Numerical studies of the polymer melt flow in the extruder screw channel and the forming tool

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Abstract. To date, polymer compositions based on polyethylene or PVC is widely used as insulating materials. These materials processing conjugate with a number of problems during selection of the rational extrusion regimes. To minimize the time and cost when determining the technological regime uses mathematical modeling techniques. The paper discusses heat and mass transfer processes in the extruder screw channel, output adapter and the cable head. During the study were determined coefficients for three rheological models based on obtained viscosity vs. shear rate experimental data. Also a comparative analysis of this viscosimetric laws application possibility for studying polymer melt flow during its processing on the extrusion equipment was held. As a result of numerical study the temperature, viscosity and shear rate fields in the extruder screw channel and forming tool were obtained.

1. Introduction
Investigation of the polymer flow in the extruder screw channel is essential, during the insulating polymer processing, because the limit of melt maximum temperature is one of the main requirements. In the plasticizing extruder metering zone, where the material is molten, take place pressure buildup, intense mixing, and homogenization of the melt, which can lead to the local material overheating. However, problems arise not only in that part of the extrusion equipment. When exiting the extruder screw channel, material enters the forming device, which also has a significant influence on the polymer processing. A sharp change in channel geometry makes a significant contribution to the character of the melt flow, causing local overheating. Therefore, determination the ways of polymer materials dissipation energy and the melt overheating volume and level reduction is one of the main problems pursued by the researchers. The aim of this work was to study flow and heat transfer processes in the extruder screw channel and forming device during production of plastic insulation and comparison of different rheological laws and geometric models.

Currently, there are a number of mathematical models describing the flow and heat transfer in extruders screw channels [1-5]. All known approaches, based on the laws of conservation, use the principle of inverse movement and turns the screw channel on a plane, that is an assumption.

A schematic illustration of the extruder is represented in figure 1. It consists of the screw, body, heating elements and a forming device. The extruder is divided into four zones: the feeding zone, a delay melting zone, a melting and metering zone. In this paper, a study was conducted with the last 5 turns of the extruder, output adapter and forming tool, because this is where the greatest overheating takes place.
2. Mathematical statement and initial data

In the construction of spatial mathematical models of flow in the extruder metering zone following assumptions were made: the process is stationary and steady at constant mass flow, the polymer melt is considered to be a purely viscous, incompressible liquid, mass forces are equal to zero.[6] In view of these assumptions, the system of differential equations has the form:

\[ \frac{\partial V_i}{\partial x_i} = 0; \]  

\[ \rho_n V_i \frac{\partial V_i}{\partial x_i} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i}; \]  

\[ \rho_n C_v V_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \lambda_m \frac{\partial T}{\partial x_i} \right) + \tau_{ij} \frac{\partial V_i}{\partial x_j}, \]  

where \( \rho_n \), \( C_v \), \( \lambda_m \) – respectively, density, heat capacity and thermal conductivity of the polymer melt; \( V_i = v_x, v_y, v_z \) — velocity component of the polymer melt movement; \( x_i = x, y, z \) – rectangular coordinates; \( \tau_{ij} \) – stress tensor deviator components; \( P \) – pressure; \( T \) – temperature.[6].

The connection between the deviator stress tensor and the strain rate tensor is given by:

\[ \tau_{ij} = \mu_3 \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \]  

where \( \mu_3 \) – effective viscosity of the polymer melt[1].

Viscosity dependence on temperature was determined by the Reynolds equation:

\[ \mu_0 = \mu_{00} \exp \left( -\beta (T - T_0) \right) \]  

The paper considered with the different rheological laws describing the dependence of the effective viscosity versus shear rate:

power law [7]

\[ \mu_3 = \mu_0 \dot{\gamma}^{\frac{n-1}{n}} \]  

Carreau model [8]

\[ \mu_3 = \left[ 1 + \dot{\gamma}^2 \dot{\gamma}^m \right]^{\frac{n-1}{2}} (\mu_0 - \mu_e) + \mu_e \]  

Cross model [7]

\[ \mu_3 = \mu_e + \frac{\mu_0 - \mu_e}{1 + \dot{\gamma}^m} \]  

where \( \dot{\gamma} \) – shear rate; \( \mu_0 \) – viscosity at zero shear rate; \( \mu_e \) – viscosity at infinite shear rate; \( n \) –
To study the processes in the extruder channel, models presented in Figure 2 were built.

![Figure 2](image_url)

**Figure 2.** Geometric models of the extruder channel: a – Flat model; b – Cylindrical model without a gap; c – Cylindrical model with a gap.

