Розроблено математичну модель процесу перероблення полімерів у двочерв'ячних екструдерах з одно- і різноспрямованим обертанням черв'яків. Модель враховує теплообмін полімеру з черв'яками й циліндром, а також реальні граничні умови (черв'яки обертаються, циліндр нерухомий).

Для аналізу процесу використано модель виділеного С-подібного об'єму, який обмежено одним витком нарізки кожного із черв'яків і в якому перебуває певний об'єм переробльованого полімеру. Така модель дає змогу описати процес перероблення як у випадку повного, так і часткового заповнення робочого каналу переробльованим матеріалом. Це особливо важливо в разі дозованого живлення екструдера полімером, що характерно для сучасного екструзійного обладнання.

Досліджено температурне поле полімеру в робочих каналах екструдерів з одно- і різноспрямованим обертанням черв'яків і виконано порівняння результатів розрахунків з експериментом. Теоретично обґрунтовано та експериментально підтверджено, що на відміну від одночерв'ячного екструдера у двочерв'ячному екструдері робочі органи спочатку потрібно інтенсивно нагрівати, а потім охолоджувати (у напрямку від завантажувальної лійки до екструзійної головки).

Розроблена методика була успішно використана під час відпрацьовування режимів перероблення різних полімерних матеріалів на двочерв'ячних екструдерах з одно- і різноспрямованим обертанням черв'яків діаметром 125 і 83 мм, відповідно.

Розбіжність розрахованого та експериментального значень температури на виході двочерв'ячного екструдера з односпрямованим обертанням черв'яків Ø83×30D не перевищує 10 %. При цьому експериментальне значення температури дещо перевищило задане значення. Це можна пояснити тим, що система термостабілізації робочих органів для досліджених режимів переробдення не могла ефективно відводити теплоту дисипації, що виділялася.

Використання розробленої математичної моделі дасть змогу краще прогнозувати ефективні режими роботи двочерв'ячних екструдерів, особливо під час перероблення матеріалів з низькою термічною стійкістю

Ключові слова: двочерв'ячний екструдер, різно- та односпрямоване обертання черв'яків, граничні умови, температурне поле

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MODELING THE PROCESS OF POLYMERS PROCESSING IN TWIN-SCREW EXTRUDERS

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1. Introduction

Manufacturers use single-screw extruders for continuous fabrication of products from thermoplastic polymers. Recently, they have also started to use twin-screw extruders. Twin-screw extruders demonstrate high productivity and mixing ability, as well as the stability of processing parameters at replacement of a forming tool (extrusion head) [1–4].

Currently, producers of equipment for processing of polymers offer many twin-screw extruders with various geometries, which significantly complicates the selection of necessary equipment. That is why mathematical modeling of the process of twin-screw extrusion acquires great importance. That makes it possible to select the most efficient equipment quickly. This possibility considerably reduces expensive experimental research and development of a polymer technology.

Many studies consider the modeling of single-screw extruders in detail (for example, papers [2, 3, 5–7]). However, there is much less attention being paid to the modeling of twin-screw extrusion.

Many authors have investigated a rather complex process of twin-screw extrusion over recent years. Authors made various assumptions to simplify a mathematical description of the process. Such an approach was acceptable for a long time, but as the productivity of extruders has increased significantly over time, many processing models became unacceptable for practical use. Therefore, modeling the process of polymer processing in twin-screw extruders, taking into account actual boundary conditions, as well as a heat exchange of a polymer with screws and an extruder barrel, is relevant.

2. Literature review and problem statement

Any thermoplastic material has certain properties. Therefore, a corresponding geometry of operation bodies (primarily screws) and a processing mode are necessary for processing of material in a twin-screw extruder. One of the ways to choose the most effective extruders, which provide the required quality of products, is mathematical modeling of processes of polymer processing [2, 3, 5]. A basis of the mathematical models developed at the early stage of twin-screw extrusion is a number of analytical solutions of a system of equations based on the classical inverse plane-parallel model for screw extrusion (screws are fixed and a barrel rotates). The model has significant disadvantages. The analysis of single-screw extrusion showed them in papers [5–7].

Processing of polymers in twin-screw extruders is much more difficult than in single-screw ones. This is explained by the presence of two rotating screws in one or opposite directions, and because of the shape of a channel of a body (barrel) of an extruder [8–10].

Researchers also point out that a lack of reliable software constrains the mathematical modeling of twin-screw extruders, so foundations for the design are experimental and practical data [9].

Due to the above, studies of twin-screw extrusion considered analysis of a process of mixing (mainly for screws, which rotate in one direction) for a long time. For example, paper [11] considers designs of mixing elements of screws with or without interlocking engagement. Paper [12] investigates effectiveness of screws with neutral and reversible pin mixing cams, and papers [13, 14] – screws with oval cams. Work [15] presents results of similar studies on screws with oval cams. Paper [16] presents classification and considers constructions of mixing-dispersing elements of screws in detail.

Authors of paper [17] studied hydrodynamics and a mixing effect of a co-rotating twin-screw extruder in detail. However, the analysis of velocity of polymer melt is in the isothermal approximation, which can lead to a significant error in processing of high-viscosity polymers.

Work [18] investigates a velocity field and pressure in a channel of a co-rotating twin-screw extruder [18]. There is no analysis of a temperature field of a polymer.

Papers [19, 20] present results of a study on the dependence of productivity of a co-rotating twin-screw extruder and pressure along its operation channel [19, 20]. There is research into screws with a channel of different geometry and different velocities of their rotation. However, the mentioned studies are relevant in the absence of a dispenser at the inlet to an extruder only, which in practice is extremely rare.

Work [21] considers the analysis of a process of mixing and distribution of pressure along an operation channel of a co-rotating twin-screw extruder Paper [22] provides similar studies (regarding screws with mixing cams). The mentioned works do not consider an influence of heat supply systems of screws and a barrel on a temperature field of processed material, which affects the quality of obtained products significantly.

Work [23] investigates melting velocity of polymer granules in a twin-screw extruder with counter-rotating screws; specifically, it determines a length of a melting zone in dependence on rotational velocity of screws. The work considers the process of processing of a polymer in the gap between the screws by analogy with the process of processing on roller machines [24]. In addition, it does not show the dependence of temperature of processed material on a length of an extruder channel, which makes difficult to analyze an influence of process parameters on the quality of obtained products.

The aim of most of experimental and practical studies is analysis of mixing ability of twin-screw extruders and determination of their productivity. At the same time, studies almost do not consider analysis of a temperature field of processed material, as well as determination of power of dissipation. However, exactly these parameters determine the quality of polymer melt and products, which we obtain in an extruder.

Due to peculiarities of the structural design of an operation channel of twin-screw extruders, heat supply systems of screws and a barrel, as well as real boundary conditions, significantly influence the process of polymer melting and provision of necessary temperature mode of processing. Given the above, a new approach is necessary for modeling of the process of twin-screw extrusion.

