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MODELING OF MELTING PROCESS IN A SINGLE SCREW EXTRUDER FOR POLYMER PROCESSING

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Розроблено математичну модель зони плавлення одночерв'ячного екструдера. Модель враховує теплообмін полімеру з черв'яком і циліндром, а також реальні граничні умови (черв'як обертається, циліндр нерухомий). Досліджено параметри зони плавлення й виконано порівняння результатів розрахунків з експериментом. Запропоновано підхід до моделювання екструдера в цілому як послідовності взаємопов'язаних між собою його функціональних зон

***Ключові слова:** одночерв'ячний екструдер, полімер, гранула, зона плавлення, граничні умови, полімерна пробка, температурне поле*

Разработана математическая модель зоны плавления одночервячного экструдера. Модель учитывает теплообмен полимера с червяком и цилиндром, а также реальные граничные условия (червяк вращается, цилиндр неподвижен). Исследованы параметры зоны плавления и выполнено сравнение результатов расчёта с экспериментом. Предложен подход к моделированию экструдера в целом как последовательности взаимосвязанных между собой его функциональных зон

***Ключевые слова:** одночервячный экструдер, полимер, гранула, зона плавления, граничные условия, полимерная пробка, температурное поле*

1. Introduction

There is a wide range of products and semi-finished products of thermoplastic polymers produced by extrusion, such as flat and tubular films, pipes, and profiles [1–3].

We can distinguish three main functional zones in the analysis of operation of single-screw extruders for processing of polymeric materials. They are feeding, melting and homogenization [2, 4, 5]. The geometry of a screw corresponds to the mentioned zones in general, therefore a classic screw is a screw with three zones, a constant step of a screw working channel and a stepless change in the specified channel along the length of a screw. In the first zone, a working channel has the greatest depth of the constant value, in the second one – it has depth, which decreases uniformly, in the third one – the smallest depth of the constant value [2–5].

Although the specified structural zones of a screw in general correspond to the functional zones of an extruder, boundaries of structural and functional zones do not always coincide. Construction of modern screw is much more complicated than a classic screw, and depends, first of all, on a material being processed [2, 4, 6, 7].

One of processes that determines quality of products obtained at a single-screw extruder is melting of polymeric material. Many authors studied the process over the past half century. They accepted various assumptions in order to simplify its mathematical description. For a long time, such an approach had been fully justified, however, in recent years, performance of extruders has increased substantially [8] and many melting models became unacceptable for practical use. Therefore, modeling of a process of melting of polymer granules in the working channel of a screw extruder, taking into consideration the actual boundary conditions, as well as heat exchange between a polymer and a screw and a cylinder of an extruder, is relevant.

2. Literature review and problem statement

Each polymer has certain properties; therefore, a corresponding geometry of working parts and a processing mode are necessary for its processing in a single-screw extruder. That is why there is a fairly large variety of extrusion equipment in the market. And there are cases where even the most advanced extruders cannot provide the desired quality of resulting products after a change of a manufacturer of the same polymer. Therefore, the modeling of processing has attracted much attention over many decades [5].

A base of the classical theory of extrusion is a solution of a corresponding mathematical model by analytic methods for a so-called inverse plane-parallel model. The given model makes possible to bring the problem to a rectangular coordinate system and consider a screw fixed and extended on the plane, and a cylinder moving along the channel of a screw and extended on the plane also.

Thus, one of the earliest works devoted to the process of polymer processing in a one-screw extruder [4] considers a simplified two-plate model in addition to the inversed plane-parallel model. In this case, the two-plate model does not even take into account the presence of ridges in a working channel between parallel plates.

Papers [2, 5] consider also the inverse plane-parallel model. The main disadvantage of the model is that processes, which actually occur near a surface of a rotating screw shift conditionally to the side of a fixed cylinder and vice versa. This is not essential for the calculation of performance, total dissipation energy and average mass temperature, but such an approach can lead to significant errors if it is necessary to take into account heat exchange between surfaces of a screw and a cylinder.

Work [9] proposes a mathematical model for polymer melting, which takes into consideration the formation of a melt film from a side of a cylinder only. Such an approach is acceptable for the inverse model, but a similar film in reality appears also near a surface of a rotating screw.

Paper [10] considers formation of melt films both near a surface of a cylinder and near a surface of a screw. However, it considers the process without taking into account systems of heat-stabilization of a screw and a cylinder. Work [11] has similar disadvantages.

Paper [12] considers both mathematical and experimental study of polymer melting in a one-screw extruder. It shows that there is a rather large discrepancy between theoretical and experimental data. This can be the result of inadequacy of the inverse plane-parallel model adopted in the paper.

Paper [13] proposes a new approach to the modeling of polymer melting process (without an analysis of a melting mechanism itself). However, authors of the paper use the inverse extrusion model as in the papers discussed.

Work [14] proposes a mechanism of melting of a polymer in the case of incomplete filling of a working channel of an extruder with polymeric granules, and work [15] presents a melting model for a more efficient barrier screw.

Papers [16, 17] study the extrusion process with a barrier screw also. Authors also used the inverse model for analysis despite the fact that the process is more complicated than the extrusion process with a use of a classic screw.

Work [18] considers experimental studies of melting of polymer mixtures. The results of experiments showed that the mechanism of melting of polymer mixtures is similar to the mechanism of melting a pure polymer.

