Modeling three-dimensional flow of the polymer melts in a converging channel

A Kuznetsov\(^1\), K Koshelev\(^2\), N Cherpakova\(^3\) and G Pyshnograi\(^1\)

\(^1\) Altai State University, avenue Lenin, 61, 656049, Barnaul, Russia
\(^2\) Institute for Water and Environmental Problems SB RAS, Molodejnaya, 2, 656049, Barnaul, Russia
\(^3\) Altai State Technical University, avenue Lenin, 46, 656049, Barnaul, Russia

E-mail: pyshnograi@mail.ru

Abstract. Temperature and volume rate impact of the polymer melt on the sizes of the vortex area has been considered. The vortex area appears during the flow at the inlet of the slotted channel. A modified Vinogradov and Pokrovskii rheological model is used for the mathematical modeling of three-dimensional flow of the melt in the convergent plane-parallel channel. This model was extended to take account of the nature of non-monotonic gradient dependence of elongation viscosity. On the solid wall the sticking conditions were used for velocity. The temperature dependence of the initial shear viscosity of the polymer melt has Arrhenius form. The initial relaxation time was rated by comparison with experimental data for a gradient based stationary viscosity in uniaxial tension, and on the basis of the molecular-kinetic approach. Discrete analogues of a system of equations of the dynamics for the polymer liquid were obtained via the method of controlling the volume with the division due to physical processes. The numerical algorithm was implemented so that the technology of parallel computing based on GPU was conveniently used. Calculations of hydrodynamic characteristics of polymer melt flows at different temperatures in a convergent channel with a rectangular cross section have shown that the sudden narrowing of the channel leads to the appearance of eddy flows. The sizes of these flows pass through a maximum with increasing melt temperature which is detected in the experiments. It also confirms that the rheological model can be used for the flows of polymer melts in areas with complex geometry. The results are proving the effectiveness of CUDA technology parallel computing for unsteady calculations of three-dimensional flows of nonlinear viscoelastic fluids with rheological law of behavior in differential form. The above calculations show that some convergent flow of polymer melts may show substantial three-dimensional picture, which manifests itself in a velocity component in a neutral flow direction. This should be taken into account when arranging experiments, as there are methods that cannot measure all velocity components. Also note that the velocity profile in the slit of the channel is set at a considerable distance from the entrance to the channel.

1. Introduction

The paper considers properties of hydrodynamic structure for 3D flows of thermoplastic melts in a plane-parallel channel with sudden convergence. Thermoplastics can be heated to melts. They solidify upon cooling in the shape of the acquired object without changing its structure. Therefore, they can undergo melting several times. Such polymers are: polyethylene, polypropylene, polystyrene, polyvinylchloride etc. The mathematical study of two and three-dimensional flows of nonlinear viscoelastic medium is of great importance in polymer melts and solutions rheology. It is known that such flows may be observed in different types of polymer processing (e.g., extrusion, casting, blowing, injection molding and others). Mathematical modeling of such flows requires refinements of
a rheological model. The accuracy of rheological models was tested by calculating two and three-dimensional flows especially in domains with complex setting.

In this paper the Vinogradov and Pokrovskii rheological model is employed to solve the problem of mathematical description for three-dimensional nonlinear viscoelastic fluid flows in a plane-equivalent channel with a sudden constriction. The control volume method including the division due to physical operations is used to obtain discrete analogs of initial particular differential equations. The numerical application is carried out via the GPU-setup equivalent calculating technology CUDA.

2. The mathematical model
It is well-defined that melts of polymers are non-linear viscoelastic media. A perfect foundation of the relaxation processes theory for polymer melts can be presented by the microscopic approach. The approach originates from researching the motion of the entangled macromolecules system. All the consequences of this approach cannot be easily calculated due to the complicated mathematics and many extra assumptions must be introduced in the calculation. The microscopic method gives justification to the phenomenological results.

To use the mesoscopic (intermediate) approach successfully in relation to polymer melts and solutions single macromolecule approximation is employed. It means that the single macromolecule is moving surrounded by other macromolecules and the solvent. It is considered to be an efficient field. Some phenomenological parameters should be introduced into the mesoscopic theory in order to characterize this effective field [1].

\[
\sigma_{ik} = -p\delta_{ik} + 2\eta_1 y_{ik} + 3\frac{\eta_0}{\tau_0} a_{ik}, \quad (1)
\]

\[
\frac{d}{dt} a_{ik} = v_i a_{jk} - v_j a_{ik} + \frac{1 + (\kappa - \beta) I}{\tau_0} a_{ik} = \frac{2}{3} y_{ik} - \frac{3\beta}{\tau_0} a_{ij} a_{jk}, \quad (2)
\]

Where \(\sigma_{ik}\) – tensor of stress for the polymer system; \(a_{ik}\) – dimensionless tensor of extra stress; \(p\) – hydrostatic pressure; \(\eta_0\) – shear viscosity initial value, \(\tau_0\) – time of initial relaxation; \(\beta\) and \(\kappa\) – coefficients of scalar anisotropy which consider shape and size of macromolecular coil; \(\eta_1\) viscosity of residual shear; \(v_{ik}\) – tensor of velocity gradient; \(y_{ik}\) – gradient tensor of symmetrized velocity; \(I\) – trace of tensor \(a_{ik}\).

