Mathematical Models of Extrusion for Control of Multi-Assortment Production of Polymeric Film

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***Abstract*— Library of configurable mathematical models for the extrusion process has been developed. The models enable us to solve the problem of control in multi-assortment production of flat and blown polymeric films. They describe the polymer melting, melt mixing, heating, and moulding. The models are constructed using laws of conservation and rheology, and allow us to calculate process throughput and energy consumption, as well as extrudate quality indicators that consumer characteristics of polymeric film depend on. Software solution, which can be adjusted according to various types of film, production method, as well as type and configuration of extruder, has been created. It allows us to realize a structural and parametric synthesis of the model so as to determine configuration and controlling actions on extruder that would ensure required film parameters given certain limits on production line throughput and energy consumption. The software solution has been tested in production on data from polyvinylchloride and polyethylene film from factories in Russia and Germany. Results of testing have confirmed workability of the software solution.**

Keywords*— mathematical modeling; numerical methods; software solution; control; multi-assortment production; extrusion processes; polymeric film

I. Introduction

Extrusion (blown or cast) and calendering are the main methods of high-tech polymeric film (PF) industrial production for foodstuff and medicine packaging. The high demand for packaging materials and 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 polyvinylchloride (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 0.022 to 1.65 mm) and width (up to 6200 mm) of a sheet of film, as well as strict quality requirements (its appearance and color). Certain PF defects are most unacceptable. These include black specks, destruction strips, 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 the large number of parameters for the raw materials, equipment, production mode, product quality, and their numerous interrelationships. For example, calender PF production is characterized by more than 100 parameters and 800 interrelationships between them [1].

Regardless 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 moulding of melt. 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 quantity of black specks, inclusion of unmelted polymer, gels per 10 m^2 of PF sheet, 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 decision based on a subjective judgement 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 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 resource and energy conservation problems of multi-assortment extrusion and calender PF production control.

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II. Object Characteristics and 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).

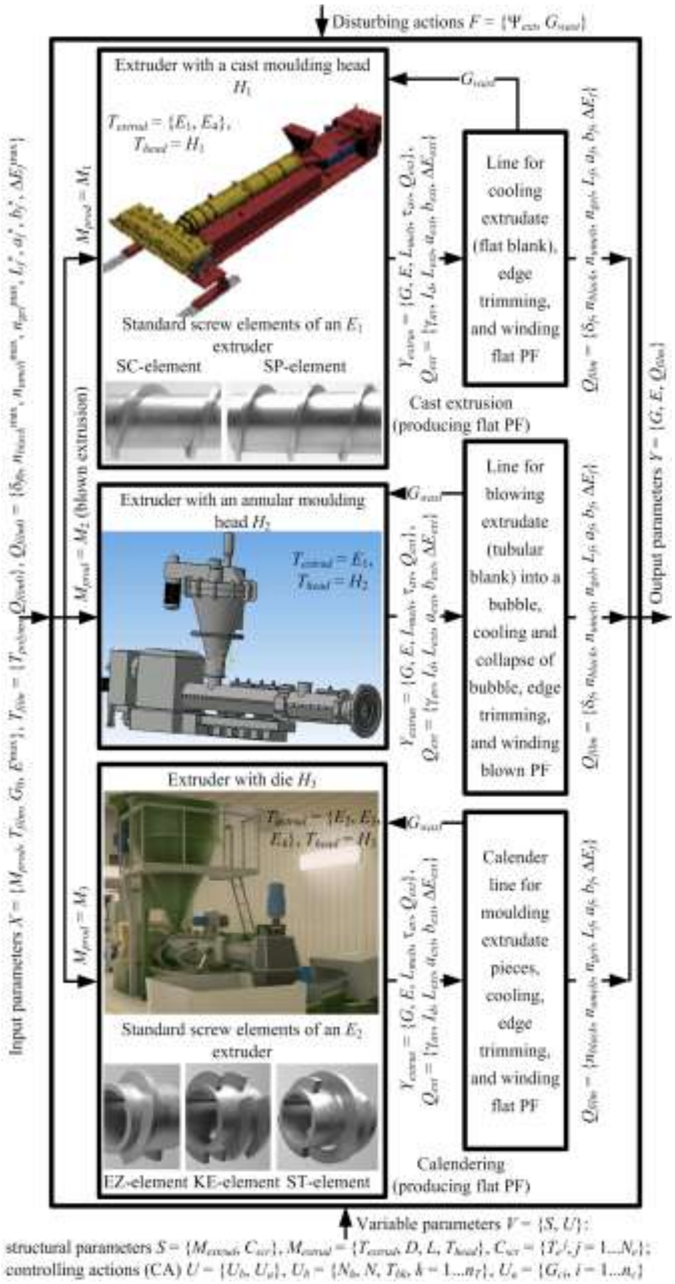

Fig. 1. Formalized description of PF production as CO.