The geometry of the channel is presented in Table 1. The body temperature was set at 200 °C, the temperature of the screw is 210°C, the temperature of the input material is 225˚C. Calculations were carried out for the screw rotation speed of 60 revolutions / min.

| Parameter                               | Value |
|-----------------------------------------|-------|
| Inner diameter of a barrel, mm         | 160.0 |
| Outer diameter of a screw, mm           | 159.4 |
| Twist, mm                              | 160.0 |
| Channel width, mm                       | 137.3 |
| Flight Wight, mm                        | 15.3  |
| Length of the dosing geometric zone, turn | 5     |
| Channel depth in the metering zone, mm  | 4     |
| Helix angle, ′                          | 17°39′|
| Radial clearance between the flight and the barrel, mm | 0.3   |

Study of the polymer melt rheological characteristics was carried out using a rotary rheometer Discovery HR-2 «TA Instruments». During the experiment, the analyzed polymer was subjected oscillating deformations in the «plate – plate» system. Thermophysical characteristics of the material and rheological models coefficients are shown in Table 2.

| Material   | Density, $\rho$ (kg/m$^3$) | Specific heat capacity, $C$ (J/kg K) | Thermal conductivity, $\lambda$ (W/m K) |
|------------|-----------------------------|-------------------------------------|----------------------------------------|
| PE 153-02K | 779                         | 2500                                | 0.182                                  |

The coefficients, used in the rheological laws $\mu_0$ (Pa·s)

- **Power law:** $\mu_0=23336.9$, $\beta=0.0124$, $n=0.34$, $T_0=433$
- **Cross model:** $\mu_0=188912$, $\beta=0.0131$, $n=0.64$, $\lambda=25.8548$, $\mu_c=51.1269$, $T_0=433$
- **Carreau model:** $\mu_0=88064.2$, $\beta=0.040424$, $n=4$, $\lambda=11.5052$, $\mu_c=124.83$, $T_0=433$
Figure 3 shows the curves of viscosity change versus shear rate, built according to the studied laws.

Figure 3. Dependence of the polymer melt effective viscosity by shear rate
- - - the experimental values; — — Carreau model; — — Cross model; — — power low

Figure 3 shows, that all shear flow curves are quite similar, with the exception of low shear rate values, where power law is significantly different. The average values deviation obtained by a power law and experimental data was 14.6%, whereas the deviation for Kerry and Cross models was 2.9 and 0.9 (%), respectively.

The equations solution (1-8) was carried out in engineering calculations package ANSYS CFX by finite element method. Construction of finite element mesh was made in ICEM CFD system.

To determine the optimal number of elements, grids with different number of elements for different channel geometries were constructed and then divergence of the maximum temperature at the channel exit was evaluated. For the deployed channel and cylindrical model without gap, a grid with a number of elements equal to 334125 was chosen. Further increase in the number of elements leads to a longer counting time, while the discrepancy becomes less than 0.2%. To solve the problem of polymer melt flow in a helical channel with a gap, a grid with a number of elements equal to 1 757 000 was required. This is due to the small size of the gap between the crest of the screw and the inner surface of the cylinder. To establish the solutions 30,000 iterations was required.

3. Results and Discussion

As a result of a numerical study of the polymer melt flow processes in the extruder dosing zone, the shear rate, temperature and viscosity fields along the channel length were received.

At the first stage of numerical studies, the fields of temperature, velocity, viscosity, and shear rate were obtained for a flat and screw channel model under conditions of reversed motion and with a screw rotation. Also a comparison of three mathematical models for different channel geometries was held. The investigations were carried out for the power law of viscosity.

The maximum and average values of temperature, viscosity and shear rates across the channel volume are shown in Table 3.
Table 3. Average values of temperature, shear rates and viscosity for power law, for various geometric models.

| Variant of calculation № | Geometric model         | Movement type | Temperature, (ºС) | Shear rate, [s⁻¹] | Viscosity, [Pa·s] |
|--------------------------|--------------------------|---------------|-------------------|-------------------|------------------|
|                          |                          |               | Max.              | Avg.              | Avg.             |
| 1                        | Flat channel             | Reversed      | 254.7             | 233.8             | 134.5            |
| 2                        | Flat channel             | Unconverted   | 302.8             | 263.8             | 257.8            |
| 3                        | Helical without a gap    | Reversed      | 250.1             | 233.5             | 134.3            |
| 4                        | Helical without a gap    | Unconverted   | 289.3             | 262.3             | 247.7            |
| 5                        | Helical with a gap       | Reversed      | 247.7             | 231.6             | 166.2            |
| 6                        | Helical with a gap       | Unconverted   | 254.1             | 235.0             | 246.5            |

In the case of reversed motion (variants 1, 3, 5), the temperature values are close, the difference in the maximum temperature does not exceed 3%, and in the average temperature is 1%, in spite of the fact that for variant 5 there are significant differences in the maximum values of the shear rate and viscosity. This is due to the presence of a gap between the crest of the screw and cylindrical body, where the highest shear rates are arise. But in view of the small channel region above the crest of the screw, this is significantly less pronounced on the temperature fields.

Figure 4. Temperature fields using the principle of reversed motion: a – Flat channel; b – Helical channel with gap.

The difference in the temperature values obtained for the flat channel model using the inverse motion principle and the helical channel model with a gap in the case of a screw movement is less than 1%, in spite of the fact that the nature of the polymer melt flow in these channels is different. In addition, the channel model with a gap in the case of a moving screw is the closest to the real conditions of polymer flow in the extruder dosing zone and allows more complete consideration of heat and mass transfer processes during polymer materials processing.