3. The aim and objectives of the study

The objective of the study is a mathematical modeling of the process of processing of polymeric materials in an operation channel of twin-screw extruders. A model should take into account dosed feeding of extruders with processed material, availability of heat supply systems for its operation elements, and also real boundary conditions (geometric ones, velocity ones and temperature conditions). This will give us a possibility to determine rational parameters of the twin-screw extrusion process to ensure the required temperature distribution of a polymer at the outlet from an extruder at its given productivity. The mentioned parameters include the method of heating or cooling of screws and an extruder body, a type of a heat-transfer agent, its temperature and volume flow, geometry of an operation channel of screws and frequency of their rotation.

It is necessary to solve the following tasks to achieve the objective:

– consideration of features of full and partial filling of an operation channel of an extruder with processed material and heat transfer of a polymer with rotating screws and a stationary barrel;

– theoretical investigation of the process of processing of a polymer in an operation channel of an extruder;

– experimental verification of adequacy of the developed mathematical model.

4. Materials and methods for studying the processes of polymer processing in twin-screw extruders

4. 1. Modeling of the process of polymer processing in a twin-screw extruder with counter-rotating screws

Among twin-screw extruders, one of the most common are extruders with counter-rotating screws and their full engagement closed both in a longitudinal direction and a transverse direction. A feature of such extruders is that spiral channels of the screws are a series of C-shaped sections almost isolated from each other, each of which has a certain volume of processed TpM (Fig. 1). We proposed a model of the separated volume limited by one turn of a screw [5, 25] for the analysis of the process of twin-screw extrusion taking into account the above.

Material that enters the C-shaped section of the operation channel of the extruder from the feeding box at rotation of screws goes in the direction of the molding head, and two C-shaped volumes of TpM come out of it in one turn. Productivity of the extruder is almost independent of resistance of the molding head [5, 26]. A depth of the cutting of screws can be relatively large, which reduces velocity of deformation of TpM and intensity of dissipation, and leads to an increase in a fraction of heat supplied to TpM from the wall of the barrel. Such scheme of motion of TpM provides equality of time of its stay in channels of screws, which is especially important for processing of heat-sensitive materials.

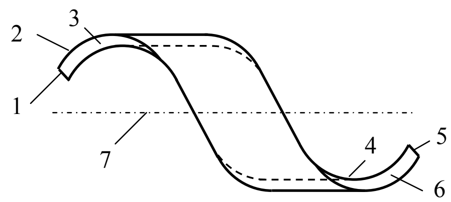
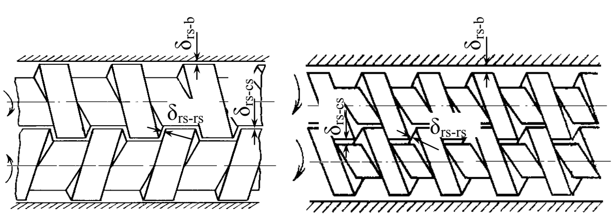


Fig. 1. Scheme of the volume of processed TpM within one turn of cutting of a screw of a twin-screw extruder: 1, 5 — surfaces of TpM limited by the corresponding volume of the neighboring screw; 2 — a surface bounded by the barrel; 3, 6 — surfaces bounded by flanges of combs of the cutting of a screw; 4 — a surface bounded by a core of a screw; 7 — longitudinal axis of a screw

Gaps between screws and between a screw and a barrel lead to some reduction in productivity, but they improve mixing of TpM. A transfer of material through the mentioned gaps from one C-shaped volume to another one depends on a pressure drop between volumes and depends on resistance of the molding head. Such gaps exist between combs of one screw and the core of a neighboring screw (roller gap) $\delta_{\text{rs-cs}}$, between lateral surfaces of combs $\delta_{\text{rs-rs}}$, and between combs of windings and the wall of a barrel $\delta_{\text{rs-b}}$ (Fig. 2).

Relative velocity of rotation of screws in $\delta_{\text{rs-rs}}$ gaps is approximately equal to zero at the counter-rotating screws, and therefore their influence on intensity of dissipation is insignificant.



a *b*

Fig. 2. A nature of the engagement of screws of a twin-screw extruder: *a* — at counter-rotating screws; *b* — at co-rotating screws

Extruders with counter-rotating screws with mutual engagement provide a high mixing effect with considerable productivity. However, in this case, radial (spreading) forces arise in twin-screw extruders. They lead to an increased wear of operation parts (primarily a barrel).

Compaction of TpM in an extruder goes due to reducing of a volume of a closed C-shaped volume in the direction of the molding head. We should note that reconsolidation and jamming of material is possible for different values of a degree of compression of screws. Therefore, a dosed feeding is necessary for twin-screw extruders operation.

Theoretically, we can define volumetric productivity of twin-screw extruders without considering of overflows as a product of two C-shaped volumes at the extruder's outlet and rotational frequency of screws [5, 26]. However, theoretical dependences give significantly higher values of productivity compared with practical data, which we can explain by presence of dispensers and the need to achieve high quality of processing. Thus, theoretical data gives an upper limit to productivity only. On the other hand, productivity of a dispenser determines productivity of an extruder at dosed feeding, and therefore determination of productivity of an extruder does not have a significant value for further calculation of an extruder, if the productivity does not exceed the maximum possible rotation frequency for the given geometry of screws.

We determine the maximum possible productivity of an extruder with dosed feeding and n_s rotational frequency of screws. In this case, only the last C-shaped sections are completely filled, and their volume, as a rule, is the smallest. For this purpose, we consider a cross section of an extruder in a plane perpendicular to longitudinal axes of screws (Fig. 3) [26].

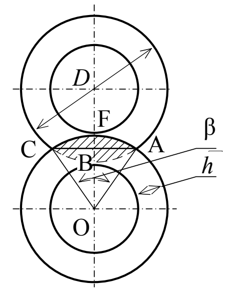


Fig. 3. A cross-section of a twin-screw extruder: *D* — diameter of a comb of cutting of screws, m; *h* — depth of the channel (depth of cutting) of each of screws, m; β is the angle of conjugation of screws, rad

For each turn of screws, a doubled C-shaped volume of TpM with a cross-section in the form of a ring of the area $\pi\left(D^2-(D-2h)^2\right)/4$ except for the shaded in Fig. 3 area of a length $(s-ke)$ in the direction of the axis of an extruder (here, e and s are a width of a comb of a turn and a pitch cutting of a screw, m, k is a number of runs of cutting of a screw) goes from an extruder.

