Computer Modeling System for Energy- and Resource-Saving Control of Multi-Assortment Polymeric Film Production

Tamara Chistyakova and Andrey Polosin

Abstract The chapter describes the questions of developing the flexible computer modeling system that allows us to realize the synthesis of mathematical models of hardware flexible extrusion processes for energy- and resource-saving control of large-capacity, multi-assortment production of polymeric films. The problem of energy- and resource-saving control, which is solved at each transition of the production to a new type of film, is to determine parameters of the extruder configuration and operating mode, ensuring the given extrudate quality when meeting the requirements for throughput and energy consumption. The library of mathematical models is the core of the system. It includes structural models of extruder elements for calculating the geometric parameters of extruders of various configurations and functional models of physical processes in the element channels. Static models for calculating throughput, energy consumption, extrudate quality indices (mixing degree, solid fraction, thermal destruction index), and dynamic models for calculating residence time in the extruder are synthesized based on the physical process models in the element channels. The structural synthesis of the models is based on a cell approach to modeling processes in partitioned apparatuses. Setting up the system is carried out using a data bank of production methods and types of films, parameters of extruders, polymer properties. A two-stage iterative algorithm is used to solve the control problem: the extruder configuration is formed in the external cycle, the extruder operating parameters, which ensure the required extrudate quality with given throughput, energy consumption, are determined in the internal cycle. Testing according to data of the polyvinyl chloride and polyethylene film productions in plants of Russia and Germany has confirmed the operability of the system and the possibility of its using as an adviser to operators.

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1 Introduction

Extrusion (cast, blown) and calendering are the main methods of the high-tech polymeric film (PF) industrial production for foodstuff and medicine packaging. The high demand for packaging materials and a multitude of packaged product types define the high-capacity multi-assortment character of extrusion and calender PF production. Thus, just one of the leading international corporations producing PF, Klöckner Pentaplast, produces 250 thousand tons of PF on 35 extrusion lines, as well as 400 thousand tons of rigid PF with a polyvinyl chloride (PVC) base on 41 calender lines per year. Packaging PF differs in its composition (in particular, the types of film-forming polymers, with PVC, polyethylene terephthalate, polypropylene, and varied density polyethylene being key among them). It is characterized by a large range of potential thickness (from 0.025 to 1.65 mm) and width (up to 6200 mm) of a sheet of film, as well as strict quality requirements (its appearance, color). Certain PF defects are most unacceptable. These include black specks, destruction strips, the inclusion of unmelted polymer, defects such as « fish-eye » (gels), and « orange peel » , as well as deviation from the required color. The difficulty in PF production control lies in a large number of parameters for the raw materials, equipment, production mode, product quality, and their numerous interrelationships [1]. For example, calender PF production is characterized by more than 100 parameters and 800 interrelationships between them. Therefore, the main innovative trend of the development of international high-technology production of the polymer industry within the framework of the Industry 4.0 concept is the creation and application of cyber-physical systems for effective control of PF production processes based on the integration of methods and technologies of computer modeling of physical processes and mining of big production data on process parameters and quality indices of semi-products and target products [2–4].

Regardless of the PF production method, the extrusion process is the key stage, which is implemented using extruders of various types and is defined by equipment flexibility (the possibility of implementing numerous screw configurations so as to produce multi-assortment PF). Extrusion includes physical processes successively following one another in the channels of the screw or screws: the heating and melting of solid polymer, heating, mixing, and molding of melt [5]. The goal is to prepare a homogenous plastic mass (extrudate) from which the PF can then be produced. The extrudate temperature, level of homogeneity, and color coordinates (hue, saturation, lightness) in large part define the most important PF consumer characteristics: the number of black points, inclusions of unmelted polymer, gels per given area of PF, and color coordinates. Extrusion PF production leads to PF thickness being dependent on the extrudate output rate, that is, on the throughput of the extruder. At the same time, only visual quality control is performed on the production line. As a result, the operators make control decisions based on a subjective judgment of extrudate quality, their own experience, and an experimentally determined set of production rules. Given the multi-assortment production conditions, this leads to errors, which lead to financial losses, resulting from an increase in defective PF, loss of resources spent on its production, an increase in time spent the line change-over, and, as a result, a decrease in throughput and increase in energy consumption.

