Hybrid computer modeling system of extrusion processes for quality control of multi-assortment polymeric films

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Abstract. A hybrid computer modeling system of extrusion processes has been developed, which includes mathematical models of various types. The system helps operators to solve the problems of quality control of multi-assortment polymeric films during change-over of production lines and in the mode of film production. The system includes a module for choice of extruder brands, a designer of virtual 3D extruder screw models, and modules for structural and parametric synthesis of mathematical models of extrusion processes and calculation of throughput, energy consumption of extruders, extrudate quality indices determining consumer characteristics of the film. The model library contains geometric models of screw elements of various types, static functional models of physical processes in channels of screw elements, empirical models of rheological properties of polymers, dynamic models for estimation of residence time, models for calculation of mixing degree, index of thermal destruction and color characteristics of extrudate. Static models have been developed on the basis of conservation and rheology laws. The method of synthesis of a cell-type hydrodynamic model with recycles has been developed. The system is adjusted according to the production method, the film type, throughput and energy consumption requirements. Modeling results are presented as tables, 2D and 3D graphs. Testing of the system according to the data of the productions of polyvinyl chloride and polyethylene films at plants in Russia, Germany has confirmed its operability.

1. Introduction

Modern productions of flat and blown packaging polymeric films for the food and pharmaceutical industry are multi-assortment systems. They are characterized by high throughput (more than 1000 kg h⁻¹), energy intensity, multiple and complex relationships between parameters of raw materials, equipment, technological regime and indices of process efficiency, as well as incomplete information on efficiency indices. Efficiency of production process is characterized by quality of polymeric film, throughput, energy consumption. Production lines realize various methods of making polymeric films: cast extrusion (for making flat films); blown extrusion (for making blown films); calendering (for making mainly polyvinyl chloride (PVC) flat films). The wide range of products is due to the many formulations of packaging polymeric films of different purpose, large ranges of thickness (0.025–1.20 mm) and width (up to 2.5 m), different requirements for consumer characteristics of films (especially the number of surface defects and color). Films are made of polymers of various types. The main film forming polymers are polypropylene (PP, 23 %), PVC (21 %), low density polyethylene (LDPE, 19 %) and polystyrene (PS, 19 %). Change-over of the line
to a new task according to the type of polymeric film and/or throughput takes place on average once a day. This significantly complicates the problem of quality control of polymeric films. As a result, the number of defects (black points, yellow-brown destruction strips, inclusions of unmelted polymer, gels) on the surface of the polymeric film and the deviation of the film color from the standard exceed the maximum permissible values. The maximum permissible values of the number of surface defects of each type (usually per 10 m² of polymeric film) and the color deviation of the film are set by quality standards (or specifications) depending on the purpose of the film. For example, the number of black points should not exceed 10 for a pharmaceutical packaging film and 20 for a food packaging film, and the number of holes should not exceed 3 for both a pharmaceutical and a food film. The respective section of the polymeric film is cut out and disposed of as non-returnable waste and the remaining sections of the film are welded. Non-returnable waste causes significant economic losses and reduced competitiveness of production. Therefore, it is necessary to develop problem-oriented computer systems to support the decision-making of managerial production staff. These systems are based on multivariate models of the control object description and help to ensure the required consumer characteristics of polymeric films, resource saving and energy saving at production.

Extrusion processes play a key role in the productions of polymeric films. In the extruders, the bulk polymer is converted into a uniform viscous flow mass (extrudate) from which the polymeric film is made. Extrusion processes are characterized by a variety of types and hardware flexibility (variable screw configurations and forming head types) of the extruders [1]. These processes determine both the consumer characteristics of the polymeric film (surface defects, color) and the safety of production. For example, up to 20% of the defects of the calendered polymeric films occur in the extrudate preparation stage. The appearance of black points and yellow-brown destruction strips on the film is a consequence of overheating and thermal degradation of the polymer in the extruder. Thermal degradation manifests itself in the breakdown of macromolecule chains and a sharp decrease in the molecular weight of the polymer. As a result, color of the extrudate changes (consistently on yellow, yellow-orange, orange-red, red-brown). In the calender production method, insufficient extruder throughput (starve feed of calender) results in an emergency situation associated with the impact of calender rolls [2]. The extrusion process is a complex object of control and is characterized by incomplete information on key characteristics (extruder throughput and direct extrudate quality indices, assessed by the operator only visually by the appearance of the extrudate).

