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Polymer Plastication during Injection Molding

Part 2 Simulations and Experiments

A computer program for the simulation of polymer plastication in screw injection molding machine created on basis of the theoretical model presented in part 1 of this paper is discussed. As simulation examples various process characteristics, e. g. solid bed, pressure and temperature profiles, are computed using the material parameters for high density polyethylene and three-zones-screw of diameter 20 mm. Effects of different geometric and operating parameters on plastication course are also demonstrated. Simulation results with respect to the screw rotation time are compared with experimental data measured for low density polyethylene, polypropylene, polystyrene, polyoxymethylene and polyamide 6. It was found that the computer program reflects correctly all features of a true plasticating system in injection molding machine. It provides also good agreement of model predictions with experimental data.

1 Introduction

The quick development in design of progressively more efficient processing devices, such as extruders and injection molding machines, requires great practical experience from designers, often supported by experimental studies. More and more frequently computer programs are also applied, as they are able to simulate the true processing course. The use of computer simulation programs for the optimization of polymer plasticization in screw processing machines is virtually restricted to extruders. This is probably due to the fact that extrusion is a typical steady-state process and it is much easier to model mathematically than the periodical, quasi-steady, screw action characteristic of injection molding machines. Hence, a number of computer programs for simulation of plasticating extrusion have been described in the literature (Tadmor and Klein, 1968, 1970; Chung, 1971; Donovan, 1971b; Lindt, 1976; Agur and Vlachopoulos, 1982; Elbirli et al., 1984; Zawadzky and Karnis, 1985; Rao, 1986; Wilczynski, 1986; Zhu and Chen, 1991; MacGregor et al., 1996). Some of them are also commercially available (EXTRUCAD, REX, SSD, SSEM). In contrast with extrusion, no complex models exist for polymer plastication during screw injection molding. As a rule, the studies known (Basow and Kazankow, 1984; Donovan et al., 1971a, 1974, Lipschitz et al., 1974; Isayev and Hieber, 1980; Rao, 1986) are restricted to some specific problems, e. g. calculation of solid bed profile after static and dynamic melting, without taking into account such fundamental factors as axial screw motion with controlled stroke, use of three-zone-screw, existence of soak times at the front and back screw positions, etc. In part I of this work, we presented and discussed in detail a mathematical model for the plasticization sequence during one injection cycle that contains most of features reflecting the true process course.

The aim of this paper is to present and discuss the simulation results with the use of a computer program that was created on the basis of this mathematical model. The effect of various geometric and operating parameters on polymer conveying and melting will be analyzed. The screw rotation time computed for different thermoplastics under various plasticating conditions will be compared with experimental measurements.

2 Simulation Results

The simulation examples presented below demonstrate the ability of the computer program to provide predictions of the most important interrelations between various geometrical, operating and material parameters and process quantities, such as solid bed width, temperature and pressure profiles, plasticization efficiency, screw torque, power requirement, screw rotation time, etc. The input data can be loaded directly or from a file. The computation results are presented in the form of diagrams or tables. They can also be stored into a file or printed. It is also possible to load few files with results and to compare the desired characteristics in diagrams.

The simulation examples presented below were obtained using the following input data:

2.1 Geometrical Parameters

Screw diameter $D = 20$ mm, screw lead $S = 20$ mm, flight width $e = 3$ mm, feed zone length (number of turns) $N_f = 14$, compression zone length (number of turns) $N_c = 5.5$, metering zone length (number of turns) $N_m = 5.5$, channel height in feed zone $H_f = 3.8$ mm, channel height in metering zone $H_m = 1.8$ mm, radial clearance $\delta_R = 0.02$ mm, distance between feed opening and the beginning of the barrel heating zone (number of turns) $N_h = 4$.

These data are valid for the plasticization system of an injection molding machine that was used for the experimental veri-

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fication of the some predictions with respect to the screw rotation time.

2.2 *Material Parameters*

Melting temperature $T_m = 408$ K, barrel friction factor $f_b = 0.5$, screw friction factor $f_s = 0{,}35$, bulk density $\rho_0 = 550\ kg/m^3$, solid density $\rho_s = 955\ kg/m^3$, melt density $\rho_m = 780\ kg/m^3$, thermal conductivity of solid $k_s = 0.42$ J/(m s K), thermal conductivity of melt $k_m = 0.26$ J/(m s K), specific heat of solid $c_s = 2.5$ kJ/(kg K), specific heat of melt $c_m = 2.0$ kJ/(kg K), heat of fusion $\lambda = 245$ kJ/kg, rheological parameters of melt: $m_0 = 11\,000$ Pa s^n, $n = 0.6$, $a = 0.01\ K^{-1}$ are the material constants of the power law of the form:

$$\eta = m_o e^{a(T-T_o)} \left(\frac{1}{2}\Pi\right)^{\frac{n-1}{2}}; \qquad (1)$$

where: η – viscosity, Π – second invariant of the rate-of-strain tensor, T_0 – reference temperature.