Thus, it is relevant to develop the flexible computer modeling system (CMS) for the synthesis of mathematical models (MM) for extrusion processes, such that they can be configured for the PF type, its production method, the type and configuration of the extruder. This would enable calculating the extrudate quality characteristics, the throughput, and energy consumption of the process, and solve the problems of energy- and resource-saving control of multi-assortment extrusion and calender PF productions.

2 Controlled Object Characteristics. Energy- and Resource-Saving Control Problem Statement

The formalized description of PF production as a controlled object (CO) is presented in Fig. 1. The extruder type T_{extrud}, diameter *D,* and length *L* of the extruder's screw are determined according to the production method M_{prod}, the type of film-forming polymer T_{polym}, and the throughput G_0 and energy consumption $E^{\max}$ requirements for the line. Extruders differ in the number of screws *q* and the way they move: single-screw extruders E_1 (the screw simply rotates at screw speed *N*), reciprocating extruders E_2 (the screw rotates and also performs oscillating motion with an amplitude S_0), twin-screw extruders with co-rotating screws (E_3) or counter-rotating screws (E_4). The screw configuration C_{scr} consists of N_e elements of various types T_e^j. The element types are determined by the type of extruder. Thus, screws of an E_1 extruder, generally, consist of elements with continuous flights and cylindrical (SC) or conical (SP) core (SP-elements are used in the melting zone). Extruders of type E_2, as a rule, have conveying elements (EZ), kneading elements (KE), and elements with a restriction ring (ST, used in the degassing zone) [6]. The extruder is assembled with a molding head of type T_{head}, the selection of which depends on the production method M_{prod}. Equipment flexibility enables us to have not only parametric control of the extruder (by changing the extrusion mode) but also structural control (by changing the screw configuration C_{scr} when reconfiguring production to a new PF type T_{film}, which is itself dependent on the polymer type T_{polym} and quality requirements Q_{film0}). Extrusion mode is switched with the help of main CA U_b: speeds of feed screw N_h and main screw *N*, barrel heating zone temperatures T_{bk}, $k = 1 \ldots n_T$. The output parameters Y_{extrus} are dependent on this extrusion mode. They include extruder throughput *G* and energy consumption *E*, which determine corresponding line characteristics, average residence time (ART) of polymer in extruder