The analysis of mathematical models of extrusion processes has showed that they are deterministic and include the equations of balances of mass, forces and heat for solid phase and melt, the rheological equation of melt and also the equations of interphase mass and heat balances (for description of melting). The melting mechanisms observed in extruders of various types are modeled: contiguous solids melting (melting of continuous solid phase – solid bed) [3–6]; dispersed solids melting [7, 8]. Models allow us to calculate the melting zone length, profiles of the solid bed width, pressure and temperature, profiles of thickness of the melt films which are formed at the barrel and screw surfaces (for contiguous solids melting), profiles of concentration and temperature of the solid particles (for dispersed solids melting), fields of flow velocities, viscous friction stresses in flows, pressure and temperature of the melt. The scope created by the mathematical models generally is limited to investigation of mass and heat transfer of polymers in extruders of separate types with classical geometry of the screw, in separate functional zones of the screw channel (solid polymer conveying [9], melting [10], melt conveying [11]) or in channels of separate elements of modular screws [12]. The mathematical models of extrusion processes, as a rule, are implemented in universal or problem-oriented software solutions for modeling (for example, ANSYS Polyflow [13], Ludovic [14] or Multiscrew System [15]). The practice of using the software solutions for modeling and investigation of various types of extrusion techniques, design of appropriate extrusion equipment types confirms their high efficiency and compliance with the level of modern production. However, the software solutions are only vaguely applicable to solving the extrudate quality control problems, as they do not allow calculating all characteristics of the extrudate quality (for example, thermal destruction degree, color characteristics), have complicated interfaces for production staff, all at a relatively high cost.
Approaches to assessment of average residence time of polymers in extruders of various types on which the extrudate quality depends have been developed. They are based on application as separate typical hydrodynamic models (for example, one-parameter axial dispersion model), and the difficult combined models of flows structure constructed on the basis of typical hydrodynamic models (plug flow reactor model, continuous stirred tank reactor model, tanks-in-series model) including with introduction of recycling flows [16]. Typical hydrodynamic models describe extruder zones with different mechanisms and intensities of mixing [17]. Recycles model back flows, in particular, the melt leakage arising owing to extruder head resistance. Thus, developed mathematical models of extrusion processes do not allow us to give a complex assessment of the extrudate quality, throughput and energy consumption of extruders in dependence on controlling actions for various types of polymers taking into account as main features of extrusion (polymer melting, melt viscosity anomaly, non-isothermal conditions), and difficult construction of extruders (screw modularity, leakages, possibility of screw reciprocation).

Thus, the development of a hybrid computer modeling system for extrusion processes, which is one of the elements of a computer control system for the production of polymeric films, is relevant. This system includes mathematical models of various types (geometric, functional, empirical) and helps managerial production staff to solve problems of resource saving, energy saving and safe control of lines for production of multi-assortment polymeric films.

Therefore, the objectives of this work are:

- development of a library of mathematical models for extrusion processes to give integrated estimation of throughput, energy consumption of extruders and quality indices of extrudate depending on controlling actions at various configurations of extruders and types of polymers;
- development of hybrid computer modeling system for determination of extruder configurations and controlling actions on extruders, which ensure specified extrudate quality guaranteeing required consumer characteristics of polymeric film.

2. Information description of the extrusion process as a control object. Statement of extrudate quality control problems

The information description of the extrusion process as a control object is shown in figure 1. It is the basis for the development of the modeling system and is built as a result of the analysis of structural and functional characteristics of extrusion processes in extrusion and calender productions of polymeric films.

Extruders are used in lines for making polymeric films of various types $T_{\text{film}}$. These lines realize different production methods $M_{\text{prod}}$ ($M_1$ is cast extrusion, $M_2$ is blown extrusion, $M_3$ is calendering). The type of produced film depends on the type of polymer $T_{\text{polym}}$ and quality requirements $Q_{\text{f}}$. Thickness $\delta_{\text{f}}$ and width $w_{\text{f}}$, maximum permissible number of black points $n_{\text{black}}$ max, inclusions of unmelted polymer $n_{\text{melt}}$ max and gels $n_{\text{gel}}$ max per 10 m$^2$ are specified indices of the polymeric film quality. If a color polymeric film is produced, the standard color coordinates of the film in CIELab space $L^*$, $a^*$, $b^*$ and maximum permissible deviation of color from standard $\Delta E_{\text{f}}$ max are further set. Brand of an extruder $M_{\text{extrud}}$ depends on the type of extruder $T_{\text{extrud}}$, diameter $D$ and length $L$ of the screw, parameters specific to extruder types (amplitude of screw reciprocation $S_0$, interaxial distance of screws $A_{\text{scr}}$), type $T_{\text{head}}$ and geometric parameters $T_{\text{head}}$ of the forming head.

