Simulation of Giesekus fluid flow in extruder using helical coordinate system

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Abstract. In the present work, it is proposed to use a helical coordinate system for mathematical modeling of non-isothermal Giesekus fluid flow in the extruder in the metric zone. The convenience of using a helical coordinate system is to reduce the three-dimensional problem to two-dimensional without the use of additional assumptions. The helical coordinate system is applicable only for steady flow conditions. Particular results of the numerical implementation of the use of a helical coordinate system are presented on the example of a Giesekus fluid flow in an extruder with a single flight, the results are compared with the flow of Newtonian fluid.

1. Introduction
The screw is a key element of the extruder and its most important part, therefore its design is crucial for the successful operation of any extrusion system [1]. The optimal design of the screw will provide a homogeneous melt with desired characteristics [2]. A detailed study of the hydrodynamics of the polymer flow in the extruder channel is the basis for modeling and understanding the extrusion process as a whole [3]. Experimental studies of liquid polymers showed a nonlinear viscoelastic nature of their behavior; therefore, almost at the same time, analytical solutions to the same problem for non-Newtonian fluids appeared. Analytical solutions of the Couette–Poiseuille flow of a viscoelastic fluid for the helical flow are known, as well as for Poiseuille flow (simpler solution for helical flow) [4]. In a number of works, for the rheological description of polymer flows, models were also used that take into account their viscoelastic properties, for example, FENE-P [5], Pom-Pom [6], Giesekus [7], PTT [8], the Leonov model [9], etc. In [10], it was proved that the PTT and Giesekus models can capture the complex nature of the polymer relaxation time at high Weissenberg numbers. Despite the complexity of the problem being solved, the use of numerical methods is important for analyzing the flow of polymers in the channels of extrusion equipment. For example, based on numerical results [11] the influence of the screw characteristics (length, diameter, pitch, normal pitch, clearance, twist angle and number of turns of the screw) and physical properties of the material (density, viscosity) on the main process were analyzed. In the general case, the velocity field of a moving fluid in a channel with a screw insert depends on three independent variables. Typically, mathematical models are used to calculate hydrodynamic fields, in which the basic system of equations is written in a Cartesian coordinate system, sometimes in a cylindrical one, whose axis coincides with the axis of symmetry of the channel. This approach is not based on helical symmetry, which is possessed by both a system of equations together with uniqueness conditions and a geometric region — a helical channel, and requires a large amount of computer memory and time for calculations in a three-dimensional setting. Using a helical coordinate system...
allows you to get the distribution of hydrodynamic fields, depending not on three, but on two variables. This significantly reduces both the memory costs and the time needed to obtain results. In this work, we used a helical coordinate system to study the processes of the Giesekus fluid flow in a channel with a non-rotating extruder.

2. Problem statement

2.1 Helical coordinate system

In this paper, we consider the flow of an incompressible viscoelastic fluid in a channel of a single-screw extruder (non-rotating) in the metric zone (fig. 1). It is assumed that the fluid motion is stationary, laminar, with a formed velocity profile at the inlet to the pipe. The temperature of the liquid does not change during its movement.

![Fig. 1 Transverse (a) and longitudinal (b) channel cross-sections: L is the lead of helical channel (length of a part of the channel which corresponds to the angular rotation of screw flight by 360°), r2 is the barrel radius; r1 is the shaft radius; h – screw thickness](image)

It is proposed to use the following helical coordinate system $$\xi^1, \xi^2, \xi^3$$

$$\begin{align*}
x &= \xi^1 \cos (\pm \alpha \xi^3) - \xi^2 \sin (\pm \alpha \xi^3) \\
y &= \xi^1 \sin (\pm \alpha \xi^3) + \xi^2 \cos (\pm \alpha \xi^3), \\
z &= \xi^3
\end{align*}$$

(1)

where \(x, y, z\) - Cartesian coordinate system, \(\omega = (2\pi)/S\), \(R\) - shaft radius, \(L\) - is the lead of helical channel. In eq. (1), the “+” sign is selected in the case when the fluid flow swirling clockwise, and the “-” sign is selected in the case of the flow swirling counterclockwise.

Note that the coordinate system (1) has no singular points, is non-orthogonal, and compared with the coordinate system presented in previous work [12] has a larger number of nonzero components of the metric tensor. It is advisable to use it in the case where the use of the system presented in the work [12] complicated by the presence of a singular point near the flow region, which leads to difficulties in numerical calculations.