The values assumed for the material parameters are characteristic of high-density polyethylene.

2.3 *Operating Parameters*

Mean barrel temperature $T_b = 200\,°C$, screw stroke (expressed as number of turns) $N_s = 3$, screw speed $N = 180\ min^{-1}$, back pressure (plastication pressure) $p_p = 10$ MPa, screw soak time in front position $t_f = 1$ s, screw soak time in the reverse position $t_b = 10$ s; the parameters could be changed during the simulations (then the changes will be described in the text). As reference temperature T_0, and melting temperature T_m were used for convenience.

Fig. 1 presents the relative solid bed widths at the moments of screw rotation end, screw rotation beginning and steady state conditions (i. e. for extrusion with constant backward screw motion). The positions of the different geometrical and dynamic zones marked with broken lines and letters are the following: A – start of screw (hopper position for screw front position), B_S – beginning of static melting, B_D – beginning of dynamic melting, T – beginning of a transient zone, F – feed zone end, C – compression zone end, M – metering zone (or screw) end.

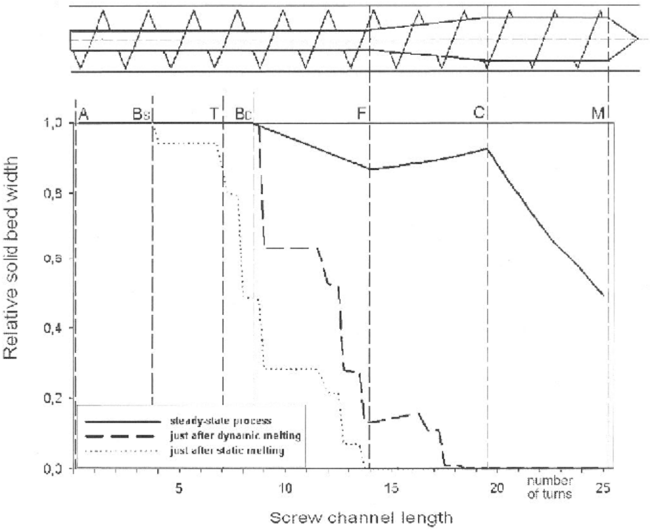

Fig. 1. Relative solid bed width during polymer plastication in injection molding, $t_b = 10$ s

It follows from Fig. 1 that under the input parameters assumed and steady-state conditions characteristic of extrusion, the screw channel at its end would be approximately 50% filled with solid polymer. However, the existence of the static melting phase causes a significant decrease in the content of solids and, therefore, the situation after dynamic melting is characterized by a much higher plasticization degree in comparison with steady-state conditions. The solid bed profiles in both cases are identical only at the initial part of the screw. The length of profiles covered depends on the screw stroke. It means that the steady-state penetrates form the back (feed opening) into the screw channel during screw rotation. The relative bed width in the compression zone (between F- and C-lines) increases because the channel cross-section area decreases more quickly than the amount of solid polymer due to melting.

It can also be seen from Fig. 1 that the solid bed profiles for injection molding are more complicated in comparison with the smooth profile characteristic of steady-state extrusion. This results from the more complicated history of solid bed motion in the screw channel in the periodical sequence of injection molding. It should be emphasized that the solid bed consists of polymer portions coming from a few consecutive injection cycles. These cycles are visible as plateaus on the solid bed distribution curve. Moreover, during the to-and-fro screw motion a part of polymer at every cycle is statically molten only in time t_f, whilst the rest of the polymer is molten in the time $t_f + t_b$. The polymer is also molten dynamically in the time t_r, depending on the operating parameters.

The absolute differences between the solid bed profiles of Fig. 1 depend strongly on the static melting times t_f and t_b for constant values of the remaining operating parameters. When $t_f \to 0$ and $t_b \to 0$ both profiles, characteristic of injection molding, gradually approach the steady-state (extrusion) profile, which is independent on t_f and t_b. This tendency is demonstrated in Fig. 2, where the solid bed profiles for injection

