Mesoscopic Rhelogical Model for Polymeric Media Flows

K Koshelev, A Kuznetcov, D Merzlikina, G Pyshnograi, I Pyshnograi and M Y Tolstykh

[1]Department of Mathematical Analysis and Applyed Mathematics, Altai State Pedagogical University, Barnaul, Russia
[2]Institute for Water and Environmental Problems, Barnaul, Russia
 [3]Department of Mathematics, Altai State Technical University, Barnaul, Russia

E-mail: pyshnograi@mail.ru

Abstract. The paper compares hydrodynamic properties of three-dimensional flows of polymer melts. A modified Vinogradov and Pokrovskii rheological model is used for the mathematical description of nonlinear viscoelastic fluid flows in a plane-parallel channel with a sudden convergence. Discrete analogs for partial differential equations were obtained via the control volume method separating physical processes. The numerical implementation is carried out using the GPU-based parallel computing technology. Velocity and pressure fields have been calculated for two samples of polyethylene melts and the circulating flow at the entrance of the slit channel is noticeable. It is shown that the size of the vortex zone depends significantly on melt rheology.

1. Introduction

Mathematical study polymer fluids flows involves two interrelated phases. Firstly, it is selection and justification of the rheological model. Secondly, it is the algorithmic implementation of the obtained equations and the numerical experiment. Regarding the first step, there are plenty of rheological models of various complexity [1,2,5-12]). All these models describe the main effects observed in viscometric experiments: gradient dependence of shear and elongation viscosity, the first and second normal stress difference and non-monotonic establishment of time dependence of shear and elongation stresses.

   All viscometric flows have a fairly simple structure, since the velocity gradient tensor is known, and all the models show similar accuracy in the description of these flows. Therefore, the issue of adequacy of the rheological model is solved via calculation of two and three-dimensional flows in areas with complex geometry.

   In this paper, we apply a modified Vinogradov-Pokrovskii rheological model to solve the problem of mathematical modeling of three-dimensional nonlinear viscoelastic fluid flows in a plane-parallel channel with a sudden contraction. The method of control volume with the division of physical processes is used upon obtaining discrete analogs. The numerical implementation is carried out using GPU-based parallel computing technology CUDA.

2. The mathematical model

It is well-known that linear polymer melts are non-linear viscoelastic media. Nowadays the equations

that take into account essential features of polymeric liquids behavior are commonly used to describe their flows [5-9]. The priority in choosing a mathematical model should be given to models which to some extent take into account the structure of polymer molecules. It is quite complicated so the most popular models are those based on the mesoscopic approach. In this case, the behavior of polymer macromolecules is replaced by the behavior of one or more relaxation oscillators, and the transition to macroscopic description is carried out via methods of statistical mechanics [5,8,9,12,13]. One such model is a modified Vinogradov and Pokrovskii rheological model [9]

$$\sigma_{ik} = -\hat{p}\delta_{ik} + 3\frac{\eta_0}{\tau_0}a_{ik},$$

$$\frac{d}{dt}a_{ik} - \nu_{ij}a_{jk} - \nu_{kj}a_{ji} + \frac{1 + (\kappa - \beta)I}{\tau_0}a_{ik} = \frac{2}{3}\gamma_{ik} - \frac{3\beta}{\tau_0}a_{ij}a_{jk}.$$

(1)

Where a_{ik} – stress tensor of the polymer system; a_{ik} – dimensionless extra stress tensor; p – hydrostatic pressure; no – initial value of shear viscosity, t_0 – initial relaxation time; κ and – scalar coefficients of anisotropy taking into account shape and size of macromolecular coil; ν_{ik} – velocity gradient tensor; y_{ik} – symmetrized velocity gradient tensor; I – trace of tensor a_{ik}.