The area of $ABCF$ segment is equal to the area of $OAFC$ sector except for the area of OAC triangle:

$$F_{ABCF}=F_{OAFC}-F_{OAC}.$$

Let us determine these areas:

$$F_{OAFC}=\frac{\pi D^2}{4}\frac{\beta}{2\pi}=\frac{D^2\beta}{8};\quad F_{OAC}=\frac{1}{2}|OB|\cdot|AC|;$$

$$|OB|=\frac{D-h}{2};\quad |AC|=2\frac{D}{2}\sin\frac{\beta}{2}=D\sin\frac{\beta}{2}.$$

Then we have:

$$F_{OAC}=\frac{D}{2}\left(\frac{D-h}{2}\right)\sin\frac{\beta}{2}$$

and

$$F_{ABCF}=\frac{D^2\beta}{8}-\frac{D}{2}\left(\frac{D-h}{2}\right)\sin\frac{\beta}{2}.$$

The cross-section area of channels of two screws is

$$S_s=\frac{1}{2}\left\{\pi\left[D^2-(D-2h)^2\right]-D\left[\frac{D\beta}{2}-(D-h)\sin\frac{\beta}{2}\right]\right\}$$

or

$$S_s=2\pi h(D-h)-\frac{D}{2}\left[\frac{D\beta}{2}-(D-h)\sin\frac{\beta}{2}\right],$$

then a volume of two C-shaped sections (m^3) is equal to

$$V_c=S_s(s-ke)=$$
$$=\left\{2\pi h(D-h)-\frac{D}{2}\left[\frac{D\beta}{2}-(D-h)\sin\frac{\beta}{2}\right]\right\}(s-ke). \qquad (1)$$

Taking into account (1), mass productivity of an extruder is

$$G_M=\rho V_c n_s=\rho(s-ke)n_s\times$$
$$\times\left\{2\pi h(D-h)-\frac{D}{2}\left[\frac{D\beta}{2}-(D-h)\sin\frac{\beta}{2}\right]\right\}, \qquad (2)$$

where G_M is mass productivity of an extruder, kg/s; ρ is density (kg/m^3) of TpM as a function of temperature T, °C; n_s is the rotational frequency of a screw, r/s.

We can determine β angle of OAFC sector by the dependence (Fig. 3)

$$\beta=2\arccos\left(\frac{|OB|}{|OA|}\right)=2\arccos\left(\frac{D-h}{D}\right).$$

At calculation of C-shaped sections that are not completely filled with material, we can define a degree of their filling as a ratio of productivity of a last section to productivity of a completely filled section in question, which we determine by a formula (2). A channel at the inlet to a roller gap will be filled completely in reality, due to a counter rotation of screws, and only the opposite part of the C-shaped section (at the outlet of the roller gap) will remain unfilled.

We can define a cross-sectional area of a TpM volume in incompletely filled sections by a dependence (2) if we know the mass productivity provided by a dispenser

$$S_s=\frac{G_M}{\rho n_s(s-ke)}. \qquad (3)$$

On the other hand, S_s area is equal to a difference in areas of sectors with R_2 and R_3 radii and an angle $(2\pi-\beta_1)$. Here β_1 is the central angle of an annular space not filled with TpM, rad; R_2 and R_3 are radii of a core of each of screws and an inner surface of a barrel, respectively, m.

Then, for two screws, we have

$$S_s=2\left[\frac{(2\pi-\beta_1)R_3^2}{2}-\frac{(2\pi-\beta_1)R_2^2}{2}\right]=(2\pi-\beta_1)(R_3^2-R_2^2)$$

or

$$S_s=(2\pi-\beta_1)(D-h)h. \qquad (4)$$

We equate dependences (3) and (4) and solve the expression obtained with respect to β_1 angle. We obtain

$$\beta_1=2\pi-\frac{G_M}{\rho n_s(s-ke)(D-h)h}.$$

Paper [5] considers a general approach to calculation of hydrodynamics and a temperature field of TpM in operation channels of a twin-screw extruder.

Then we determine total dissipation power ΔQ_{dis} in a volume of two C-shaped sections. We take into account that intensity of dissipation q_{dis} (W/m^3) varies along the radius only for the accepted assumptions. So, according to the Simpson's numerical integration formula, we obtain

$$\Delta Q_{\text{dis}}=\frac{2}{3}(2\pi-\beta_1)\Delta r(s-ke)\times$$
$$\times\left(q_{\text{dis}\,0}R_2+q_{\text{dis}\,m}R_3+4\sum_{i=1}^{m-1}q_{\text{dis}\,i}\,r_i+2\sum_{j=2}^{m-2}q_{\text{dis}\,j}\,r_j\right)$$

or

$$\Delta Q_{\text{dis}}=\frac{2}{3}(2\pi-\beta_1)\Delta r(s-ke)\times$$
$$\times\left(q_{\text{dis}\,0}\left(\frac{D}{2}-h\right)+q_{\text{dis}\,m}\frac{D}{2}+4\sum_{i=1}^{m-1}q_{\text{dis}\,i}\,r_i+2\sum_{j=2}^{m-2}q_{\text{fis}\,j}\,r_j\right), \qquad (5)$$

where

$$i=1,3,\ldots,m-1;\quad j=2,4,\ldots,m-2;$$

r_i and r_j are radii of corresponding elements Δr, m; m is a number of nodes in the Simpson's formula.

We determine $q_{dis\,i}$ and $q_{dis\,j}$ values, which are parts of dependence (5), from formula

$$q_{\text{dos}}=\mu(\dot\gamma)\left(\dot\gamma_r^2+\dot\gamma_z^2\right),$$

where μ is the dynamic viscosity of TpM, Pa·s; $\dot\gamma$, $\dot\gamma_r$ and $\dot\gamma_z$ is the shift rate and its components in the direction of r and z axes, respectively, s^{-1}.

In addition, drive power acts to deform melt in $\delta_{rs\text{-}b}$, $\delta_{rs\text{-}cs}$ and $\delta_{rs\text{-}rs}$ gaps (Fig. 2, *a*). Since the rotation of screws is opposite-directional, there is almost no shear deformation in $\delta_{rs\text{-}rs}$ lateral gaps of engagement, and therefore we do not consider them. Power costs in $\delta_{rs\text{-}cs}$ roller gap also have no significant effect on results of engineering calculations as shown by calculations performed with a use of the method of calculation of roller machines [24]. The greatest power costs take place in $\delta_{rs\text{-}b}$ radial gap between a comb of a turn and a wall of a barrel. As we already noted, an influence of a pressure gradient on a velocity profile is insignificant due to a small size of a gap, and we can consider a flow in the gap as a flow between a stationary surface and a moving surface with linear velocity distribution. Then the shear rate in the gap is $\dot\gamma=W_s/\delta_{\text{rs-b}}$, and we can determine the dissipation power from dependence

$$q_{\text{dis rs-b}}=\mu\left(\dot\gamma_{\text{rs-b}},T_{\text{rs-b}}\right)\dot\gamma_{\text{rs-b}}^2=\mu\left(\dot\gamma_{\text{rs-b}},T_{\text{rs-b}}\right)\left(\frac{W_s}{\delta_{\text{rs-b}}}\right)^2,$$

where $T_{rs\text{-}b}$ is the average temperature TpM in a gap between a comb of a screw and a barrel, which we take as equal to temperature of TpM near a surface of a barrel T_b, °C, W_s is the circumferential velocity of a comb of each of screws ($W_s=\pi D n_s$), m/s.

