Mathematical modeling of a biopolymer melt flow in the extruder forming

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Abstract. The universal extrusion process is increasingly used in the food industry, displacing some of traditional types of food technology. Despite this fact, we still have limited knowledge of mathematical models describing the behavior of the biopolymer melt in the forming channels of the extruder die, of the predie zone, and even of the screw channel of the extruder metering zone, even if we take into account simplifying assumptions. Moreover, the development of mathematical models of mediums flow in the extruder forming channel is complicated by the structural, rheological and physicochemical transformations that the biopolymer undergoes in this zone. This paper presents a developed mathematical model that describes a particular case of the melt flow process in the forming channel of a single-screw extruder. The model considers the stationary flow of a biopolymer melt, the rheological properties of which obey the power law, inside of a cylindrical forming channel of a constant section extruder die. Using the obtained equations, it is possible to determine the values of the melt flow rate of the biopolymer and the temperature in the cross sections of the extruder forming channel, and thereby to justify the optimal operating modes of the apparatus in order to obtain a homogenized product with the required quality indicators, as well as to select the most rational geometric parameters of the extruder die.

1. Introduction
The extrusion process has found wide application in various industries, including the food industry, since on the one hand it allows the production of a wide range of food products, and on the other hand, it is possible to replace a set of technological equipment with one apparatus, which is an extruder [1, 2]. In a number of food productions, the extrusion process has supplanted traditional technologies for processing raw materials, and analysts predict an increase in the share of extrusion equipment used [3]. At present, screw extruders that have found greater application, are the ones the die of which is stationary, since it is mounted on the extruder body [4]. It should be noted that in order to obtain extruded food products of consistently high quality, it is necessary to select the optimal parameters of the technological process and the rational design of equipment for specific industries. The fulfillment of this requirement is complicated by the interconnection of hydro-mechanical, rheological and heat and mass transfer processes that occur during extrusion and determine its effectiveness [5].

Modeling and scaling of the extrusion process is used in order to predict technological parameters of the process, such as pressure and temperature along the screw length and the cross section of the channel, the filling factor, the residence time distribution and the power on the shaft, under various operating conditions [6, 7]. Currently, most industrial designs of extruders and their main working
bodies are developed on the basis of empirical studies, since specifics of the transformations in the extrusion process are not well understood. The main goals of mathematical modeling of the extrusion process in various zones of the extruder are to deepen the physical understanding of the process and its quantitative description with the closest possible approximation to real technological practice [8]. Mathematical models are developed separately taking into account the specifics of the process for each zone of the extruder. All of the existing mathematical models consider the processes occurring in the extruder zones where calculations are much easier to be performed, in zones where no phase transformations of the biopolymer can be observed, but only grinding, mixing and compression processes [9-13]. Models can be conditionally divided into five subgroups as for the sign of increasing mathematical complexity: one-dimensional flow of Newtonian fluids; one-dimensional flow of non-Newtonian fluids under simple shear conditions; one-dimensional flow of non-Newtonian fluids under complex shear conditions; two-dimensional flow of non-Newtonian fluids; three-dimensional flow of non-Newtonian fluids [5, 14, 15]. A common drawback of most models is the lack of solutions to the problem of assessing the quality of the polymer melt and, accordingly, of the finished product, which can be achieved by stabilizing the main parameters of the extrusion process, which are productivity, pressure, and temperature [16, 17]. A significant contribution to the development of mathematical models and methods for calculating single-screw extruders was made by U.L. Wilkinson, D.M. Mc Kelvey, D.H. Chang, G.V. Vinogradov, N.B. Uryev, Yu.A. Machikhin, S.A. Machikhin, B.M. Azarov, B.A., Nikolaev, G.K. Berman, G.G. Zurabishvili, A.N. Ostrikov, G. Schenkel, E. Bernhardt, Z. Tadmore, J. Maze, R.V. Thorner., M.L. Booy, V.S. Kim, V.V. Skachkova, A.A. Tatarnikova, O.I. Skulsky, J.P. Melcion, P. Colonna, J.L. Rossen, R.C. Miller, J.M. Harper, D. Hammer, T.F. Tsao, V.V. Lukyanov, I.E. Gruzdev, B.M., Gorbatov, V.P. Yuriev, A.N. Bogatyrev and others [1, 4-6, 16, 20].