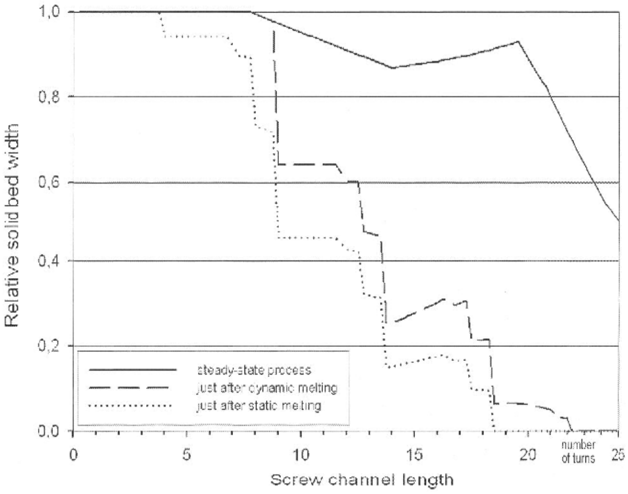

Fig. 2. Relative solid bed width during polymer plastication in injection molding, $t_b = 2$ s

molding are computed for $t_b = 2$ s instead of $t_b = 10$ s, as in Fig. 1. It can be seen that the degree of filling of the screw channel with solid polymer increases and the differences between both profiles become smaller, as expected.

Fig. 3 presents the temperature profile just before the end of dynamic melting, i. e. just before screw rotation stops. It shows that the quick temperature rise appears at the early plasticization stages, when the screw channel is mainly filled with solids. In the melt conveying section the temperature increases much more slowly. Such behavior is typical not only of injection molding, but also of extrusion (Tadmor and Klein, 1970). The corresponding pressure profile is shown in Fig. 4. The exponential pressure rise at the end of the solid conveying zone is qualitatively similar to the results of previous experimental studies (Bernhardt, 1959; Tadmor and Klein, 1970; Donovan, 1971b; Diakun, 1991). In the transient (delay) zone, between points T and B_D, the exponential pressure rise is apparently restrained, and in the melting zone the pressure increases almost linearly up to the maximal value. The existence of a pressure maximum in the screw channel appears as a rule in the compression zone (between F and C points). It depends usually on the values of the operating parameters, especially on the back (plastication) pressure p_p assumed, i. e. the pressure at the screw tip (point M).

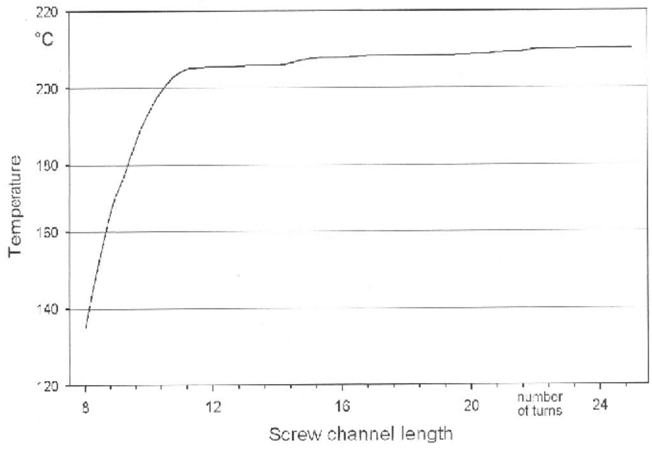

Fig. 3. Temperature profile during polymer plastication in injection molding

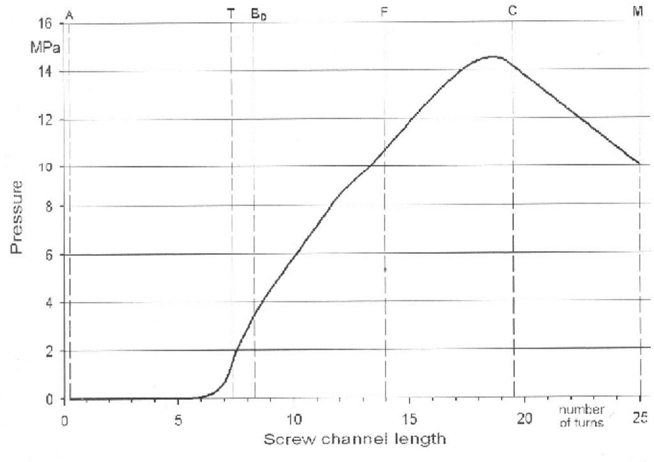

Fig. 4. Pressure profile during polymer plastication in injection molding

Simulation results reflecting the effects of some operating and geometrical parameters on various characteristics of the plasticization process are presented below.

The effect of screw speed on the relative solid bed width at the end of screw rotation, i. e. after the dynamic melting, is shown in Fig. 5. It can be seen that increasing screw speeds lead to an increase in the degree of filling of the screw channel with solid polymer. This expected effect is more pronounced at lower screw speeds. Qualitatively, very similar results, i. e. increase in degree of filling of the screw channel with increasing screw speed, follow from different extrusion models, e. g. from Tadmor model (Tadmor and Klein, 1970). This is obviously due to a quicker rise in the conveying rate of solid polymer than the rise in its melting rate with increasing screw speed.

