The mathematical models and program complex for synthesis of reciprocating extruders with adjustable configurations

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Abstract. The program complex which enables solving tasks of structural and parametrical synthesis of reciprocating extruders with adjustable configurations has been developed. The complex includes modules for extruder brand choice, assembly and visualization of 3D model of extruder screw, calculation of geometrical parameters of elements and sections of assembled screw configurations, synthesis of a mathematical model of extrusion, and calculation of its output parameters. The complex is configured to various types of polymeric films, as well as throughput and energy consumption requirements. The combined modeling method is implemented by the complex. It consists of synthesis of a static model for calculation of polymeric material state parameters, extruder throughput and energy consumption, indices of extrudate quality and a dynamic model for calculation of average residence time. Calculation results are visualized in the form of 3D graphs of criterion indices’ dependence on controlling influences. The complex is an effective tool for helping production personnel determine screw configurations and extruder regime parameters, ensuring required extrudate quality when performing restrictions for throughput and energy consumption for various types of films.

1. Introduction
The current state of world market of packing materials is characterized by strengthening of competition and toughening of ecological requirements. It leads to continuous growth of the output of rigid films on the basis of polypropylene (PP), polyvinylchloride (PVC), low density polyethylene (LDPE), etc. Already now the output exceeds 2.5 million tons per year. At the same time the steady tendency of growth by 5–7 % annually is observed. More than 50 % of rigid films are used for packing of pharmaceutical medicines (15 %) and foodstuff (38 %) that defines essential increase in requirements to their quality.

The main way of flat rigid polymeric films production is the extrusion-calender method. This method in comparison with an extrusion method is characterized by high throughput, wide range of thickness and flexibility of change-over on the new thickness and width of polymeric film. The method consists in preparation of the homogeneous plastic substance (extrudate) in the screw mixer and kneader (extruder) and further formation of this substance in polymeric film on multiple-roll calender. Therefore consumer characteristics of polymeric film substantially depend on extrudate quality — thermal condition and degree of uniformity. According to experts, up to 30 % of film surface defects arise at stage of extrudate preparation. The least acceptable
of these defects for consumers are impurities of unmelted polymer, yellow, brown destruction strips, black points, unevenness of coloring and deviation of color from standard (for colored films).

Productions of polymeric films are multi-assortment. They are characterized by incompleteness of information on direct indices of extrudate quality. Besides, there are no program complexes allowing to predict quality on the basis of mathematical models and to form the relevant advice to production personnel on change-over of production lines on new tasks and also on quality control in the mode of product manufacture. As a result operators are forced to make control decisions on the basis of subjective visual evaluation of surface condition and color of extrudate pieces coming to feeding calender gap. At the same time they are based on experimentally determined production procedures and own know-how. Change-over time upon transition to new type of polymeric film is 30 min, upon transition to new color — up to 3 h. With growth of change-over time the throughput decreases, the share of spoilage and returnable waste increases.

Extruders of different types are used to preparation of the extrudate in the modern productions of polymeric films. They differ in number of screws (single-screw and twin-screw, planetary-roller extruders) and nature of their motion (rotational, simultaneous rotational and reciprocating motion). But hardware flexible reciprocating extruders are widely used (approximately in 60 % of the extrusion-calender lines). They are the most difficult from the point of view of product quality control. This type of extruders is characterized by high throughput (up to 3000 kg h\(^{-1}\)) and big expenditure of energy (power consumption more than 1000 kW). The kinematic feature of reciprocating extruders is that the screw along with rotation makes axial reciprocating motion. At the same time one complete revolution around an axis corresponds to one reciprocal stroke. Origin of backflows of polymeric material in the extruder intensifies melting and mixing of material, promoting increase in homogeneity of extrudate. On the other hand, residence time of the polymeric material which is characterized by low thermal stability increases. It leads to growth of material destruction danger in case of high temperatures in the extruder and also to increase in transition time from one processed material to another and time necessary for the extruder cleaning. The screw of extruder has variable modular configuration [1]. It is assembled from elements of different types that enables adjusting extruder to different types of polymeric materials, but also complicates quality control of polymeric films.

