Mathematical modeling for resource and energy saving control of extruders in multi-assortment productions of polymeric films

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Abstract. In this article, the authors describe mathematical modeling of polymer processing in extruders of various types used in extrusion and calender productions of film materials. The method consists of the synthesis of a static model for calculating throughput, energy consumption of the extruder, extrudate quality indices, as well as a dynamic model for evaluating polymer residence time in the extruder, on which the quality indices depend. Models are adjusted according to the extruder type (single-screw, reciprocating, twin-screw), its screw and head configuration, extruder’s work temperature conditions, and the processed polymer type. Models enable creating extruder screw configurations and determining extruder controlling action values that provide the extrudate of required quality while satisfying extruder throughput and energy consumption requirements. Model adequacy has been verified using polyolefins’ and polyvinylchloride processing data in different extruders. The program complex, based on mathematical models, has been developed in order to control extruders of various types in order to ensure resource and energy saving in multi-assortment productions of polymeric films. Using the program complex in the control system for the extrusion stage of the polymeric film productions enables improving film quality, reducing spoilage, lessening the time required for production line change-over to other throughput and film type assignment.

1. Introduction

Modern productions of packing and technical polymeric films are difficult large-tonnage power-intensive technological systems. So, the capacity of the European market of films exceeds 10 million tons per year. At the same time, the tendency of constant growth of the annual outputs is observed (for 10–12 %). Films are made of polymers of various types. Basic types of polymers for films are polypropylene (PP, 23 %), polyvinylchloride (PVC, 21 %), low density polyethylene (LDPE, 19 %). Films are characterized by a variety of formulas, according to their application. More than 50 % of packing films are applied in food and pharmaceutical industry, therefore strict requirements are imposed on their quality (appearance, color). The least acceptable defects of film surface are black points, destruction strips, inclusions of unmelted polymer, unevenness of coloring. The wide variety of films, varying according to their formulas (including types of film-forming polymers \( T_{\text{polym}} \) and requirements placed on their thickness \( \delta_f \), width \( w_f \), and consumer characteristics (color, shrinkage), leads to a variety of film production methods \( M_{\text{prod}} \), types of extruders \( T_{\text{extrud}} \) and extrusion heads \( T_{\text{head}} \).
In figure 1, the following designations are used: HDPE – high density polyethylene; PVC – plasticized PVC and rigid PVC; PS – polystyrene; PET – polyethylene terephthalate; $I_{\text{extrud}}, I_{\text{scrv}}, I_{\text{head}}$ – geometric parameters of the extruder, its screw and its head; $M_{\text{extrud}}$ – extruder brand; $C_{\text{scrv}}$ – screw configuration; $D, L$ – diameter and length of the screw (m); $q$ – number of screws; $S_0$ – amplitude of screw oscillation (m); $D_{\text{rot}}$ – direction of screw rotation; $T_{\text{extrud}}^j$ – $j$-th screw element’s type; $N_0$ – number of screw elements; $T_{\text{extrud}}^j$ – geometric parameters of $j$-th screw element; $U$ – controlling actions on the extruder; $N_h, N$ – speeds of the feed hopper screw and the extruder screw (s$^{-1}$); $T_{\text{extrud}}^k$ – temperature of $k$-th thermal zone of the extruder barrel (ºC); $n_T$ – number of thermal zones; $Y$ – output parameters of extrusion; $G$ – extruder throughput (kg s$^{-1}$); $E$ – energy consumption (EC) of the extruder (J kg$^{-1}$); $\gamma$ – average mixing degree of the extrudate (shear units); $I_d$ – destruction index of the extrudate (%).

Figure 1. Polymeric film production methods.

Extrusion consists of obtaining the homogeneous plastic mass (extrudate) by heating, melting, and mixing bulk polymeric material in the screw channel, which is continuously fed into the extruder. The
resulting polymer melt is forced through the forming opening of the extrusion head [1].

The extruders differ in the number of screws and the nature of their movement: 

- E₁ – single-screw extruders, their screw only rotates ($q = 1, S_0 = D_{rot} = 0$);
- E₂ – reciprocating extruders, their screw rotates and makes axial reciprocating motion simultaneously ($q = 1, S_0 \neq 0, D_{rot} = 0$);
- twin-screw extruders with screw co-rotation ($q = 2, S_0 = D_{rot} = 1$) and counter-rotation ($E_3; q = 2, S_0 = 0, D_{rot} = 2$).