The inverse extrusion model proved to be quite satisfactory for relatively low speeds of processing of traditional polymeric materials. Therefore, it is spread quite widely even at the beginning of the third millennium [2, 5].

Development of computer technology made it possible to refine these models to study the effect of previously ignored factors on the melting process. At the same time, coefficients used are associated with certain difficulties and almost do not affect a final result. In addition, complexity of models for engineering calculations is often inappropriate, since we cannot always fully take account the actual properties of materials processed in theoretical models [19].

At the same time, analysis of calculations, as well as experimental and practical data, showed disadvantages of well-known models [20, 21]. The explanation of the above disadvantages is first of all the fact that classical solutions of the screw extrusion were meant for a plane-parallel model with a fixed screw and a rotating cylinder. Therefore, processes, which occur actually near the surface of a rotating screw, shift conditionally to a side of a fixed cylinder and vice versa. This is not essential for calculation of performance, dissipation intensity and average mass temperature, but such an approach can lead to significant errors if it is necessary to take into account a heat exchange with surfaces of a screw and a cylinder.

For a model with a rotating screw, in comparison with the inverse model, intensity of dissipation at the surface of a screw is greater than that of the cylinder surface. Therefore, if the energy supplied from external heaters is commensurable with the dissipation energy, then we must take this fact into account when calculating a heat transfer process of a polymer with surfaces of a screw and a cylinder. This is especially important when processing polymers with low viscosity or high humidity. An increase in a share of external heaters in the process of melting of a polymer requires an increase in the surface of a heat transfer, that is, a length of a screw, or reduction of extruder performance. Therefore, a range of processing modes that provide the required quality of the resulting product is substantially narrowed for an extruder with a screw of a predetermined length. Taking into account the above, we need a new approach to model the process of screw extrusion, and above all to model melting of a polymer.

3. The aim and objectives of the study

The aim of present study is mathematical modeling of the process of melting of polymer granules in a working channel of an extruder, taking into account heat supply systems of its working parts, as well as real boundary conditions – geometric conditions, speed conditions, and temperature. This will make it possible to determine rational parameters of both the melting process and the extrusion process in general to provide the desired polymer temperature distribution at the extruder output at its predetermined performance. The parameters include a method of heating or cooling of a screw and an extruder body, a type of a heat carrier, its temperature and a volume expense, a geometry of a screw channel and its rotational frequency.

We must solve the following tasks to achieve the objective:

– to develop a mathematical model of the polymer melting process in a screw extruder taking into account heat transfer between a polymer with a screw and a cylinder, rotation of a screw and a fixed cylinder, as well as a cylindrical shape of a working channel of an extruder;

– to theoretically investigate the process of melting of polymer granules in a working channel of an extruder;

– to verify experimentally the adequacy of the developed mathematical model.

4. Materials and methods to study melting processes in a single-screw extruder

Fig. 1 shows schematic of an extruder with a classic three-zone screw [2–5]. The working channel of such an extruder has the greatest depth of the constant in the feed zone, the decreasing depth in the melting zone and the smallest depth of the constant in the homogenization zone.

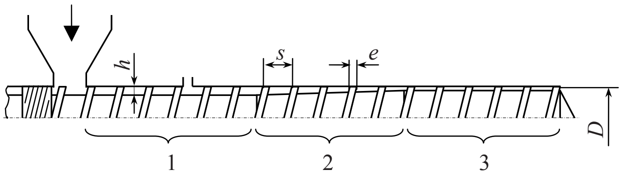

Fig. 1. Schematic of the classical three-zone single-screw extruder: 1, 2, 3 – feeding, melting and homogenization zones; *D*, *h* and *e* – a diameter, a height and a width of the ridge of the screw thread, m; *s* – a step of angular thread, m

Photograph of the screw extracted from an extruder cylinder (we removed solid granules remaining in the working channel of the screw for a better representation of the melting process, Fig. 2) illustrates the mechanism of the melting process, which is typical for most single-screw extruders. We chose polyethylene of high pressure (low density polyethylene) – one of the most common polymers processed in screw extruders – for the study [1, 8, 12].

Fig. 2. Physical appearance of the screw extracted from an extruder body (light color highlights the melt solidified in the screw channel)

From the photograph shown above, it is evident that there is a separation of a polymer in the melting zone into the melt area, which accumulates on the side of the pushing shoulder of the ridge of the angular thread of the screw channel and the area of a solid polymer (Fig. 3).

There are five areas distinguished conditionally in the working channel of the melting zone of an extruder: A – a solid polymer layer ("solid bed"); B – a main melt layer between the front (pushing) shoulder and the ridge of the screw channel and the "solid bed"; C – a melting layer between the surface of the cylinder wall and the "solid bed"; D – a melting layer between the back shoulder of the screw channel the "solid bed" (they are usually neglected at consideration of a melting zone); E – a melt layer between the surface of the screw and the "solid bed".

Let us consider the process of melting of material in a cylindrical coordinate system z, r, ϑ (Fig. 4). At the same time, we will consider the process within the allocated volume equal to one step of a screw thread. Such cylindrical coordinate system is motionless relatively to the allocated volume and moves along L axis with it. We consider motion of the most isolated volume in x, y, z system of Cartesian rectangular coordinates [20, 21].

