A generalized mathematical model of the heat/mass transfer in the polymer in the channel of a plasticating extruder

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Abstract. A mathematical model capable of describing the heat transfer in the metering zone of the extruder is offered. The results obtained by this model were compared to the predictions made by other models, and a good agreement between them was noted. Based on the present model and previously developed models [1,2], we elaborated a generalized model for a classical single-screw extruder. This model allows the description of the polymer movement and the heat transfer in the polymer in the feed, melting delay, melting and metering zones of the extruder. The data on velocity, temperature, pressure and their derivatives are provided for each point of the extruder screw in the cross and down channel directions. The performance of each extruder zone is evaluated numerically under different technological conditions (input parameters).

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Introduction

Our earlier works [1,2] present the mathematical models for the first three zones of the extruder performance: feed, melting delay and melting zones. In order to describe the plasticating extruder on the whole, we need to study the processes taking place in the metering zone, where the polymer is in the liquid phase. By now, there are lots of mathematical models capable of describing the flow and heat transfer in the channels of extruder pumps, including those in the metering zone of the extruder. The earlier works taking into account the viscosity anomaly and non-isothermal flow, were devoted to the analysis of Couette flow between parallel plates [3-6]. Further development of the extrusion theory allowed in [7-12] consider two-dimensional mathematical model of the polymer flow, which does not take into account the effect of the channel side walls. Development of computer-technology have allowed to solve the problem of heat transfer in the metering zone of the extruder in three-dimensional formulation [13-17], which takes into account the circulation of the polymer melt in the channel cross section. However, since our purpose in this paper is to develop a generalized model of the plasticizing extruder, the mathematical description of the heat/mass transfer in the metering zone should be done using the same notation and spatial approach as for the other extruder zones. Besides, we should elucidate the relation between the extruder zones in order to take into account the change in one of the zones and its effect on the other zones.

In the frame of the problem formulation given in work [1], for the metering zone we take the boundary conditions for the flow function ψ, by assuming that the channel walls are impenetrable and there is no slip at them:

$$\psi\left[x(\tau),y,z\right]_{z=0}=\psi\left[x(\tau),y,z\right]_{z=1}=0,$$
$$\psi\left[x(\tau),y,z\right]_{y=0}=\psi\left[x(\tau),y,z\right]_{y=S/H}=0.$$

where $x=\overline{x}/H,\ y=\overline{y}/H,\ z=\overline{z}/H$ is the dimensionless coordinates [1] $\tau=tv_0/H$ are the dimensionless "convective time", v_0 is the peripheral screw speed, *H, S*are the depth and width of the channel screw, and *t* is the true time.

The boundary conditions for the vortex function ω are found as in [1], i.e., in terms of the Wouds formula of the second order of accuracy.

The boundary conditions for the temperature of the polymer melt in the metering zone are written as

$$T\big|_{z=1}=T_B,\ T\big|_{z=0}=T\big|_{y=0}=T\big|_{y=S/H}=T_S,$$

where T_B, T_S are the temperature of the extruder barrel and that of the screw.

A peculiarity of the proposed model regarding the metering zone is its quasistationarity (quasithree-dimensionality). In equations of conservation of mass, momentum and energy [1], the derivative with respect to coordinate *x* (in the down channel direction) in the convective terms is replaced by the time derivative. In such a case, the transition from the time to the longitudinal coordinate in the melting zone is implemented through the values of the velocity of the solid bed u

$$\bar{x} = tu$$

For determining the longitudinal coordinate in the metering zone of the extruder, we use the average values of the melt velocity in the cross-channel direction v_{xa}

$$\bar{x} = tv_{xa}$$

It should be noted that the average melt velocity v_{xa} in the channel height (polymer melting is completed at the channel section of constant depth, i.e., H=const) is equal to the velocity of the solid bed u. The calculation procedure in this case is analogous to that for the melting zone, when $v_{xa} = u$.