The important factor in the study of polymer flow processes is the choice of rheological laws that describe the change in viscosity from shear rate and temperature. Since the viscometric curves constructed according to the described above models (Fig. 3) have a significant discrepancy in the region of low shear rates, it was necessary to analyze the effect of the selected rheological law on the polymer flow in the extruder screw channel.

Shear rates values realized in the channel for all three rheological laws under equal conditions and assumptions are differ by not more than 3% (see Table 4). Using the power law in describing the polymer flow in a channel is possible, because there are no shear rates in the dosing zone at which this model does not correctly describe the viscosity change. When considering models with regard to the rotation of the screw, shear rates of less than 1 s⁻¹ are arise. This, certainly, goes beyond the range of
adequate description of the viscosity change, however, regions with such values of shear rates are small and do not significantly influence on the investigations results. The difference between the maximum and average temperatures at the exit from the extruder channel does not exceed 2°C. Thus, the use of a power law to describe the polymer flow in an extruder channel is possible.

Table 4. Average values of temperature, shear rate and viscosity in terms of volume for the flat channel.

| Rheological law  | Movement type | Shear rate, s⁻¹ | Viscosity, Pa·s⁻¹ |
|-----------------|---------------|-----------------|-------------------|
|                 |               | Avg.  | Max.  | Min.  | Avg.  | Max.  | Min.  |
| Power law       | Reversed      | 134.5 | 317.7 | 35.7  | 578.0 | 1172.0| 165.5 |
|                 | Unconverted   | 257.8 | 1030.0| 1.1   | 757.1 | 6219.0| 40.8  |
| Carreau model   | Reversed      | 134.4 | 324.1 | 36.1  | 606.3 | 1229.0| 165.1 |
|                 | Unconverted   | 244.1 | 1170.0| 0.9   | 810.8 | 6170.0| 34.0  |
| Cross model     | Reversed      | 134.5 | 320.2 | 35.8  | 577.9 | 1178.0| 157.7 |
|                 | Unconverted   | 253.0 | 1078.0| 1.0   | 745.6 | 5331.0| 36.1  |

In order to more fully study the processes which occur during the polymer compositions processing on extrusion equipment, a full model was constructed (see Figure 3).

Since the helical channel model with a gap in the case of screw rotation yields the most adequate results, it was chosen to study the polymer melt flow processes in a full model which consists of dosing zones, output adapter and cable heads.

Heat and mass transfer processes in the output adapter are the most interesting in studying the polymer flow within the framework of the described above model, because in this area the polymer melt flow is reconstructed. This occurs because channel geometry is changing and material is heating due to the energy dissipation. In the course of numerical investigation, the temperature field in the adapter was obtained (see Figure 5). It should be noted that in the middle of this area the maximum temperature value increases by 10°C. Depending on the geometric features of the output adapter, in particular the angle of the conical part, overheating can reach 30°C, which can be critical for a number of polymer materials. Such increase in the temperature of the melt is associated with the appearance of a circulation movement at the end of the screw. Figure 6 shows the flow functions that allow you to see the path of the material movement and identify the areas of the vortex flow in the output adapter.
Pressure is the most important parameter in choosing the rational operation mode of the extrusion equipment. Figure 7 shows the pressure and flow rate characteristics of the extruder and forming tool. The pressure values obtained by calculating the model, taking into account the output adapter and the forming tool (marked with dots), quite well coincide with the operating points, which are determined on the basis of the flow-rate characteristics separately for the extruder and cable head. The difference does not exceed 4%. The complete model allows to obtain pressure values directly at the manometer installation site in a real extruder.

4. Conclusion
As a result of the study, a number of conclusions can be done. Since for a number of processed polymers the value of the maximum melt temperature is essential, it is important to adequately describe the polymers viscosity dependence on the shear rate and temperature during calculations. Despite the fact that the viscometric flow curves built from the Kerry and Kross models differ quite strongly from the power law, the temperature, viscosity and shear rate fields obtained in the study are quite close. In addition, the power law has a significant advantage, which lies in the simplicity of its use and the small number of empirical coefficients.

An analysis of the mathematical model with different channel geometries of the dosing zone allows us to conclude that they are valid for the case of reversed motion. Thus, the shape of the channel (flat or screw) has little effect on the flow process, while the choice of the movable wall (rotation of the body or screw) has a significant effect on the calculation results.
Using the principle of reversed motion leads to a change in the polymer flow nature, which accordingly affects the temperature, viscosity and shear rates in the channel of the extruder. The possibility of using the principle of inverted motion depends on the chosen mathematical model (channel geometry).

The calculation of the full model makes it possible to consider the heat and mass transfer processes, which are close to reality, both in the main channel of the extruder and in the forming tool. In addition, it becomes possible to determine the rational mode of extrusion equipment operation by means of one model calculation.

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