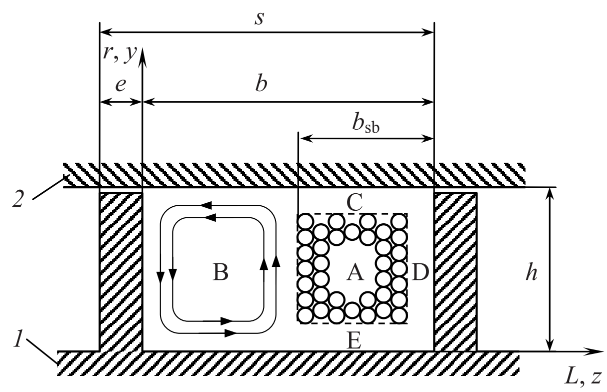

Fig. 3. The mechanism of melting of a polymer in the working channel of a single-screw extruder: *1* – a screw; *2* – a cylinder; A, B, C, D, E – areas of the working channel in the boundaries of the melting zone of the extruder; *z*, *L* – coordinates directed along the axis of the screw, m; *r*, *y* – coordinates directed along the height of the channel of the screw, m; *b* – a width of the screw channel, m; b_{sb} – a width of a solid polymeric "solid bed", m

In analysis of the process, we will assume that a width of the "solid bed" of non-melted polymer b_{sb} is constant and equal to its average value within one step of calculation. In this case, we can consider the melting process as axisymmetric process.

When analyzing a process in the allocated volume (within the limits of the calculation step under consideration), the value of z coordinate varies from 0 to b, and we can determine the speed of the allocated volume along the axis of the screw w_L from the previously obtained expression [20, 21].

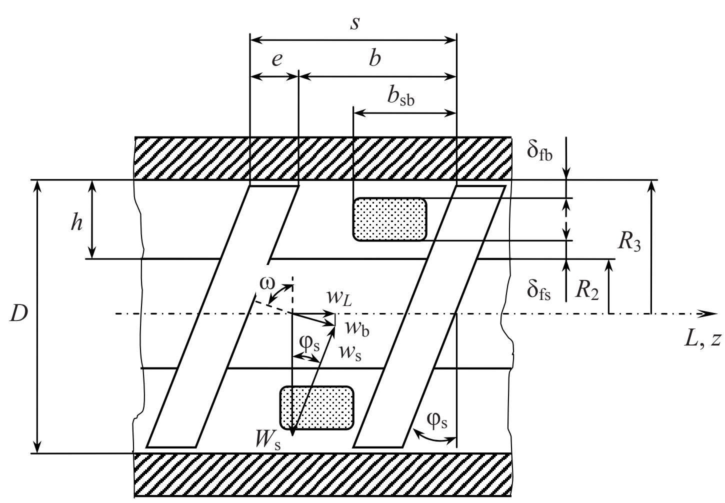

Fig. 4. For formulation of the mathematical model of the melting process: R_2 and R_3 – radii of a core of the screw and an internal radius of the cylinder, m; δ_{fs} and δ_{fb} – thicknesses of melt films near the surface of the screw and the cylinder, m; W_s is a linear speed of the surface of the ridge of the screw thread, m/s; w_s and w_b – components of a speed of the "plug" relative to the screw and the cylinder, m/s; w_L – speed of the allocated volume along the axis of the screw, m/s; φ_s – angle of inclination of the screw thread, °; ω – angle between speed component w_b and speed W_s, °

$$w_L = \frac{G}{\rho\left\{\frac{\pi}{4}\left[D^2-(D-2h)^2\right]-\frac{eh}{\operatorname{tg}\phi_s}\right\}}, \quad (1)$$

where G is the mass output of the extruder, kg/s; ρ is density (kg/m^3) of a polymer as a function of temperature T, °C.

Since the ratio of L coordinate to the speed w_L, $t = L/w_L$, determines the time t of a shift of the allocated volume along L coordinate, we can write energy conservation in the form

$$\rho c w_L \frac{\partial T}{\partial L} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda\frac{\partial T}{\partial r}\right]+\frac{\partial}{\partial z}\left[\lambda\frac{\partial T}{\partial z}\right]+q_V, \quad (2)$$

where c, λ are mass heat capacity (J/(kg·K)) and thermal conductivity (W/(m·K)) of a polymer as a function of temperature; t – time, s; q_V – is volume density of a heat flow of internal energy sources of a polymer, W/m^3.

Melt films of δ_{fs} and δ_{fb} thicknesses formed near surfaces of the screw and the cylinder (areas E and C in Fig. 3) surround a solid polymer. There is a dissipation of energy in these films, due to shear deformation, while there are no internal energy sources in the volume of the "solid bed" (unmelt polymer, area A in Fig. 3). Then, for the solution of equation (2) within the "solid bed", the boundary conditions take the form:

$$T\big|_{L=0} = T_{in};$$

$$T\big|_{z=b-b_{sb}} = T_m;$$

$$T\big|_{z=b} = T_m;$$

$$T\big|_{r=R_2+\delta_{fs}} = T_m;$$

$$T\big|_{r=R_3-\delta_{fb}} = T_m,$$

where T_{in} and T_m are the temperatures of a polymer at the entrance to the melting zone and the melting point of a polymer, °C.