If the channel height in the metering zone is varying (polymer melting is completed in the tapered section of the screw), then the channel is changed by a stepwise one [2], and for each step we calculate its own average velocity and, hence , the length of the examined section.

As the initial values of functions in the beginning of the metering zone, we assume the values at the exit from the melting zone.

To support the validity of the described transition from the variable $\bar{x}$ to the variable t and the proposed model of the metering zone in general, we examined the metering zone of the extruder (ME-160) of geometry, polymer properties and operating conditions (variant 1) provided in work [2]. Calculations were made in terms of the proposed model [1], the model of complex shear [18] and the two-dimensional model, which does not take into account temperature changes in the channel depth [8]. A comparison of the results obtained by the above models was made for the average temperature of the polymer melt and the pressure gradient at the end of the metering zone. The results are summarized in Table 1, where, for the channel with varying height H_1 / H_2 =2, and the channel length being the same as in the case H=const, i.e. 6 turns (for the geometry of the extruder ME-160 see work [2]).

Inspection of the results given in the Table discloses that the proposed approach can be used for changing the variables in the three-dimensional model, notwithstanding the fact that the results obtained for the pressure gradient with the aid of the two-dimensional model are different from the rest significantly.

Table 1: Comparison of different models of the flow in the metering zone

channel shape	Model	$\partial p / \partial x \cdot 10^{-6}$, N/m³	T, □C
H = const	N1	1.2	218.9
	N2	1.6	222.7
	N3	1.4	218.4
H = var	N1	-1.66	219.5
	N2	-1.46	223.4
	N3	-1.54	222.7

To sum up, the theory of heat/mass transfer in the plasticating extruder channel is based on the models developed for separate zones and presented in works [1,2]. A generalized model of the extruder involves earlier developed mathematical models and interrelates them so that the temperature fields, obtained in the end of the feed zone, are assumed to be input data for calculating the processes in the melting delay zone. The fields of temperature, velocities and pressure in the end of this zone define the initial values for the melting zone and so on.

For the feed zone, we calculate the three-dimensional temperature field and pressure in a solid bed. At the instant the thin melt layer is generated near the barrel surface, we record the length of the channel, which specifies the length of the feed zone. Then the equations of energy (heat conductivity) are supplemented with the equations of hydrodynamics for liquid phase and, hence, the solution to the problem of the polymer movement and heat transfer in it under phase transition is found. When the desired thickness of the melt film (greater than the clearance between the screw fights and the inner barrel surface) is attained, we introduce the hydrodynamic equations to evaluate the circulating flow of the melt. Temperature of the solid phase of the polymer is calculated as before, i.e. in terms of the heat conductivity equation. The completion of polymer melting and the length of the melting zone are defined by the cross section where the solid bed disappears. For the remaining part of the channel length, we solve the hydrodynamic equations. Similarly to the previous zones, the values calculated in the end of the melting zone are taken as the conditions at the beginning to the metering zone.

Discussion

Numerical analysis has been performed for the ME-160 extruder the geometry of which is described in work [2]. The properties of polyvinylchloride plasticate used in calculations are also given in this work.

Since the effect of different parameters on the processes of heat/mass transfer and polymer melting in each zone of the extruder was considered at great length in work [2], here we examine these processes for extruder as a whole through simultaneous variation of two-three factors (input parameters of the process). This affects chiefly technological parameters of the process.

The results of calculations are summarized in Table 2 where each number of computational variant corresponds to a particular set of the input parameters. The following notation is used in the Table 2: $T_{\max}$ is the maximum value of temperature of a liquid phase in the melting zone; z_S is the number of screw turn corresponding to $T_{\max}$; $T_{B1}, T_{B2}, T_{B3}, T_{B4}$ are temperatures of the screw barrel with respect to a heating zone (Fig. 1) The figures given in the second column of Table 2 specify screw geometry. Three versions of screw configuration are presented in Figure 1. The examined variants of the barrel temperature variation are given in Figure 2. Variant 7 in Table 2 is taken as a reference or basic computational variant. L_{z1}, L_{z2}, L_{zm} denote, respectively, the end of the feed, melting delay and melting zones.