It should be noted that it is the forming zone of the extruder that complex physical, mechanical and rheological processes take place, which ultimately determine the structural, mechanical and qualitative characteristics of the finished product [16]. However, a very limited number of works [1, 5, 15, 16, 18-20] are devoted to the subject of modeling processes in this extruder zone, which can be explained by the complexity of the structural, rheological, and physicochemical transformations that the product undergoes. The difficulty in formulating the problem leads to the use of simplifying assumptions in modeling, which do not contradict the physics of the process and are generally accepted [19]. These assumptions include the following: the process is considered as stationary at a constant mass flow rate; there is no heat transfer due to heat conduction along the channel axis; the medium is considered incompressible, elastic processes in the melt are not taken into account; mass forces and inertia forces are neglected; the dimensions of the channel along the entire length are constant. Mathematical models of the processes occurring in the extruder forming zone are based on the same laws as for other zones: laws of conservation of mass, motion and of energy [5, 15]. The description of the process is considered complete in case the velocity vector and thermodynamic parameters, such as pressure and temperature, are known at any moment of time at any point in the flow [16]. In order to obtain the listed values, the equations of conservation laws are combined with the basic equations establishing relations between the parameters describing kinetics of motion, on the one hand, with individual thermodynamic parameters of motion, on the other.

However, we note that the behavior of the biopolymer melt of the prescription mixture from food raw materials in the forming channels of the die, the predie zone, and even the screw channel of the metering zone of the extruder remains poorly understood. Thus, it becomes an urgent task to develop mathematical models of the extrusion process that describe the change in temperature and speed of abnormally viscous food media in these zones, which directly affect the quality of the finished product. Creation of such a mathematical model would make it possible to predict the quality of the finished product and to take into account the required indicators when calculating or selecting the geometric parameters of the die.

2. Results and Discussion

The model describes the stationary flow of an incompressible non-Newtonian fluid in the forming channel of the extruder matrix, the geometry of which is shown in Figure 1.
Figure 1. Sketch of the forming channel of the die extrude.

The temperature and pressure of the biopolymer melt at the input to the forming channel are taken as the input parameters of the model. The thermo-physical properties of the food mixture melt under study, the thermo-physical characteristics of the materials of the forming zone as well as the ambient air are considered known. The change in the melt temperature of the biopolymer during its stay inside the forming channel is associated with heating due to viscous dissipation and to the heat removal into the environment.

The basic system of model equations includes the continuity equation, the motion equation, the energy equation and the rheological equation. Let us write down the basic system of equations in the Cartesian coordinate system (x, y, z):

The continuity equation is the following:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_x)}{\partial x} + \frac{\partial (\rho v_y)}{\partial y} + \frac{\partial (\rho v_z)}{\partial z} = 0 \]

where: \( \rho \) is the melt density of the biopolymer, t is time, x, y, z are Cartesian coordinates, \( v_x, v_y, v_z \) are projections of the biopolymer melt velocity on the corresponding coordinate axes.

The motion equation in rectangular coordinates in the projections on the coordinate axis, respectively, is the following:

\[ \rho \left( \frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right) = - \frac{\partial P}{\partial x} + \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) + \rho g_x \]

\[ \rho \left( \frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right) = - \frac{\partial P}{\partial y} + \left( \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) + \rho g_y \]

\[ \rho \left( \frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) = - \frac{\partial P}{\partial z} + \left( \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) + \rho g_z \]

where: \( \tau \) are components of the shear stress tensor, \( P \) is the pressure.

The energy equation is as follows:

\[ \rho C_v \left( \frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = \]

\[ = - \left( \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right) - AT \left( \frac{\partial P}{\partial t} + \frac{\partial P}{\partial x} \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) \right) \]

\[ + A \left[ \tau_{xx} \frac{\partial v_x}{\partial x} + \tau_{yy} \frac{\partial v_y}{\partial y} + \tau_{zx} \frac{\partial v_z}{\partial z} \right] \]

\[ + \tau_{xy} \left( \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) + \tau_{xz} \left( \frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right) + \tau_{yz} \left( \frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right) \]

Since the geometrical shape of the forming zone of the extruder is conical with a rotating cylindrical section, we pass to the cylindrical coordinate system (r, \( \theta \), z). Then the basic system of equations will take the following form:

The continuity equation can be presented as follows:
The motion equation is following:

Projection on the direction $r$:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial (\rho r v_r)}{\partial r} + \frac{1}{r} \frac{\partial (\rho v_r)}{\partial \theta} + \frac{\partial (\rho v_z)}{\partial z} = 0$$

The energy equation is as follows:

$$\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + v_\theta \frac{\partial v_r}{\partial \theta} - \frac{v_r^2}{r} + v_z \frac{\partial v_r}{\partial z} \right) = \frac{\partial P}{\partial r} + \left( \frac{1}{r} \frac{\partial (r \tau_{rr})}{\partial r} + \frac{1}{r} \frac{\partial \tau_{r\theta}}{\partial \theta} + \frac{\partial \tau_{rz}}{\partial z} \right) + \rho g_r$$