In the area of the melt, for the solution of equation (2), the boundary conditions have the form:

$$T\big|_{L=0} = T_{in};$$

$$T\big|_{z=0} = T_s;$$

$$T\big|_{z=b-b_{sb}} = T_m;$$

$$\lambda\frac{\partial T}{\partial z}\bigg|_{(z=b-b_{sb})_f} = \lambda\frac{\partial T}{\partial z}\bigg|_{(z=b-b_{sb})_{sb}}; \quad (3)$$

$$\lambda\frac{\partial T}{\partial r}\bigg|_{r=R_2} = q_s; \quad T\big|_{r=R_2} = T_s;$$

$$\lambda\frac{\partial T}{\partial r}\bigg|_{r=R_3} = q_b; \quad T\big|_{r=R_3} = T_b,$$

where q_s and q_b are specific heat flows from external systems of thermostabilization of the screw and the cylinder, W/m^2; T_s and T_b are the temperatures of screw and cylinder working surfaces, °C.

Condition (3) means that a temperature on the surface of the "melt-solid polymer" contact is equal to the melting point T_m, as well as the equality of thermal flows through this surface is respected.

To determine intensity of dissipation in the volume of the melt q_V it is necessary to know speed fields in this volume.

Let us consider processes that occur in melt films in more detail. By analogy with the feed zone, we consider components of speed of non-melted polymer solid bed [21] (Fig. 4).

The screw rotates at a speed $W_s = \pi D n_s$, while the "solid bed" slips on melt films at a speed of w_s relatively to the screw and at speed of w_b relative to the cylinder. We can obtain the following expressions for determining the speed components from geometric relations (Fig. 4):

$$w_L = W_s \frac{\operatorname{tg}\phi_s \operatorname{tg}\omega}{\operatorname{tg}\phi_s + \operatorname{tg}\omega};$$

$$w_b = \frac{w_L}{\sin\omega};$$

$$w_s = \sqrt{W_s^2 + w_b^2 - 2W_s w_b \cos\omega}.$$

If mass production of an extruder G is known, then, after determination a value of the speed w_L by equation (1), it is possible to find an angle ω (rad)

$$\omega = \operatorname{arctg}\left(\frac{w_L \operatorname{tg}\phi_s}{W_s \operatorname{tg}\phi_s - w_L}\right).$$

Since thickness of films δ_{fs} and δ_{fb} is small, we can neglect a curvature of melting surfaces of the "solid bed" and consider processes in films not in a cylindrical, but in a rectangular coordinate system by directing y axis along the thickness of films. Let us assume that the relative speed in melt films varies linearly from 0 to w_s at the surface of the screw and from 0 to w_b at the surface of the cylinder. We will also assume that, within dL element, a speed and thermophysical properties of the film melt are constant and determined by average values of temperature and shift speeds both from the side of the screw $\dot{\gamma}_{fs} = w_s/\delta_{fs}$, and from the side of the cylinder $\dot{\gamma}_{fb} = w_f/\delta_{fb}$. Then the energy conservation equations in the assumption that only thermal conductivity transmits heat through film thickness, take the form:

– for a film at the surface of the screw

$$\lambda_{fs}\frac{\partial^2 T}{\partial y^2} + \mu_{fs}\left(\frac{w_s}{\delta_{fs}}\right)^2 = 0; \quad (4)$$

– for a film at the surface of the cylinder

$$\lambda_{fb}\frac{\partial^2 T}{\partial y^2} + \mu_{fb}\left(\frac{w_b}{\delta_{fb}}\right)^2 = 0, \quad (5)$$

where λ_{fs} and λ_{fb} are the thermal conductivities of the melt in films near the screw and the cylinder as a function of temperature, W/(m·K); μ_{fs} are μ_{fb} are the speeds of the melt in films near the surfaces of the screw and cylinder, Pa·s.

The boundary conditions for equations (4) and (5) take the form:

– for equation (4):

$$-\lambda_{fs}\frac{\partial T}{\partial y}\bigg|_{y=0} = q_s; \quad T\big|_{y=0} = T_s;$$

$$T\big|_{y=\delta_{fs}} = T_m;$$

– for equation (5):

$$T\big|_{y=0}=T_{\mathrm{m}}; \tag{6}$$

$$\lambda_{\mathrm{fb}}\frac{\partial T}{\partial y}\bigg|_{y=\delta_{\mathrm{fb}}}=q_{\mathrm{b}};\;\; T\big|_{y=\delta_{\mathrm{fb}}}=T_{\mathrm{b}}. \tag{7}$$

Heat coming from surfaces of the melt to non-melted polymer will consist of:

– for a film at the surface of the screw

$$q_{\mathrm{fs}}=-\lambda_{\mathrm{fs}}\frac{\partial T}{\partial y}\bigg|_{y=\delta_{\mathrm{fs}}} b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}\frac{\Delta L}{\sin\phi_{\mathrm{s}}}=$$

$$=-\lambda_{\mathrm{fs}}\frac{\partial T}{\partial y}\bigg|_{y=\delta_{\mathrm{fs}}} b_{\mathrm{sb}}\Delta L\mathrm{ctg}\phi_{\mathrm{s}}; \tag{8}$$

– for a film at the surface of the cylinder

$$q_{\mathrm{fb}}=\lambda_{\mathrm{fb}}\frac{\partial T}{\partial y}\bigg|_{y=0} b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}\frac{\Delta L}{\sin\phi_{\mathrm{s}}}=\lambda_{\mathrm{fb}}\frac{\partial T}{\partial y}\bigg|_{y=0} b_{\mathrm{sb}}\Delta L\mathrm{ctg}\phi_{\mathrm{s}}. \tag{9}$$

