Mathematical model of the polymeric composition melt flow in the middle layer extruder of the coextrusion equipment

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Abstract. The paper analyzes the urgency of using coextrusion technology while recycling the secondary polymeric raw material. The balance equation in the melt flow tensions is obtained. The connection between the tensor of tensions and tensor of deformation rates components is determined. The generalized power law is used as a rheological equation of state. The energy balance equation is worked out for the stable regime of the melt flow. The limiting conditions for the complete differential model of extrusion are determined. The equation for determining the effective output of the middle layer extruder is worked out based on the efficiency of the whole extrusion machinery which depends on the characteristics of the rest four extruders and the head’s characteristics.

1. Introduction
Every year ecological problems are becoming more and more burning. The significant part of these problems is the environmental pollution with polymeric materials waste. This waste has a considerable period of decomposition in the soil, thus, for polypropylene bags this period is more than 500 years. While utilizing such waste by burning, toxic gas emissions, harmful for the atmosphere, are produced. Thereby, the method of secondary processing is the safest for the ecology.

Despite the variety of methods of processing polymeric materials into products we cannot use all the polymeric materials as possible waste. It is caused by the worsening of the polymer properties while secondary processing, by classification complexity of secondary polymers into separate types and brands, by bad quality of the obtained secondary product, by the limitation of the application field of the product, produced from such waste, by the high cost of the secondary polymeric materials’ preparation for recycling, etc.

The most perspective method for waste recycling is the coextrusion method. This method allows processing the secondary polymeric materials into a new product, having a complex of valuable operational properties. This result is achieved due to the multilayer structure of the obtained product. The middle layer is made of the waste, and the outer layers provide the safe contact with the surrounding or the substance, being inside the product (e.g. in case of package).

A precise description of the processes going on in the extruder of the middle layer, while processing the secondary polymeric materials, is needed for an effective designing of modern coextrusion equipment.

2. The problem statement
During the implementation of waste recycling polymeric materials cover a definite distance in the extruder and the moulding head, going through structural changes.
A great number of scientific papers are dedicated to the research of homogeneous materials flow in the extrusion equipment [1, 2, 3, 4]. Different kinds of extrusion equipment are minutely studied [5-7]. The properties of the combined materials, going on in the coextrusion equipment, are researched insufficiently. That is why the objective of the paper is the theoretical description of coextrusion processes and working out a mathematical model of heterogeneous polymeric materials’ movement under pressure in the middle layer extruder.

3. Theory
To describe satisfactorily the extrusion process in the main extruder of the coextrusion equipment the mathematical model of the melt flow within the zone of batching has to meet at least the following requirements: to take into consideration the anomaly of viscosity existence (polymeric material has a heterogeneous structure); to consider the mutual influence of circulating and onward flows; to consider the influence of the heat, released as a result of the internal friction, on the effective viscosity of the melt; to take into consideration the heat exchange between the surroundings.

Evidently, it does not matter to the extruder’s operation if the worm screw rotates inside the motionless framework or, on the contrary, the framework rotates relatively to the worm screw. For this reason for simplicity we will consider the framework rotating [8].

The arrangement of the motionless system of reference axes x, y, z and the auxiliary axis l, connected with the worm screw, is presented in figure 1. The axis z is directed along the axis of the screw channel of the worm screw, the axis l is directed along the axis of the worm screw.

![Figure 1. The scheme of the arrangement of the reference axes and designation of the geometrical parameters of the worm screw.](image)

Considerable simplification is achieved if to ignore the curvature of the channel. It is possible due to infinitesimality of the ratio of the screw channel depth \( h \) to the radius \( R \) which in most machineries [9] is \( 0.005 - 0.05 \). Using this simplification, the worm screw channel can be displayed on the plane, as it is shown in figure 2. Along with this the extruder’s framework will be presented as an infinite plane, moving above the displayed channels in the perpendicular direction to the worm screw axis. The flow is considered to be settled. We ignore the mass force and the inertial force. Taking into consideration these assumptions, we get the balance equations in the tensions of the following type:

\[
\begin{align*}
\frac{\partial P}{\partial x} &= \frac{\partial p_{yx}}{\partial y} + \frac{\partial p_{xz}}{\partial z}, \\
\frac{\partial P}{\partial y} &= \frac{\partial p_{xy}}{\partial x} + \frac{\partial p_{yz}}{\partial z}, \\
\frac{\partial P}{\partial z} &= \frac{\partial p_{yz}}{\partial y} + \frac{\partial p_{zz}}{\partial z}
\end{align*}
\]  

(1)
Figure 2. The sweep of the worm screw channel on the plane: 1 – the channel wall; 2 – the worm screw sweep; 3 – the surface of the framework; 4 – the channel.