The complexity of extrusion is caused by the hardware flexibility of reciprocating extruders, existence of backflows of polymeric material owing to reciprocation of screw and hydraulic resistance of extrusion head, existence of different physical processes (heating, melting, mixing of the material moving in the screw channel), coexistence of solid phase and melt of material, nonlinearity of rheological properties of melt, heat exchange of material with barrel and screw of the extruder. Therefore task solution of computer-aided structural and parametrical synthesis of reciprocating extruders in case of design and control of multi-assortment polymeric films productions requires an integrated approach. Such approach is based on knowledge of main extrusion features, configurations of extruders, the modes of their functioning and application of methods of mathematical modeling and computer technologies [2].

The mathematical models (MM) of polymeric materials processing in reciprocating extruders described in literature are determined and constructed on the basis of laws of physical substances conservation (mass, pulse, energy) and rheology [3, 4]. They allow to calculate distributions of flow velocities, distributions of viscous friction stresses in flows, distributions of pressure and temperature of melt as in channels of separate screw elements of different types, and in channel of modular screw. These models adequately describe object only in narrow area of functioning owing to accepted assumptions, for example, about Newtonian behavior of melt and isothermal nature of process [5], smallness of melt leakages [6], absence of screw reciprocation [7]. Models, as a rule, are implemented using simulation software (for example, Polyflow) which enables
solving investigation tasks preferentially, has difficult user interface for production personnel, is closed system, has high cost of procurement and maintenance.

Any of models does not describe melting in reciprocating extruders. At the same time melting determines extrusion velocity, energy consumption of extruder and has strong influence on quality of extrudate and quality of polymeric film (impurities of unmelted polymer are one of polymeric film defects which are least acceptable for consumers). Experimental studies have shown that in reciprocating extruders transition of polymer to viscous-flow state proceeds on the dispersed solids melting mechanism with formation of two-phase polymer system “solid particles (dispersed phase) — melt (dispersive phase)” [8]. It is promoted by reciprocating motion of screw and kneading pins in internal wall of extruder barrel.

Approaches to evaluation of residence time in extruders have been proposed. In work [9] the model of reciprocating extruder is constructed by combination of ideal hydrodynamic models (continuous stirred tank reactor model, tanks-in-series model, plug flow reactor model). Each ideal model describes the screw section made of elements of one type. The model type choice is defined by type of functional zone of extruder in which the section is situated, and intensity of polymeric material mixing in the section. The mixing intensity depends on number of axial cuts in flights of the section elements and number of kneading pins of extruder barrel adjacent with the section. Backflows are modeled by recycling flows. In work [10] it is proposed to describe each section of extruder screw by tanks-in-series model with various number of cells (continuous stirred tank reactors) regardless of elements types of which the section consists, and the section arrangement in functional zone of reciprocating extruder.

However there is no modeling method allowing to give complex evaluation of extrudate quality, throughput and energy consumption of reciprocating extruders depending on controlling influences for various types of polymeric materials taking into account both the main regularities of extrusion, and the complex construction of reciprocating extruders.

In this regard the purpose of this work is to solve urgent task of development of the flexible program complex allowing on the basis of multivariant (information, mathematical) models to carry out structural and parametrical synthesis of the reciprocating extruders used in multi-assortment productions of polymeric films. Such synthesis consists in formation of configuration of modular screw and determination of regime parameters values of extruder ensuring the required indices of extrudate quality when performing restrictions for throughput and energy consumption of extruder for various types of polymeric materials. The program complex is intended for solution of change-over tasks of operating extrusion-calender lines (as the decision support system of production personnel) and design tasks of new hi-tech productions of polymeric films taking into account requirements for resource- and energy saving.

2. Structure of program complex. Combined method for modeling of extrusion

The analysis of configurations of screws and geometrical parameters of reciprocating extruders, properties of polymeric materials, technological regimes of extrusion, characteristics of extrudate has allowed to propose the information description of reciprocating extruder as object of synthesis, shown in figure 1 in form of set of vectors of input parameters \(X\), varied parameters \(V\) and output parameters \(Y\). This description is basis for development of program complex.