At the expense of heat, the value of which we can determine in accordance with dependences (8) and (9), heating and gradual melting of a certain amount of a solid polymer with an increase in its enthalpy by the value $(i_{\mathrm{m}}-i_{\mathrm{in}})$, occurs, where i_{m} and i_{in} are mass enthalpies of a polymer at a temperature T_{m} and T_{in}, J/kg. Under stationary conditions, the resulting melt passes to the main melt area near the pushing shoulder of the ridge of the screw channel (area B in Fig. 3) completely, and thickness of films is set to provide this transition. The average speed of the melt in the direction perpendicular to the ridge of the screw will equal:

– for a film at the surface of the screw:

$$\frac{w_{\mathrm{s}}}{2}\mathrm{tg}\phi_{\mathrm{s}};$$

– for a film at the surface of the cylinder:

$$\frac{w_{\mathrm{b}}}{2}\sin(\omega+\phi_{\mathrm{s}}).$$

Then, for a growth of the mass expense of a melt, we can write the following dependences:

– for a film at the surface of the screw

$$\Delta G_{\mathrm{fs}}=-\lambda_{\mathrm{fs}}\frac{\partial T}{\partial y}\bigg|_{y=\delta_{\mathrm{fs}}} b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}\frac{\Delta L}{\sin\phi_{\mathrm{s}}}\frac{1}{(i_{\mathrm{m}}-i_{\mathrm{in}})}=$$

$$=\rho_{\mathrm{fs}}\frac{w_{\mathrm{s}}}{2}\mathrm{tg}\phi_{\mathrm{s}}\frac{\Delta L}{\sin\phi_{\mathrm{s}}}\delta_{\mathrm{fs}}$$

or

$$\Delta G_{\mathrm{fs}}=-\lambda_{\mathrm{fs}}\frac{\partial T}{\partial y}\bigg|_{y=\delta_{\mathrm{fs}}}\frac{b_{\mathrm{sb}}\Delta L\mathrm{ctg}\phi_{\mathrm{s}}}{(i_{\mathrm{m}}-i_{\mathrm{in}})}=\frac{\rho_{\mathrm{fs}}w_{\mathrm{s}}\Delta L\delta_{\mathrm{fs}}}{2\cos\phi_{\mathrm{s}}}; \tag{10}$$

– for a film at the surface of the cylinder

$$\Delta G_{\mathrm{fb}}=\lambda_{\mathrm{fb}}\frac{\partial T}{\partial y}\bigg|_{y=0} b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}\frac{\Delta L}{\sin\phi_{\mathrm{s}}}\frac{1}{(i_{\mathrm{m}}-i_{\mathrm{in}})}=$$

$$=\rho_{\mathrm{fb}}\frac{w_{\mathrm{b}}}{2}\sin(\omega+\phi_{\mathrm{s}})\frac{\Delta L}{\sin\phi_{\mathrm{s}}}\delta_{\mathrm{fb}}$$

or

$$\Delta G_{\mathrm{fb}}=\lambda_{\mathrm{fb}}\frac{\partial T}{\partial y}\bigg|_{y=0}\frac{b_{\mathrm{sb}}\Delta L\mathrm{ctg}\phi_{\mathrm{s}}}{(i_{\mathrm{m}}-i_{\mathrm{in}})}=\rho_{\mathrm{fb}}w_{\mathrm{b}}\Delta L\delta_{\mathrm{fb}}\frac{\sin(\omega+\phi_{\mathrm{s}})}{2\sin\phi_{\mathrm{s}}}. \tag{11}$$

In the general case, the channel depth of a screw h varies along L coordinate, but we can assume it as a constant within the allocated volume ΔL for the given calculation step. That is, we can replace a continuous change in the depth of the channel h with a step one. At the same time, we assume that the value of a width of a "solid bed" of the non-melted polymer b_{sb} decreases in proportion to the ratio of expends of the non-melted polymer and the melt.

The average temperature of melt films is:

– for a film at the surface of the screw

$$\bar{T}_{\mathrm{fs}}=\frac{1}{\delta_{\mathrm{fs}}}\int_0^{\delta_{\mathrm{fs}}}T\mathrm{d}y; \tag{12}$$

– for a film at the surface of the cylinder

$$\bar{T}_{\mathrm{fb}}=\frac{1}{\delta_{\mathrm{fb}}}\int_0^{\delta_{\mathrm{fb}}}T\mathrm{d}y. \tag{13}$$

Accordingly, the power consumed in films will equal:

– for a film near the screw

$$\Delta N_{\mathrm{fs}}=\rho_{\mathrm{fs}}w_{\mathrm{s}}\sin\phi_{\mathrm{s}}\pi R_2\delta_{\mathrm{fs}}\left(\bar{i}_{\mathrm{fs}}-i_{\mathrm{in}}\right);$$

– for a film near the cylinder

$$\Delta N_{\mathrm{fb}}=\rho_{\mathrm{fb}}w_L\pi R_3\delta_{\mathrm{fb}}\left(\bar{i}_{\mathrm{fb}}-i_{\mathrm{in}}\right),$$

where ΔN_{fs} and ΔN_{fb} are the powers consumed in films near the screw and the cylinder, W; ρ_{fs} and ρ_{fb} are melt densities in films near the screw and the cylinder as a function of temperature, kg/m^3; $\bar{i}_{\mathrm{fs}}$ and $\bar{i}_{\mathrm{fb}}$ are the mass enthalpies of a polymer at average temperatures $\bar{T}_{\mathrm{fs}}$ and $\bar{T}_{\mathrm{fb}}$, J/kg.