Fig. 6 demonstrates the effect of screw speed on the pressure profile under similar conditions. As expected, the pressure differences within the channel become larger for higher screw speeds.

The effect of screw speed on the temperature distribution in the screw channel is shown in Fig. 7. In this case, somewhat different input data were used ($D = S = 60$ mm, $H_f = 12$ mm, $H_m = 4$ mm, $N_s = 4$, $N_h = 3$, $t_b = 3$ s, $p_p = 20$ MPa, $T_b = 473$ K) to increase the differences (but not the trends) between temperature profiles corresponding to various screw speeds. It can be seen that higher screw speeds lead to the rise of mean melt

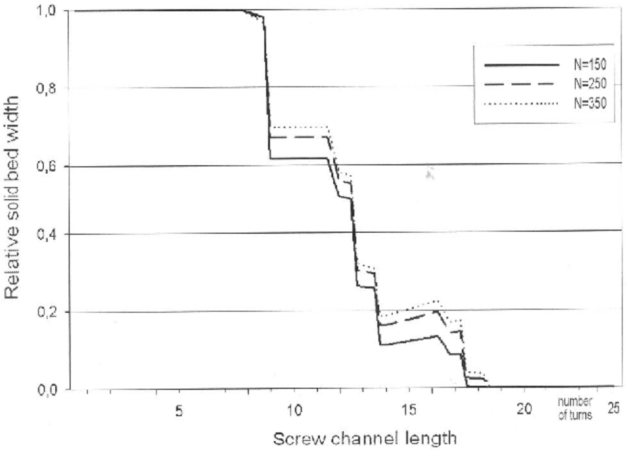

Fig. 5. Effect of screw speed on relative solid bed profile just before stop of screw rotation

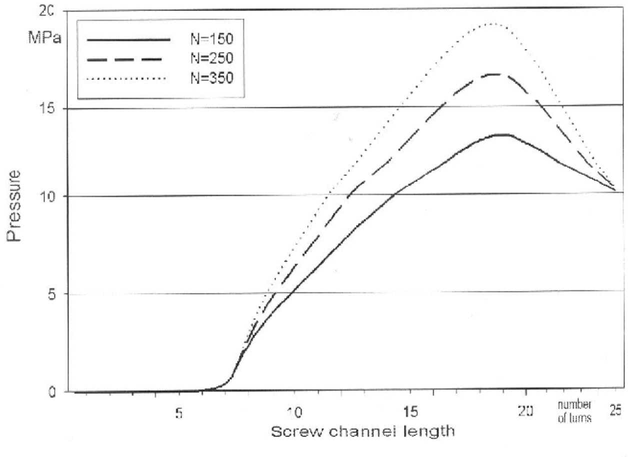

Fig. 6. Effect of screw speed on pressure profile just before stop of screw rotation

temperatures in the channel, as a result of more intense viscous heating. Such behavior is really observed (Tadmor and Klein, 1970; Basow and Kazankow, 1984; Wilczynski, 1986).

Fig. 8 compares the effect of screw speed on various quantities, such as maximal melt temperature, screw power requirement, energy consumption per unit melt mass and screw rotation time, which characterize the polymer plasticization route during injection molding. The results show that all quantities (except screw rotation time) increase with increasing screw speed. The above trends are also in accordance with the expectations.

The effect of soak time of screw in the backside position t_b on the relative solid bed width, just after the screw stopped rotating is demonstrated in Fig. 9. It is visible that for a longer t_b (a part of the total time of static melting) the relative solid bed width decreases as expected. The changes in the solid bed profile are especially significant in the compression and metering zones, reflecting the important role of the static melting phase in the plasticization process.

Fig. 10 shows the effect of the screw stroke on the solid bed width distribution in the screw channel after dynamic melting. A larger screw stroke, i.e. more volume of solid polymer drawn into the screw channel, increases the relative solid bed width over the whole channel length. Such behavior is also consistent with expectations.