The surrounding is considered to be incompressible:

\[ \frac{\partial \psi_x}{\partial x} + \frac{\partial \psi_y}{\partial y} + \frac{\partial \psi_z}{\partial z} = 0. \]  

(2)

The connection between the tensor of tensions \( p_{ij} \) and the tensor of deformation rates \( \varepsilon_{ij} \) is determined by the formula:

\[ p_{ij} = \eta \cdot 2 \varepsilon_{ij} (i, j = x, y, z), \]

(3)

or in the extended form:

\[ p_{xx} = \eta \left( \frac{\partial \psi_x}{\partial x} + \frac{\partial \psi_x}{\partial y} \right); \]

\[ p_{yy} = \eta \left( \frac{\partial \psi_y}{\partial y} + \frac{\partial \psi_y}{\partial z} \right); \]

\[ p_{zz} = \eta \left( \frac{\partial \psi_z}{\partial z} + \frac{\partial \psi_z}{\partial x} \right); \]

\[ p_{xz} = p_{xy} = p_{yz} = P. \]

As a rheological equation of the state the generalized power law is used:

\[ \eta = \mu_0 \cdot b^{(T-T_0)} \left( \frac{1}{2} I_2 \right)^{\frac{1-n}{2n}}, \]

(5)

where \( \mu_0, n \) are the constants of the material;

\( b \) is the temperature coefficient of viscosity;

\( I_2 \) is a quadratic invariant of the deformation rates tensor [8].

The energy balance equation, worked out for the settled regime in the assumption that all thermalphysical characteristics do not depend on the temperature, is as follows:

\[ \rho c_p \left( v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = -k_m \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + p_{xx} \frac{\partial \psi_x}{\partial x} + p_{xy} \frac{\partial \psi_y}{\partial y} + \]

\[ + p_{xz} \frac{\partial \psi_z}{\partial z} + p_{yy} \left( \frac{\partial \psi_x}{\partial y} + \frac{\partial \psi_y}{\partial x} \right) + p_{zz} \left( \frac{\partial \psi_x}{\partial z} + \frac{\partial \psi_z}{\partial x} \right) + p_{yz} \left( \frac{\partial \psi_y}{\partial z} + \frac{\partial \psi_z}{\partial y} \right), \]

(6)

where \( \rho \) is the density of the melt;

\( C_p \) is the heat capacity of the melt;

\( T \) is the temperature of the melt;

\( k_m \) is the coefficient of the heat conductivity of the melt.
The limiting conditions for such a complete differential extrusion model are of the following type:

\[ u_x = u_y = u_z = 0 \text{ with } y = 0, \]
\[ T = T_r, \text{ with } x = 0 \text{ and } x = \omega (\text{for all } y), \]
\[ u_x = U_x, u_z = U_z; T = T_w \text{ with } 0 < x < \omega \text{ and } y = h, \]
\[ T = T_b \text{ with } z = 0, \]

where \( T_r \) and \( T_b \) are correspondingly the temperatures of the worm screw and the wall of the framework.

The equations (1) - (6) make up the complete equation system relative to eight functions (\( P, p_i, v_i, T \)) and quite strictly describe the task of the “power” liquid movement if there is heat exchange. However, as the scientific papers show [10-14], their solutions can be obtained by the numerical method. For designing the model, allowing an analytical solution, we make the following assumptions:

1. The flow in the direction to the axis \( y \) exists only in immediate proximity to the walls of the channel. In the rest part of the channel section the flow in the direction to the axis \( y \) is absent (\( u_y = 0 \)).
2. The dimensions of the channel along the whole length are constant, consequently, the values \( u_x \) and \( u_z \) do not depend on \( z \).
3. The temperature gradient in the diametrical direction because of the circulating flow is negligibly small in comparison to the lengthwise gradient. Thereby, \( \partial T/\partial x = \partial T/\partial y = 0; \partial T/\partial z \neq 0 \).
4. Along the whole length of the channel there is evenly mixed and melted blend of several polymers and a filler.