In paper [10] the two- and three-dimensional flows under the constant pressure gradient are considered in channels with a rectangular cross-section. The pressure field gradient has been known. In paper [15] an axisymmetric circular channel was used to model the input flows. However, an attempt to use the numerical method [15] for calculating flat channels failed. For calculating real flows on the basis of this model the following equations of momentum conservation and mass should be added to (1)

$$\rho\Big(\frac{\partial}{\partial t}v_i + v_k\frac{\partial}{\partial x_k}v_i\Big) = \frac{\partial}{\partial x_k}\sigma_{ik}, \qquad \frac{\partial}{\partial x_k}v_k = 0.$$

(2)

Here p - the density of the polymer; v_i - i-th component of the velocity vector.

The system of equations (1, 2) is closed with respect to variables a_{ik}, v_i, p. To solve the problem initial and boundary conditions are required. We first discuss the computational domain to establish these conditions.

The computational domain involves two 3D boxes. The first reservoir is channel 14 x 14(mm) with a square section, the second a slotted channel with a cross section of 14 x 1(mm). Lengths of the parallelepipeds are selected sufficiently large -80 < x < 80(mm) to eliminate the influence both of the input into the tank and output from the slotted channel. It is expected that within this area the flow will be three-dimensional, i.e. different directions in different axes. In this case, the main flow is directed along axis *Ox;* whereas along axis Oy a strong flow compression will occur. This can cause vortices though along axis *Oz* changes will be immaterial. Therefore, we call axis *Ox* - the flow direction, axis *Oy* - the direction perpendicular to the flow, and axis *Oz* - the direction neutral to the flow.

The main boundary conditions are stick conditions on a solid surface for velocity: $v_i = 0$.

The boundary conditions for the dimensionless stresses are obtained by substituting these conditions in (1) and discarding the corresponding terms.

The boundary conditions $z = 0$ and $y = 0$ are used for terms of symmetry or vanishing of the corresponding partial derivatives. At the entrance to the reservoir at x = -80 for the velocity components we use expressions $v_2(-80,y,z) = v_3(-80,y,z) = 0$ and $vi(-80,y,z) = 9V(z - 7)^2(y - 7)^2/5488$(mm/s), where V - volume flow rate.

Flows in a plane-parallel channel with a sudden contraction, are commonly referred to as converging flows or input flows. In order to calculate such flows via model (1, 2) it is necessary to determine the numerical values of the parameters for the rheological model: κ, P, no and To . To do this, we turn to the experimental data on the dependence of steady-state shear viscosity on the shear rate [18] where flows of two samples of polyethylene melts were applied - linear low density polyethylene (LLDPE) and low density polyethylene (LDPE). The model parameters were chosen to

give the best agreement between the experimental and theoretical curves. For LLDPE sample we obtained no = 14500(Pa · s), $T_0 = 0.2$(s), and for the LDPE $n_o = 18500$(Pa · s), $T_0 = 2$(s). Anisotropy parameters P = 0,1 and к = 0,12 were the same. Density values were given in [18] and account for 918(kg/m^3) for LDPE and 926(kg/m^3) for LLDPE.

The numerical method is constructed for relatively easy implementation when creating a computer model using technologies GPU NVIDIA and CUDA. The finite-difference approach is employed to find the solution. For the difference approximation the method of control volume was used that does not cause difficulties in a relatively simple geometry of the domain.

3. Mathematical modeling for exit flows

To compare the results of calculations we used the experimental data [18] where flows of two samples of polyethylene melts were applied LLDPE and LDPE. The differences between these two examples is that LLDPE shear viscosity changes less than for LDPE, and LLDPE relaxation time is shorter than that of LDPE. We found out that there is an explicit secondary flow for LDPE flows in the corners of the flow channel, which is not observed for LLDPE. These vortices change their shape in the channel cross-sections parallel to the axis, which characterizes the three-dimensional nature of the flow field. Furthermore, it is noted that within the investigated vortex flow there is a helical stream, which is directed to the tank wall. Particular attention is paid to the distribution of velocity along the symmetry axis of the channel. It was found that LDPE maximum velocity is observed directly in the entrance portion of the channel slot. This effect does not appear for LLDPE under the same conditions.