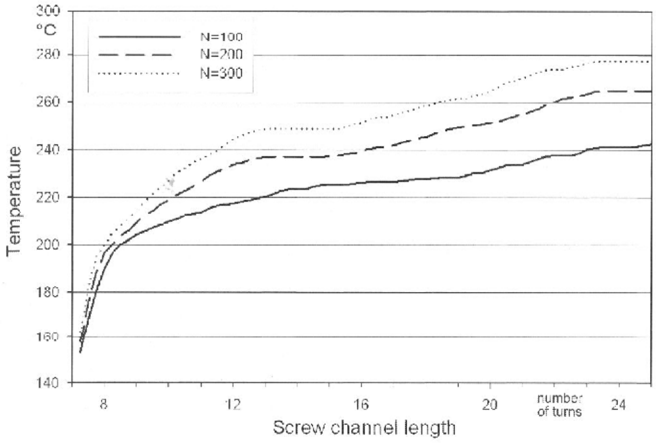

Fig. 7. Effect of screw speed on temperature profile just before stop of screw rotation

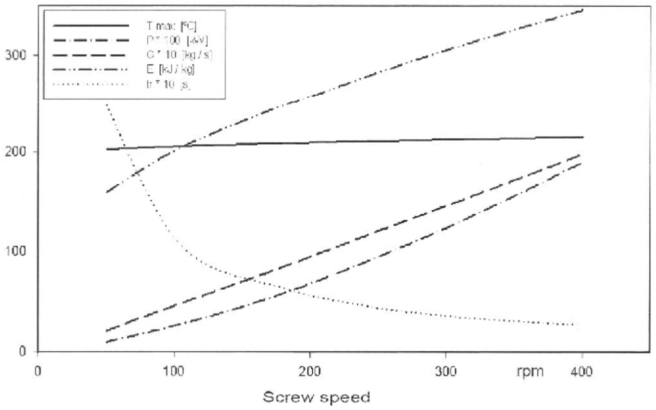

Fig. 8. Effect of screw speed on different characteristics of plastication process (maximal melt temperature in channel, power requirement by screw, melt mass flow rate, energy consumption per mass unit of polymer, screw rotation time)

Fig. 11 presents the simulated effects of channel depth ratio $R = H_f/H_m$ on the solid bed profile just before the end of dynamic melting. It demonstrates that screws with a higher compression ratio promote melting in terms of reducing somewhat the relative solid bed width.

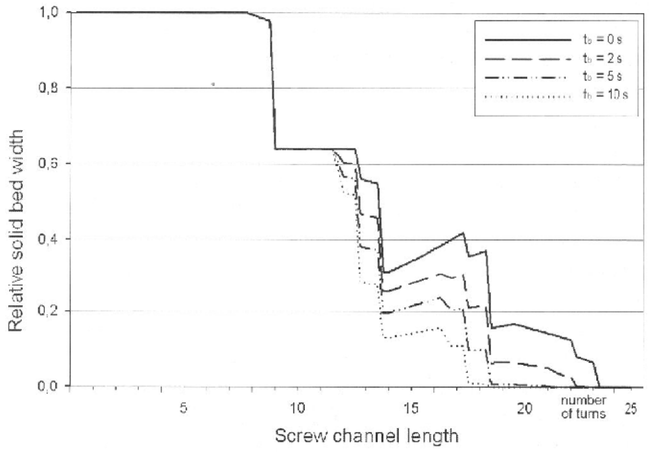

Fig. 9. Effect of screw soak time in back position on relative solid bed profile just before stop of screw rotation

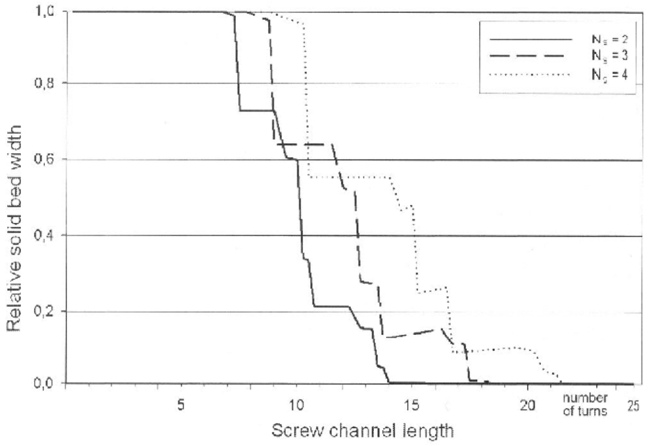

Fig. 10. Effect of screw stroke on relative solid bed profile just before stop of screw rotation (screw stroke values are given in number of turns)

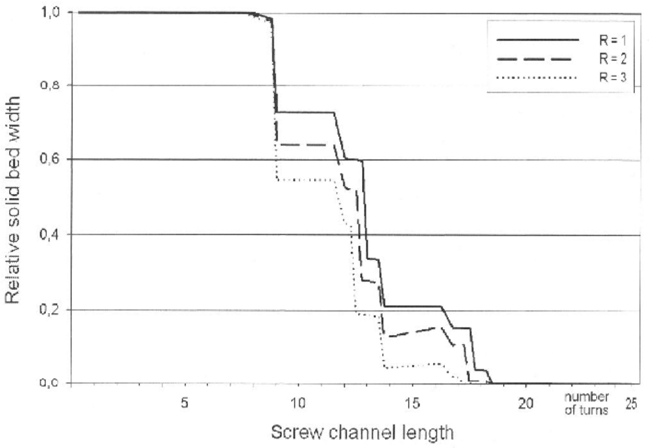

Fig. 11. Effect of channel depths ratio on solid bed profile just before stop of screw rotation