It can be expected that this model tested on simple flows will be suitable for the numerical study of polymer behavior in difficult conditions of deformation, which are typical for polymer processing. These are steady and unsteady flows in circular ducts, flows in channels with a sharply varying cross-sectional area and flows with a free surface. An essential feature of such flows is their two- and three-dimensional character. Earlier attempts of modeling such flows on the basis of the model have been made [1-3].

Work [3] considers the two- and three-dimensional flows under the constant pressure gradient in channels with a rectangular cross-section. For calculating real flows on the basis of this model the equations of momentum and mass conservation should be added to the rheological model.

3. Results and Discussion
Temperature is one of the most important parameters affecting the quality of products made of polymers. The influence of polymer melts temperature on the size of the vortex area, appearing in the flow at the slit channel entrance was studied.

Model parameters (\(\beta = 0.1\) and \(p_0 = 0.005\)) were obtained by investigating similarity between numerical data and theoretical dependences for shear and elongation viscosity. The comparative results for these curves are shown in Figure 1. Recalculation of values \(\eta_0\) and \(\tau_0\) for pure shear is made by the following equations:

\[
\eta_0(T) = \eta_0(T_0) \cdot 10^{\frac{E_a}{R} \frac{1}{T_0} \left(\frac{1}{T} - \frac{1}{T_0}\right)}, \quad \tau_0(T) = \frac{\eta_0(T) \cdot M}{\rho R T}, \quad (3)
\]

Here \(R\) – the ideal gas constant, \(E_a = 58\) KJ/mol – activation energy, \(T_0 = 150^\circ C\).
Values of $\tau_0$ have been chosen so that the initial section of elongation viscosity growing has been described properly, while values of $p_0$ have been selected for the decreasing region of elongation viscosity.

Let us notice that the influence of $p_0$ parameter on the view of stationary and non-stationary viscometric functions was studied in [2]. They have shown that this parameter slightly affects the stationary shear viscosity function. It has been added for the description of non-monotonic type of the stationary viscosity function under axial tension.

The value of density was given in [4] and it is 918 kg/m$^3$ for the low density polyethylene. Note, that this parameter has an insignificant effect on the final solution, since the Reynolds number for the described flows is rather small (about $10^5$). As for residual viscosity $\eta_1$, its values were obtained according to $\eta_1 = 0.005 \cdot \eta_0$ and its influence is not visible in Figure 1. This parameter was added to the model for preventing a rheological model from transition into a perfect fluid model under large velocity gradients. It can be observed when velocity field and stress field undergo significant transformations. For residual viscosity detection in polymer melts at viscometric experiments, a range of shear velocities needs to be extended significantly at the same time as this parameter for concentrated solutions can be obtained easily and is not only a viscosity solvent. It also depends on polymer concentration. The effect on final results of $\eta_1$ is negligible but it provides a much bigger time step at the first computation period when the available approximation needs significant realignment.

We refer to paper [4] for comparison between experimental data and computation results. Firstly, it should be noted that stationary values could have been attained neither at calculations nor at experiments because calculated velocity, stress and pressure profiles fluctuate near stationary values. The magnitude of these fluctuations which does not exceed 10 percent for velocity vector components allows making comparison with an experiment. This comparison is shown in Figure 1 ($T=180$ °C). The vortex area before the slit channel entrance has been detected both in the experiment and in the calculation. Because of the irregular mesh type in the numerical research, the small scale is applied for velocity vector display at the right image. In reality velocity vector modules are close, which is granted by a good match between volume rates.

Figure 1. Comparing theoretical and experimental dependences on elongation speed of stationary shear viscosity and stationary tension viscosity at different temperatures.
So the size or the vortex area is an essential characteristic of the studied flows. Paper [4] offers to calculate the vortex area via the following technique.

Firstly values of $f(x)$ are obtained, for which $\int_{-7}^{f(x)} u(y) dy = 0$, and then the area under $f(x)$ curve. Let’s notice that good results can be obtained by this approach only if the velocity vector component at the direction neutral to the flow is much lower than at two other directions.