Each of the capacities ΔN_{fs} and ΔN_{fb} is a sum of the corresponding dissipation power and power supplied from an external thermal stabilization (cooling or heating) system. Then the dissipation power will equal:

– for a film at the surface of the screw

$$\Delta N_{\mathrm{dis\,fs}}=\Delta N_{\mathrm{fs}}-q_{\mathrm{s}}\Delta L b_{\mathrm{sb}}\mathrm{ctg}\phi_{\mathrm{s}}; \tag{14}$$

– for a film at the surface of the cylinder

$$\Delta N_{\mathrm{dis\,fb}}=\Delta N_{\mathrm{fb}}-q_{\mathrm{b}}\Delta L b_{\mathrm{sb}}\mathrm{ctg}\phi_{\mathrm{s}}.$$

In equation (14), q_{s} value has a plus sign in the case of screw's heating and a minus sign if it is cooled.

It is necessary to add functions that determine a dependence of thermophysical properties on a temperature, as well as viscosity of a shift rate and temperature to the dependences described above, which describe the melting process in a single-screw extruder [19, 22].

Let us consider equations that describe the processes in melt films.

As a result of solving equation (4) for a film near the screw, we obtain:

$$T=T_{\mathrm{m}}+\frac{\mu_{\mathrm{fs}}}{2\lambda_{\mathrm{fs}}}\left(\frac{w_{\mathrm{s}}}{\delta_{\mathrm{fs}}}\right)^2\left(\delta_{\mathrm{fs}}^2-y^2\right)+\frac{q_{\mathrm{s}}}{\lambda_{\mathrm{fs}}}(\delta_{\mathrm{fs}}-y). \tag{15}$$

We can determine an average film temperature by substituting relation (15) in expression (12), after integration of the latter

$$\overline{T}_{\mathrm{fs}} = T_{\mathrm{m}} + \frac{\mu_{\mathrm{fs}} w_{\mathrm{s}}^2}{3\lambda_{\mathrm{fs}}} + \frac{q_{\mathrm{s}}\delta_{\mathrm{fs}}}{2\lambda_{\mathrm{fs}}}. \tag{16}$$

Accordingly, we determine a surface temperature of the screw by substitution of the value of $y = 0$ coordinate into dependence (15)

$$T_{\mathrm{s}} = T_{\mathrm{m}} + \frac{\mu_{\mathrm{fs}} w_{\mathrm{s}}^2}{2\lambda_{\mathrm{fs}}} + \frac{q_{\mathrm{s}}\delta_{\mathrm{fs}}}{\lambda_{\mathrm{fs}}}. \tag{17}$$

Then a temperature gradient near the melting surface ($y = \delta_{\mathrm{fs}}$) will equal

$$\left.\frac{\partial T}{\partial y}\right|_{y=\delta_{\mathrm{fs}}} = -\frac{\mu_{\mathrm{fs}} w_{\mathrm{s}}^2}{\lambda_{\mathrm{fs}}\delta_{\mathrm{fs}}} - \frac{q_{\mathrm{s}}}{\lambda_{\mathrm{fs}}}. \tag{18}$$

By substituting expression (18) in dependence (10), we obtain

$$\left(\frac{\mu_{\mathrm{fs}} w_{\mathrm{s}}^2}{\delta_{\mathrm{fs}}} + q_{\mathrm{s}}\right) b_{\mathrm{sb}} \cos\phi_{\mathrm{s}} \frac{1}{\left(i_{\mathrm{m}} - i_{\mathrm{in}}\right)} = \rho_{\mathrm{fs}} \frac{w_{\mathrm{s}}}{2} \mathrm{tg}\,\phi_{\mathrm{s}} \delta_{\mathrm{fs}}. \tag{19}$$

After transformation of expression (19), we can obtain a dependence for the determination of thickness of a melt film from the side of the screw

$$\delta_{\mathrm{fs}} = \frac{q_{\mathrm{s}} + \sqrt{q_{\mathrm{s}}^2 + \dfrac{2\rho_{\mathrm{fs}}\mu_{\mathrm{fs}} w_{\mathrm{s}}^3 \left(i_{\mathrm{m}} - i_{\mathrm{in}}\right)\mathrm{tg}\,\phi_{\mathrm{s}}}{b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}}}}{\dfrac{\rho_{\mathrm{fs}} w_{\mathrm{s}} \left(i_{\mathrm{m}} - i_{\mathrm{in}}\right)\mathrm{tg}\,\phi_{\mathrm{s}}}{b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}}}.$$

We obtain a function, which describes a temperature profile in a melt film near the cylinder by integration of an equation (5) and definition of integration constants from the boundary conditions (6) and (7)

$$T = T_{\mathrm{m}} + \frac{\mu_{\mathrm{fb}}}{\lambda_{\mathrm{fn}}}\left(\frac{w_{\mathrm{b}}}{\delta_{\mathrm{fb}}}\right)^2 \left(\delta_{\mathrm{fb}} y - \frac{y^2}{2}\right) + \frac{q_{\mathrm{b}} y}{\lambda_{\mathrm{fb}}}. \tag{20}$$