Bulk polymeric material of type \(T_{\text{polym}}\) with initial pressure \(P_0\) and temperature \(T_0\) is moved by the screw of feed hopper 1, rotating with speed \(N_h\), to the channel of the modular screw of extruder 2 of brand \(M_{\text{extrud}}\). The screw has diameter \(D\), length \(L\), configuration \(C_{\text{scr}}\) and consists of \(N_e\) elements. The type of each element \(T_i^j\) corresponds to one of common types: element with continuous flights (SC) 4; conveying element (EZ) 5; kneading element (KE) 6; restriction ring adapter (ST) 7 with restriction ring 10. Elements of various types differ in geometrical parameters (number of flights, number of axial cuts in flights 3, number of kneading pins in extruder barrel 8 with which flights 9 interact). Therefore various elements have different
degree of strain influence on polymeric material. It enables carrying out structural adjustment of extruder (by variation of screw configuration) on various types of polymeric materials. The screw rotates with speed \( N \), at the same time during each turn (operating cycle) being displaced in axial direction at first towards extrusion head (die) at stroke \( S_0 \), and then coming back to starting position. Temperature condition of extruder work is implemented by zoned heating of the barrel by the heat transfer agent 12 (as a rule, oil) up to temperature \( T_{b k} \) in each of \( n_T \) thermal zones and cooling of the screw with the water 13 circulating in channel 11 up to temperature \( T_{\text{scr}} \). At movement in screw channel the solid polymeric material heats up, transits to viscous-flow state, resulting melt heats up, mixes up and is pressed through openings of die as extrudate 14, being feed for calender. Sources of heating are: the viscous heat generation in the polymer melt; the heat conducted into the screw channel (through extruder barrel).

Output parameters of extrusion are parameters \( S \), characterizing state of solid phase (particle radius \( R^s_j \), volume fraction \( \phi^s_j \), temperature \( T^s_j \)) and melt (velocity of cross-channel flow \( v^i_{\text{mx}} \), velocity of down-channel flow \( v^d_{\text{mx}} \), pressure \( P^m_{\text{in}} \), temperature \( T^m_{\text{in}} \), viscosity \( \eta^j \)) of polymeric material, and criterion indices. Criterion indices characterizing efficiency of extrusion are throughput \( G \), specific energy consumption \( E \), average residence time in extruder \( \bar{\tau} \) and indices of extrudate quality \( Q_{\text{ext}} \) which depend on residence time. For quantitative evaluation of extrudate quality are proposed: average degree of mixing \( \bar{\gamma} \); index of thermal destruction \( I_d \). Average degree of mixing characterizes material uniformity of extrudate. It is determined by total shear strain which is accumulated in all small volumes of polymeric material during their residence in extruder. Index of thermal destruction characterizes degree of irreversible changes in polymeric material under influence of high temperature during residence in extruder:

\[
I_d = \frac{\bar{\tau}}{\tau_d} \exp \left[ \frac{E_d (T_{\text{ext}} - T_d)}{8.31 \left( T_{\text{ext}} + 273 \right) \left( T_d + 273 \right)} \right] 100, \tag{1}
\]

where \( \tau_d \), \( T_d \) — time (s) and temperature (°C) of beginning of changes of polymeric material color at destruction; \( E_d \) — activation energy of destruction (J mol\(^{-1}\)); \( T_{\text{ext}} \) — extrudate temperature (°C).

On the basis of the information description the task of structural and parametrical synthesis
of reciprocating extruder is formulated: at change-over of production line on new operations assignment $Y_0 = \{T_{\text{film}}, G_0, E^{\max}\}$: to choose extruder brand $M_{\text{extrud}}$ and to form procedural ranges of controlling influences on extruder $[U^{\min}, U^{\max}]$ for production of extrudate with throughput $G \geq G_0$ and specific energy consumption $E \leq E^{\max}$ from polymeric material of type $T_{\text{polym}}$; to create screw configuration $C_{\text{scr}}$ and to determine values of controlling influences on extruder $U \in [U^{\min}, U^{\max}]$, which provide extrudate of required quality $\gamma \geq \gamma^{\min}$, $I_d \leq I_d^{\max}$, guaranteeing observance of the customer requirements to the corresponding characteristics of quality of polymeric film surface, where $T_{\text{film}} = \{T_{\text{polym}}, n_{\text{umelt}}^{\max}, n_{\text{black}}^{\max}\}$ — film type; $n_{\text{umelt}}^{\max}$, $n_{\text{black}}^{\max}$ — maximum numbers of unmelted particles and black points on $10 \text{ m}^2$ of film surface depending on film destination; $G_0$ — throughput of the extrusion-calender line $(\text{kg s}^{-1})$; $E^{\max}$ — maximum specific energy consumption $(\text{J kg}^{-1})$; $R_{\text{conf}}$ — set of admissible configurations of the screw; $\gamma^{\min}$ — minimum degree of mixing at which uniform free from unmelted particles melt turns out (that guarantees, in particular, uniformity of film coloring) (shear unit); $I_d^{\max}$ — maximum index of thermal destruction depending on requirements to number of black points (%).