2.2. Giesekus model

To describe the rheological behaviour of viscoelastic fluid it is used the Giesekus model [13]

$$\begin{align*}
\sigma = \sigma_v + \alpha_N \sigma_N + \alpha_G \sigma_G
\end{align*}$$

$$\begin{align*}
\sigma_v + \lambda \sigma_v + \frac{\alpha_G}{\mu_v} \sigma_N \cdot \sigma_v = 2\mu_v D_v
\end{align*}$$

(2)

where \(\sigma = \frac{d\sigma}{dt} - \sigma \cdot \nabla V^T - \nabla V \cdot \sigma = \frac{\partial \sigma}{\partial t} + \nabla \sigma \cdot V - \sigma \cdot \nabla V^T - \nabla V \cdot \sigma\) - upper convective derivative of the tensor; \(\sigma\) - stress tensor deviator; \(\alpha_N, \alpha_G\) - viscous and elastic components of the tensor \(\sigma\); \(D_v\) - strain rate tensor; \(\mu_v\) - viscosity; \(\lambda\) - relaxation time; \(\alpha_G\) - rheological parameter; \(V\) - velocity vector.
2.3. Governing equation

Based on assumption, the system of equations for the transfer of momentum and continuity in the coordinate system (1) can be written as follows

\[
\text{Re}^* \left( \left( \frac{\partial v^i}{\partial \eta^j} \begin{pmatrix} \mu \eta^j & \eta^j \\ 0 & \eta^j \end{pmatrix} \frac{\partial v^j}{\partial \eta^j} \right) v^i + \left( \frac{\partial v^i}{\partial \eta^j} \begin{pmatrix} \mu \eta^j & \eta^j \\ 0 & \eta^j \end{pmatrix} \frac{\partial v^j}{\partial \eta^j} \right) v^j - \kappa^2 \eta^j \left( v^j \right)^2 \right) = - \frac{\partial p^*}{\partial \eta^j} + \frac{\delta s_{1j}^1}{\partial \eta^j} + \frac{\delta s_{3j}^2}{\partial \eta^j} \mu \kappa \eta_s^3,
\]

(3)

\[
\text{Re}^* \left( \left( \frac{\partial v^2}{\partial \eta^j} \begin{pmatrix} \mu \eta^j & \eta^j \\ 0 & \eta^j \end{pmatrix} \frac{\partial v^3}{\partial \eta^j} \right) v^j \pm 2 \kappa^2 \eta^j \left( v^j \right)^2 \right) = - \frac{\partial p^*}{\partial \eta^j} + \frac{\delta s_{1j}^1}{\partial \eta^j} + \frac{\delta s_{3j}^2}{\partial \eta^j} \pm \kappa \eta_s^3,
\]

(4)

\[
\text{Re}^* \left( \left( \frac{\partial v^1}{\partial \eta^j} \begin{pmatrix} \mu \eta^j & \eta^j \\ 0 & \eta^j \end{pmatrix} \frac{\partial v^2}{\partial \eta^j} \right) v^j + \left( 1 + \kappa^2 \left( \left( \eta^j \right)^2 + \left( \eta^j \right)^2 \right) \right) \frac{\partial v^3}{\partial \eta^j} \right) v^j + \frac{\partial v^2}{\partial \eta^j} = \frac{\partial p^*}{\partial \eta^j} + \frac{\delta s_{1j}^1}{\partial \eta^j} + \frac{\delta s_{3j}^2}{\partial \eta^j} \mu \kappa \eta_s^1 + \kappa^2 \eta_s^1 \eta_s^3 + \kappa^2 \eta_s^3 \eta_s^2 + \kappa^2 \eta_s^3 s_s^1.
\]

(5)

\[
\frac{\partial v^i}{\partial \eta^j} + \frac{\partial v^j}{\partial \eta^i} = 0,
\]

(6)

here \( \kappa = \omega R \), \( \frac{\partial p^*}{\partial \eta^j} = \text{const} \), \( \eta^j = \zeta / R (i = 1, 2, 3) \) - dimensionless variables; \( u^i = V^i / V^* (i = 1, 2, 3) \) dimensionless contravariant velocity components; \( p^* = \rho R / \left( \mu_n + \mu_v \right) \) - dimensionless pressure; \( \text{Re}_H^* = V^* R / \left( \mu_n + \mu_v \right) \) - modified Reynolds number; \( V^* \) - specified velocity.