Due to a large ratio of the screw channel width to its depth, and due to the peculiarity of the circulating flow, we may assume that at a certain distance from the channel walls the rates \( u_x \) and \( u_z \) do not depend on \( x \). Thereby:

\[ \frac{\partial u_x}{\partial x} = 0, \quad \frac{\partial u_z}{\partial z} = 0, \quad \frac{\partial u_x}{\partial y} = 0, \quad \frac{\partial u_z}{\partial z} = 0, \quad \frac{\partial u_z}{\partial x} = 0. \]

(8)

If \( u_x = u_x(y) \) and \( u_z = u_z(y) \), then the velocity field depends only on the coordinate \( y \). That is why the value of the quadric invariant \( I_2 \) turns out to be equal:

\[ I_2 = \left( \frac{\partial u_x}{\partial y} \right)^2 + \left( \frac{\partial u_z}{\partial y} \right)^2. \]

(9)

The substitution of partial derivatives by regular derivatives is the consequence of the term (8). Along with this, from (4) and (5) we have:

\[ p_{xy} = \eta_x \frac{\partial u_x}{\partial y}; \quad p_{yz} = \eta_x \frac{\partial u_z}{\partial y}; \quad p_{yx} = 0. \]

(10)

Thus, the components of the tensions \( p_{xy} \) and \( p_{yz} \) turn out to be the functions of only \( y \) and \( z \), and the latter dependence is possible only in case if \( T = T(z) \). Taking into consideration (10), we get the following instead of (1):

\[ \frac{\partial P}{\partial x} = \frac{\partial p_{xy}}{\partial y} = \frac{\partial p_{xy}}{\partial y} = \frac{\partial p_{xy}}{\partial z} = \frac{\partial p_{xy}}{\partial z}. \]

(11)

Along with this, the integration of quasi-static equations is done independently, as in (11) the number of equations corresponds to the number of the required functions. The distribution of the rates is determined by the integration of another dependent system of coupling equations.

While recording the energy balance equations, we will consider that the heat transmission for account of heat conductivity along the channel axis is negligibly small because of the filler’s presence in the complex polymeric composition, consisting of secondary polymers. However, the same filler brings the changes in the heat balance of the polymeric composition as a result of differences in thermal physic properties of every polymer and the filler. In this case the equation (6) will be as follows:
Presented in this form, the equation (6) in essence turns into the heat release equation. During its integration it is necessary to satisfy the thermal conditions on the surface of the polymeric stream, taking into consideration that the surface temperature depends on the heat exchange with the surroundings. Thereby, during the direct integration of the heat conductivity equation, or in this case heat release, the heat emission through the walls of the framework will become a limiting condition. We may integrate the equation (12) according to the coordinate $y$ similar to what has been done in the scientific papers [15-19]. In this case instead of differential formula for the elementary volume we will get:

$$\frac{Z}{Q} = p_{cp} \cdot C_p + V \cdot \Delta P + \lambda,$$  

(13)

where $Z$ is the total power consumed for the polymer extrusion ($Z = Z_{of\ worm\ screw} + Z_{of\ the\ heater} - Z_{of\ cooling}$);

$Q$ is the mass polymer consumption for the polymer extrusion;

$P_{cp}$ is the polymer density;

$C_p$ is the specific heat of the polymer;

$V$ is the specific volume of the polymer ($V = 1/p$);

$\Delta P$ is the difference between the pressure in the head and the pressure at the extruder’s input;

$\lambda$ is the melting heat of the polymer.

During the coextrusion of the five-layer product through the coextrusion head the equation (13) for the middle layer extruder will be as follows:

$$\frac{Z_{cp}}{Q_{cp}} = p_{cp} \cdot C_{cp} + V \cdot \Delta P_{cp} + \lambda_{cp},$$  

(14)

where $Z_{cp}$ is the total power consumed for the polymer extrusion in the middle layer extruder;

$Q_{cp}$ is the polymer consumption of the middle layer extruder at the head output;

$P_{cp}$ is an average polymer density;

$C_{cp}$ is an average heat capacity of the polymer in the head;

$\lambda_{cp} = \lambda_1 + \lambda_2 + ... + \lambda_n$ is the total heat of polymer melting;