Now let us calculate vortex area areas in $z = \text{const}$ section plane. Comparing experimental and calculated dependences of the vortex size on the distance to the channel axis as shown in Figure 2, it can be concluded that the intensity of vortex flows increases while removing from the channel axis. This fact may be explained by the Weissenberg effect. From the above comparison it may be stated that the experimental results and the numerical data agree qualitatively. It is noted that the calculations given for Newton’s law of behavior ($\tau_0 = 0; \beta_0 = P_0 = 0$) show the absence of vortex areas where as the calculations for Oldroyd-B viscoelastic fluid ($\beta_0 = P_0 = 0$) demonstrate understated values for vortex area and absence of the increase in vortex intensity while the section plane removes from the axis of the channel [3].

![Figure 2. Vortex size at different section planes at T=180°C.](image)

Let us consider the influence of the polymer melt temperature on the vortex area size. The computed values of the vortex area in the axial section plane at different temperatures are shown in Figure 3. Since the temperature affects both initial shear viscosity $\eta_0$ and initial relaxation time $\tau_0$, it leads to the reduction of these parameters during the temperature increase. Thus, the temperature influence is quite complicated. Initially the vortex size grows alongside with the temperature increase but then, after going through the maximum it starts to decrease. Such a non-monotonic view of dependence is also observed at experiments, the results shown in Figure 3 too.
The analysis of the results shown in Figures 2 and 3 reveals the discrepancy between theoretical and experimental dependences (which can differ by a factor of two). Can this be considered acceptable? Or does such accuracy suggest the inadequacy of rheological model (1)?

Let us notice that in modeling viscometric functions calculated on the basis of model (1) as showed in [1, 2]. These discrepancies can reach 5-10 times for simple shear stress and when axial elongation stress is plateaued. This can also be seen in Figure 1 for stationary shear viscosity at the shear rate of 0.7 s$^{-1}$. This disadvantage of the model is easily overcome by the transition to the multi-mode approximation [5]. Herewith several relaxation processes are introduced for consideration, their time scales can differ by 4 orders. If it is not difficult in the viscometric flows modeling due to their simplicity, in the three-dimensional flows modeling this fact can not only lead to significant increase in calculation time but also makes the calculations impossible because of the increased "hardness" of the solved system. Also it should be noted that the paper [3] the vortex area size has fallen to zero when the initial relaxation time changes from 2 s to 0.2 s. In other words, errors in the definition of the relaxation time can change the flow pattern essentially. Thus the computation accuracy, obtained in Figures 2 and 3 can be considered acceptable. Anyway this issue needs comprehensive study both in terms of the convergence for numerical schemes and adequate description for the studied processes.

Therefore, model (1) describes experiments mentioned here in qualitatively, and the differences between experimental and theoretical curves can be attributed to both inaccuracy in defining $\tau_0$ parameter, the single-mode nature of model (1) and the oscillatory character of the solutions obtained. Perhaps this is a consequence of instability inherent in the examined flows. Velocity vector oscillations are possible both in the absolute value and in the direction that allows to average the observed values over the period of oscillation. Despite this, it should be noted that the studied flow is not turbulent, in other words, the observed oscillations are regular and not chaotic. Anyway, these issues need further thorough research to be carried out in the following works.

4. Conclusion.
Thus, the paper has compared the polymer melt flows with different rheological characteristics in a convergent channel with a rectangular cross section. It has shown that an increase in the relaxation time of the polymer sample gives rise to the eddy flow which is detected in the experiments.
Therefore, it confirms the applicability of a modified rheological Vinogradov and Pokrovskii model for describing the dynamics of polymer melts in areas with complex geometry. Also, the results obtained in this paper prove the effective application of parallel computing CUDA technology at unsteady calculations for three-dimensional flows of nonlinear viscoelastic media with rheological law of behavior in a differential form.

However, this paper does not discuss many issues related to flows in converging channels. For example, it doesn’t state that the channel geometry, the molecular structure of the polymer or the temperature can affect the flow pattern. These and other issues can be explored in subsequent papers on the basis of the developed mathematical models and numerical methods tested here.

5. References
[1] Altukhov Yu A, Golovicheva I E, Pyshnograi G V 2000 Fluid Dynamics 35 1
[2] Altukhov Yu A, Pokrovskii V N, Pyshnograi G V 2004 J. Non-Newtonian Fluid Mech. 121 73
[3] Koshelev K B, Pyshnograi G V, Tolstykh M Yu 2015 Fluid Dynamics 50 16
[4] Hertel D, Valette ., Münstedt H 2008 J. Non-Newtonian Fluid Mech. 153 82
[5] Merzlikina D A, Pyshnograi G V, Pivokonskii R, Filip P 2016 Journal of Engineering Physics and Thermophysics 89 652