Mixed dimensionless components of the stress tensor deviator \( s = \frac{R}{\left( \mu_n + \mu_v \right) V^*} \sigma \) in the coordinate system (1) have the form

\[
s_i^j = 2(1 - \beta) d_i^j + \beta s_v^j,
\]

(7)

here \( \beta = \frac{\mu_v}{\mu_n + \mu_v} \); \( d_i^j \) - mixed components of the dimensionless strain rate tensor,

\[
d = \frac{R}{\left( \mu_n + \mu_v \right) V^*} \Delta; \ s_v^j \) mixed components of dimensionless elastic part, \( s_v = \frac{R}{\left( \mu_n + \mu_v \right) V^*} \sigma_v \) stress tensor deviator.

3. Results and discussion

The numerical implementation of the problem was carried out in the «Comsol Multiphysics». The package allows you to rewrite the governing equations in the helical coordinate system (1). The numerical results were made for the case \( \text{Re}_H \to 0 \) and \( \text{Re}_H = 150 \), \( \text{We}_H = 0.04 \), \( \alpha = 0.7 \), \( \beta = 0.3 \), \( \delta = 0.66 \left( \frac{\delta}{r_i / r_i} \right) \), \( L = 3D \) (\( \text{We}^* = 2V^* / R \) - Weissenberg number). The Reynolds and Weissenberg numbers are calculated using the equivalent diameter, calculated from the channel cross-section.
Fig. 2 shows the distribution of the contours of the dimensionless axial velocity for two Reynolds numbers \( \text{Re}_H \to 0 \) and \( \text{Re}_H = 150 \). For comparison, the same figure shows the distribution of the same component for the case of a Newtonian fluid flow at \( \text{Re}_H = 150 \) and \( \text{We}_H = 0 \). As can be seen from the figure, with increasing the Reynolds number, the maximum value of the dimensionless axial velocity shifts toward the screw wall under the action of centrifugal forces. The distributions of the axial velocity for the Giesekus fluid and the Newtonian fluid has qualitative coincidence, but for the same Reynolds number it can be seen that the contours for the Giesekus fluid flow are more elongated in the tangential direction and narrow in radial direction.

Fig. 3 and 4 shows contours of the dimensionless component of the elastic part of the stress tensor \( s_{13} \) and \( s_{23} \). At small Reynolds numbers these distributions are symmetric, then with increasing Reynolds numbers it becomes asymmetric under the influence of a similar change in the velocity field. The maximum values of these components, as expected, are located near the walls. Especially strongly with increasing Reynolds number, the modulus of the component in the region of the screw flight on the side of the incoming flow increases.

Fig. 3. The contours of the dimensionless component of the elastic part of the stress tensor \( (s_{13}) \). Designations are similar fig. 2.
Fig. 4. The contours of the dimensionless component of the elastic part of the stress tensor (s²). Designations are similar fig. 2.

Reference

[1] Kim VS 2005 Theory and practice of polymer extrusion (Moscow: Chemistry, KolosS)
[2] Roland W, Kommenda M, Marschik C and Miethlinger J 2019 Polymers 11 (2) 334
[3] Wilczynski K, Buziak K, Wilczynski KJ, Lewandowski A and Nastaj A 2018 Polymers 10 (3) 295
[4] Cruz DOA and Pinho FT 1983 J. Non-Neut. Fluid Mech. 13 109-143.
[5] Barrett J and Boyaval S 2017 Finite Element Approximation of the FENE-P Model hal-01501197
[6] Hawke LDG, Huang Q, Hassager O and Read DJ 2015 Journal of Rheology 59 995-1017
[7] Mokarizadeh H, Asgharian M and Raisi A 2013 J. Non-Neut. Fluid Mech. 196 95–101
[8] Cruz DOA and Pinho FT 2012 J. Non-Neut. Fluid Mech. 167 95-105
[9] Leonov AI 1976 Rheol. Acta 15 85–98
[10] Holmes LT 2010 Modeling 3D viscoelastic secondary flows in extrusion (Madison: The University of Wisconsin)
[11] Siregar AN, Mahmod WMFW, Ghani JA, Haron CHC, and Rizal M 2014 Res. J. Appl. Sci. Eng. Tech. 7 (10) 2098-2105
[12] Vachagina EK and Kadyirov AI 2014 Q. J. Mech. Appl. Math. 67 (4) 553–566
[13] Giesekus H 1982 J. Non-Neut. Fluid Mech. 11 69–109

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