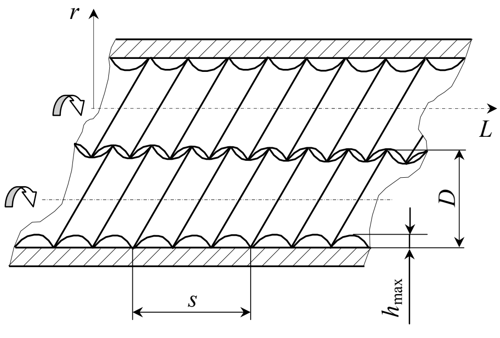
Then, power costs in gaps of two adjacent C-shaped sections of both screws are equal to

$$\Delta Q_{dis\ rs\text{-}b}=2q_{dis\ rs\text{-}b}(2\pi-\beta_1)(D-h)e\delta_{rs\text{-}b}.$$

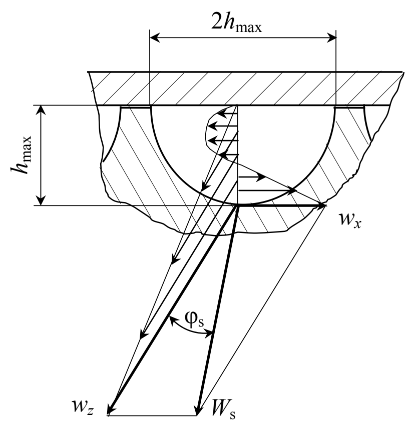
4. 2. Modeling the process of polymer processing in a co-rotating twin-screw extruder

Rotation of screws of a twin-screw extruder in one direction increases their rotational frequency and excludes possible jamming of screws. Accordingly, productivity increases at high quality mixing of TpM and self-cleaning of screws. In many cases, screws have an opposite-run profile with a semicircular cutting, which promotes better mixing of melt.

Let us consider a three-run screw (Fig. 4). We use a model of the allocated volume limited by one turn of each of screws as for a counter-rotating twin-screw extruder to analyze the process.



a



b

Fig. 4. Design model of a co-rotating twin-screw extruder: *a* — nature of engagement of screws with a semicircular profile of cutting; *b* — velocity components in a channel of a screw (D — diameter of a comb of cutting of screws, m; s — pitch of cutting of screws, m; h_{max} — maximum depth of an operation channel (radius of cutting of each of screws), m; r, L — coordinates directed along a height of cutting of screws and along the axis of each of screws, respectively, m; φ_s — angle of spiral cutting of screws, rad, w_x and w_z — velocity components along the x and z axes, respectively, m/s; W_s — circumferential velocity of each of screws, m/s)

Fig. 4 shows that a TpM flow is redistributed between adjacent channels of their cuttings at the contact point of screws, and the motion of TpM is similar to its motion in a single-screw extruder for the remaining length of channels. Since twin-screw extruders operate under the condition of dosed feeding, only the last few turns of cutting of screws are completely filled, which provide the necessary pressure at the outlet from an extruder. A volume of a channel of each of screws decreases along its axis both due to a decrease in depth, and due to a reduction in a pitch of cutting. Such a reduction occurs usually stepwise along the length of a screw in a point of contact of several structural zones of a screw with each other. Since a TpM flow is redistributed continuously, and melt in the melting zone is mixed with solid material, we assume that there is no clearly defined melting zone as in a counter-rotating twin-screw extruder. And shear deformation takes place in the entire volume of TpM along the entire length of screws.

A volume of the C-shaped section is not isolated (Fig. 4, *a*) in this case, unlike the counter-rotating twin-screw extruders. However, material fills the last cutting sections completely, and therefore we can define velocity of its axial motion w_L in these sections from the mass flow equation

$$G_M = \rho S_s w_L, \qquad (6)$$

where w_L is the velocity of an axial motion of TpM, m/s.

We consider that the profile of a channel is semicircular with h_{max} cutting radius for two screws with a k-turn cutting, so we have

$$S_s = 2k\frac{\pi h_{max}^2}{2\sin\phi_s}, \qquad (7)$$

where S_s is the cross-sectional area of channels of two screws, m.

We substitute an expression (7) with dependence (6) and solve it with respect to w_L. And we obtain

$$w_L = \frac{G_M \sin\phi_s}{k\rho\pi h_{max}^2}, \qquad (8)$$

where we calculate an angle of a rise of screw cutting of screws from formula

$$\phi_s = \mathrm{arctg}\left(\frac{s}{\pi D}\right).$$

We refine average material velocity w_L calculated from (8) for the last sections of screws at calculation of their remaining sections by multiplication of w_L velocity by the ratio of a cutting pitch of the section to a cutting pitch of the last section.

We determine the equivalent depth h of a channel of a semicircular shape by replacing it with a rectangular one, if areas of their cross sections are equal (Fig. 4, *b*)

$$\frac{\pi h_{max}^2}{2} = \left(2h_{max}\right)h,$$

from which the equivalent depth of a channel will be equal to (m)

$$h = \frac{\pi h_{max}}{4}.$$

We can determine the equivalent depth of a channel at the site of their location similarly in the presence of mixing cams.

Equivalent cutting in cross section forms an annular space not completely filled with material, the area of which in the diametric section for two screws is approximately equal to

$$S_s = 2(2\pi - \beta_1)h\frac{D-h}{2}, \quad (9)$$

where β1 is the central angle of a cross-section of a C-shaped section not filled with TpM, rad.

We substitute expression (9) with dependence for mass productivity (6) and solve the expression obtained with respect to β_1 angle. And we obtain

$$\beta_1 = 2\pi - \frac{G_M}{\rho w_L (D-h)h}.$$

Productivity of an extruder is equal to productivity of a dispenser at dosed feeding, but it cannot exceed the maximum productivity $G_{M\max}$, which depends on frequency of rotation of screws n_s and geometry of completely filled last sections. Since the C-shaped sections are not completely isolated from each other in the case of unidirectional rotation, we use a single-screw extrusion theory to determine productivity of the last sections. For a plane-parallel screw model with a pressure gradient close to zero, the productivity will equal

$$G_{\max} = k\rho\frac{\pi h_{\max}^2 G_M w_z}{2}, \quad (10)$$

where

$$w_z = \pi D n_s \cos\phi_s$$

is the velocity component along a screw deployed on the plane of a screw channel, m/s.