Extruder types differ in number of screws $n_{\text{scr}}$ and the nature of their movement. Being applied:

- single-screw extruders ($E_1$), the screw of which only rotates (for $M_{\text{prod}} = M_1 \lor M_2$);
- reciprocating extruders ($E_2$), the screw of which simultaneously rotates and reciprocates axially with amplitude $S_0$ (for $M_{\text{prod}} = M_3$);
intermeshing co-rotating twin-screw extruders \((E_3, \text{for } M_{\text{prod}} = M_1)\) and intermeshing counter-rotating twin-screw extruders \((E_4, \text{for } M_{\text{prod}} = M_3)\).

**Figure 1.** Information description of the extrusion process as a control object.

The type of extruder head depends on the production method: cast head \((D_t)\) if \(M_{\text{prod}} = M_1\);
annular head \((D_2)\) if \(M_{prod} = M_2\); die \((D_1)\) if \(M_{prod} = M_1\). The set of geometric parameters of the head depends on the type of head. For example, for head of type \(D_1\) such parameters are thickness, width, and length of the forming gap. Values of the geometric parameters of the head in which the melt is formed directly into the film (heads of types \(D_1\) and \(D_2\)) depend on the specified thickness \(\delta_{st}\) and width \(w_{st}\) of polymeric film.

The solid polymer is fed into the channel of the screw typically cooled (with water or oil) to a temperature \(T_{scr}\). As it progresses through the screw channel, the polymer is heated and converted into a viscous fluid (melt). The melting mechanism depends on the type of extruder. Melting of continuous solid phase (solid bed) of the polymer by the Maddock–Street's mechanism takes place in extruders of type \(E_1\) [1, 3, 4, 6]. A melt film is formed at the surface of the solid bed in contact with the heated inner surface of the extruder barrel and flows into the screw channel displacing the solid bed. In most cases, the solid bed is pushed against the passive screw flight flank and the melt starts to accumulate in a melt pool between the solid bed and the active screw flight flank. Melting of individual polymer solids suspended in the melt occurs in extruders of types \(E_2–E_4\) [1]. Design of these extruders (kneading pins on the barrel surface of extruder of type \(E_2\), flights of the second screw in extruders of types \(E_3\) and \(E_4\)) interferes with formation of the solid bed [7, 8, 18]. Polymer melt is transported to forming head. The presence of melt leakage flows (through radial clearance between barrel surface and screw flights 2, axial cuts in screw flights 3, calender clearances 4 and side clearances 5) is the main feature of the melt conveying zone. The leakage flows are superimposed on the down-channel flow 1. Leaks result, on the one hand, in reduced extruder throughput and, on the other hand, in increased melt mixing intensity. This contributes to a more uniform (gel free) extrudate.

Variable parameters of the extrusion process are the modular screw configuration \(C_{scr}\) and the controlling actions \(U\) – the main controlling actions \(U_b\) and the additional controlling actions \(U_a\).

Extruder screw consists of \(N_e\) elements of various types \(T_{scr}^j\). The screw elements of different types differ in geometric parameters. Therefore, screw elements of different types have different transport and mixing capabilities and are used in different functional zones of an extruder. The main types of screw elements are:

- elements with continuous flights SC (with constant height of the channel) and SP (with decreasing height of the channel) for extruder of type \(E_1\);
- elements with interrupted flights EZ (single flighted element with one axial cut), KE (double flighted element with three axial cuts) and ST (combination of KE element and restriction ring) for extruder of type \(E_2\).

Linking screw elements of one type in screw section and combining screw sections of various types, it is possible to adjust an extruder for processing of various types of polymers.