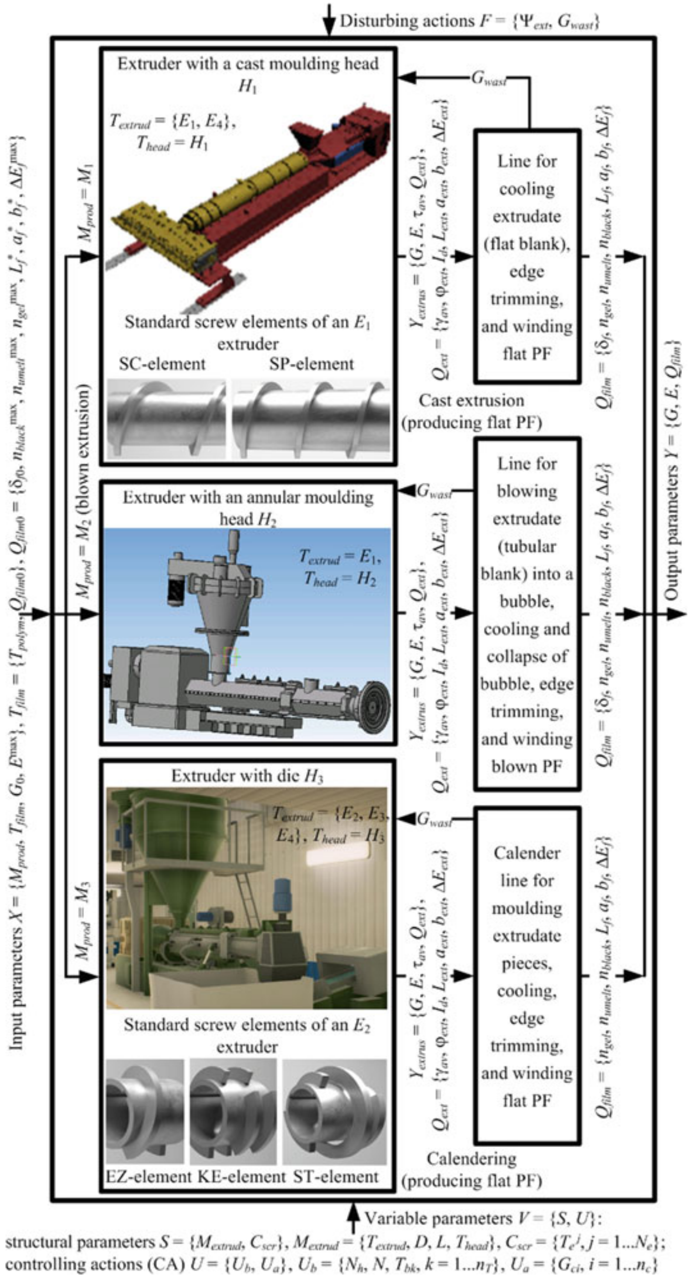

Fig. 1 Formalized description of PF production as CO

τ_{av} and extrudate quality indices Q_{ext} (average mixing degree γ_{av}, a solid fraction φ_{ext}, thermal destruction index I_d).

Film thickness δ_f is dependent on throughput (if $M_{prod} = M_1 \vee M_2$). Raising a solid fraction above a certain upper bound $\varphi_{ext}^{\max}$ indicates the presence of unmelted particles n_{umelt} in PF. Other extrudate quality indices (γ_{av}, I_d) determine corresponding PF quality indices Q_{film} – number of gels n_{gel} and black points n_{black}.

During the production of a colored film, feeding wasted supplies back in the extruder (shredded PF sheet trim) at a flow rate G_{wast} and oscillation in the extrudate supply Ψ_{ext} within the feeding trough of calender lead to a deviation of the PF color coordinates L_f, a_f, b_f from the required values L_f^*, a_f^*, b_f^* due to a deviation in the extrudate color coordinates L_{ext}, a_{ext}, b_{ext}. This color coordinate drift ΔE_f passes a preset upper bound $\Delta E_f^{\max}$, which requires correction via additional CA U_a: flow rates of liquid colorants fed into an extruder, G_{ci}, $i = 1 \ldots n_c$.

The analysis of the CO allowed us to formulate the problems of PF production control during line change-over and during active production.

The control problem during change-over of the line, which is implementing the production method M_{prod}, to a new task $Y_0 = \{T_{film}, G_0, E^{\max}\}$ consists of selecting extruder brand M_{extrud}, forming its screw configuration C_{scr} and admissible values for main CA $U_b^* \in [U_b^{\min}; U_b^{\max}]$, which ensure the maintenance of quality indices $\gamma_{av} \geq \gamma^{\min}$, $\varphi_{ext} \leq \varphi_{ext}^{\max}$, $I_d \leq I_d^{\max}$, that ensure compliance with the restrictions on the number of PF defects ($n_{gel} \leq n_{gel}^{\max}$, $n_{umelt} \leq n_{umelt}^{\max}$, $n_{black} \leq n_{black}^{\max}$), while maintaining line requirements $G \geq G_0$, $E \leq E^{\max}$. Here, $\gamma^{\min}$ and $I_d^{\max}$ are the boundary values for extrudate quality, which depend on requirements for their corresponding PF defects.

Control problems while in active production (with the presence of disturbing actions G_{wast} and Ψ_{ext}), consisting of determination (depending on the current extruder throughput G) of flow rates G_{ci}^*, $i = 1 \ldots n_c$, so as to ensure fulfillment of extrudate color deviation $\Delta E_{ext} \leq \Delta E_{ext}^{\max} \pm \Delta_{\max}$ requirements, have been defined in prior work [7]. Here $\Delta E_{ext}^{\max}$ is the limit deviation of the extrudate color from the standard, determined depending on the PF color requirement ($\Delta E_f^{\max}$), $\Delta_{\max}$ is color measurement error.

Due to the incompleteness of the information regarding the extrusion process state parameters and extrudate quality indicators attainable with CO, solving multi-assortment PF production control problems requires using MM, which enables us to provide a comprehensive evaluation of extrudate quality, extruder throughput, and energy consumption in response to the CA.

3 Library of Mathematical Models for Extrusion Processes

In order to take into account the variety of extruder types and their equipment flexibility, the multitude of polymer types, as well as the complex diagram of motion, melting, and heat exchange within the screw channel, a complex modeling method has been proposed. It is based on a MM library of extrusion processes, rules, and an algorithm for the structural and parametric synthesis of the control model.

