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Potential Applications for Computer-aided Extruder Design

The simulation method is able to relieve the engineer of experimental work during the planning of extrusion plant and thus clearly reduces the development time. Sufficiently precise determination of the calculable parameters is possible with the process models developed so far. The empirical knowledge of the engineer is, of course, necessary as well in order to estimate the impact of influencing parameters that are not taken into account in the calculation models. The presented simulation program REX can perform these complex calculations in a comprehensive manner, with its simple and comfortable user interface. The program, however, can be employed as a valuable tool only if it is in the hands of an expert operator who can, and indeed must, be able to interpret the results as well.

1 Introduction

Scale-up rules derived from the similarity theory have proved largely successful when it comes to the design of extruder series in practice, taking a known machine as a basis. The drawback to this approach, however, is that it is necessary to know the behaviour of the basic machine for the particular material in question. This makes it impossible for the method to be used in process or machine optimisation. Such optimisation calls physico-mathematical process models, which relate the parameters of interest in thermoplastic extrusion to the geometrical and process parameters and make appropriate allowance for the material laws.

The models that describe the pressure/throughput behaviour and the melting behaviour in rectangular channels have been familiar from the literature for a long time [1, 2]. On account of their in part complex structure and the structural viscosity of the plastics, which leads to non-linear material laws, it is no longer possible for the user to conduct a mathematical analysis of the models without assistance, particularly in the light of the complex screw geometries that are employed today. Computer simulation is a method that provides a solution to this problem. Computer simulation saves the user from the complex calculation and thus makes it possible for the models to be calculated.

Over the past few years, a number of papers have been published on the computer-simulation of the extrusion process [3 to 5]. Most of these programs use FE or FD methods so that the coupled differential equations can be suitably solved with non-linear material laws. This method either involves the use of mainframe computers or requires long computing times. When it comes to application in industry, where engineers require programs that will provide rapid answers without necessitating a lengthy familiarisation time, these programs are only of limited benefit.

2 Simulation software

A program for the computer-aided design of extruders (REX) has been developed by the Plastics Technology Group at the University of Paderborn, in cooperation with 18 industrial companies (Table 1) [6]. The program works with analytical equation solutions and can thus be used on a PC with acceptable computing times.

The following principles were taken into account in order to provide a solution suitably tailored to practice [7]:
- the principle of a simple model,
- the principle of a model solution that is readily comprehensible in mathematical terms,

Table 1. Computer-aided extruder design project participants

Company	Location
Alpine	Augsburg/Germany
Arenz	Meckenheim/Germany
BARMAG	Remscheid/Germany
BASF	Ludwigshafen/Germany
Battenfeld GmbH	Meinerzhagen/Germany
Bayer	Leverkusen/Germany
Bekum Maschinenfabrik	Berlin/Germany
Breyer	Singen/Germany
ER-WE-PA	Erkrath/Germany
Hüls	Marl/Germany
B. Ide	Ostfildern/Germany
Kiefel Extrusionstechnik	Worms/Germany
Krauss-Maffei	München/Germany
Maag Pump Systems	Zürich/Switzerland
Reifenhäuser	Troisdorf/Germany
F. Theysohn	Bad Oeynhausen/Germany
P. Troester Maschinenfabrik	Hannover/Germany
Windmöller & Hölscher	Lengerich/Germany

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Table 2. Calculable simulation results

Scalar results	Throughput Torque Drive power Melt temperature Residence times Mixing constants Melting length
Data fields	Pressure profile Melting profile Temperature profile Local power requirements Heating/cooling capacity Wall shear stresses

Table 3. Main assumptions

The melt adheres to the wall.
The solid bed behaviour is described by plug flow.
The screw-channel is viewed as a flat channel.
The flow over the screw-flights is neglected.
The polymer melt is incompressible.
The flow behaviour obeys the power law $\eta(\dot{\gamma},T) = K\, e^{-\beta T} \dot{\gamma}^{n-1}$, the coefficients of the power law result from local analysis of the Carreau-function $\eta(\dot{\gamma},T) = \frac{Aa(T)}{(1 + B\dot{\gamma}a(T))^C}$.

Table 4. Main models

Throughput pressure	One-dimensional, non-isothermal flow in a flat channel, correction factors in consideration of the two-dimensional real flow and the influence of the flights
Melting behaviour	Maddock/Tadmor model with a variable melt layer thickness at the barrel wall, special solution for non-Newtonian flow
Temperature	Analytical solution for the energy equation $\varrho c \bar{v}_z \frac{\partial T}{\partial z} = \lambda \frac{\partial^2 T}{\partial y^2} + (\tau\dot{\gamma})$
Drive power	Local analysis of $P = \iint (\tau v)\, dx\, dz$

- the principle of a mathematically closed solution, even if this calls for strict simplifications,
- the principle of the linearisation of intermediate results on a semi-logarithmic or double-logarithmic plot, so that a closed solution can be achieved for a succession of differential equations,
- the principle of the approximation of numerical solutions if precise solutions are no longer possible,
- the principle of describing stochastic processes through well-defined distribution functions, if possible.