The solution of task of industrial reciprocating extruders synthesis by practical consideration without application of methods and technologies of computer modeling is led to big expenses of expensive material and energy resources, essential increase in time of change-over of the extrusion-calender lines. Therefore the problem-oriented program complex including information, geometrical, functional models of extruders and being the tool for synthesis of reciprocating extruders has been developed. Its functional structure is shown in figure 2.

The program complex includes subsystem for structural synthesis and subsystem for parametrical synthesis. These subsystems interact with the data bank including the database (DB) of geometrical parameters and 3D models for functional elements of reciprocating extruders, DB of types of films, physical properties of polymeric materials and requirements to extrudate quality, DB of technological parameters of extrusion. The interface allows the operator of the extruder to adjust program complex to type of film, requirements to throughput and energy consumption, to input extruder screw configuration and controlling influences.

The choice of extruder brand is carried out from the DB of equipment on the basis of rules for the choice. The set of brands of extruders $R_{\text{mark}}$ is formed, each of which is admissible for processing of given type of polymeric material $T_{\text{polym}}$ at production of film with required throughput $G_0$ and energy consumption which is not exceeding maximum energy consumption $E^{\max}$. Rules for the extruder brand choice have been formed as productional rules of type "IF condition, THEN consequence". At the validity of condition the consequence is accepted. Example of the rule: IF $T_{\text{polym}} = "\text{PP}" \land G_0 = 1500 \text{ kg h}^{-1} \in [800 \text{ kg/h}; 2500 \text{ kg/h}] \land E = 1500 \text{ kJ kg}^{-1} < E^{\max} = 2700 \text{ kJ kg}^{-1}$, THEN $M_{\text{extrud}} = \{D = 0.2 \text{ m}, L = 2.2 \text{ m}, S_0 = 0.03 \text{ m}\}$.

For the extruder brand chosen by the operator $M_{\text{extrud}} \in R_{\text{mark}}$ in the virtual designer the computer-aided assembly of 3D model $M_{3Dscr}$ for the screw of given configuration $C_{\text{scr}}$ is carried out. The language of design has been developed for this purpose. Elements of the language are virtual models for screw elements of various types, and operations of the language are choice, placement, removal. The operations are carried out with the virtual models. The 3D scene with the 3D model for the screw core located in it is automatically created. Assembly of virtual model for the screw is similar to assembly of the real screw. Every time the operator chooses 3D model for the screw element of the required type from DB and places it on 3D model for the screw core, packing with 3D model for the previous element. At the same time the current total length of the grouped elements which should not exceed screw length $L$ is checking. Length of each attached element $L_j$ is determined from DB of geometrical parameters depending on its type $T_d^j$ and screw diameter $D$. Assembly is carried out by means of rules for placement and packaging. These rules allow to place and pack 3D model for chosen $(j + 1)$-th element
Figure 2. Functional structure of program complex for synthesis of reciprocating extruders.

with 3D model for already placed j-th element, if type of the chosen element \(T_{j+1}\) belongs to set of admissible types for packaging with jth element of the screw. Besides, the condition of conjugation of screw elements on height of their channels has to be satisfied: \(H_{\text{in}}^{j+1} = H_{\text{out}}^{j}\), where \(H_{\text{in}}^{j+1}\) — height of the channel at entrance in \((j+1)\)-th element (m); \(H_{\text{out}}^{j}\) — height of the channel at exit from j-th element (m).

The configuration of the screw created on the basis of the rules for placement and packaging is admissible: \(C_{\text{conf}} \in R_{\text{conf}}\). For it set of element parameter values of the screw \(\Gamma_{e} = \{L_{j}, B_{j}, z_{j}, e_{j}, H_{\text{in}}^{j}, H_{\text{out}}^{j}, \delta_{0}, m_{j}, s_{j}\}, j = 1 \ldots N_{e}\) and the die \(T_{\text{die}}\) is formed from DB of geometrical parameters. Here \(B_{j}\), \(e_{j}\) — pitch and width of flights (m); \(z_{j}\) — number of flights; \(\delta_{0}\) — radial clearance (m); \(m_{j}\) — number of axial cuts in flights; \(s_{j}\) — cut width (m).