We determine an average film temperature from the cylinder side after substituting expression (20) in equation (13) and integration of it

$$\overline{T}_{\mathrm{fb}} = T_{\mathrm{m}} + \frac{\mu_{\mathrm{fb}} w_{\mathrm{b}}^2}{3\lambda_{\mathrm{fb}}} + \frac{q_{\mathrm{b}}\delta_{\mathrm{fb}}}{2\lambda_{\mathrm{fb}}}.$$

We find a temperature of the side of the cylinder by substituting the value $y = \delta_{\mathrm{fb}}$ in expression (20)

$$T_{\mathrm{b}} = T_{\mathrm{m}} + \frac{\mu_{\mathrm{fb}} w_{\mathrm{b}}^2}{2\lambda_{\mathrm{fb}}} + \frac{q_{\mathrm{b}}\delta_{\mathrm{fb}}}{\lambda_{\mathrm{fb}}}. \tag{21}$$

We should note that if T_{b} value is less than the set value, cylinder heaters are included and a heat flow q_{b} is equal to the heat flow from heaters. If T_{b} temperature exceeds the set value, a cooling system switches on, while q_{b} value is equal to the heat flow to the cooling medium and has a minus sign. We differentiate expression (20) at the value $y = 0$ and substitute the obtained dependence in expression (11), then we obtain

$$\left(\frac{\mu_{\mathrm{fb}} w_{\mathrm{b}}^2}{\delta_{\mathrm{fb}}} + q_{\mathrm{b}}\right) \frac{b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}}{\left(i_{\mathrm{m}} - i_{\mathrm{in}}\right)} = \rho_{\mathrm{fb}}\delta_{\mathrm{fb}} \frac{w_{\mathrm{b}}}{2} \sin\left(\omega + \phi_{\mathrm{s}}\right),$$

from which it is possible to obtain an expression for the determination of film thickness δ_{fb}

$$\delta_{\mathrm{fb}} = \frac{q_{\mathrm{b}} + \sqrt{q_{\mathrm{b}}^2 + \dfrac{2\rho_{\mathrm{fb}}\mu_{\mathrm{fb}} w_{\mathrm{b}}^3 \left(i_{\mathrm{m}} - i_{\mathrm{in}}\right)\sin\left(\omega + \phi_{\mathrm{s}}\right)}{b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}}}}{\dfrac{\rho_{\mathrm{fb}} w_{\mathrm{b}} \left(i_{\mathrm{m}} - i_{\mathrm{in}}\right)\sin\left(\omega + \phi_{\mathrm{s}}\right)}{b_{\mathrm{sb}}\cos\phi_{\mathrm{s}}}}.$$

Expressions (17) and (21) make it possible to calculate temperature of the working surfaces of the screw and the cylinder T_{s} and T_{b} under condition that heat flows q_{s} and q_{b} are given. On the other hand, the same equations make it possible to determine heat flows that provide the set values of temperatures T_{s} and T_{b}.

5. Results of numerical modeling of the melting process in a single-screw extruder

The purpose of calculation of a melting zone of an extruder is to determine a temperature field in material to be processed, coordinates of the melting process completion, as well as energy costs.

We carried out numerical modeling of the melting process for polyethylene of high pressure (low density) under the initial data given in work [12].

Fig. 5 shows the results of calculation of a temperature field of a polymer in the working channel of the extruder along the length of the screw, and Fig. 6 shows the comparison of results of the calculation according to the developed method with experimental data given in work [12].

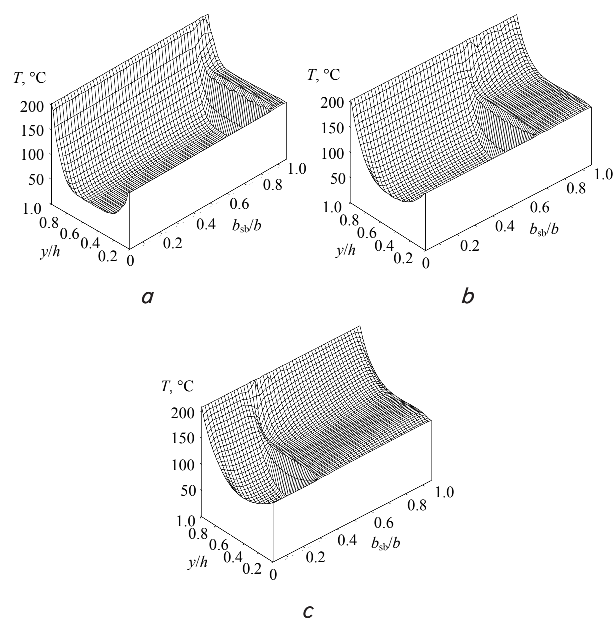

Fig. 5. Temperature fields in the screw channel at different values of the dimensionless coordinate L/D: *a* — 6.0; *b* — 8.0; *c* — 12.5 (b_{sb}/b — dimensionless width of the "solid bed"; y/h — dimensionless height of the working channel)