The main controlling actions are screw speed \(N\) and temperature of each thermal zone of barrel \(T_{bi}\) (here \(n_t\) is number of thermal zones of barrel). In the production of color polymeric film, flow rates of liquid colorants \(G_{ci}\), \(i = 1…n_c\) (here \(n_c\) is number of colorants) are added to the main controlling actions.

The main disturbing actions of the extrusion process \(F\) include fluctuations in the quality of the feed to the extruder (in any production method) and fluctuations in the stock (level) of the extrudate in the calender feed gap \(\Psi_{ext}\) (if \(M_{prod} = M_3\)). Raw material quality fluctuations are caused by feed of returnable waste flow (crushed edges of produced polymeric film) at flow rate \(G_{wast}\).

The efficiency of the extrusion process is characterized by throughput \(G\), energy consumption \(E\), average residence time of polymer in extruder \(\tau_{av}\), extrudate temperature \(T_{ext}\) and extrudate quality indices \(Q_{ext}\). To evaluate the extrudate quality there have been offered:
• average mixing degree \( \gamma_{av} \) (average shear strain accumulated by polymer melt during residence time) and solids fraction \( \varphi_{ext} \), which characterize material uniformity of the extrudate;
• index of thermal destruction \( I_d \), describing the degree of irreversible changes in polymer under temperature and time influence on it;
• color coordinates \( L_{ext}, a_{ext}, b_{ext} \), color deviation from standard \( \Delta E_{ext} \) [19–21].

Analysis of the operating modes of the production system and the acting disturbances has allowed formulating the problems of extrudate quality control in the following modes:
• under change-over of the line that realizes specific production method \( M_{prod} \) to new production task \( \{P, G_T, S_{film}\} \);
• under polymeric film production (under the returnable waste \( G_{wast} \) and under the extrudate stock fluctuations \( \Psi_{ext} \)).

The problem of control under production line change-over is as follows:
to choose the extruder brand \( M_{extrud} \), create its screw configuration \( C_{scr} \) and determine the permissible values of the main controlling actions \( U_b \in \{U_{b_{min}}; U_{b_{max}}\} \), which ensure the required extrudate quality \( \gamma_{av} \geq \gamma_{av_{min}}, \varphi_{ext} \leq \varphi_{ext_{max}}, I_d \leq I_{d_{max}} \) under performance of restrictions for the extruder characteristics \( G \geq G_b, E \leq E^{max} \).

The problem of color control under polymeric film production is to determine the flow rates of liquid colorants \( U_c \in \{U_{c_{min}}; U_{c_{max}}\} \), which ensure that the extrudate color matches the standard \( \Delta E_{ext} \leq \Delta E^{max} \).

Here \( U^{min} = \{U_{b_{min}}, G_{i_{min}}, i=1...n_i\} \), \( U^{max} = \{U_{b_{max}}, G_{i_{max}}, i=1...n_i\} \) are procedural restrictions for the controlling actions. \( \Delta E^{max} = \Delta E^{max}_{f} \) if \( M_{prod} = M_1 \neq M_2 \); \( \Delta E^{max} = \Delta E^{max}_{ext} \) if \( M_{prod} = M_3 \). \( \Delta E^{max}_{ext} \) is the maximum deviation of the extrudate color from the standard determined depending on the film color requirement (\( \Delta E^{max}_{f} \)).

Implementation of requirements to mixing degree, solids fraction and thermal destruction index of the extrudate guarantees observance of restrictions for number of superficial defects of the polymeric film – gels, inclusions of unmelted polymer and black points respectively.

The multi-assortment nature of productions of polymeric films, many types and hardware flexibility of extruders, incompleteness of information on the extrusion process and the extrudate quality, complexity of relationships between control object parameters demand application of mathematical modeling methods and computer technologies for solution of the control problems.

3. Functional structure of hybrid computer modeling system. Library of mathematical models of extrusion processes
The functional structure of the hybrid computer modeling system of extrusion processes to solve the extrudate quality control problems is shown in figure 2.

The modeling system includes a module for choice of extruder brand and forming procedural ranges of controlling actions on it, a designer of virtual 3D models of modular extruder screws, modules for structural and parametric synthesis of mathematical models of extrusion processes and calculation of throughput, energy consumption of extruders, average residence time of polymers in extruders and extrudate quality indices. Modeling results are visualized as 2D and 3D graphs at the researcher interface.