The simulation results presented above show that the predicted behavior of the system caused by changes in the operating conditions or screw geometry are at least qualitatively consistent with those observed in a real process (Tadmor and Klein, 1970). In conclusion, the computer model created reflects correctly the dynamics and all specific features of polymer plasticization during injection molding. A more quantitative appraisal of the model requires its experimental verification, as presented below.

3 Experimental Measurements

A versatile experimental verification of the model, including measurements of solid bed, pressure and temperature profiles in the screw channel and simultaneous determination of other important process characteristics such as power requirement, screw torque, energy consumption, etc., requires the availability of a well instrumented injection molding machine. Since such an equipment could not be used, the experimental studies were restricted to measurements of the screw rotation time as a function of different operating parameters, such as the screw speed and back pressure, for a few thermoplastics. The screw rotation time t_R, i. e. the time for dynamic melting, is a complex dynamic quantity (in contrast with the time of static melting), that depends on geometrical, operating and material parameters. Therefore, the differences between the predicted and measured rotation times under various conditions can be treated as a general quality measure of the simulation program. However, it should be recognized that such a restricted experimental verification of the theoretical model cannot be treated as a truly convincing validation, as more complex measurements would be necessary.

The measurements of screw rotation time were carried out in a Arburg 221M Allrouder 250-55 injection molding machine, with a screw diameter of $D = 20$ mm. Other geometrical parameters were defined at the beginning of the previous section. The rotation times were measured for a few thermoplastic polymers, such as LDPE, PP, PS, POM and PA6, injected under different screw speeds N (64, 128, 192, 256, 320 min^{-1}) and back pressures p_p (8, 16, 24 MPa). Other operating parameters, such as mean barrel temperature, screw soak times in the back and front positions and screw stroke remained constant for each polymer. They were selected in such way to prevent a correct course of the molding process. The barrel temperature was not really constant, but the maximal temperature differences between five barrel heating zones remain within 10–20 K. The screw stroke was limited by the mold volume (approximately 20 cm^3). The material parameters for LDPE, PP, PS, POM and PA6 taken from literature or from the data provided by the producer, are summarized in Table 1. The rheological parameters (m_o, n, a) were determined by means conventional capillary rheometry.

Before each rotation time measurement (for any polymer and operating conditions) several shots were done to stabilize the process conditions. The screw rotation time was determined as the arithmetic mean of consecutive ten injection cycles (the maximal fluctuations of rotation time within any measurement series did not exceed 3 to 5 %).

Fig. 12 compares the measured and computed rotation times for PP under different operating conditions. The agreement is almost perfect for the back pressure of 8 MPa. For the back pressure 24 MPa the differences are somewhat larger, but as a rule smaller than 30 %. In both cases, the rotation times resulting from the computer model are smaller than the values measured for higher screw speeds, while for lower speeds the opposite tendency is observed.

Parameter \ Polymer	LDPE	PP	PS	POM	PA6
T_m [°C]	115	165	130	180	215
f_b	0.40	0.45	0.50	0.30	0.50
f_s	0.35	0.40	0.45	0.20	0.45
ρ_0 [kg/m^3]	550	550	600	700	650
ρ_s [kg/m^3]	915	905	1055	1410	1150
ρ_m [kg/m^3]	780	750	955	1100	950
k_s [J/(m s deg)]	0.34	0.19	0.15	0.29	0.35
k_m [J/(m s deg)]	0,25	0.21	0.19	0.35	0.21
λ [kJ/kg]	138	234	–	236	230
c_s [kJ/(kg deg)]	2.4	2.0	1.3	1.5	1.8
c_m [kJ/(kg deg)]	2.4	2.5	2.2	2.3	2.8
m_0 [kPa s^n]	140	10	700	18	3.8
n	0.28	0.44	0.27	0.72	0.65
a [1/deg]	0.015	0.01	0.04	0.01	0.04