The scheme of screw element with continuous flights is shown in figure 3.

The formed parameters are used for calculation of geometrical parameters of channels of
elements $\Gamma_{\text{ch}}^j = \{\varphi^j, Z_e^j, H^j, W^j, V_c^j, Z_s^j\}$ (they are calculated by use of analytical geometrical model for the channel developed at assumption about trifle of the channel curvature) and sections $\Gamma_{\text{st}}^i = \{Z_{\text{st}}^i, V_{\text{st}}^i\}, i = 1 \ldots N_{\text{st}}$ of the screw:

$$\varphi^j = \arctan\left(\frac{B^j}{\pi D}\right), Z_e^j = \frac{L_e^j}{\sin \varphi^j}, H^j = H_{\text{in}}^j - \left(H_{\text{in}}^j - H_{\text{out}}^j\right) \frac{z}{Z_e^j}, 0 \leq z \leq Z_e^j,$$

$$W^j = \left(B^j - z_e^j e^j\right) \frac{\cos \varphi^j}{z_e^j}, V_c^j = 0.5 \left(H_{\text{in}}^j + H_{\text{out}}^j\right) W^j Z_e^j, Z_s^j = m^s s^j,$$

(2)

$$Z_{\text{st}}^i = \sum_{j=1}^{N_e^i} Z_e^j, V_{\text{st}}^i = \sum_{j=1}^{N_e^i} V_c^j,$$

(3)

where $\varphi^j$ — pitch angle (rad); $Z_e^j$ — channel length (m); $H^j$ — height depending on down-channel coordinate $z$ (m); $W^j$ — width (m); $V_c^j$ — volume (m$^3$); $Z_s^j$ — width of through channels in flights (m); $N_e^i$ — number of elements of one type; $N_{\text{st}}$ — number of sections in the screw.

Thus, the subsystem for structural synthesis forms a vector of values of geometrical parameters $\Gamma_{\text{extrud}}$ of the extruder of chosen brand $M_{\text{extrud}}$, including parameters $\Gamma_{\text{scr}} = \{z_e^j, e^j, \delta_0^j, \Gamma_{\text{ch}}^j, j = 1 \ldots N_e, \Gamma_{\text{st}}^i, i = 1 \ldots N_{\text{st}}\}$ of the screw of created configuration $C_{\text{scr}}$ and parameters of the die $\Gamma_{\text{die}}$.