The hybrid nature of the modeling system is due to the fact that the system contains in its structure multivariate models of extrusion process description. These are:
- mathematical models of screw elements and sections, polymers and physical processes in extruders;
- information models (relational databases of extrusion process characteristics);
- models of knowledge representation (bases of production rules for choice of hardware design of extrusion stage, assembly of virtual models of screws, structural and parametric synthesis of mathematical models of extrusion processes).

Figure 2. Structure of hybrid modeling system of extrusion processes (examples of module interfaces for choice of extruder brand, assembly of 3D model and calculating geometric parameters are shown in Russian, since the Russian version of the system has so far been developed).

For the task $S_M$ created by the researcher the set of extruder brands is formed on the basis of database of extruders and choice rules of hardware design of extrusion processes. Each extruder brand is acceptable for processing a given type of polymer $T_{polym}$ at production of polymeric film by preset method $M_{prod}$ with the required throughput $G_0$ and energy consumption not exceeding the maximum permissible value $E_{max}$. Example of the rule: IF $M_{prod} = M_1 \land T_{polym} = PVC \land G_0 = 900 \text{ kg h}^{-1} \in [800 \text{ kg h}^{-1}$;
\[ 2500 \text{ kg h}^{-1} \land E = 250 \text{ kJ kg}^{-1} < E_{\text{max}} = 360 \text{ kJ kg}^{-1}, \text{THEN } M_{\text{extrud}} = \{ L_{\text{extrud}} = 4.2 \text{ m}, D = 0.2 \text{ m}, L = 2.2 \text{ m}, S_p = 0.03 \text{ m}, T_{\text{head}} = D_{3}\}. \]

Assembly of 3D screw model \( M_{3\text{dscr}} \) for screw configuration \( C_{\text{scr}} \) based on assembly rules is carried out in the virtual model designer for the extruder brand \( M_{\text{extrud}} \) chosen by the researcher from formed set of extruder brands. Assembly rules of 3D screw model allow us to place and link the 3D model of the current screw element with the 3D model of the screw element already placed on the 3D model of the screw core, if certain conditions are met. These conditions require that the type of the current screw element belongs to set of valid types for linkage with the placed screw element and the screw elements mate in channel height [19]. If the placement and linkage rules are not executed, the 3D model of the current screw element is painted red. This indicates that the operation (placement, linkage) cannot be performed. In addition, during 3D screw model assembly the current total length of the placed screw elements is checked. It must not exceed the screw length specified by the extruder brand choice.

The mathematical model library allows us to implement a combined method of modeling extrusion processes. The method consists in structural and parametric synthesis of static and dynamic mathematical model of the extrusion process [19, 20]. A static model is necessary to calculate state parameters of the polymer solid phase and melt in the screw channel, solids fraction in the extrudate, throughput and energy consumption of the extruder. A dynamic model is necessary to estimate average residence time in the extruder on which quality indices of the extrudate depend.

The model library includes mathematical models of various types:

- geometric models of screw elements and sections for extruders of various types, which allow us to assemble 3D model of screw of arbitrary configuration and to calculate geometric parameters (height, width, length, volume) of channels of both individual elements of screw and sections of screw;
- static functional models of physical processes in channels of extruder elements (polymer melting, melt mixing, heating and forming);
- dynamic models for estimating residence time of polymers in extruders;
- empirical models of the rheological properties of polymers (rheological models of two-phase systems “solid particles – melt” and melts);
- models for calculation of quality indices (average mixing degree, thermal destruction index, color characteristics) of the extrudate.