Table 2: Operating conditions of extruder ME-160 for polyvinylchloride plasticate

variant no.	Input parameters								Zone length			$T_{\max}$, □C	z_S turns
	N, rpm	$G \cdot 10^5$ kg/s	Variants of barrel heating	T_{B1}, □C	T_{B2}, □C	T_{B3}, □C	T_{B4}, □C	μ_0, $Pa \cdot s^n$	L_{z1} turns	L_{z2} turns	L_{zm} turns		
1	60	786	1	170	180	190	190	23635	4.68	5.18	15.88	332	9.8
2	60	786	2	170	180	180	180	23635	4.68	5.18	16.28	224	12.62
3	60	786	2	170	180	180	180	23635	4.68	5.18	16.14	239	6.52
4	60	786	3	170	180	190	180	23635	4.68	5.18	16.28	225	12.61
5	70	860	2	170	180	180	180	13000	5.15	5.79	13.32	243	11.87
6	70	860	2	170	180	180	180	23635	5.15	5.65	16.58	224	7.11
7	60	786	2	170	180	180	180	23635	4.68	5.18	16.28	225	12.62
8	70	860	4	180	190	180	180	23635	3.26	3.89	13.88	280	10.8
9	60	786	5	170	190	190	190	23635	4.68	5.18	15.79	264	7.16
10	50	700	2	170	180	180	180	23635	4.17	4.67	14.42	306	9.7
11	60	786	6	170	160	160	160	23635	4.7	5.18	17.32	276	12.52
12	80	940	7	180	180	180	180	23635	3.56	4.15	16.30	320	10.23
13	100	1572	8	180	170	170	170	23635	5.95	7.06	22.91	235	21.03
14	115	2358	9	200	170	170	170	23635	5.95	7.11	plugging of the channel		
15	95	1179	2	170	180	180	180	23635	7.02	plugging of the channel			

It should be noted that the examined operations regimes of the extruder which in most cases correspond to real conditions essentially affect not only the length of all zones but also the state of the polymer melt both in the zone of melting and in the zone of metering. However in the zone of melting delay no appreciable changes in the melt behavior and temperature are recorded.

The analysis of temperature fields in the melt has shown that after completion of melting the temperature fields continue to change in the down-channel direction. The latter reach a steady state rather quickly (along the length of ½ turn) as soon as the polymer is pushed out of the tapered portion of the extruder.

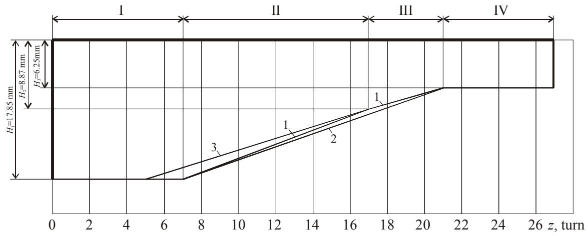

Fig. 1. Channel depths and lengths of the heated zones of the ME-160 extruder barrel (in screw turns)