These data are transferred to subsystem for parametrical synthesis. Kernel of the subsystem is MM of extrusion which is adjusted to configuration of screw and type of polymeric material. For creation of such model the combined method has been proposed. It consists in synthesis of static model for calculation of polymeric material state parameters, throughput and energy consumption of extruder, indices of extrudate quality and dynamic model for calculation of average residence time in extruder [11]. Kernel of static model is the basic model describing the movement, heating, melting of polymeric material in the channel of element, representing the system of the equations constructed on the basis of laws of conservation and rheology and allowing to calculate distributions of state parameters of material phases on the channel of element.
the equations for calculation of radius and temperature of the solid phase particles
\[
\rho_s c_{\text{ms}}^j \frac{dR_s^j}{dz} = -\varphi_s \xi_{\text{ss}-m}^j, \quad z^{j-1} \leq z \leq z^j + Z_s^j; \tag{4}
\]
\[
\varphi_s \rho_s c_{\text{ms}}^j \frac{dT_s^j}{dz} = \varphi_s \xi_{\text{ss}-m}^j (T_s^j - T_s^j_T) - \varphi_s \xi_{\text{s}-m}^j c_s (T_s^j - T_s^j_T); \tag{5}
\]
the equations for calculation of flow velocities, pressure and temperatures of the melt
\[
\int_0^{H^j} v_{\text{mix}}^j dy = \dot{Q}_s^j + Q_s^j, \quad W^j \int_0^{H^j} v_{\text{mix}}^j dy = Q^j, \quad Q = z^j Q^j - (Q_s^j + Q_s^j); \tag{6}
\]
\[
\frac{\partial P_m^j}{\partial x} = \frac{\partial}{\partial y} \left( \eta^j \frac{\partial v_{\text{mix}}^j}{\partial y} \right), \quad \frac{\partial P_m^j}{\partial z} = \frac{\partial}{\partial y} \left( \eta^j \frac{\partial v_{\text{mix}}^j}{\partial y} \right), \quad 0 < y < H^j; \tag{7}
\]
\[
(1 - \varphi_s^j) \rho_m c_{\text{pm}} v_{\text{mix}}^j \frac{\partial T_m^j}{\partial z} = \lambda_m \frac{\partial^2 T_m^j}{\partial y^2} - \varphi_s \xi_{\text{s}-m}^j (T_m^j - T_s^j) - \varphi_s \xi_{\text{s}-m}^j c_p (T_m^j - T_s^j) + \eta^j \left[ \left( \frac{\partial v_{\text{mix}}^j}{\partial y} \right)^2 + \left( \frac{\partial v_{\text{mix}}^j}{\partial y} \right)^2 \right], \quad z^{j-1} \leq z \leq z^j + Z_s^j; \tag{8}
\]
the equation for calculation of viscosity of the two-phase system "solid particles | melt" 
\[
\eta^j = \mu^j \left[ \left( \frac{\partial v_{\text{mix}}^j}{\partial y} \right)^2 + \left( \frac{\partial v_{\text{mix}}^j}{\partial y} \right)^2 \right]^{(n-1)/2}; \tag{9}
\]
the equation for calculation of specific rate of melting \( \xi_{\text{s}-m}^j \) (Stefan condition)
\[
\alpha_{\text{m}}^j (T_m^j - T_s^j) = \alpha_s^j (T_s^j - T_s^j_T) + \xi_{\text{s}-m}^j [(1 - h_p) c_s (T_s^j - T_s^j_T) + h_j]; \tag{10}
\]
boundary conditions at entrance in the channel of the element
\[
z = 0: \quad R_s^1 = 0.5 d_s, \quad v_s^1 = \varphi_s^0, \quad T_s^1 = T_0, \quad P_m^1 = P_0, \quad T_m^1 = T_s^j - T_s^j_T, \quad j = 1; \tag{11}
\]
\[
z = z^{j-1}: \quad R_s^j = R_s^j_{\text{out}}, \quad v_s^j = v_s^{j-1}, \quad T_s^j = T_s^{j-1}_{\text{out}}, \quad P_m^j = P_m^{j-1}_{\text{out}}, \quad T_m^j = T_m^{j-1}_{\text{out}}, \quad j = 2 \ldots N_e; \tag{12}
\]
boundary conditions at bottom and cover of the channel
\[
y = 0: \quad v_{\text{mix}}^j = 0, \quad v_{\text{mz}}^j = 0, \quad -\lambda_m \frac{\partial T_m^j}{\partial y} = q_{\text{scr}}; \tag{13}
\]
\[
y = H^j: \quad v_{\text{mix}}^j = \pi N \left( -D \sin \varphi^j + S_0 \sin \varphi_{\text{osc}} \cos \varphi^j \right), \quad v_{\text{mz}}^j = \pi N \left( D \cos \varphi^j + S_0 \sin \varphi_{\text{osc}} \sin \varphi^j \right), \quad -\lambda_m \frac{\partial T_m^j}{\partial y} = q_{bk}, \quad k = 1 \ldots n_{\Gamma}, \tag{14}
\]
where \( \rho_s, \rho_m \) — densities of solid phase and melt (kg m\(^{-3}\)); \( v_{\text{mix}}^j \) — average velocity of down-channel flow (m s\(^{-1}\)); \( z, y \) — cross-channel and normal coordinates (m); \( z^{j-1} \) — coordinate of entrance in the channel (m); \( c_s, c_{\text{pm}} \) — average specific heats of solid phase and melt (J kg\(^{-1}\)°C\(^{-1}\)); \( \varphi_s^j \) — particle surface area (m\(^2\)); \( \alpha_s^j \) — heat transfer coefficient from surface
into particle (W m$^{-2}$ °C$^{-1}$); $T_{k-m}$ — melting temperature (°C); $\dot{Q}_s^j + \dot{Q}_d^j$ — total intensity of leakages through clearance $\delta_s^j$ and axial cuts $s^j$ (m$^2$ s$^{-1}$); $\dot{Q}^j$ — flow rate in the channel without leakages (m$^3$ s$^{-1}$); $Q$ — flow rate in extruder determining throughput (m$^3$ s$^{-1}$); $\dot{Q}_s^j + \dot{Q}_d^j$ — total flow rate of leakages (m$^3$ s$^{-1}$); $\lambda_m$ — thermal conductivity of melt (W m$^{-1}$ °C$^{-1}$); $\alpha_m$ — heat transfer coefficient from surrounding melt to surface of particles (W m$^{-2}$ °C$^{-1}$); $F_{\rho}^{\phi} = f_{\rho}^e (\varphi_{s}^j)$ — correction factor considering increase in energy dissipation; $\mu^j$ — consistency index (Pa s$^n$); $n$ — power law index; $h_p$ — coefficient allowing to adjust MM to polymer class; $r$ — melting enthalpy (J kg$^{-1}$); $d_s$ — average equivalent diameter of solid particles (m); $\varphi_{c0}$ — initial volume fraction of solid phase; $R_{s,out}^{j-1}$, $\varphi_{s,out}^{j-1}$, $T_{s,out}^{j-1}$, $P_{m,out}^{j-1}$, $T_{m,out}^{j-1}$ — state parameters of material phases at exit from the channel of $(j-1)$-th element; $q_{ext}$, $q_{hk}$ — densities of heat fluxes from polymeric material to screw and from $k$-th thermal zone of barrel to polymeric material (W m$^{-2}$); $\Phi_{osc} = f_N (N)$ — oscillation phase (rad).