Static mathematical models have been developed on the basis of conservation laws of physical substances (mass, momentum, energy) for solid phase, melt and interfacial boundary. Assumptions about low curvature of the screw element channel, steady down-channel movement of the polymer, constant (temperature-independent and pressure-independent) thermal properties and non-compressibility of the melt, low inertia and mass (body) forces, melt adhesion to the walls of the channel have been taken into account [1, 3–8]. At synthesis of the static mathematical model of the extrusion process mathematical models of polymer melting (contiguous solids melting or dispersed solids melting) and flow of its melt in the screw element channel are linked with mathematical models for calculation of flow rates of melt leakages, viscosity of polymer, densities of external heat fluxes (heat fluxes from polymer to screw and from \( k \)-th thermal zone of barrel to polymer) [19]. These models are chosen depending on types of extruder, screw element and polymer grade, and temperature condition of extruder work. According to preset configuration of screw, formed mathematical models of polymer movement, melting and mixing in channels of screw elements of various types are linked between each other. At that, compliance with conditions of mathematical models conjugation is provided. Conjugation conditions determine equality of pressure and temperature of polymer at inlet of channel of \((j + 1)\)-th screw element with pressure and temperature of polymer at outlet of channel of \( j \)-th screw element. The constructed mathematical model of movement, melting and mixing of the polymer in the channel of the modular screw is linked with the flow model in the extruder head chosen depending on the type of head. As a result, mathematical model is formed, which is a system of nonlinear algebraic and differential equations. This system includes the equations of mass balance,
balance of friction and pressure forces (momentum balance), heat balance for solid phase and melt of polymer, the equations of mass and heat balances for interfacial boundary, the rheological equation of polymer state [19, 20]. The system of equations is closed by boundary conditions at the screw channel inlet and screw channel walls. Parametric adjustment of the static model is carried out by forming values of geometric parameters of screw elements and forming head (using database of geometric parameters of screw elements and forming heads, and depending on extruder brand) and parameters of polymer phase properties (using polymer properties database and depending on type of film forming polymer). Values of model coefficients are forming by used the mathematical model library. These coefficients are the rheological model coefficients of the polymer, the heat transfer coefficients from the polymer to the screw and from the barrel to the polymer, the heat transfer coefficients from the interfacial boundary to the solid phase of the polymer and from the polymer melt to the interfacial boundary. Numerical (finite-difference) solution [22, 23] of the mathematical model allows us to calculate distributions of polymer phases state parameters (velocities, pressures, temperatures) over channels of extruder screw elements, solids fraction in the extrudate $\phi_{\text{ext}}$, throughput $G$ and energy consumption $E$ of the extruder.

To estimate the average residence time $\tau_{av}$, on which the extrudate quality indices $\gamma_{av}$ and $I_d$ depend, the dynamic mathematical model of the extrusion process is synthesized. This model consists of typical hydrodynamic models with recycles, taking into account melt leakages and screw reciprocation (in extruder of type $E_1$) [19, 24]. Typical hydrodynamic models (continuous stirred tank reactor model, tanks-in-series model, plug flow reactor model) describe the flow structure in screw sections with different mechanisms and intensities of mixing. The residence time distribution function in the extruder under Dirac pulse at the extruder inlet is calculated using the mathematical model. For this purpose the formed system of equations of mass balance on flows and tracer is solved numerically (using the finite-difference method). The average residence time of the polymer in the extruder $\tau_{av}$ is calculated by the moment method as the first moment of the residence time distribution function.

Rules for the synthesis of mathematical models include:

rules for choice and adjustment of structure of mathematical models for extrusion process components (mathematical models of polymer melting and melt flow, mathematical models of leakages, rheological models, mathematical models of external heat exchange) depending on type of extruder and head, types of screw elements, polymer grade, thermal mode of extrusion process;

module linkage rules when constructing static and dynamic mathematical model of extrusion process.

The following mathematical models have been developed to calculate characteristics of material uniformity and thermal destruction of the extrudate:

$$
\gamma_{av} = \frac{\tau_{av}}{Z} \sum_{j=1}^{N} \left( \int_{x_{j-1}}^{x_j} \int_{z_{j-1}}^{z_j} \left( \frac{1}{W^j H^j} \sum_{n=1}^{N} \left[ \left( \frac{\gamma_{av}}{\tau_{av}} \right)^n \left( \gamma_{av} \right)^{n-1} \right] \right) dx \right) dy \right) z \right) dz \right)
$$

(1)

$$
I_d = \frac{\tau_{av}}{\tau_d} \exp \left[ \frac{E_d (T_{ext} - T_d)}{8.31(T_{ext} + 273.15)(T_d + 273.15)} \right] 100
$$

(2)

where $Z$ is the screw channel length (m); $z_{j-1}$ is the channel inlet coordinate of $j$-th screw element (m); $Z_j$ is the channel length of $j$-th screw element (m); $W^j$ is the channel width of $j$-th screw element (m); $H^j$ is the channel height of $j$-th screw element (m); $\gamma_{av}$ is the shear strain rates in the cross-channel and down-channel melt flow (s$^{-1}$); $\gamma'_{av}$ are the cross-channel and down-channel melt flow velocities (ms$^{-1}$); $x$, $y$, $z$ are coordinates along channel width, height and length (m); $\tau_d$ is the time of beginning of polymer color changes due to thermal destruction (s); $E_d$ is the energy of thermal destruction activation (J mol$^{-1}$); $T_d$ is the temperature of beginning of
polymer color changes due to destruction (°C).