$\lambda_1, \lambda_2 ... \lambda_n$ is the heat of melting of each polymer, respectively, constituting the composition.

$$Q_{cp} = \frac{Z_{cp}}{p_{cp} \cdot C_{cp} + V \cdot \Delta P_{cp} + \lambda_{cp}}.$$  

(15)

As the efficiency of the coextrusion machine is determined by the sum of each layer efficiency, we have got:

$$Q_{sum} = Q_{ol1} + Q_{ol2} + Q_{cp} + Q_{il1} + Q_{il2},$$  

(16)

where $Q_{sum}$ is the efficiency of the coextrusion machinery;

$Q_{ol1}, Q_{ol2}$ is the efficiency of the first and second outer layer, respectively;

$Q_{il1}, Q_{il2}$ is the efficiency of the first and second inside layer, respectively.

The real efficiency of the coextrusion machinery is determined by the reciprocal influence of the worm screw characteristics and the head characteristics. The value of the consumption through the coextrusion head is described by the equation [20]:

$$Q_i = k_i \cdot \frac{\Delta P_i}{\mu_i},$$  

(17)

where $i$ is the polymer layer in the head;

$k_i$ is the constant coefficient, depending on the geometric sizes of the head for the corresponding layer;

$\Delta P_i$ is the pressure drop in the head for the corresponding layer;

$\mu_i$ is the viscosity of the polymer in the head for the corresponding layer.
Substituting the formula (15) in (16) we get:

\[ Q_{\text{sum}} = (Q_{ol1} + Q_{ol2} + Q_{il1} + Q_{il2}) = \frac{Z_{cp}}{P_{cp} \cdot C_{cp} + V \cdot \Delta P_{cp} + \lambda_{cp}}. \]  

(18)

Substituting instead of \( Q_{ol1}, Q_{ol2}, Q_{il1}, Q_{il2} \) in the equation (17) corresponding formulas, considering the geometric channels of the head for each layer, we work out the final formula:

\[ Q_{\text{sum}} = \frac{Z_{cp}}{p_{cp} \cdot C_{cp} + V \cdot \Delta P_{cp} + \lambda_{cp}} + k_{ol1} \frac{\Delta P_{ol1}}{\mu_{ol1}} + k_{ol2} \frac{\Delta P_{ol2}}{\mu_{ol2}} + k_{il1} \frac{\Delta P_{il1}}{\mu_{il1}} + k_{il2} \frac{\Delta P_{il2}}{\mu_{il2}}. \]  

(19)

From the equation (19) it follows that the middle layer worm screw characteristics can be represented by the efficiency of the whole coextrusion machinery, which, in its turn, depends on the characteristics of the rest extruders.

An analysis of the parameters and characteristics of coextrusion based on the simulation results, shows that the extrusion performance of each layer is only slightly dependent on temperature during the coextrusion of non-Newtonian fluids. As, despite the fact that the values of the viscosity of the material in the worm and the head due to the difference in the magnitude of the velocity gradients are not the same, their ratio with the temperature changes remains almost constant. It happens because of the viscosity values in the worm and head are changing approximately the same with the changing of the temperature. Worms and heads characteristics are shown in the figure 3. The each extruder "operating points" on the graphs are determined by the intersection of these characteristics. This method allows depicting the variety of possible modes of coextrusion of multilayer structures in one setup diagram. The figure 3 shows the characteristics of the extruders at the different screw speeds.

![Figure 3](image_url)

**Figure 3.** The extruders and heads operating characteristics, the thickness of each layer in MPM is 0.33 mm; \( T=1700^\circ\text{C} \); 1, 1′, 1″ – points, that determine the necessary frequency of the screws rotation; \( N1 = 0.72 \text{ rps} \); \( N2 = 1.04 \text{ rpm} \); \( N3 = 1.45 \text{ rps} \)

The productivity of a co-extrusion machine is primarily determined by the rotational speed of the screws, as far as it has shallow channels and the countercurrent flow (back pressure in the head) does not significantly reduce the productivity level.

4. Conclusions
We worked out the energy balance equation and the limiting extrusion conditions in the form of a complete differential model, made up for the settled regime in the assumption that all the thermalphysic characteristics do not depend on the temperature. We worked out the equation for calculating the real efficiency of the middle layer extruder based on the efficiency of the whole coextrusion machinery which depends on the characteristics of the rest four extruders and the head characteristics.

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