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). The extruder is assembled with a moulding 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, melting zone length (MZL) L_{melt}, average polymer residence time (ART) in the extruder τ_{av} and such extrudate quality indicators Q_{ext} as average mixing degree γ_{av} and thermal destruction index I_d. Film thickness δ_f is dependent on throughput (if $M_{prod} = M_1 \vee M_2$). Raising MZL above a certain upper bound $L_{melt}^{\max}$, dependent on T_{extrud} and T_{polym}, indicates the presence of unmelted particles n_{umelt}. The indicators Q_{ext} determine the PF quality indicators Q_{film} – number of gels n_{gel} and black specks n_{black}. During production of colored film, feeding wasted supplies back in 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 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 line change-over, which is implementing the production method M_{prod}, to a new task $Y_0 = \{T_{film}, G_0, E^{\max}\}$ consists of selecting extruder model 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 maintenance of quality indicators $\gamma_{av} \geq \gamma^{\min}$, $I_d \leq I_d^{\max}$ and MZL $L_{melt} \leq L_{melt}^{\max}$, that ensure compliance with the restrictions on the number of PF defects ($n_{gel} \leq n_{gel}^{\max}$, $n_{black} \leq n_{black}^{\max}$, $n_{umelt} \leq n_{umelt}^{\max}$), 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 of flow rates G_{ci}^*, $i = 1 \ldots n_c$, so as to ensure fulfillment of extrudate color deviation ΔE_{ext} requirements, have been defined in a prior work [2]. 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 enable us to provide a comprehensive evaluation of extrudate quality, extruder throughput and energy consumption in response to the CA.

III. Extrusion Process Model Library

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, 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. Analysis of the published MM of extrusion processes in various aggregates, whether built using conservation and rheology laws [3, 4] or using ideal hydrodynamic models [5, 6], 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 (IHM), describing flow structure in the channels of the screw sections of various types (dependent on element types);

MMs for calculating extrudate quality indicators Q_{ext}.

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

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

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

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

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

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

$$P^j\Big|_{z=z^{j-1}} = P_{out}^{j-1},\ T^j\Big|_{z=z^{j-1}} = T_{out}^{j-1}, \tag{6}$$

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

$$v_z^{\,j}\Big|_{x=0} = v_z^{\,j}\Big|_{x=W^j} = v_z^{\,j}\Big|_{y=0} = \varphi_2\left(q, D, N\right), \tag{8}$$

$$v_z^{\,j}\Big|_{y=H^j} = \varphi_3\left(q, D, N, S_0, \Phi_{osc}\right), \tag{9}$$

$$-\lambda\partial T^j/\partial y\Big|_{y=0} = q_{scr}^{\,j}\left(T_{scr}, T^j\right), -\lambda\partial T^j/\partial y\Big|_{y=H^j} = q_{bk}^{\,j}\left(T_{bk}, T^j\right), \tag{10}$$

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 flow rate through the element (m^3/s); Q is flow rate through the extruder with 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 the extrusion MM, the MM (1)–(10) is integrated 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. The used rheological model takes the form:

$$\eta^j = \mu^j\left(T^j\right)\left[\left(\dot{\gamma}_{xy}^{\,j}\right)^2 + (q-1)\left(\dot{\gamma}_{zx}^{\,j}\right)^2 + \left(\dot{\gamma}_{zy}^{\,j}\right)^2\right]^{(n-1)/2}, \tag{11}$$

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

The dependence of μ^j on the fraction of solid particles is described by the Maron–Pierce equation. 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.

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 extruder head, selected depending on the head type. 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), MZL L_{melt}, throughput G and energy consumption E of the extruder.

In order to evaluate ART τ_{av}, upon which quality indicators γ_{av} and I_d are dependent, dynamic MM of the extruder is synthesized (Fig. 2). The MM consists of IHM, covered by recycling, taking into account the leakages and oscillation [2, 5]. 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 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.

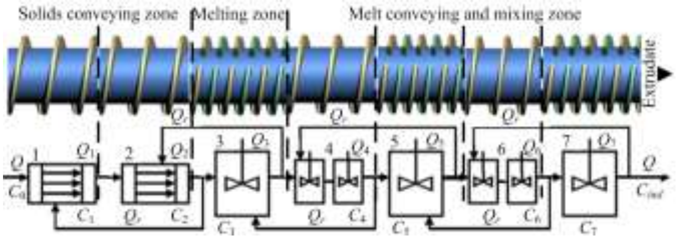

Fig. 2. Example of a structural scheme of a dynamic MM for ART evaluation.

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}. The CIELab model is used for calculating the color deviation of extrudate ΔE_{ext}.

The MMs have been evaluated by comparing the calculated and measured values of extrudate temperature, MZL, 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, polypropylene, and low density polyethylene (LDPE). The adequacy of the models has been confirmed by checking the data with the mean squared error and Fisher's criterion.

Configurable software solution has been developed. It includes modules for selecting extruder model M_{extrud} (depending on the production method M_{prod} and parameters of task Y_0), 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 bounds of CA) and visualization of the modeling results [7]. The software information ware 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 bounds for the 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. The software solution allows us to select an extruder model for a given production method of a given PF type, with given throughput and energy consumption requirements for production line. Then, using the synthesized MM of the extrusion process, we can determine a screw configuration and CA for the extruder of selected model, so as to ensure the given extrudate quality requirements are met (which, in turn, guarantees meeting quality requirements for the PF consumer characteristics), while meeting the throughput and energy consumption requirements for the line.

The software solution has been tested using data from calender lines producing flat PF with PVC as the core constituent and extrusion lines producing blown PF with LDPE as the core constituent at factories in Russia and Germany. Testing has confirmed its workability for control of multi-assortment PF production, both during the change-over mode and during active production. The application of this software solution helps ensure extrudate quality, ensuring PF quality in the process, and lower the extrusion process energy consumption. It also helps lower the time spent the line change-over by determination of reasonable CA values for the extruder, which help prevent extrudate quality requirement failures.

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