To estimate the color coordinates of the extrudate \( L_{ext} \), \( a_{ext} \), \( b_{ext} \) the nonlinear regression models obtained by processing the results of active production experiments (using the least square method) are used:

\[
L_{ext} = c_0 + c_1 k_{c_1} + c_2 k_{c_2} + c_3 k_{c_3} + c_4 k_{c_4} k_{c_2} + c_5 k_{c_5} k_{c_3} + c_6 k_{c_6} k_{c_3} + c_7 k_{c_7}^2 + c_8 k_{c_8}^2 + c_9 k_{c_9}^2 \tag{3}
\]

\[
a_{ext} = d_0 + d_1 k_{c_1} + d_2 k_{c_2} + d_3 k_{c_3} + d_4 k_{c_4} k_{c_2} + d_5 k_{c_5} k_{c_3} + d_6 k_{c_6} k_{c_3} + d_7 k_{c_7}^2 + d_8 k_{c_8}^2 + d_9 k_{c_9}^2 \tag{4}
\]

\[
b_{ext} = f_0 + f_1 k_{c_1} + f_2 k_{c_2} + f_3 k_{c_3} + f_4 k_{c_4} k_{c_2} + f_5 k_{c_5} k_{c_3} + f_6 k_{c_6} k_{c_3} + f_7 k_{c_7}^2 + f_8 k_{c_8}^2 + f_9 k_{c_9}^2 \tag{5}
\]

where \( c_i, d_i, f_i, l = 0 \ldots 9 \) are empirical coefficients depending on type of film forming polymer, types of colorants and extruder brand; \( k_{ci} = G_{ci}/G \), \( i = 1 \ldots 3 \) are fractions of colorant flow rates in extruder throughput.

Equations (3)–(5) are given for three colorants fed to the extruder (typically the number of colorants \( n \) used to form color of polymeric film does not exceed 2–3 [21]).

Calculation of the color deviation \( \Delta E_{ext} \) is carried out by using CIELab model:

\[
\Delta E_{ext} = \sqrt{\left[ L' - L_{ext} \right]^2 + \left( a' - a_{ext} \right)^2 + \left( b' - b_{ext} \right)^2} \tag{6}
\]

where \( L' = L_{t}^* \), \( a' = a_{t}^* \), \( b' = b_{t}^* \) if \( M_{prod} = M_{i} \lor M_{j} \); \( L' = L_{ext}^* \), \( a' = a_{ext}^* \), \( b' = b_{ext}^* \) if \( M_{prod} = M_{3} \);

\( L_{ext}^* \), \( a_{ext}^* \), \( b_{ext}^* \) are the standard color coordinates of the extrudate.

The standard color coordinates of the extrudate are determined (at each change-over of the calender line to new standard of the film color) as the values of the extrudate color coordinates \( L_{ext} \), \( a_{ext} \), \( b_{ext} \), at which the values of the film color coordinates correspond to the standard values \( L_{t}^* \), \( a_{t}^* \), \( b_{t}^* \).

The modeling system has been created taking into account the principles of system unity, compatibility and evolution. It has provided integrity of the modeling system (due to integration of its modules on the basis of the uniform data bank), solution hierarchy of the problems of extruder brand choice, forming of extruder screw configuration and synthesis of mathematical model for investigation and control of extruder quality, openness of the modeling system and its integrability in the computer-aided systems of scientific investigations of extrusion and quality control of polymeric films. The open architecture of the modeling system ensures expansion of its functionality due to development and connection of additional program modules [24]. The modeling system allows us to fill up the data bank, the bases of rules and the mathematical model library for expansion of class of modeled extrusion processes.

The tool of visual programming (programming environment Visual Studio, programming language C#), the tools for development of the information ware components (database management system SQLite) and the program interfaces (structured query language SQL), the construction tool of the virtual 3D models of objects (CAD system 3ds Max), the tool for work with interactive 3D graphics (software environment Unreal Engine) have been used for creation of the modeling system. The modeling system has been developed with use of the object-oriented programming technology on the basis of the principles of encapsulation, inheritance and polymorphism.