We substitute this expression with dependence (10) and obtain

$$G_{\max} = \frac{1}{2}\pi^2 k\rho h_{\max}^2 D n_s \cos\phi_s.$$

It is necessary to determine deformation rate at nodal points (by analogy with counter-rotating twin-screw extruders) to determine intensity of dissipation q_{dis} in TpM volume. It is necessary to take into account that C-shaped sections are not locked and there is no circulation in the longitudinal direction in them when determining the deformation rate component $\dot{\gamma}_z$ as it is in the case with counter-rotating screws. But for unfilled sections, the pressure gradient in z direction is close to zero, so we can assume that the velocity along the channel height changes linearly, and the deformation rate is, respectively

$$\dot{\gamma}_z = \frac{w_z}{h} = \frac{\pi D n_s \cos\phi_s}{h}.$$

We determine the dissipation power by integration of dissipation intensity q_{dis} by the TpM volume, which is in the section under consideration

$$\Delta Q_{\text{dis}} = 2\int_0^{2\pi-\beta_1}\int_0^{s}\int_{(D-2h)/2}^{D/2} q_{\text{dis}}\,\mathrm{d}r\,\mathrm{d}L\,\mathrm{d}\theta, \quad (11)$$

where r, θ, z are the cylindrical coordinates.

Since q_{dis} depends only on the radius, expression (11) takes the form

$$\Delta Q_{\text{dis}} = 2(2\pi - \beta_1)s\int_{(D-2h)/2}^{D/2} q_{\text{dis}}\,\mathrm{d}r. \quad (12)$$

We calculate the integral in expression (12) by the Simpson's numerical integration formula (by analogy with expression (5))

$$\Delta Q_{\text{dis}} = \frac{2}{3}(2\pi - \beta_1)s\Delta r \times$$
$$\times\left(q_{\text{dis}\,0}R_2 + q_{\text{dis}\,m}R_3 + 2\sum_{i=1}^{m-1} q_{\text{dis}\,i}\,r_i + 4\sum_{j=2}^{m-2} q_{\text{dis}\,j}\,r_j\right).$$

We determine $q_{dis\,i}$ and $q_{dis\,j}$ values at the nodal points by a technique similar for a counter-rotating twin-screw extruder.

The profile of cutting has the shape of a segment in contrast to a counter-rotating twin-screw extruder, and therefore TpM deformations do not matter much for calculation of drive power in $\delta_{rs\text{-}cs}$, $\delta_{rs\text{-}rs}$ and $\delta_{rs\text{-}b}$ gaps (Fig. 2, *b*). We can reduce an error caused by not taking into account deformation in the mentioned gaps by integration of dissipation intensity over the entire volume of the C-shaped section filled with the processed material (that is, under condition $\beta_1 = 0$).

5. Results of numerical modeling of the process of polymer processing in twin-screw extruders

5. 1. Results of modeling a counter-rotating twin-screw extruder

Let us analyze the results of calculation of the process of processing of TpM on a counter-rotating twin-screw extruder with a diameter of 125 mm and an operation length of 30*D* for productivity of 500 kg/h and a rotational frequency of screws of 50 rpm. We performed calculations for two options: at a given temperature of surfaces of screws and a barrel, and in the absence of heat exchange with surfaces of screws and a barrel (the adiabatic mode). We assumed the exponent of n degree rheological equation as 0.3 and 1.0.

Fig. 5 shows a temperature dependence of a dimensionless y/h channel height for three cross sections at the first, fifteenth and thirtieth turns of screws at $n=1$ and $n=0.3$ values of the exponent for the adiabatic mode. We can also see on Fig. 5 that more intense heating of TpM takes place near a surface of each of screws, and temperature inhomogeneity of TpM can reach 30...50 °C. At the same time, a temperature level of processing decreases at an increase in deviation from Newtonian behavior, which occurs due to a decrease in intensity of the melt circulation.

Fig. 6 shows a temperature change along a dimensionless y/h channel height under boundary conditions of the first kind (given temperatures of operation surfaces of screws and a barrel) for the indicated sections of screws. It follows from Fig. 6 that it is necessary to heat TpM, and then to cool surfaces of screws and a barrel to maintain the given temperature at the first turns.

A need to maintain such a thermal mode follows from Fig. 7, 8, which show curves of a change in a heat flow along the length of the extruder q_b that must be brought or removed from surfaces of the barrel and each of the screws. It is possible to determine and select a necessary temperature mode for processing using these curves. Geometry of screws causes some jumps in heat flows at 5th, 13th and 19th turns.

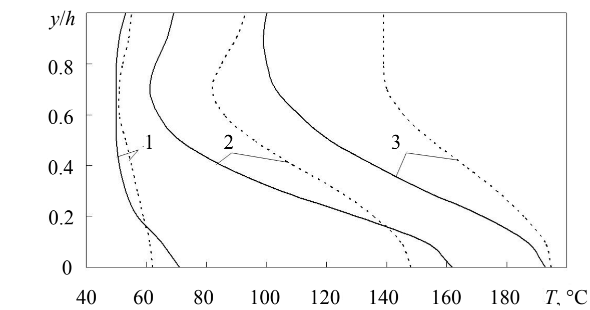


Fig. 5. A temperature change along the height of the channel of screws for the adiabatic mode at n=0.3 (solid lines) and n=1 (dashed lines) along the length of screws: 1 — at the beginning; 2 — in the middle; 3 — at the end of screws; y — a coordinate directed along the height of a working gap ($y=\overline{0,h}$)

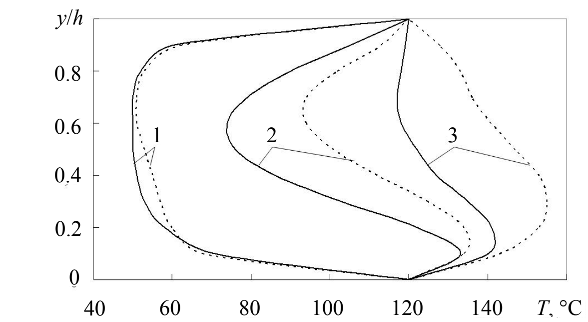


Fig. 6. A temperature change along the height of the screw channel for the given temperatures of the screw and the barrel at n=0.3 (solid lines) and n=1 (dashed lines) along a length of the screws: 1 — at the beginning; 2 — in the middle; 3 — at the end of screws

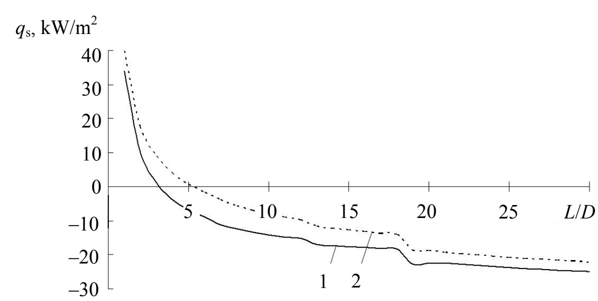


Fig. 7. A heat flow, which must be brought to a screw (or away from a screw) along its length at values n=0.3 (1) and n=1 (2)

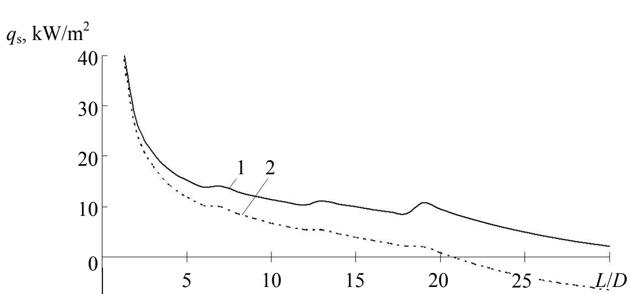


Fig. 8. The heat flow, which must be brought to a barrel (or away from a barrel) along its length for values n=0.3 (1) and n=1 (2)

Fig. 9 shows a temperature change of TpM along a dimensionless height of a y/h channel for three cross sections at the beginning, in the middle and at the end of the screws. We performed the analysis for productivity of 200 kg/h, the adiabatic processing mode and two values of the equivalent thermal conductivity [5]: normal one and doubled one, that is, for different mixing modes.