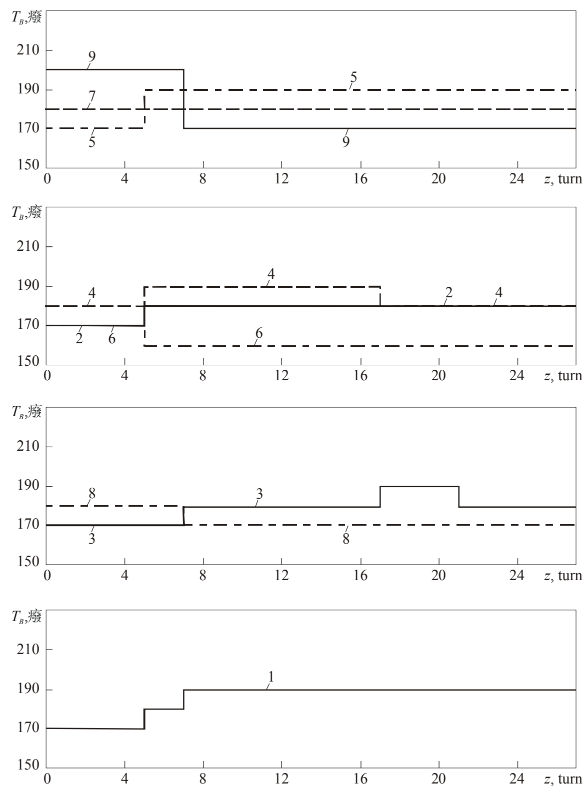

Fig. 2. Variation in the barrel temperature T_B for different extruder zones

The established temperature field is quite uniform and on the average equals 199ºC. In a steady-state process the melt temperature in the metering zone is different for various computational versions. The diagram of average temperature values in the metering zone (Fig. 3) shows that the maximum difference is 12ºC for computational variants 1 and 11. These calculations give the lowest and highest values of the barrel temperature compared to the other variants (curve 1 and 6 in Figure 2), which evidently specifies the melt temperature at the end of the metering zone. For these operating conditions, variation of the average melt temperature in the down-channel direction is shown in Figure 4. As it is readily seen the values of the average temperature differ essentially.

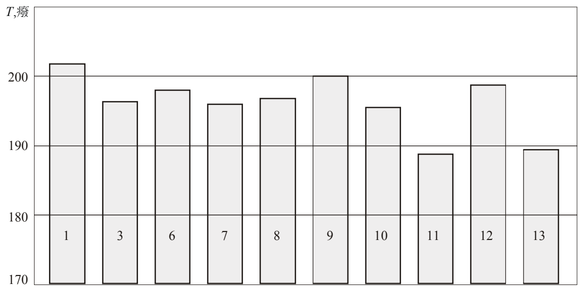

Fig. 3. Variation in the average values of the polymer melt temperature in the end of the metering zone of the extruder. Figures correspond to the numbers of calculation variants from Table 2

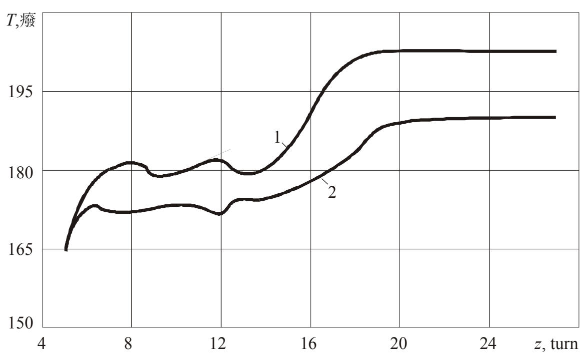

Fig.4. Variation in the average temperature of the polymer melt along the screw

The diagram in Figure 5 shows the ratio and variation of lengths of the feed L_{z1}, melting delay L_{z2} and melting L_{zm} zones expressed in terms of the screw turns at different conditions of polymer processing. The figures on the diagram correspond to the numbers of computational variants given in Table 2. The shortest total length of channel zones was obtained for variant 8 in which the mass flow rate was assumed greater, the screw speed was 10% larger, and the barrel temperature T_B in the first and second heating zones was $10^{\circ}C$ higher than in the reference variant. In this case, in spite of the fact that the solid bed moves along the channel with a greater velocity, an increase in the power of the external heat source proved to be quite sufficient for heating the solid bed and enhancing the activity of the melting process. The largest value of the total zone length L_{z1}, L_{z2}, L_{zm} corresponds to the computational variant 13, in which the mass flow rate is 2 times as greater as in the reference variant 7and the barrel temperature is varied in the down-channel direction. In this case polymer melting is completed in the metering zone. As it follows in the diagram in Figure 5, in some cases the output of the extruder can be essentially increased by rising the temperature of its functional zones. However while doing this one should concentrate on the temperature field of the melt in the course of melting and at the channel exit. Thus overheating of the material is especially detrimental to the quality of the finite product. The lowest values of the maximum temperature were obtained for the reference variant 7. Compared to the other computational variants , here there are no regions with the values of dimensionless temperature equaling 1.7 and 1.9. For computational variant 7 the melt temperature during melting is rather homogeneous and relatively low. It is clear that selection of technological parameters in this case is optimal. Essential overheating is common to regimes with lower mass flow rate and higher temperature of the barrel (variant 10). The melt with temperature $T = \overline{T} / T_m$ occupies a larger volume. The computational variant 8 yields intermediate values of polymer temperature. Here an increase in temperature occurs in parallel with the growth of throughput.