All these effects are found during the numerical experiment. The calculations imply that the increase in speed in the slit of the channel happens due to the three-dimensional nature of the flow field and the stress caused by the increase in the flow of LDPE compared with a sample of LLDPE. The three-dimensional nature of LDPE flow is confirmed by the presence of the neutral component of velocity in the flow direction, which was not observed for LLDPE flow. This additional component of velocity results in increasing the volumetric flow along the centerline at the entrance to the slit channel.

Thus, the velocity, pressure and stress fields were calculated in a steady flow. Herewith circulating areas were found at the entrance of the slit channel. As seen from Figure 1 for LLDPE sample ($T_0 = 0,2$(s)), the reverse flow zone is negligible. For LDPE sample ($T_0 = 2$(s)) this zone, as seen from Figure 2 is much larger. Note that the value of viscous parameter n_o in these samples is approximately the same and the difference in their behavior should be attributed to time parameter T_0.
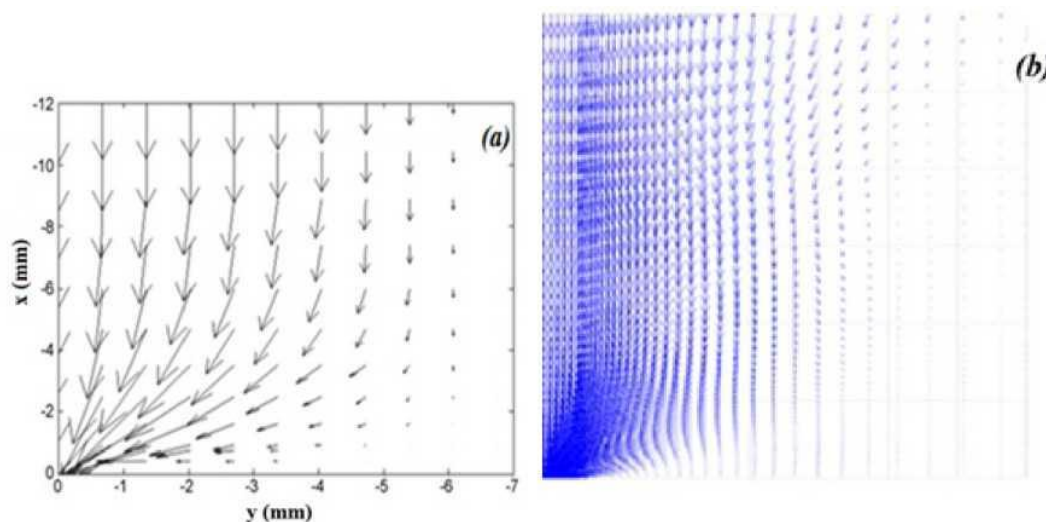

Figure 1. Comparison of experimental (a) and theoretical (b) LLDPE velocity vector fields in a slit entrance channel (V = 0, 20 [cm^3/s])

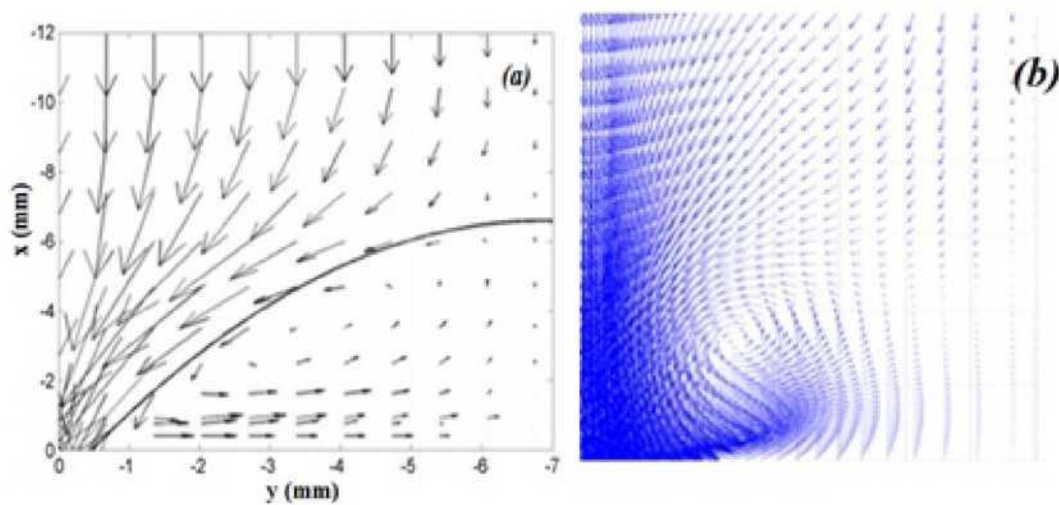**Figure 2.** Comparison of experimental (a) and theoretical (b) LDPE velocity vector fields in a slit entrance channel (V = 0,20 [cm^3/s])