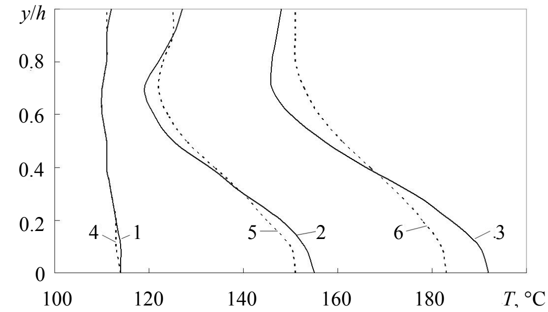
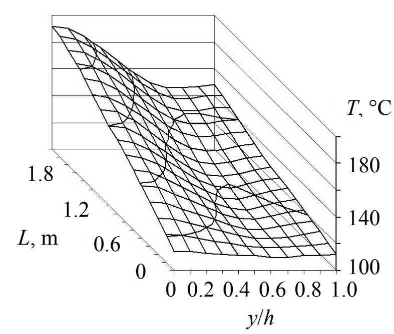
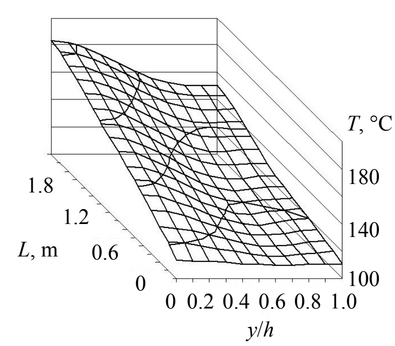


Fig. 9. A dependence of melt temperature along the height of the screw channel at the beginning (1, 4), in the middle (2, 5) and at the end (3, 6) of the screw for different values of the equivalent thermal conductivity — ordinary one (1–3) and doubled one (4–6)

Fig. 9 shows that temperature values are rather close to each other in certain places along a length of the extruder for different values of the equivalent thermal conductivity. Thus, intensity of dissipation at certain points in the TpM volume determines temperature fields. Similarity of the temperature fields obtained as a result of calculations for the adiabatic mode confirms this as well (Fig. 10).



a



b

Fig. 10. A temperature field for the adiabatic mode of the extrusion process: *a* — for the usual equivalent thermal conductivity of melt; *b* — for the doubled equivalent thermal conductivity of melt

We should note that it is necessary to supply a screw and a barrel with a considerable amount of heat on the first turns to maintain a given temperature mode, which is not always possible, since a heat exchange area of operation bodies is limited. Therefore, it is expedient to perform calculations for the case with boundary conditions of the second kind (we know heat flows on operation surfaces of screws and a barrel) firstly, and to select values of temperatures on surfaces of operation bodies according to the results. It is expedient to use mixing elements to reduce temperature inhomogeneity of TpM melt in the operation channel of an extruder [16].

5. 2. Results of modeling a co-rotating twin-screw extruder

We performed verification of the developed model during selection and refinement of TpM processing modes on the basis of high-pressure polyethylene with filler (aluminum hydroxide) and additives. We used this material as a self-extinguishing electrical insulation for cable products. We compared the results of the numerical modeling with the experimental data obtained by granulating of the composition in JSC Kyivkhimvolokno (Kiev, Ukraine) on a twin-screw extruder with a screw of a diameter of 83 mm and an operation length of 30*D*. The composing screws had three-runs sections with a cutting pitch of 120, 90 and 60 mm with a semicircular cutting profile of a radius of 12, 8 and 6 mm, respectively, as well as mixing cams of triangular shape. We carried out the experiments at the productivity of 50 kg/h and rotational frequency of the screws of 40 and 25 rpm. We maintained the temperature of a barrel wall by a liquid system of thermal stabilization with four autonomous zones along its length. During the experiments, we recorded values of wall temperature of the barrel T_b, temperature of TpM at the outlet from the extruder, productivity and rotation frequency of the screws continuously.

We determined the temperature of the barrel wall of the extruder by thermoelectric converters TKhK-259 and TKhK-539 (HCX L, the measuring range is 0...400 °C). In addition, the measuring kit included automatic potentiometers of A-565-001-01 type (0.15/0.05 accuracy class, the measuring range is from –50 to 800 °C, digital sampling rate is 0.1 °C).

We determined the temperature of the melt at the exit from the extruder with a help of thermoelectric converters of K1 needle type (analogue TP174, HCX L, the measuring range is from –40 to 200 °C). In addition, the measuring kit included automatic potentiometers of A100-H-1 type (a 0.5 accuracy class, the measuring range is 0...200 °C, digital sampling rate is 0.1 °C).

Fig. 11 shows the calculated temperature profiles along the dimensionless height of y/h channel on the 7th, 14th, 21st and 28th turns for the productivity of 50 kg/h and the rotational frequency of the screws of 40 rpm as an example. A system of thermal stabilization maintained the temperature of the barrel wall in zones. The temperature was 160, 160, 180, and 180 °C, and we assumed it as given one during calculations.

Fig. 11 shows that the temperature near the surface of the barrel drops sharply to a predetermined value due to a large value of a heat flow removed by a thermal stabilization system. The temperature of the material at the outlet of the extruder was 220 °C, which is close to the calculated value. A comparison of the calculation results with the experimental data showed that the actual temperature (approximately 210 °C) was close to the average TpM temperature and exceeded the given value. This fact indicates that a thermal stabilization system cannot remove heat of dissipation during this processing mode effectively.

Fig. 12 shows similar dependencies obtained for the same performance, but with a reduced to 25 rpm rotation frequency and the given temperature of the barrel wall in the zones of 140, 140, 140 and 160 °C, respectively. Fig. 13 shows the temperature field of TpM for boundary conditions of the first kind at the barrel wall temperature by zones of 140, 140, 160 and 160 °C.

