

\[ \frac{dx}{dt} = u, \quad \frac{dy}{dt} = v. \] (2)

The analysis of the classical mathematical model of fluid dynamics using the motion equations, natural boundary conditions on the free surface, and no-slip conditions on the moving contact line for the values of the dynamic contact angle, which is not equal to 0 and \(\pi\), has shown that in the determination of the dynamic characteristics of the flows, singularities arise that lead to an infinite increase in the flow parameters as the three-phase contact line (TPCL) is approached \([8, 9]\). Therefore, the problem formulation takes into account that at the contact point \(C\) the condition of the shear stress absence is realized (1), the normal velocity is equal to zero, and in the small vicinity of the contact line the tangential velocity on the wall decreases asymptotically from the value at the point \(C\) to zero. It is supposed, that the flow regime and the interaction behavior of the phases on the contact line correspond to the edge angle equal to \(\pi\) with an insignificant capillary effects in comparison with inertial, viscous, and gravitational forces in the flow. Using such a boundary conditions eliminates the speciality of the traditional formulation of the problem and at the same time has a little effect on the kinematic characteristics of the flow is a small vicinity of the contact point \([10]\).

3. Method of solution

The formulated problem is solved using a finite-difference method. A staggered difference grid covers the solution domain. The SIMPLE algorithm \([11]\) is applied to calculate the unknown variables at the internal nods. Near the free surface the irregular nodes appear. In these nodes, the values of unknown variables are defined using linear interpolation of data from the free surface and regular nodes. The free boundary is represented as a set of uniformly distributed marker particles: the first marker is located on the line of symmetry and the last marker is on the TPCL. The velocity components are calculated using the method of invariants \([12]\), which is based on the assumption of no shear stresses and the continuity equations for each marker that designate the free boundary at a given time moment. The markers of the free surface, except for the last one, move in accordance with the discrete analog of the kinematic condition (2). The motion of the contact point is implemented in accordance with the slip condition and the value of the dynamical edge angle is equal to \(\pi\).

The calculation method was tested on the problem of power-law fluid flow in a planar channel at a specified flow rate with consideration for dissipative heating and exponential temperature dependence of viscosity. The parabolic velocity profile and zero temperature were specified at the inlet of a channel, and the soft boundary conditions were specified at the outlet of a channel. On the rigid walls, the no-slip boundary conditions were realized and the temperature was set to zero. In this case, a length of the channel was selected that it was sufficient to set steady state flow in the cross section of the outlet.

The results of calculations were compared with the solution of a one-dimensional problem that described the nonisothermal fluid flow in the infinite channel at a specified flow rate. The mathematical statement of that problem included the following system of equations:

\[ \frac{d}{dx} \left( e^{-\alpha T} \frac{dv}{dx} \right) = -\alpha p, \quad \frac{d^2 T}{dx^2} + \text{Br} e^{-\alpha T} \frac{dv}{dx} \bigg|_{m+1} = 0, \] (3)
and the boundary conditions on the rigid wall were similar to the conditions of two-dimensional mathematical statement. Here, $\delta p$ is the pressure drop along the channel. The equation for the temperature calculation [7] is carried out from the differential equation system (3)

$$\frac{d^2T}{dx^2} + Br \exp(CT/m)(\delta p x)^{1+m} = 0.$$ 

The approximate solution of this equation with required accuracy is obtained using the sweep method. For calculation of the velocity the numerical integration of the first equation in system (3) is implemented. The comparison of the calculated data with a solution of the one-dimensional problem is shown in Fig. 2. Table 1 contains a quantitative confirmation of approximation convergence based on the values of the relative errors $e_1$ and $e_2$, which are defined using the formulas

$$e_1 = \frac{v_{\text{numerical}} - v_{\text{approximate}}}{v_{\text{approximate}}} \cdot 100\%,$$

$$e_2 = \frac{T_{\text{numerical}} - T_{\text{approximate}}}{T_{\text{approximate}}} \cdot 100\%,$$

where $v_{\text{numerical}}$, $T_{\text{numerical}}$ are the values on the centerline at the outlet boundary; $v_{\text{approximate}}$, $T_{\text{approximate}}$ are the results of a one-dimensional problem solution.

![Figure 2. Distributions of the velocity (a) and temperature (b) at the outlet boundary](image)

**Table 1.** Values of the relative errors $e(h)$, where $h$ is a step of the square computational mesh

| $h$   | $e_1(h)$ | $e_2(h)$ |
|-------|----------|----------|
| 1/10  | 0.102    | 0.186    |
| 1/20  | 0.083    | 0.046    |
| 1/40  | 0.075    | 0.027    |

4. Results and discussion

According to the flow behavior, the stream can be separated into a three-dimensional flow zone near the free surface and a one-dimensional flow zone far away from it. A parabolic longitudinal velocity profile typical for a steady state flow in the channel is realized in a one-dimensional flow zone. The deceleration of liquid particles that approach the flow front leads to the appearance of transverse velocity component, and the velocity vector turns towards the rigid wall. In course of time, the stable state distribution of the characteristics is developed in the fountain flow zone (Fig. 3).
The effect of the Br parameter and nonlinearity degree $m$ on the steady state temperature distribution near the free surface is shown in Fig. 4. It is evident that the temperature maximum is located in a fountain flow zone and its value increases with an increase of Br.

**Figure 3.** Distribution of the transverse velocity (a), longitudinal velocity (b), pressure (c), apparent viscosity (d) 
(Re=0.1, Pe=100, $m=0.9$: $C=1$, Br=1, W=5)

**Figure 4.** Temperature distribution as a function of Br parameter 
(Re=0.1, Pe=100, $m=0.9$, W=5: $C=1$, a – Br=1, b – Br=1.5, c – Br=2)

**Figure 5.** Temperature distribution as a function of nonlinearity degree 
(Re=0.1, Pe=100, Br=1, W=5: $C=1$, a – m=1, b – m=0.8)
5. Conclusions
The numerical simulation has shown a separation of the flow into a two-dimensional flow zone in the vicinity of the free surface and a one-dimensional flow zone away from it, where the temperature maximum is located in two-dimensional flow zone. The effect of a viscous dissipation and rheology on the temperature distribution was demonstrated. With an increase of Br from 1 to 2 the temperature maximum increases from 0.67 to 1.11, and with a decrease of nonlinearity degree from 1 to 0.8 the temperature maximum decreases from 0.72 to 0.61.

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