The analysis of MMs of extrusion processes described in literature has shown that they are constructed on the basis of conservation laws of physical substances and include the equations of balances of mass, forces, and energy for solid phase and melt, a rheological equation of state of melt and also the equation of an interphase material and heat balance (for the description of melting) [8]. Different melting mechanisms are modeled: contiguous solids melting (melting of continuous solid phase – solid bed) in extruders of type E_1 [9–13]; dispersed solids melting (melting of dispersed solid phase) in extruders of types E_2–E_4 [5, 14–16]. Models allow us to calculate the melting zone length, profiles of width (concentration of solid particles for dispersed solids melting) and temperature of the solid phase, fields of flow velocities, stresses of viscous friction inflows, pressure, and temperatures of melt. The scope created by MM generally is limited to a research of patterns of processes of a heat mass transfer of polymers in extruders of separate types with classical geometry of the screw [17], in separate functional zones of the channel of the screw (solid polymer conveying [18], melting, melt conveying [19–22]) or in channels of separate elements of modular screws [23]. Results of modeling allow obtaining information necessary for the design of extruders, but not for quality control of the extrudate. Approaches to assessment of ART in extruders of different types are based on application as separate standard hydrodynamic models (for example, one-parameter axial dispersion model [24]), and the difficult combined models of the structure of the flows. These models are constructed on the basis of standard hydrodynamic models (plug flow reactor model, continuous stirred tank reactor model, tanks-in-series model) including the introduction of recirculating flows modeling melt leakages [25, 26]. Standard models describe extruder zones with the different mechanisms and intensity of mixing [27]. However, MMs do not allow to give a complex assessment of the quality of the extrudate, throughput, and energy consumption of extruders in dependence on CA for different types of polymers taking into account the difficult construction of extruders and main patterns of the extrusion process.

Performed analysis has allowed us to develop a MM library. It includes: basic MMs, describing polymer motion, melting, and mixing in the screw channel, and enabling us to calculate distributions of melt flow velocities v_x^j, v_z^j and shear rates $\dot{\gamma}_{xy}^j$, $\dot{\gamma}_{zx}^j$, $\dot{\gamma}_{zy}^j$, as well as distributions of polymer phase pressure P^j and temperature T^j;

MMs of melt flows in gaps of various kinds (radial, side, calender) and axial cuts in element flights to calculate corresponding leakage flow rates Q_δ^j, Q_s^j, Q_r^j, Q_c^j;

MMs for calculating melt viscosity η^j;

MMs for calculating densities of heat fluxes given heat exchange between the melt and the barrel q_{bk}^j, as well as the melt and the screw q_{scr}^j;

MMs of melt flow in extruder heads of various types for calculating melt-pressure drop;

Ideal hydrodynamic models, describing flow structure in the channels of the screw sections of various types (dependent on element types of which the sections are compiled);

MMs for calculating extrudate quality indices Q_{ext}.

The structure of the basic MM, describing shear flow in the channel of the j-th screw element, takes the form:

$$\int_0^{H^j} v_x^j \, \mathrm{d}y = \dot{Q}_\delta^j + \dot{Q}_c^j, \quad (1)$$

$$z_f^j \left[(2-q) W^j \int_0^{H^j} v_z^j \, \mathrm{d}y + (q-1) \int_0^{W^j} \int_0^{H^j} v_z^j \, \mathrm{d}y \, \mathrm{d}x \right] = (2-q) Q^j - (q-1)\left(2Q_s^j + Q_r^j\right), \quad (2)$$

$$Q^j = q^{-1} Q + \left(Q_\delta^j + Q_c^j\right) + (q-1)\left(2Q_s^j + Q_r^j\right), \quad (3)$$

$$\frac{\partial P^j}{\partial x} = \frac{\partial}{\partial y}\left(\eta^j \dot{\gamma}_{xy}^j\right), \ \frac{\partial P^j}{\partial z} = (q-1)\frac{\partial}{\partial x}\left(\eta^j \dot{\gamma}_{zx}^j\right) + \frac{\partial}{\partial y}\left(\eta^j \dot{\gamma}_{zy}^j\right),$$
$$\frac{\partial P^j}{\partial z} = (q-1)\frac{\partial}{\partial x}\left(\eta^j \dot{\gamma}_{zx}^j\right) + \frac{\partial}{\partial y}\left(\eta^j \dot{\gamma}_{zy}^j\right) \quad (4)$$