Projection on the direction $\theta$:

$$\rho \left( \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + v_\theta \frac{\partial v_\theta}{\partial \theta} - \frac{v_r v_\theta}{r} + \frac{\partial v_\theta}{\partial z} \right) = -\frac{1}{r} \frac{\partial P}{\partial \theta} + \left( \frac{1}{r^2} \frac{\partial (r^2 \tau_{r\theta})}{\partial r} + \frac{1}{r} \frac{\partial \tau_{\theta\theta}}{\partial \theta} + \frac{\partial \tau_{\theta z}}{\partial z} \right) + \rho g_\theta$$

Projection on the direction $z$:

$$\rho \left( \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + v_\theta \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{1}{r} \frac{\partial P}{\partial z} + \left( \frac{1}{r} \frac{\partial (r \tau_{rz})}{\partial r} + \frac{1}{r} \frac{\partial \tau_{\theta z}}{\partial \theta} + \frac{\partial \tau_{zz}}{\partial z} \right) + \rho g_z$$

The relationship between the shear stress and the change in the velocity gradient caused by it, can be expressed through the following equation:

$$\tau = \mu \frac{dv}{dh}$$

where: $h$ is the height of the fluid layer, $\mu$ is the proportionality ratio (viscosity).

Since the model assumes a viscous-plastic incompressible non-Newtonian fluid with rheological properties obeying the Ostwald-de Waele power law, a functional empirical dependence is used in order to describe fluids of this type, in which the viscosity is related to the shear rate by the following relation:

$$\tau = m \gamma^n$$

where: $m$ is a measure of the consistency of the liquid (the higher the viscosity of the liquid is, the greater the $m$ value becomes), $n$ is the flow index that characterizes the degree of non-Newtonian behavior of the material (the more $n$ differs from unity, the more clearly its non-Newtonian properties are manifested).

For incompressible non-Newtonian fluids, the rheological equation takes the following form:

$$\tau = \eta \cdot \Delta + \frac{1}{2} \eta_c (\Delta; \Delta)$$

where: $\eta_c$ is the shear viscosity coefficient, $\Delta$ is the strain rate tensor, it has components defined by the following equation:

$$\Delta_{ij} = \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}$$

In general, the power law is written as follows:

$$\eta = \eta_0 \left( \frac{\Delta; \Delta}{\gamma^2} \right)^{1-n} \quad (1)$$

where: $\eta_0$ is the viscosity at a unit shear rate $\gamma = 1 \text{s}^{-1}$.

The scalar value $(\Delta; \Delta)$ is the invariant of the strain rate tensor, which remains unchanged when the coordinate axes rotate in a cylindrical coordinate system, it has the following form:
This is the way the basic system of equations of the model is written in.

In the general setting, the mathematical model is very complex and it is not possible to obtain a general solution to it. Therefore, we introduce simplifying assumptions regarding the extruder forming channel and the nature of the flow of the biopolymer melt and we solve this system in a particular case.

Let us suppose that a laminar axisymmetric melt flow of a biopolymer, modeled by an incompressible non-Newtonian fluid, whose viscosity is assumed to obey a power law, is established in the forming channel of the extruder. We will model the forming channel of the extruder with a long circular tube of a radius \( R \). We assume that the temperature of the forming channel walls of the extruder is kept constant and equal to \( T_w \). It is required to determine the distribution of speed and temperature in the cross sections of the forming channel of the extruder, which are so remote from the entrance that neither temperature nor speed depend on the longitudinal coordinate \( z \).

In such an approximate, simplified formulation, all derivatives of temperature, velocity, and components of the voltage deviator with respect to the variables \( \theta, z, \) and \( t \) are equal to zero that is, the process is considered stationary. The velocity components \( v_{\theta} \) and \( v_r \) are also equal to zero. Due to the incompressibility of the fluid, \( \left( \nabla \cdot v \right) \) is equal to 0. Then, under such assumptions, the equations of motion and energy take the following form, in which the viscosity coefficient \( \eta \) is determined from the following equation (1):

\[
\frac{1}{2} (\Delta : \Delta) = 2 \left( \frac{\partial v_r}{\partial r} \right)^2 + \frac{1}{r} \left( \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right)^2 + \left( \frac{\partial v_z}{\partial r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} \right)^2 + \left( \frac{\partial v_z}{\partial z} \right)^2 + \left( \frac{\partial v_r}{\partial z} \frac{\partial v_z}{\partial r} \right)^2
\]

where:

\[
\Delta = \frac{1}{2} \left( \frac{\partial v_r}{\partial r} \right)^2 + \frac{1}{r} \left( \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right)^2 + \left( \frac{\partial v_z}{\partial r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} \right)^2 + \left( \frac{\partial v_z}{\partial z} \right)^2 + \left( \frac{\partial v_r}{\partial z} \frac{\partial v_z}{\partial r} \right)^2
\]

Therefore, the viscosity coefficient \( \eta \) is determined as follows:

\[
\eta = \eta_0 \left| \dot{\gamma} \right|^{n-1}
\]

where the reduced shear rate \( \dot{\gamma} \) is chosen equal to 1 c\(^{-1}\).