Table 1. Material parameters for various thermoplastic polymers

A similar comparison is shown in Fig. 13 for LDPE. Here, the computed values are smaller than the measurements for all back pressures and screw speeds, the average differences reaching approximately 30 %, and they somewhat increase with increasing values of back pressure. It should be noted that the typical back pressure range for a screw of diameter $D = 20$ mm is approximately 5 to 15 MPa. For pressures above this range the differences are as a rule larger than for pressures within the range. Such tendency was already observed in the case of PP. It is also observed for PS and POM, as clearly follows from Figs. 14 and 15. Fig. 14 demonstrates that the mean differences between theoretical and experimental values of rotation times for PS are generally comparable to those of LDPE shown in Fig. 13. A qualitative similarity exists also between the corresponding relations for PP and POM (Figs. 12 and 15). In both cases (PP and POM), the theoretical and experimental values of the screw rotation time agree very well for $p_p = 8$ MPa, especially for higher screw speeds. It should also

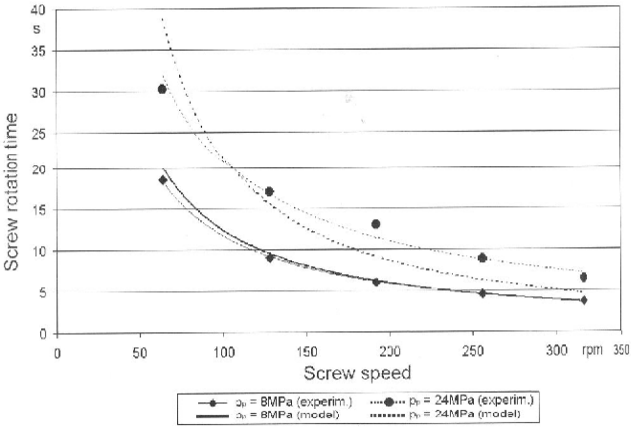

Fig. 12. Comparison of experimental and theoretical screw rotation times for polypropylene

be noted that in this screw speed region, both the predicted and measured rotation times depend little on back pressure.

Fig. 16 refers to PA6. The data corresponds only to a back pressure 8 MPa, because the experiments showed that a back pressure 24 MPa was too high to enable the axial screw motion during its rotation at any screw speed. It should be emphasized that such behavior was also predicted by the model. The simulations have shown that the maximal pressure that can be reached in front of the rotating screw was approximately 15 MPa. Experiments performed at $p_p = 16$ MPa seemed to confirm this result, because at the highest screw speeds only a very slow screw axial displacement was observed. The results of the experiments with a back pressure 16 MPa are not shown in Figs. 12 to 15 for clarity reasons. They confirm the trends observed for back pressures of 8 and 24 MPa.

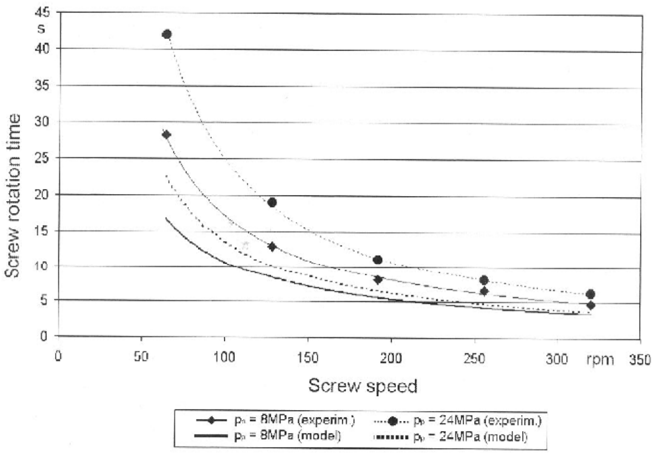

Fig. 13. Comparison of experimental and theoretical screw rotation times for low density polyethylene

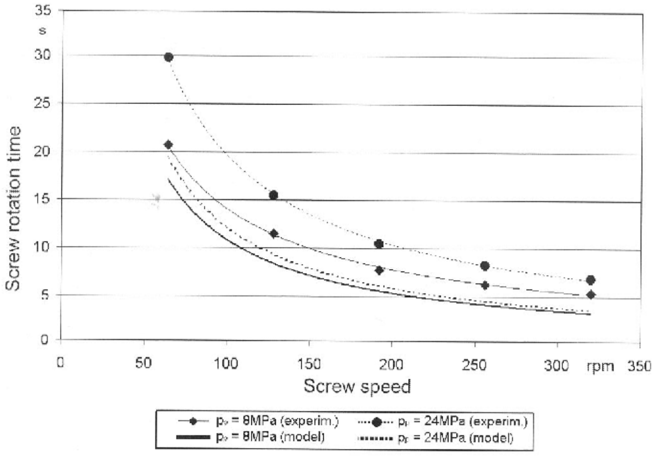

Fig. 14. Comparison of experimental and theoretical screw rotation times for polystyrene