$$\rho \, c_P v_z^j \frac{\partial T^j}{\partial z} = \lambda \frac{\partial^2 T^j}{\partial y^2} + \eta^j \left[\left(\dot{\gamma}_{xy}^j\right)^2 + (q-1)\left(\dot{\gamma}_{zx}^j\right)^2 + \left(\dot{\gamma}_{zy}^j\right)^2 \right], \quad (5)$$

$$P^j\big|_{z=z^{j-1}} = P_{out}^{j-1}, \ \ T^j\big|_{z=z^{j-1}} = T_{out}^{j-1}, \quad (6)$$

$$v_x^j\big|_{y=0} = 0, \quad v_x^j\big|_{y=H^j} = \varphi_1(q, D, N, S_0, \Phi_{osc}) \quad (7)$$

$$v_z^j\big|_{x=0} = v_z^j\big|_{x=W^j} = v_z^j\big|_{y=0} = \varphi_2(q, D, N), \ \ v_z^j\big|_{y=H^j} = \varphi_3(q, D, N, S_0, \Phi_{osc}), \quad (8)$$

$$-\lambda \, \partial T^j / \partial y\big|_{y=0} = q_{scr}^j\left(T_{scr}, \ T^j\right), \ -\lambda \, \partial T^j / \partial y\big|_{y=H^j} = q_{bk}^j\left(T_{bk}, \ T^j\right), \quad (9)$$

where x, y, z are coordinates along the width W^j, height H^j and length of the channel (m); $z_f{}^j$ is number of flights; Q^j is the flow rate through the element (m^3/s); Q is flow rate through the extruder with the head (equivalent to throughput, m^3/s); ρ, c_P, λ are melt density (kg/m^3), specific heat (J/(kg·°C)), thermal conductivity (W/(m·°C)); z^{j-1} is channel entrance coordinate (m); P_{out}^{j-1}, T_{out}^{j-1} are pressure (Pa) and temperature (°C) at channel exit of the (j–1)-th element; Φ_{osc} is screw oscillation phase in a type E_2 extruder (rad); T_{scr} is screw temperature (°C).

In the process of synthesizing MM of extrusion, the MM (1)–(9) is assembled with MMs for calculating the leakage flow rates, viscosity, densities of external heat fluxes, selected depending on extruder type, screw element type, polymer type, and extrusion heat mode [28, 29]. The used rheological model takes the form:

$$\eta^j = \mu^j(T^j)\left[\left(\dot{\gamma}_{xy}^j\right)^2 + (q-1)\left(\dot{\gamma}_{zx}^j\right)^2 + \left(\dot{\gamma}_{zy}^j\right)^2\right]^{(n-1)/2}, \tag{10}$$

where μ^j is consistency index, taking into account the influence of the volume fraction of solid polymer particles in the melt (for dispersed solids melting) and temperature on viscosity (Pa·s^n); n is the power law index.

The dependence of μ^j on the fraction of solid particles is described by the Maron–Pierce equation [16]. In order to describe its dependence on temperature, the Williams–Landel–Ferry equation and Reynolds equation (depending on the polymer type and process temperature range) are used [30].

In accordance with the presented screw configuration, the formed MMs for polymer motion, melting, and mixing in the channels of the screw elements of various types are assembled. The conditions for the MM conjugation defined by (6) are satisfied when assembling MM. The created MM for polymer motion, melting, and mixing in the channel of a modular screw is integrated with the MM for melt flow in the extruder head, selected depending on the head type [29]. As a result, MM is created for calculating the polymer phase state parameters (v_x, v_z, $\dot{\gamma}_{xy}$, $\dot{\gamma}_{zx}$, $\dot{\gamma}_{zy}$, P, T, η), throughput G, and energy consumption E of the extruder.

The end of the melting zone is defined by a condition when the fraction of solid phase (the solid bed width carried to the width of the channel at contiguous solids melting or a fraction of solid particles in the melt at dispersed solids melting) becomes less maximum permissible $\varphi_{ext}^{\max}$ [28]. The corresponding value of a fraction of solid phase defines the maintenance of a solid phase in the extrudate φ_{ext}.