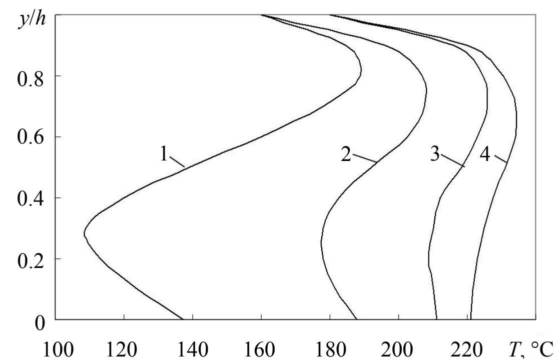


Fig. 11. Temperature profiles of TpM along the cutting height of screws for n_s=40 rpm (1–4 on the length of the screws, which corresponds to the numbers of turns of cutting No. 7, 14, 21 and 28)

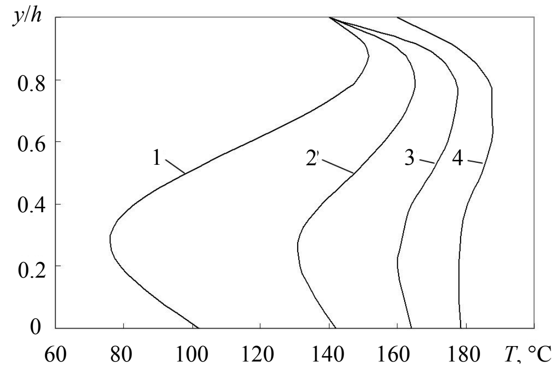


Fig. 12. Temperature profiles along the height of the channel for n_s=25 rpm (1–4 on the length of the screws, which corresponds to the numbers of turns of the cutting No. 7, 14, 21 and 28)

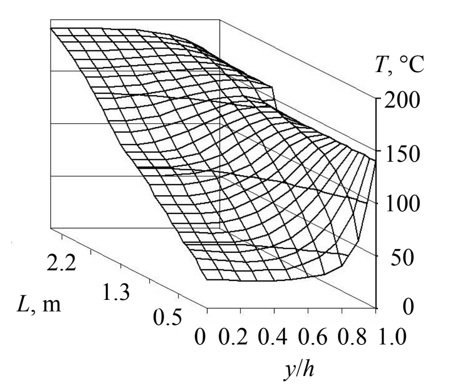


Fig. 13. A temperature field of TpM in a co-rotating twin-screw extruder under boundary conditions of the first kind

A comparison of the theoretical and experimental values of the wall temperature of the barrel showed that a cooling system removes heat necessary to maintain a given wall temperature in the first three zones. A significant amplitude of regulation indicates that TpM temperature in general is higher than the given wall temperature. In the fourth zone, where the wall temperature was 160 °C, the amplitude of control oscillations was smaller, since the wall temperature was closer to the TpM temperature. The calculated material temperature of 180 °C was close to the experimental value of the wall temperature in this zone.

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

Analysis of the results of numerical modeling showed that they agree with the experimental data satisfactorily. The discrepancy between calculated temperature values and measured temperature values at the outlet of a co-rotating twin-screw extruder with screws Ø83×30*D*, which is acceptable for engineering calculations, does not exceed 10 %. The measured temperature values were slightly higher than the given value. Because of the fact that systems of thermal stabilization of the barrel and screws could not remove evolving heat of dissipation for modes under study efficiently.

We can explain a good concordance between the results of numerical modeling and experimental data by taking into account partial filling of the initial section of the operation channel with the processed material, as well as the correctness of the accepted boundary conditions (velocity and temperature ones).

Neglecting partial filling of the initial section of the operation channel with a polymer would lead to an increase in the calculated dissipation power and the temperature of the processed material.

We also took into account real velocities on surfaces of operation bodies of the extruder: the zero velocity on the surface of the fixed barrel and the corresponding velocities on surfaces of the rotating screws. Taking into account heat exchange conditions on the outer surface of the barrel and the internal surfaces of the screws, this made possible to clarify temperature of the polymer both at surfaces of the barrel and the screws, and in the volume of the operation channel as a whole.

We showed that it is necessary to use mixing elements for mixing of materials with clearly expressed Newtonian properties in the operation channel of a twin-screw extruder. We also showed that intensity of energy dissipation in certain places of processed material determines temperature fields in the volume of processed material.

We consider the fact there were an experimental verification of adequacy of the developed models for one size of an extruder only as a disadvantage of the conducted studies. A lack of complete experimental data for other extruders did not make possible to perform a more detailed analysis of effectiveness of the developed calculation methodology.

In addition, the obtained dependences are valid for the analysis of the process of twin-screw extrusion of an "exponential" liquid only. Nevertheless, the proposed approach makes possible to obtain similar dependences for melts of polymers. Other rheological equations describe their behavior under load.

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

We plan further research to analyze the process of grinding of polymers and elastomers wastes in screw machines [27], as well as processes of processing of polymeric materials in disk, combined and cascade extruders with operation bodies of various design.

7. Conclusions

1. We developed models for the processing of polymers in co- and counter-rotating twin-screw extruders based on the generalized mathematical model of screw extrusion. A base of the proposed models is the analysis of an allocated C-shaped volume, which is limited by one turn of cutting of each of screws and in which there is a certain volume of a processed polymer. Such model gives possibility to describe the process of processing both in the case of complete and partial filling of an operation channel with processed material. This is especially important in case of dosed feeding of an extruder with a polymer, which is typical for modern processing equipment.

In addition, the proposed models take into account real boundary conditions on operation surfaces of rotating screws and a stationary barrel, which gives possibility to choose parameters of thermal stabilization systems of operation elements of an extruder unambiguously.

2. We studied the process of melting of polymer granules in an operation channel of an extruder screw. The results of the study showed that it is necessary to use mixing elements at an increase of deviation of the behavior of processed material from the Newtonian behavior in an operation channel of screws. We established that intensity of energy dissipation at certain points in the volume of a processed polymer determines temperature fields in the volume of processed material.

We substantiated that, firstly, an intensive external energy supply to screws and a barrel with their subsequent gradual cooling is necessary during the processing of a polymer on twin-screw extruders in contrast to single-screw extrusion.

3. We verified the adequacy of the developed model by comparison of the results of the numerical modeling with the experimental data in processing of a composition based on high-density polyethylene filled with aluminum hydroxide in a twin-screw extruder Ø83×30 with co-rotation screws. We carried out studies for the industrial production of 50 kg/h and the rotational frequencies of screws of 25 and 40 rpm.

The proposed model of twin-screw extrusion gives possibility to determine main parameters of the equipment and the process and to estimate temperature heterogeneity of melt at the design calculation for a given productivity and the required final temperature of polymer melt. The parameters include the geometry of operation elements, frequency of rotation of screws and required minimum drive power. It is possible to determine rotational frequency of screws and thermal conditions of extruder working elements at verification calculation of an extruder for a given geometry of screws.