At creation of basic model the assumptions about inverse motion of extruder barrel and screw, trifle of curvature of the channel of screw, stationarity of extrusion, steady down-channel movement of polymeric material, independence of thermal properties of material phases on temperature and pressure have been accepted. The concentrated suspension which is formed when melting polymeric material is considered as monodisperse system. Particles of dispersed phase of the suspension are not deformable spheres. Interaction and collisions between particles are negligible; there are no processes of their crushing and adhesion. Therefore the number of particles remains constant (numerical volume concentration of dispersed phase $n_0$ is constant), and reduction of a fraction of solid phase is consequence of particles radius reduction at polymer melting. Particles do not move and do not rotate relatively melt. Influence of cross-channel movement on temperature of particles is negligible. The heat transferred from melt to solid phase is equally distributed between all particles therefore melting rate in all points of surface of each particle is identical. Melt is incompressible inelastic liquid; there are no radial flow, inertial and mass forces, temperature gradient in cross-channel flow, sliding of melt on the channel walls. Along normal coordinate heat transfer by conductivity prevails.

Program synthesis of structure of static model $S_{st}$ includes the following stages:

— the choice (from library of MM) of the equations for calculation of flow rates of leakages $Q_s^j, Q_d^j$ (depending on element type $T_{s}^j$), the equations for calculation of densities of heat fluxes $q_{ext}$, $q_{hk}$ (depending on temperature condition of extruder work), the equations for calculation of consistence index $\mu^j$ (depending on polymer class);

— packaging of chosen equations with the equations of basic model (4)–(10) for formation of structure of models which describe the movement and heat transfer of polymeric material in channels of elements of various types making the extruder screw;

— packaging of constructed MM of elements of all types according to configuration of the screw and at observance of conjugation conditions (12).

Parametrical setup of static model $K_s$ includes formation of physical property values $H_{polym} = \{d_s, \rho_s, c_s, T_{k-m}, r, \rho_m, n, c_{polym}, \lambda_m, \tau_d, T_d, E_d\}$ (from DB of polymeric materials) and heat transfer coefficients (from library of MM) depending on polymeric material type $T_{polym}$.

The structure of dynamic model $S_{md}$ is synthesized by packaging of hydrodynamic models describing flows in the channel sections. In the model recycling flows describing backflows are introduced between zones. The library of hydrodynamic models includes plug flow reactor model (describes extruder feed zone sections), continuous stirred tank reactor model (describes sections of zones of melting and mixing), tanks-in-series model (describes melt conveying zone sections). Parametrical setup of dynamic model $K_d$ includes formation of coefficients values of dependences of recycling ratio and degree of the channel fill on controlling influences.