In order to evaluate ART τ_{av}, upon which quality indices γ_{av}, I_d are dependent, dynamic MM of the extruder is synthesized (see Fig. 2). The MM consists of standard hydrodynamic models, covered by recycling, taking into account the leakages and oscillation [26, 28].

Various standard models (plug flow reactor model, continuous stirred tank reactor model, tanks-in-series model) describe the structure of flows in sections of various

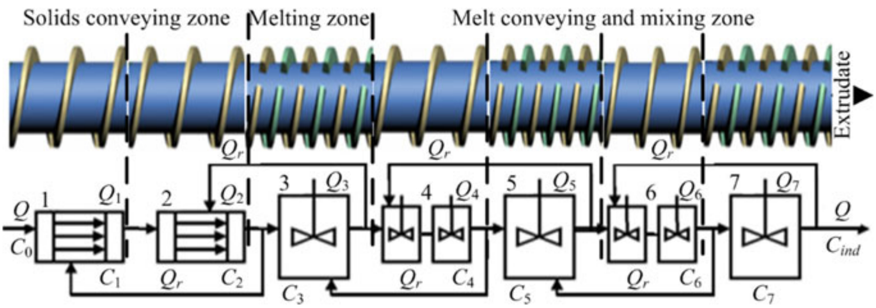

Fig. 2 Example of a structural scheme of a dynamic MM for ART evaluation

types. For example, in the extruder of type E_2 the section consisted of KE-elements is described by a continuous stirred tank reactor model and the section consisted of EZ-elements is described by a tanks-in-series model. The C-shaped chambers in extruders of types E_3 and E_4 are described by the continuous stirred tank reactor model. Distribution of tracer output concentration C_{ind} over time is calculated given pulse disturbance in the composition of the input flow C_0. It depends on the polymer flow rates Q_l and tracer concentrations C_l, $l = 1 \ldots N_s$ (in the example in Fig. 2 $N_s = 7$) in the screw sections, as well as the recycling flow rates Q_r. ART τ_{av} is calculated using a C-curve and the method of moments.

The mixing degree γ_{av} and the thermal destruction index I_d are calculated using the shear rates, temperature, and ART. The mixing degree is determined as the average shear strain accumulated by the polymer. The thermal destruction index is determined as a mapping of the dependence of the destruction degree on time given some temperature-time mode in the extruder, on the dependence derived experimentally for the specific polymer type given isothermal conditions. Regression MMs attained by data processing of active production experiments are used for evaluating the color coordinates of extrudate L_{ext}, a_{ext}, b_{ext}, and the CIELab model is used for calculating the color deviation of the extrudate ΔE_{ext} [31, 32].

The MMs has been evaluated by comparing the calculated and measured values of extrudate temperature, throughput and ART for extruders of various types (E_1–E_4) and configurations (C_{scr}), using corresponding heads (H_1–H_3), during the processing PVC, polystyrene, polypropylene, and low density polyethylene (LDPE). The adequacy of the models has been confirmed by checking the data with Fisher's criterion and mean squared deviation which does not exceed 3% for the temperature and 10% for the ART.

4 Software Package of Model Synthesis for Extrusion Control and Results of Its Testing

CMS is implemented in the form of a flexible software package. It includes modules for selecting extruder brand M_{extrud} (depending on the production method M_{prod} and parameters of task Y_0), the formation of the extruder's screw configuration C_{scr}, structural synthesis, and parametric setup of the MM for calculating extrusion process output parameters Y_{extrus} (within the procedural ranges of CA) and visualization of the modeling results. The information ware of the package includes a databank of PF production parameters, a rule base for extruder model selection, a rule base for placement and assembly of 3D models for screw elements, and a rule base for extrusion process MM synthesis. The databank includes databases of PF production methods and geometric parameters of extruders, screw elements, and extruder heads. It also includes databases of PF types, quality requirements for extrudate and PF, properties of film-forming polymers, and procedural ranges of CA. The visualization module enables presenting the results in the form of 3D models for screws of formed configurations, 3D graphs of polymer phase state parameter distribution along the screw channel, 3D graphs of the dependence of extrudate quality indicators, extruder throughput, and energy consumption on the CA, trends of extrusion process output parameters.