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References

1. Schenkel G. Schneckenpressen für kunststoffe. München: Carl Hanser Verlag, 1959. 467 p.
2. Tadmor Z., Gogos C. G. Principles of polymer processing. 2nd ed. Hoboken: John Wiley & Sons, 2006. 961 p.
3. Rauwendaal C. Polymer extrusion. 5th ed. Carl Hanser Verlag GmbH & Co. KG, 2014. 950 p. doi: https://doi.org/10.3139/9781569905395
4. Mikulionok I. O. Classification of Processes and Equipment for Manufacture of Continuous Products from Thermoplastic Materials // Chemical and Petroleum Engineering. 2015. Vol. 51, Issue 1-2. P. 14–19. doi: https://doi.org/10.1007/s10556-015-9990-6
5. Mikulionok I. O., Radchenko L. B. Screw extrusion of thermoplastics: I. General model of the screw extrusion // Russian Journal of Applied Chemistry. 2012. Vol. 85, Issue 3. P. 489–504. doi: https://doi.org/10.1134/s1070427211030305
6. Mikulionok I. O., Radchenko L. B. Screw extrusion of thermoplastics: II. Simulation of feeding zone of the single screw extruder // Russian Journal of Applied Chemistry. 2012. Vol. 85, Issue 3. P. 505–514. doi: https://doi.org/10.1134/s1070427211030317
7. Mikulionok I., Gavva O., Kryvoplias-Volodina L. Modeling of melting process in a single screw extruder for polymer processing // Eastern-European Journal of Enterprise Technologies. 2018. Vol. 2, Issue 5 (92). P. 4–11. doi: https://doi.org/10.15587/1729-4061.2018.127583
8. Todd D. B. Improving incorporation of fillers in plastics. A special report // Advances in Polymer Technology. 2000. Vol. 19, Issue 1. P. 54–64. doi: https://doi.org/10.1002/(sici)1098-2329(20000117)19:1<54::aid-adv6>3.0.co;2-#
9. Potente H., Kretschmer K. In 60 Sekunden optimiert // Kunststoffe. 2001. Issue 9. P. 76, 78, 80–81.
10. Mikulyonok I. O. Equipment for preparing and continuous molding of thermoplastic composites // Chemical and Petroleum Engineering. 2013. Vol. 48, Issue 11-12. P. 658–661. doi: https://doi.org/10.1007/s10556-013-9676-x
11. Rauwendaal C. The geometry of self-cleaning twin-screw extruders // Advances in Polymer Technology. 1996. Vol. 15, Issue 2. P. 127–133. doi: https://doi.org/10.1002/(sici)1098-2329(199622)15:2<127::aid-adv2>3.0.co;2-x
12. Shearer G., Tzoganakis C. Distributive mixing profiles for co-rotating twin-screw extruders // Advances in Polymer Technology. 2001. Vol. 20, Issue 3. P. 169–190. doi: https://doi.org/10.1002/adv.1014
13. Avalosse T., Rubin Y. Analysis of Mixing in Corotating Twin Screw Extruders through Numerical Simulation // International Polymer Processing. 2000. Vol. 15, Issue 2. P. 117–123. doi: https://doi.org/10.3139/217.1586
14. Bravo V. L., Hrymak A. N., Wright J. D. Numerical simulation of pressure and velocity profiles in kneading elements of a co-rotating twin screw extruder // Polymer Engineering & Science. 2000. Vol. 40, Issue 2. P. 525–541. doi: https://doi.org/10.1002/pen.11184
15. Non-Newtonian Fluid Mixing in a Twin-Screw Mixer Geometry: Three-Dimensional Mesh Development, Effect of Fluid Model and Operating Conditions / Rathod M. L., Ashokan B. K., Fanning L. M., Kokini J. L. // Journal of Food Process Engineering. 2014. Vol. 38, Issue 3. P. 207–224. doi: https://doi.org/10.1111/jfpe.12154
16. Mikulionok I. O. Screw extruder mixing and dispersing units // Chemical and Petroleum Engineering. 2013. Vol. 49, Issue 1-2. P. 103–109. doi: https://doi.org/10.1007/s10556-013-9711-y
17. Eitzlmayr A., Khinast J. Co-rotating twin-screw extruders: Detailed analysis of conveying elements based on smoothed particle hydrodynamics. Part 1: Hydrodynamics // Chemical Engineering Science. 2015. Vol. 134. P. 861–879. doi: https://doi.org/10.1016/j.ces.2015.04.055
18. Numerical simulation of 2D unsteady shear-thinning non-Newtonian incompressible fluid in screw extruder with fictitious domain method / He Q., Huang J., Shi X., Wang X.-P., Bi C. // Computers & Mathematics with Applications. 2017. Vol. 73, Issue 1. P. 109–121. doi: https://doi.org/10.1016/j.camwa.2016.11.005
19. Experimental characterization and modeling of twin-screw extruder elements for pharmaceutical hot melt extrusion / Eitzlmayr A., Khinast J., Hörl G., Koscher G., Reynolds G., Huang Z. et. al. // AIChE Journal. 2013. Vol. 59, Issue 11. P. 4440–4450. doi: https://doi.org/10.1002/aic.14184
20. Eitzlmayr A., Matić J., Khinast J. Analysis of flow and mixing in screw elements of corotating twin-screw extruders via SPH // AIChE Journal. 2017. Vol. 63, Issue 6. P. 2451–2463. doi: https://doi.org/10.1002/aic.15607
21. Hétu J.-F., Ilinca F. Immersed boundary finite elements for 3D flow simulations in twin-screw extruders // Computers & Fluids. 2013. Vol. 87. P. 2–11. doi: https://doi.org/10.1016/j.compfluid.2012.06.025
22. Numerical simulation and experimental validation of mixing performance of kneading discs in a twin screw extruder / Zhang X.-M., Feng L.-F., Chen W.-X., Hu G.-H. // Polymer Engineering & Science. 2009. Vol. 49, Issue 9. P. 1772–1783. doi: https://doi.org/10.1002/pen.21404
23. A composite model for an intermeshing counter-rotating twin-screw extruder and its experimental verification / Lewandowski A., Wilczyński K. J., Nastaj A., Wilczyński K. // Polymer Engineering & Science. 2015. Vol. 55, Issue 12. P. 2838–2848. doi: https://doi.org/10.1002/pen.24175
24. Mikulionok I. O. Technique of parametric and heat computations of rollers for processing of plastics and rubber compounds // Russian Journal of Applied Chemistry. 2011. Vol. 84, Issue 9. P. 1642–1654. doi: https://doi.org/10.1134/s1070427211090333
25. Wilczyński K., Lewandowski A. Study on the Polymer Melt Flow in a Closely Intermeshing Counter-Rotating Twin Screw Extruder // International Polymer Processing. 2014. Vol. 29, Issue 5. P. 649–659. doi: https://doi.org/10.3139/217.2962
26. Basov N. I., Kazankov Yu. V., Lyubartovich V. A. Raschet i konstruirovanie oborudovaniya dlya proizvodstva i pererabotki polimernyh materialov. Moscow: Himiya, 1986. 488 p.
27. Mikulionok I. O. Pretreatment of recycled polymer raw material // Russian Journal of Applied Chemistry. 2011. Vol. 84, Issue 6. P. 1105–1113. doi: https://doi.org/10.1134/s1070427211060371