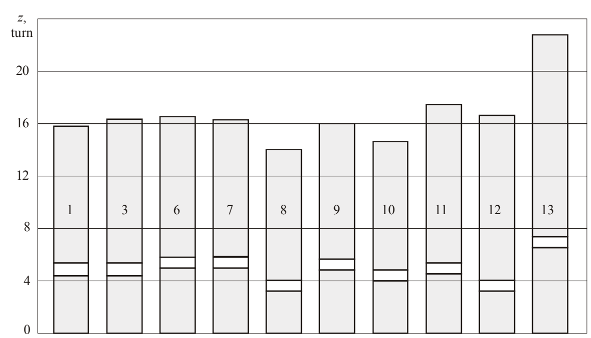

Fig.5. Changes in the lengths of the operation zones of the extruder. Figures correspond to the numbers of variants from Table 2

In the context of temperature distribution problem it is also of interest to define temperature maximum and its location in the polymer melt throughout the screw channel. Table 2 gives the calculated values of $T_{\max}$ for each computational variant. In this respect, most unfavorable is the operating regime obtained from the variant 1 with considerably increased barrel temperature (see, curve 4 in Figure 2). The maximum temperature occurs in the section of the channel where the shear rate reaches its maximum value, namely along the first 1/3 length of the melting zone, which is also typical for other operating regimes. The smoothest variation of $T_{\max}$ was obtained for the basic computational variant 7. Variation of $T_{\max}$ in the down-channel direction for variants 7 and 12 is shown in Figure 6.

The proposed mathematical model allows us to calculate extrusion processes for any screw geometry. Inessential changes in the screw geometry (see variant 2 in Figure 1) produce little effect on mass/heat transfer processes, hence the lengths of the zones L_{z1}, L_{z2}, L_{zm} and also the temperature fields in the melting and metering zones remain unaltered. Then it follows that II and III zones of the extruder may have identical taper angles. Calculations made for the screw with increased length of the taped section (variant 3, Figure 1) but with the same degree of tapering show that melting processes undergo some changes. Although the length of the melting zone decreases (approximately by 1%) the value of the temperature maximum in the melt increases by 31ºC, the temperatures in the metering zone being practically the same.

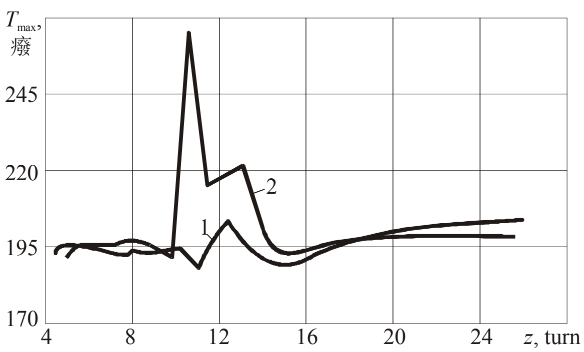

Fig.6. Distribution of the maximum temperature of the melt polymer along the screw: 1 – variant 1; 2 – variant 12

A 10% increase in the output of the extruder (and the screw speed , respectively) under the conditions of invariable barrel temperature does not affect the total length of the zones (computational variants 5, 6 and 7).This is attributed to the fact that at the increased throughput the velocity of the solid bed becomes higher and it is transported more rapidly to the tapering zone where melting processes proceed more intensively.