The synthesized MM of the extrusion process allows us to solve the investigation problem of CA influence on extrudate quality indices Q_{ext} and the determination problem of CA U_b on the extruder of configuration C_{scr} ensuring given quality at the implementation of requirements to throughput G and energy consumption E. A two-stage iterative algorithm is used to solve the energy- and resource-saving control problem: the extruder's screw configuration C_{scr} is formed in the external cycle, the CA U_b, which ensures the required extrudate quality with given throughput and energy consumption, are determined in the internal cycle.

The software package has been tested using data from calender lines producing flat PF with PVC as the core constituent (the extruders of types E_2 and E_4) and extrusion lines producing blown PF with LDPE as the core constituent (the extruders of type E_1) at plants in Russia and Germany. Testing has confirmed its operability for the solution of control problems of multi-assortment PF productions, both during the change-over mode and during active production. Examples of the software package work results are presented in Fig. 3.

5 Conclusion

The flexible CMS has been developed that allows us to select the extruder brand for a given production method, type of PF, production line throughput, and energy consumption requirements. CMS also allows us based on the synthesized MM of extrusion process to determine the configuration of screw/screws and CA on the extruder, which ensures the specified extrudate quality characteristics (which guarantees the specified consumer characteristics of PF) when meeting the production line performance requirements.

The test results have confirmed the operability of CMS and the possibility of its use as part of industrial cyber-physical systems for efficient energy- and resource-saving control of the extrusion stage at multi-assortment productions of flat and blown PFs in the mode of operator's adviser. CMS was introduced into pilot operation at plants for the production of multi-assortment PF for packaging pharmaceuticals and food products in Russia (Klöckner Pentaplast Rus LLC) and Germany (Klöckner Pentaplast Europe GmbH and Co. KG).

The application of CMS within the framework of the Industry 4.0 concept allows us to ensure the specified quality of the extrudate, and therefore the quality of PF, reduce defects and energy consumption of the extrusion process, reduce the time spent the production line change-over by determination of rational screw configuration and CA values on the extruder, which help prevent abnormal situations associated with impaired extrudate quality.

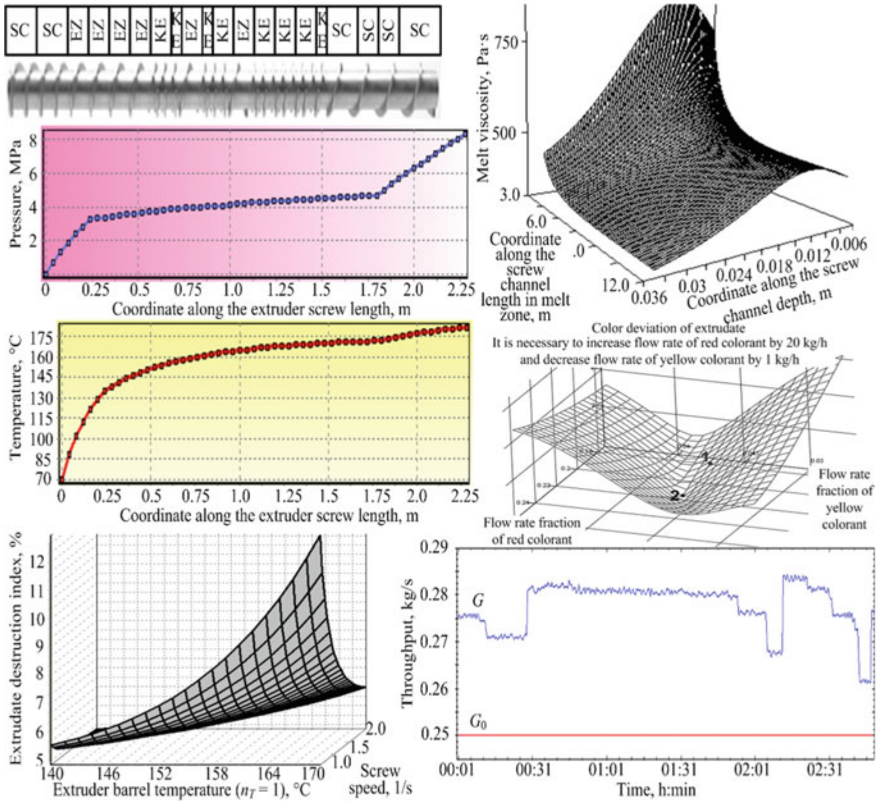

Fig. 3 3D model of the screw and calculated characteristics of the process in the extruder of type E_2

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