The hardware flexibility is a feature of the extruders: the modular screws are assembled from elements of different types $T_j$ (conveying elements – EZ, kneading elements – KE, restriction ring adapters – ST, etc.). These elements differ in their geometric parameters $T_j$ (length $Z_j$, width $W_j$, and height $H_j$ of the channel, number of flights $z_j$, number of axial cuts in the flights, etc.). The elements have different degrees of strain influence on the polymeric material, and are used in different functional zones of the extruder. The hardware flexibility permits us to carry out not only parametric control of the extruder (by changing the extrusion mode $U$), but also structural control (by changing the configuration of the screw or screws $C_{scr}$, in case of production change-over to a new film type).

Regardless film production method $M_{prod}$, extrusion is a key stage of production, as the film surface quality depends on the extrudate thermal condition and a degree of uniformity. At the same time, only visual evaluation of the extrudate appearance occurs during production. Therefore, control decisions made by operators, based on subjective evaluation of the extrudate quality, inevitably lead to film surface defects. It promotes an increase in exit of rejected film, growth of material and power losses.

Thus, it is urgent to develop extrusion mathematical models (MM) allowing us to calculate extrudate quality characteristics (mixing degree, destruction index), throughput, EC, as well as to solve problems of resource and energy saving control of extruders of various types with adjustable configurations in multi-assortment extrusion and calender productions of polymeric films.

### 2. Formulating the problem of resource and energy saving control of extruders

The problem of resource and energy saving control of extruders consists in the following: during change-over of line utilizing production method $M_{prod}$ to assignment $Y_0 = \{T_{polym}, n_{umelt}^{max}, n_{black}^{max}, G_0, E^{max}\}$, it is necessary for us to create screw configuration $C_{scr}$, and determine controlling actions $U \in [U^{min}, U^{max}]$ for the extruder of a given brand $M_{extrud}$, to satisfy extrudate quality, extruder throughput and specific EC requirements:

$$\bar{I}_{min} \leq I_{d} \leq I_{d}^{max}, \ G \geq G_0, \ E \leq E^{max}$$

where $I_{d}^{min}$ – the minimum mixing degree characterizing extrudate uniformity; $I_{d}^{max}$ – the maximum destruction index; $G_0$ – the given production line throughput; $E^{max}$ – the maximum EC.

Satisfying quality indices’ requirements guarantees resource saving, that is, film production with uniform characteristic distribution (in particular uniform coloring). At the same time, there is a satisfaction of restrictions on the number of film surface defects (inclusions of unmelted polymer, black points, and destruction strips) arising because of irrational extruder configuration and/or operating mode. The restriction on EC is created as a result of the demand for an increase in power production efficiency, as the extruder is a very power-intensive element of the line (for example, the power consumption of industrial reciprocating extruders with screw diameter $D = 0.2$ m is 300–500 kW).

The MM for extrusion control have to consider the main extrusion features: polymer melting, both per the contiguous solids melting (CSM) mechanism and the dispersed solids melting (DSM) mechanism; dependence of melt viscosity on shear rate; mutual influence of down-channel and cross-channel flows of melt; melt leakages through the radial clearance, the axial cuts in element flights, and the gaps of screws gearing; influence of energy dissipation and heat exchange with the barrel and the screw on material temperature and viscosity; head hydraulic resistance. The MM of polymeric material melting and flow in extruders of various types described in literature are determined and constructed based on the mass balance, momentum balance, and energy balance equations for solid phase and melt, the rheological equation for melt, Stefan’s condition, and interphase mass balance equations (for the melting zone). The MM allow us to calculate the length of the melting zone, distributions of flow velocities, viscous friction stresses in flows, pressure and temperature of the melt.
3. Polymer extrusion mathematical models

The analysis of existing approaches to modeling of physical processes in extruders of various types has allowed us to offer a complex method for extrusion modeling. The method consists of the synthesis of MM of two types: a static model for calculating material state parameters in the extruder, and indices of extrudate quality; a dynamic model for evaluating average residence time of the material in the extruder, which the quality indices depend on. The static model represents a set of models describing motion and heat exchange of materials in the channels of the screw elements (melting and melt conveying zones) and the extrusion head.

Melting characteristics are calculated using the CSM and DSM models [7]. The CSM (Maddock–Street’s mechanism) occurs in single-screw extruders, and is characterized by the formation of a compacted solid phase of polymer. The DSM occurs in reciprocating and twin-screw extruders, and is characterized by the formation of a two-phase polymer system “solid particles – melt” [8].