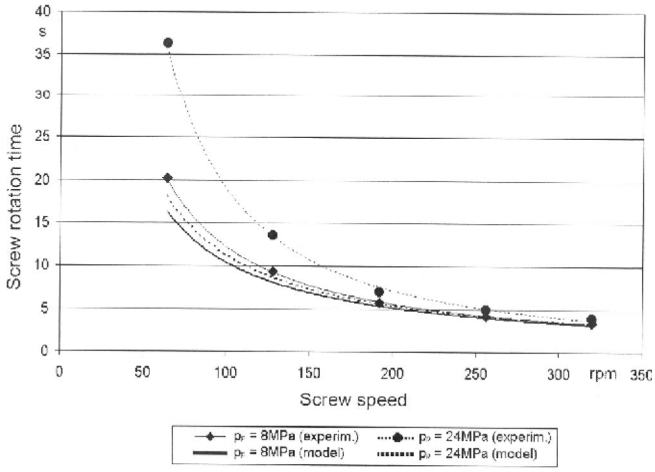

Fig. 15. Comparison of experimental and theoretical screw rotation times for poly(oxymethylene)

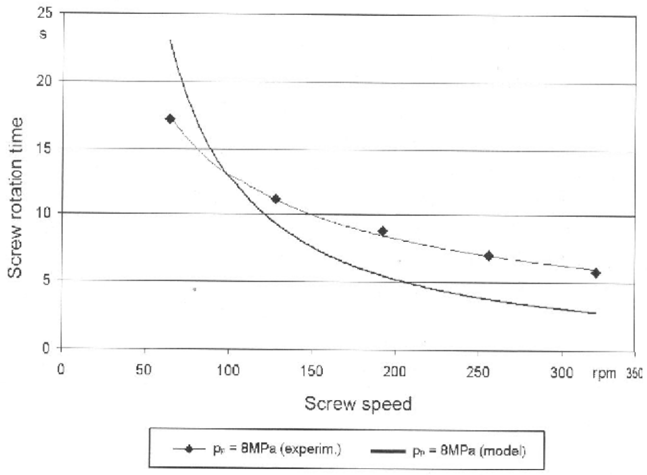

Fig. 16. Comparison of experimental and theoretical screw rotation times for polyamide 6

4 Final Remarks and Conclusions

Generally, it can be stated that the computer model created of polymer plasticization during injection molding reflects qualitatively very well the dynamics of the process and provides a relative good quantitative consistency with experimental results with respect to screw rotation time for different polymers. The predicted rotation time values are somewhat lower than the experimental ones, but the average discrepancies do not exceed 25 %. They become smaller with decreasing the back pressure p_p. The smallest differences between simulations and experiments are observed for back pressures below 10 MPa and screw speeds above 150 min^{-1}, i.e. under the operating conditions that are typical of a real plasticization process when using a 20 mm three-zone-screw. These differences should be due to the following assumptions:

- Constant speed of axial screw motion U, that was determined under process conditions corresponding to the moment of the screw rotation break. Experimental observations show that the velocity of the screw backward displacement is not constant during screw rotation. For this reason, the axial motion velocity should be rather determined as an average calculated from instant velocities corresponding to various transient solid bed profiles during the screw rotation. This statement is also valid for other process quantities, e.g. energy consumption or power requirement, which have an "integral character". The calculations of such integral quantities are also possible within the presented model, but they require much longer computation times. In the case of screw rotation time, they lead to (a not very significant) consistency improvement of simulation and experimental results.

- The rheological properties of the melt are described by the "power law", that reflects the properties of a pure viscous liquid, while a polymer melt is clearly viscoelastic. In contrast to extrusion, polymer plasticization during injection molding is a typical unsteady-state process, that proceeds as a rule more intense due to a higher screw speed and its axial motion. For this reason, various viscoelastic phenomena, such as secondary flows, may become important. Moreover, different material parameters used in the model (that depend on pressure, temperature, shear rate, etc.) are assumed as constant to simplify (and in some cases to actually make possible) the calculations.
- Constant temperatures in the heated and non-heated barrel sections assumed in the model do not exist in a real injection process. However, such simplification allows the analytical solutions describing time evolution of solid bed and temperature profiles. Furthermore, the model neglects leakage flow in the radial clearance, although is well known that this changes the pressure distribution in the screw channel.

Most of the simplifications discussed determine in some cases the possibility of describing polymer plasticization during injection molding, but they are a potential source of differences between experimental results and model predictions. These simplifying assumptions are usually not necessary to obtain a satisfactory analytical or numerical solution of steady-state extrusion. This fact is probably the main reason why complex computer models of polymer plasticization in injection molding are so rare.

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