If the \( z \) axis is oriented so that the pressure increases with increasing \( z \), then the fluid will flow in the direction of negative \( z \) values, and the shear rate is positive for all \( r \) values. Therefore, the sign of the absolute value in equation (6) may be omitted. Substituting (3) in (2), we obtain the following equation:

\[
\frac{\partial \sigma}{\partial z} = \frac{\eta_0}{r} \frac{\partial}{\partial r} (r \dot{\gamma}^n)
\]
Integrating equation (7), we obtain the following:

\[ \dot{\gamma} = \frac{\partial \nu_z}{\partial r} = \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \frac{1}{r} - \frac{c_1}{r} \quad (8) \]

Given the initial conditions, namely, that the shear rate on the axis of the pipe should be zero, we obtain that the integration constant \( C_1 \) is equal to 0.

Integrating equation (8), we obtain the following:

\[ \nu_z = \frac{n}{n+1} \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \frac{1}{r} R \frac{n+1}{n} + C_2 \quad (9) \]

The integration constant \( C_2 \) is determined from the condition (4).

After calculating the integration constant \( C_2 \), the equation (9) takes the following form:

\[ \nu_z = -\frac{n}{n+1} \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \frac{1}{r} R \frac{n+1}{n} \left[ 1 - \left( \frac{r}{R} \right)^{n+1} \right] \quad (10) \]

The velocity on the axis of the pipe \( \nu_0 \) obtained by substituting \( r = 0 \) in equation (10) is determined by the following expression:

\[ \nu_0 = -\frac{n}{n+1} \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \frac{1}{r} R \frac{n+1}{n} \]

Then the velocity distribution equation can be written as follows:

\[ \nu = \nu_0 \left[ 1 - \left( \frac{r}{R} \right)^{n+1} \right] \]

In order to obtain the temperature distribution value, we substitute expressions (6) and (8) in equation (3). After a single integration, we get the following:

\[ \frac{\partial T}{\partial r} = -\frac{\eta_0}{k} \frac{n}{3n+1} A \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \left[ \frac{n+1}{n} R \frac{2n+1}{n} + C_3 \right] \quad (11) \]

In equation (11), the constant \( C_3 \) should be taken as being equal to zero, since the temperature gradient on the pipe axis is equal to zero. Integrating equation (11), we obtain the following:

\[ T = -\frac{\eta_0}{k} \left( \frac{n}{3n+1} \right)^2 A \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \left[ \frac{n+1}{n} R \frac{2n+1}{n} + C_4 \right] \quad (12) \]

The integration constant \( C_4 \) is calculated from the initial condition (5), where \( T_w \) is the temperature of the extruder forming channel wall. Then, from the expression (12) we find:

\[ T - T_w = \frac{\eta_0}{k} \left( \frac{n}{3n+1} \right)^2 A \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \left[ \frac{n+1}{n} R \frac{2n+1}{n} + C_4 \right] \quad (13) \]

The temperature difference of the fluid on the axis of the forming channel of the extruder and on the wall is obtained by substituting \( r = 0 \) in equation (13) and is determined by the following expression:

\[ T_0 - T_w = \frac{\eta_0}{k} \left( \frac{n}{3n+1} \right)^2 A \left( \frac{1}{2\eta_0} \frac{\partial \rho}{\partial z} \right) \left[ \frac{n+1}{n} R \frac{2n+1}{n} \right] \]

Therefore, equation (13) can be written in equivalent form:

\[ \frac{T - T_w}{T_0 - T_w} = 1 - \left[ \left( \frac{r}{R} \right)^{n+1} \right] \]

Thus, the melt flow rates of the biopolymer and the temperature changes are determined.

3. Conclusion
Improving the theory and methods of calculating extrusion technology ensures optimal design of the main components of the apparatus for obtaining finished products of the required quality level and a stable flow of the process. Thus, there is a need for mathematical modeling of the extrusion process, which is widely used in the modern world.

As a result of the study, an analytical solution is obtained for a mathematical model of the flow of an incompressible non-Newtonian fluid, the viscosity of which is assumed to be subject to a power law in the forming zone of a single-screw extruder, considered in a particular case. Using the obtained equations, it is possible to determine the values of the melt flow rate of the biopolymer and the temperature in the cross sections of the extruder forming channel, and thereby to justify the optimal operating modes of the apparatus for producing homogenized product with required quality indicators, as well as to select the most rational geometry of the forming channel of the extruder die.

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