General assumptions have been made during the creation of the element’s channel melt flow model. These include the inverse motion of the extruder barrel and screw, minor channel curvature, the channel being fully filled, melt incompressibility, process stationarity, steady down-channel flow, as well as a lack of radial flow, inertial forces, body forces, temperature gradient in the cross-channel flow, and melt slip on the channel walls. It is assumed that the prevailing heat transfer is radial thermal conduction. The basic model describing non-isothermal melt flow in the channel of j-th screw element can be written as:

mass balance, balance of pressure forces and internal friction forces, and heat balance equations:

\[ \int_0^{x_j'} v_j \, dy = \frac{\dot{Q}}{\rho} + \frac{\dot{Q}'}{\rho}, \quad z_j = \left[(2-q)W_j' + (q-1)\int_0^{x_j'} \frac{v_j \, dy}{dx}\right] = (2-q)Q - (q-1)(2Q_j + Q_j') \]

\[ Q_j' = q \frac{\dot{Q}}{\rho} + (Q_j + Q_j') + (q-1)(2Q_j + Q_j') \]

\[ \frac{\partial P_j'}{\partial x} - \frac{\partial}{\partial y} \left[ (\eta_j \dot{\gamma}_j) + (q-1) \frac{\partial}{\partial y} (\dot{\gamma}_j \dot{\gamma}_j) \right], \quad 0 < x < W_j', \quad 0 < y < H_j', \quad z_j' < z \leq z_j' + Z_j' \]

\[ \rho v_j \frac{\partial T_j'}{\partial z} = \lambda \frac{\partial^2 T_j'}{\partial y^2} + \eta_j' \dot{\gamma}_j'^2, \quad z_j' < z \leq z_j' + Z_j' \]

a rheological equation of the melt:

\[ \eta' = \mu' (T_j'), \quad |\dot{\gamma}_j'| = \left[ (\dot{\gamma}_j) + (q-1)(\dot{\gamma}_j') \right] \left[ \frac{\partial^2}{\partial y^2} \right], \quad \dot{\gamma}_j = \frac{dv_j}{dy}, \quad \dot{\gamma}_j' = \frac{dv_j}{dy} \]

kinematic and temperature boundary conditions:

\[ v_s \big|_{x=0} = 0, \quad v_s \big|_{x=W_j'} = \pi N (-D \sin \varphi + (2-q)S_0 \sin \Phi_{osc} \cos \varphi'), \quad v_s \big|_{x=0} = \pi N = v_s \big|_{x=W_j'} = -\frac{\pi D N (\cos \varphi')}{4} \]

\[ v_s \big|_{x=W_j'} = \pi N [(2-q)(D \cos \varphi' + S_0 \sin \Phi_{osc} \sin \varphi') - (q-1)D x \tan \varphi' \sin \varphi'] \]
where \( x, y, z \) – the cross-channel, normal and down-channel coordinates (m); \( v_x^{j}, v_y^{j}, v_z^{j} \) – the cross-channel and down-channel velocities (m/s); \( Q_\text{ax}^{j}, Q_\text{cy}^{j} \) – the intensity of leakages through the radial clearance (in extruders of all types) and the axial cuts in element flights (in the extruder of type \( E_d \)) (m\(^3\)/s); \( Q \) – the flow rate in the down-channel direction (m\(^3\)/s); \( Q_\text{ax}^{j}, Q_\text{cy}^{j} \) – the flow rates of leakages through the side and the calender gaps in the extruders of types \( E_3 \) and \( E_4 \) (m\(^3\)/s); \( Q \) – the flow rate determining the extruder throughput (m\(^3\)/s); \( Q_\text{ax}^{j}, Q_\text{cy}^{j} \) – the flow rates of leakages through the radial clearance and the axial cuts (m\(^3\)/s); \( P \) – pressure (Pa); \( \eta \) – melt viscosity (Pa s); \( \delta \) – the coordinate of the entrance to \( j \)-th element channel (m); \( \rho, c_p, \lambda \) – density (kg m\(^{-3}\)), heat capacity (J kg\(^{-1}\) K\(^{-1}\)), and thermal conductivity (W m\(^{-1}\) K\(^{-1}\)) of the melt, which are independent of its pressure and its temperature; \( T \) – temperature (°C); \( \mu' \) – consistency index (Pa s); \( n \) – power law index; \( \phi \) – helix angle (rad); \( \Phi_\text{osc} \) – screw oscillation phase in extruder \( E_2 \) (rad); \( q_\text{ax}^{j}, q_\text{cy}^{j} \) – the densities of heat flows from the melt to the screw and barrel (in \( k \)-th thermal zone) (W m\(^{-2}\)); \( T_\text{scr} \) – screw temperature (°C).