An increase of the barrel temperature in I and II zones (Figure 1) at higher value of the mass flow rate (computational variant 8 in Table 2) reduces the length of each zone and their total length by 17 %. In this case, the maximum temperature $T_{\max}$ increases by 36%.

Variation in the barrel temperature in the III heated zone (computational variant 4) results in nonuniform temperature fields approximately at turn 20 of the screw (see Figure 7), with all other parameters of the extrusion process being the same.

The computational software developed on the basis of the proposed model (1) allows us to define the pressure distribution in the down-channel direction. Figure 8 gives variation of pressure with the screw length for various computational variants. Curve 1 corresponds to the variant considering refined screw geometry (see variant 3 of the screw geometry in Figure 1). In this case the pressure at the exit of the screw channel reaches its minimum because an increase of the tapering zone length assists in reducing the value of positive pressure gradient. It should be noted that in all variants considered the pressure gradient $\partial p / \partial x$ was positive and did not change the sign all along the channel length. This is attributed to the relation between the value of the mass flow rate and frequency of screw rotation for preset screw geometry and material properties. The largest value of $\partial p / \partial x$ and accordingly of p was obtained for the computational variant 8 at the increased mass low rate and frequency of screw rotation.

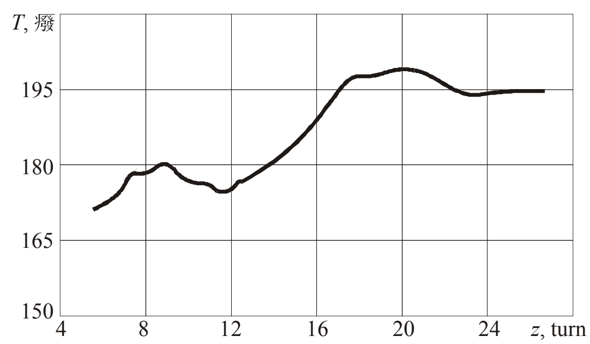

Fig.7. Variation in the average temperature of the polymer melt along the screw for variant 4

From the practical view point it is of particular importance to identify the worst-case working conditions which may lead to channel blocking and to exclude them from the range of technological parameters To this end we made calculations for variants 13, 14 and 15. At invariable barrel temperature in the feed zone and 1.5 rise in the flow rate (computational variant 15 the effect of channel plugging occurs already at the 8-th turn from which the channel tapers off. Increasing of the barrel temperature by 10ºC (variant 13) and the flow rate by 2 times does not cause channel plugging despite the fact that the barrel temperature in the zones II, III, and IV was reduced. Although in this case the melting process finishes at the mid of the metering zone the melt does not experience any significant overheating and the temperature maximum does not exceed 235ºC.

The variant 14, in which calculations have been made for the8th variant of heating regime for the extruder barrel (Fig. 2) and for a threefold flow rate, allows us to avoid plugging of the channel at the beginning of the tapering zone. This is due to the fact that an essential increase in the barrel temperature in the feeding zone facilitates good heating of the solid bed despite a threefold increase in the mass flow rate. Nevertheless, plugging of the channel does occur at the 12th turn of the screw where the second tapering zone with greater tapering degree (zone III) begins.

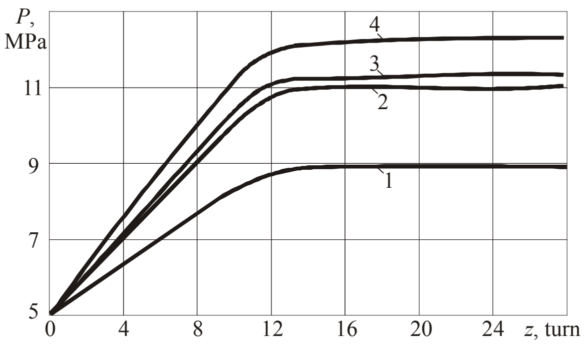

Fig.8. Pressure change along the screw: 1 – variant 3; 2 – variant 4; 3 – variant 7; 4 – variant 8

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