The solution of the equations of static model enables calculating the work point of extruder determining throughput $G$. The computing procedure including external and internal iterative
cycles has been realized for this purpose. In external cycle calculation of flow rate $Q$ determining extruder throughput is carried out. In internal cycle there is calculation of flow rate $Q^i_j$ in the channel of each element which in the presence of leakages from the channel ensures given flow rate $Q$ in external cycle. At each new value of flow rate $Q$ the flow rates $Q^i_j$ and distributions of state parameters along length of each screw element are calculated. The calculation is carry out taking into account conditions at entrance in the channel (11) and conditions of conjugation of elements (12). For this purpose the equations (4)–(10) taking into account boundary conditions (13), (14) are solved. For the solution of the equations (4), (5) Runge–Kutta method is used. For the solution of the equations (6)–(8) the computing scheme based on the theory of flat asymmetrical flows in non-isothermal conditions is used [11]. The end of melting is determined by disappearance of solid phase when the volume fraction of particles in suspension keeps within limits of admissible error of calculation. The corresponding down-channel coordinate remains and on its basis melting zone length is determined. The external cycle proceeds, the condition of conjugation of screw and die determining equality of pressure at exit from the channel of screw to pressure at entrance in the forming zone of die will not be satisfied yet.

With the calculated throughput the pulse characteristic of extruder is determined by dynamic model. The finite difference Lax–Wendroff method (the equations of plug flow reactor model) and Runge–Kutta method (the equations of continuous stirred tank reactor model and tanks-in-series model) are used to solve the model equations. On the basis of the pulse characteristic the average residence time $\bar{\tau}$ is calculated by use of moments method.

On the basis of residence time and state parameters $S$ the indices of extrudate quality $\bar{\gamma}, \, I_d$ are calculated depending on controlling influences $U$, varied in the procedural ranges $[U^\min; U^\max]$, formed from DB of technological parameters. The analysis of 3D graphs of these dependences allows us to determine admissible values of controlling influences on the extruder of brand $M_{extrud}$ with the screw of configuration $C_{scr}$. At the values of controlling influences restrictions for quality indices $Q_{ext}$, ensuring suitability of extrudate for formation on calender and lack of film defects over extrusion are observed.

The program complex has been developed using the following computer technologies: object-oriented programming environment Visual Studio; data manager SQLite; CAD system 3ds Max (for creation of 3D models for elements of screws); software for work with interactive 3D graphics Unreal Engine (for creation of the designer of virtual models for screws).

3. Results and discussion

Results of check have confirmed adequacy of MM (by Fisher criterion) and operability of the program complex for industrial and laboratory reciprocating extruders of various configurations when processing materials on basis of PP, PVC, LDPE. The results of work of the program complex are shown in figure 4 and figure 5: for industrial extruder of PR-200 brand ($D = 0.2 \, \text{m}, \, L = 2.28 \, \text{m}$), in which PVC is processed, the screw configuration is created, distributions of pressure and temperature of polymeric material along screw length are calculated, external characteristics of the screw and die and also dependence of the specific energy consumption on the controlling influences are constructed. The point of intersection of the external characteristics determines work point of extruder.

The analysis of the results of modeling allows us to determine the rational mode of functioning extruder of assembled configuration at which requirements to extrudate quality, throughput and energy consumption of extruder are fulfilled. For given example such analysis gives the following results: $N_h = 0.2 \, \text{s}^{-1}, \, N = 1.67 \, \text{s}^{-1}, \, T_b = 150 \, ^\circ\text{C}, \, \bar{\gamma} = 9374$ shear units ($\gamma^\min = 3000$ shear units), $I_d = 7.2 \% (I_d^\max = 10 \%), \, G = 982 \, \text{kg/h}.$
4. Conclusion
The method for mathematical modeling of polymeric materials processing in reciprocating extruders with adjustable configurations has been proposed. The method considers the main features of extrusion (reciprocation and modularity of the screw, phase transition and anomaly...
of viscosity of polymeric material, leakages, non-isothermal process, etc.) and allows us to calculate efficiency characteristics (throughput and energy consumption of extruder, indices of extrudate quality) depending on the process regime parameters.

The simulating program complex which allows us to solve tasks of screw configuration creation and determination of controlling influences on reciprocating extruders ensuring extrudate of given quality in case of observance of requirements to throughput and energy consumption has been developed. The complex is configured to different types of polymeric materials and geometrical characteristics of reciprocating extruders.

Use of the program complex in control system for extrusion in multi-assortment polymeric films productions allows us to increase their efficiency due to improvement of product quality, reduction of spoilage, resource- and energy saving, decrease in change-over time of production lines. The program complex can be used (in case of the appropriate extension of DB, bases of rules and libraries of MM) for control of extruders in similar hi-tech productions (for example, productions of linoleum, foam plates, sorbents and catalytic agents).

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