The melt flow and heat exchange model synthesis procedure includes the following stages: choosing (from a library of models) equations for calculating leakages’ flow rates, consistency index, heat flows’ densities, and the integration of these equations to the basic model equations (2)–(4); coupling the constructed MM for flow and heat exchange in the elements according to the screw configuration; coupling the model for flow and heat exchange in the screw with the chosen head model. The equations are chosen depending on the types of the extruder, head, and screw elements, the polymer class, and the thermal mode. Conditions (5) are used to integrate the MM for flow and heat exchange in the elements.

The synthesis of the dynamic model consists of choosing and combining the hydrodynamic models describing flow in standard sections of screws made of elements of the same type. In order to account for the back axial mixing in the extruder, recycling flows are introduced between section models [9]. The library of the hydrodynamic models includes plug flow reactor model (for description of sections in the solids conveying zone), continuous stirred tank reactor model (for sections in the melting and mixing zones), tanks-in-series model (for sections in the melt conveying zone).

The MM allow us to calculate the distributions of material state parameters in screw elements’ channels (\( Q, v_x^{j}, v_y^{j}, v_z^{j}, P, T, \eta \)), the extruder throughput \( G \) (by calculating the work point of the extruder using the static model), and the average residence time of polymer in the extruder depending on the throughput \( \tau \) (using the dynamic model). Extrudate quality indices are defined as:

\[
\tau = \frac{T}{Z} \sum_{i=n}^{j} \left[ \left( \frac{1}{H} \right)^{H} \right]^{H} \int_{z}^{H} \Phi dy \, dz, \quad \tau_d = \exp \left[ \frac{E_d (T_{\text{ext}} - T_d)}{8.3 \, (T_{\text{ext}} + 273) \, (T_d + 273)} \right] \quad 100
\]

where \( Z \) – the screw channel length (m); \( \tau_d, T_d \) – time (s) and temperature (°C) of the beginning of polymer color change at destruction; \( E_d \) – activation energy (J/mol); \( T_{\text{ext}} = T^\text{b}(Z) \) – extrudate temperature (°C).

Model adequacy verification is accomplished by comparing the calculated and the measured values of extrudate temperature, as well as throughput and residence time for extruders of various types (\( E_1 \)– \( E_4 \)) and configurations during production of PP, LDPE, and PVC films. Figure 2 shows calculated (1, 3) and measured (2, 4) dependencies of extrudate temperature on screw speed of the reciprocating extruder: 1. \( 2 - D = 0.046 \) m, screw configuration 1, \( T_{\text{polym}} = \text{PP}, T_{\text{scr}} = 150 ^\circ C, T_b = 200 ^\circ C; 3, 4 - D = 0.2 \) m, screw configuration 2, \( T_{\text{polym}} = \text{PVC}, T_{\text{scr}} = 120 ^\circ C, T_b = 150 ^\circ C \). The extrudate temperature increases with increasing screw speed. As a result of the screw speed increasing, the shear rate increases, leading to growing dissipative heat generation. The results of statistical processing of the data have confirmed the MM adequacy as per Fisher’s criterion and coefficient of determination.
4. Program complex for extruder modeling and control

The program complex (PC) includes the subsystem for screw configuration creation and extruder geometric parameter calculation, the modeling subsystem for calculation of the output parameters of extrusion $Y$ in the procedural ranges $[U_{\text{min}}, U_{\text{max}}]$ of controlling actions $U$, the databank of extrusion characteristics, the visualization subsystem [10]. The database allows us to adjust the PC for various production methods $M_{\text{prod}}$ and assignments $Y_0$. The visualization subsystem enables representing the results as 3D models of the screws of created configurations, 3D graphs for distributions of material state parameters in the screw channel, and 3D graphs for the dependencies of output parameters on controlling actions (figure 3). The analysis of the created dependencies enables us to determine the values of controlling actions that ensure the implementation of criterion restrictions (1).

5. Conclusion

The MM and PC have been developed for resource and energy saving control of extruders of various types used in productions of polymeric films. The PC adjusts according to the configuration of the extruder screw and head, as well as the type of polymer. Testing has confirmed the functionality of the PC and the possibility of its use for production personnel decision support. Using the PC enables us to ensure the required extrudate quality and, as a result, the film quality. It enables us to reduce extruder EC, and lower the time required for production line change-over to a new assignment by determining the appropriate values for the extruder regime parameters, which prevent extrudate quality violations.

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