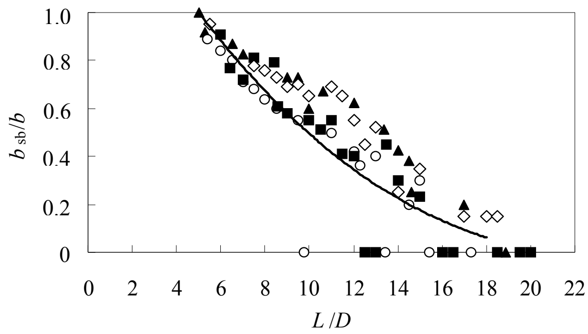

Fig. 6. Comparison of experimental data [12] with the calculation results according to the developed method (screw rotation speed 40 rpm, mass performance 32.6 kg/h; markers show the results of measurements of four series of experiments)

Results of the calculation, shown in Fig. 6, of a dimensionless width of the "solid bed" b_{sb}/b from the dimensionless coordinate L/D along the axis of the screw (shown as a continuous curve) agree satisfactorily with experimental results presented in work [12]. At the same time, the calculated values were somewhat lower than the measured values. Probably the reason of the difference is the fact that thermophysical properties of a polymer in work [12] are given in the form of constants. At the same time, the properties depend not only on temperature [22], but even on a polymer manufacturer of the given mark [19].

6. Discussion of the results of numerical modeling of the melting process in a single-screw extruder

The analysis of the results of numerical modeling showed that they are in good agreement with experimental data. The difference between calculated and measured values of a dimensionless width of a polymeric "solid bed" from a dimensionless coordinate along the axis of the screw does not exceed 15 %. This is significantly lower than in the case of the traditional approach to melting modeling [12] and is acceptable for engineering calculations.

We can explain the good agreement of the results of numerical modeling with experimental data, first of all, by correctness of the accepted boundary conditions.

First of all, we took into account a curvilinear form of the working channel in a diametrical section of the screw. Since the channel depth at the beginning of the melting zone was 9.39 mm at the screw diameter of 63.5 mm (that is 14.8 %), neglecting a curvature of the channel would increase a calculation error.

We also took into account real speeds on surfaces of working parts of the extruder: a zero speed on the surface of the fixed cylinder and a corresponding speed on the surface of the rotating screw. Taking into account heat transfer conditions on the outer surface of the cylinder and the inner surface of the screw, this gave possibility to specify a temperature of a polymer both at surfaces of the cylinder and the screw, as well as in the volume of the working channel as a whole.

We conducted studies for one size type of extruders, which is a disadvantage of the conducted studies. A lack of complete experimental data for other extruders did not give possibility to analyze effectiveness of the developed calculation methodology in more detail. This would be especially true for extruders with large diameter of screws (90 mm and larger), for which a curvature of a working channel in a diametrical section of a screw decreases with an increase in a diameter.

In addition, the obtained analytical dependencies are valid for an analysis of the extrusion process of the "power" liquid only. At the same time, the proposed approach makes possible to obtain similar dependencies for melts of polymers, behavior of which under load is described by other rheological equations.

We would also like to note that calculation of the melting zone must be performed together with calculation of other functional zones of an extruder. In this case, parameters of a polymer being processed at the output of a previous zone are taken as raw data for calculation of each subsequent zone. It is precisely such approach to analyzing of the extrusion process as a whole, taking into account interconnection of all zones, is an effective tool for the correct design of a new or a choice of existing equipment for the processing of a particular polymer.

We tested the developed method successfully in the design of industrial extruders developed by PJSC NPP Bolshevik "(Kiev, Ukraine) (JSSPC " Bolshevik").

We plan to carry out further studies to analyze processes of processing of polymer materials in twin-screw extruders with co-rotating and counter-rotating screws. At the same time, it is necessary to investigate a behavior of material in gaps between screws (specifically, between co-rotating screws) that are in mutual engagement. However, relevant experimental studies may face technical difficulties.

7. Conclusions

1. We developed a mathematical model of the polymer melting process in a single-screw extruder. The model includes differential energy equations for a "solid bed" of the non-melted polymer and melt films at surfaces of the rotating screw and the fixed cylinder of the extruder, as well as the corresponding initial and boundary conditions. The boundary conditions take into account an effect of the heat exchange of a polymer with the screw and the cylinder on a polymer temperature.

2. We investigated the process of melting of polymer granules in the working channel of a screw extruder theoretically. The results of the study showed that the use of the developed model makes possible to take into account speeds and temperatures of screw and cylinder surfaces on the melting process. We established that we can observe the maximum intensity of dissipation near the surface of the screw in the proposed model with a rotating screw, while the classical model with a movable cylinder determines the maximum intensity of dissipation near the surface of the cylinder. In the processing of materials characterized by low thermal resistance, this feature of the developed model becomes determinative.

3. The comparison of the results of numerical modeling with experimental data at the processing of high pressure polyethylene (low density) on a single-screw extruder Ø 63.5×25 verifies the adequacy of the developed mathematical model. We carried out the study for the screw rotational speed of 40 rpm and the mass productivity of 32.6 kg/hr. The developed model makes possible to calculate a coordinate of the completion of the polymer melting process, which means

to determine a coordinate of the beginning of the subsequent functional zone of an extruder – a zone of homogenization, as well as choose a place of introduction of different additives in a polymer. The given model also gives possibility to determine rational thermal modes of working parts of an extruder, a speed of a screw and energy costs for processing of various polymer materials.

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