4. Results and discussion

The modeling system is adjusted according to the production method, the type of polymeric film, extruder throughput and energy consumption requirements. Modeling results are visualized as tables and graphs of distributions of polymer phases state parameters, dependences of extrudate quality indices on controlling actions on the extruder, trends of controlling actions, extruder throughput and extrudate quality indices (figure 3).
Figure 3. Examples of the modeling system interfaces and the extrusion process modeling results (dynamic mnemonic scheme and interface for input of polymer properties are shown in Russian).

Adequacy check of the static mathematical models of the extrusion processes has been executed by comparison of the measured and calculated values of the extrudate temperature, the melting zone length and the extruder throughput. Extruders of various types ($E_1$–$E_4$) have been investigated, having different screw configurations and head types ($D_1$–$D_4$). The extruded polymers are PP, LDPE and PVC. Variable parameters are screw speed and temperature of thermal zones of extruder barrel. Besides, the measured and calculated distributions of the PVC temperature along the screw length for the industrial and laboratory extruders of type $E_2$ with various configurations of the screws has been compared. For adequacy check of the dynamic mathematical models the comparative analysis of the
measured and calculated values of the residence time distribution function and the average residence time in extruders of various types and configurations when processing PP, PVC, PS has been made. Results of statistical data processing have confirmed adequacy of the mathematical models by the Fischer’s criterion and the standard deviation that does not exceed 3 % for the extrudate temperature and 10 % for the average residence time [19, 20, 24].

Analyzing the modeling results allows us to determine rational extrusion regime which ensures the extrudate quality, extruder throughput and energy consumption requirements for polymer of given type and extruder of given configuration are met.

Testing of the hybrid computer modeling system has been carried out according to the data of the productions of unpainted and colored flat PVC films and unpainted blown LDPE films at plants in Russia and Germany. Testing results have confirmed the modeling system operability for this class of modeling and control objects.

The modeling system can be used in the control system of the extrudate preparation stage under change-over of the production line to new production task and the polymeric film production. It helps technologists, operators to determine extruder screw configurations and controlling actions on extruders that ensure the specified extrudate quality indices guaranteeing the required consumer characteristics of the polymeric film while meeting throughput and energy consumption requirements. Application of the modeling system increases efficiency of production due to improvement of polymeric film quality, reduction of spoilage (non-returnable waste), lessening time required for production line change-over and energy consumption.

Integration of the modeling system into computer simulators for managerial production staff of polymeric film productions allows developing skills of resource saving control of complex extrusion processes at various training scenarios (production methods and types of polymeric films, requirements to extruder throughput and energy consumption) [25].

5. Conclusion
The hybrid computer modeling system of hardware flexible extrusion processes based on multivariate models of description of extrusion process (mathematical models, information models, models of knowledge representation) has been developed with use of modern information technologies.

The system implements combined method of mathematical modeling extrusion processes developed on the basis of the information description of the extrusion process at flexible multi-assortment productions of polymeric films as control object. The method is based on use of the static and dynamic mathematical models of the processes in extruders of various types (single-screw, reciprocating and twin-screw extruders). It allows us to give integrated estimation of throughput, energy consumption of the extruders and quality indices of the extrudate taking into account hardware flexibility of the extruders, features of the polymer melting and melt flow.

The modeling system allows solving the problems of synthesis of mathematical models for investigation and control of the extrudate quality, on which quality of products of flexible extrusion and calender productions of multi-assortment packaging polymeric films depends.

The modeling system has been successfully tested according to the data of modern high-tech extrusion and calender productions of packaging multi-assortment polymeric films at plants in Russia and Germany. The results of the testing have showed that the use of the modeling system as advisor for the managerial production staff allows increasing its professional competence and, as a result, lessening time required for making decisions on the quality control of the polymeric films under change-over of the production lines and the polymeric film production. This contributes to improvement of consumer characteristics of the polymeric films, resource saving (reduction of non-returnable waste and corresponding increase of the yield of standard film), energy saving, and therefore, to increase of the efficiency and competitiveness of polymeric film production due to determination of rational configurations of the extruder screws and controlling actions on the extruders.
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