We note that the values of the Reynolds number calculated using the formula (Re = pv_oh/n_o) for the considered currents in the slot channel do not exceed 0, 02. Such flows are fairly well understood in the classical Newtonian model, and eddy zones in this case are not observed.

Thus, converging flows for some polymer melts may exhibit a substantial three-dimensional picture that is shown by the presence of velocity components in the direction neutral to the flow. This should be taken into account in the design of the experiment, as there are methods that are not able to measure all the components of velocity.

Also one should mention the fact of long-term relaxation of the velocity profile in the gap. Calculations showed that the steady velocity profile is observed at a considerable distance from the entrance slit. This should be considered when conducting measurements in a narrow channel portion.

Previously, it was noted the presence of eddy currents in the corners of the flow channel, the size of which depends strongly on the temperature of the melt and on specific consumption.
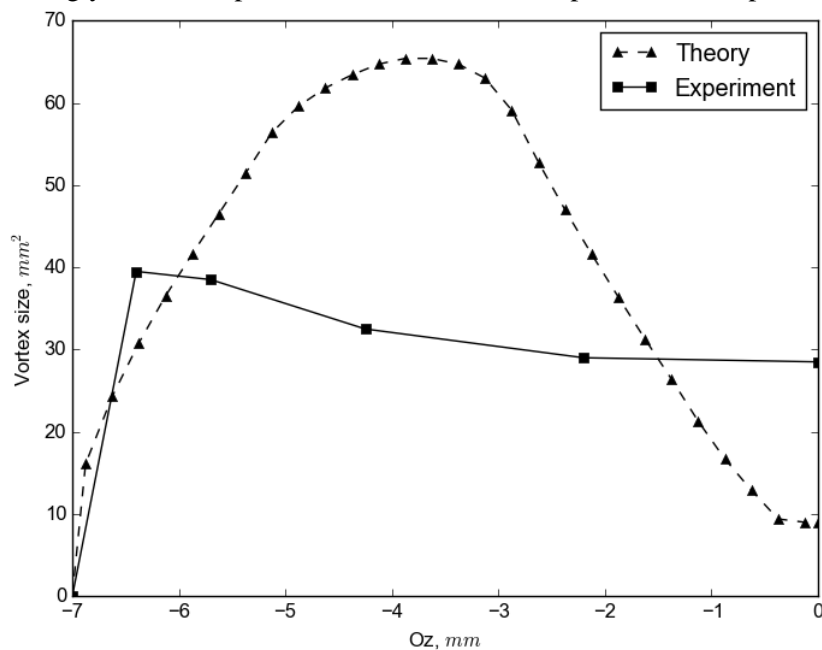

Figure 3. The size of the vortex in different sections

One of the essential characteristics of the test flow is the size of the vortex. We calculated the area of the vortex zones when flow section planes z = *const*. Comparing shown in Figure 3 the calculated and experimental vortex sizes depending on the distance from the axis of the channel may be concluded that an increase in the intensity of the vortex flows away from the axis of the channel. This fact can be explained by Weissenberg effect. From this comparison it can be concluded qualitative agreement of the experimental and the payment data. Note that in the calculations carried out for the Newtonian law of behavior (тO = 0; $P_0 = p_0 = 0$) demonstrate the absence of vortex zones, and calculations for viscoelastic Oldroyd-B ($P_O = p_0 = 0$) show low values of the vortex area and the lack of increase in the intensity of the vortex when you remove the cross section on the axis of the channel.

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