The fact of cooperation with partners from industry meant that a number of constraints had to be borne in mind in terms of both the hardware and the software to be employed. More specifically, these involved specifications for the hardware platform, the operating system and the programming language. As far as the hardware platform was concerned, it was specified that the program had to be able to run on an IBM or compatible PC, under MS-DOS, with the standard graphics cards. Turbo Pascal was laid down as the programming language.

Apart from these external constraints, particular attention was paid during development work to achieving a complete realisation of the model and a rapid and precise calculation. In order to counter the application problems set out above, particular value was placed on a clear structure and a comfortable user interface. A modular structure also guarantees the possibility of incorporating new or extended models (new shear and mixing sections, barrier screws) as well as interfaces to other software systems.

Table 2 shows the simulation results that can be calculated. The results can be obtained in the form of graphs or tables [8]. The theory underlying the calculation is set out in [9]. The main assumptions for the analysis of the flow of the polymer are shown in Table 3. Starting from these assumptions, the calculation of throughput, pressure, melting, temperature, homogeneity and drive power is carried out with various mathematical models for the different screw zones and the various state of the material. Table 4 contains the main models.

The models have been verified in a large number of papers. Figure 1 is intended to serve as an example of a calculation for a conventional extruder. This figure shows a comparison of measured throughputs and throughputs calculated with REX. Where the experimental and theoretical results coincide, the points are positioned on the lines of agreement. The two additional straignt lines indicate relative deviations of $\pm 10\,\%$. The tests were performed on an extruder with a diameter of 45 mm using four different screws and varied process parameters. The material used was LDPE 1810 H. It is seen that the throughput can be calculated with a good degree of accuracy for a broad range of processing conditions.

The same applies for Fig. 2. This contains a plot of the theoretically calculated dimensionless throughput over the experimental dimensionless throughput for a grooved bush machine operating in the solids conveying range.

The experimental investigations of Bruker and Balek [13] were employed in order to verify the melting model [11, 12]. A good level of agreement was achieved, as can be seen from Figs. 3 and 4.

3 Sample applications

Potential applications exist for computer-aided extruder design in a large number of fields [7]. On the one hand, the

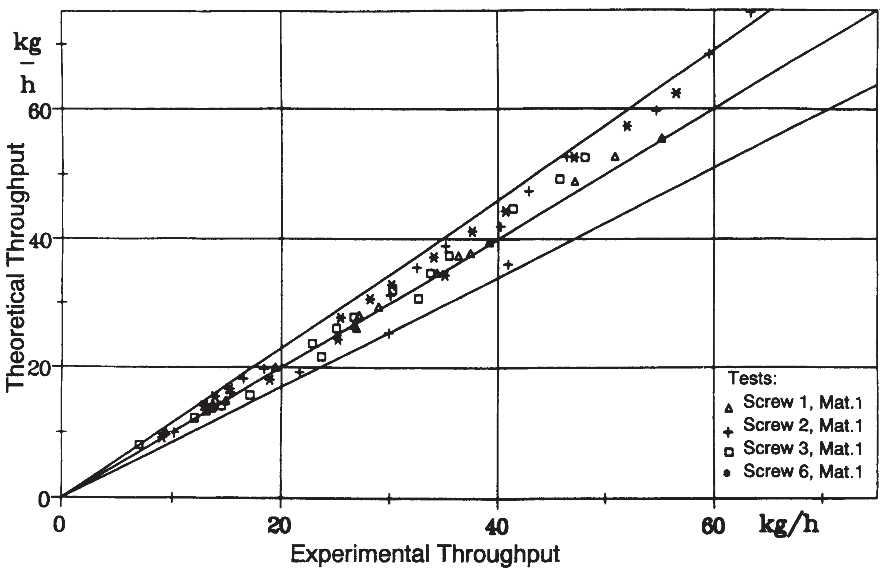

Fig. 1. Comparison of theoretical and experimental throughput

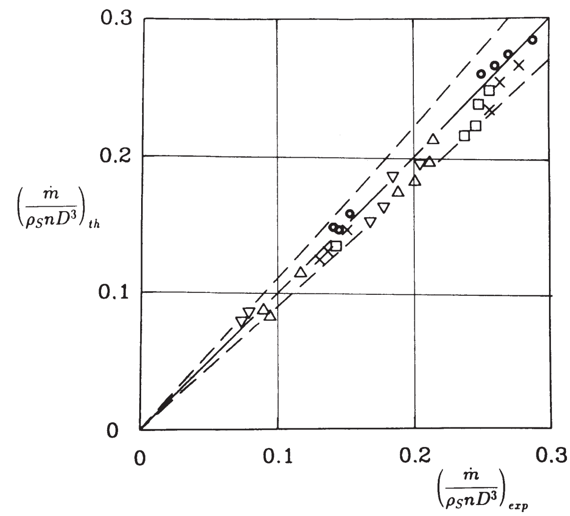

Fig. 2. Comparison of theoretical and experimental dimensionless throughput

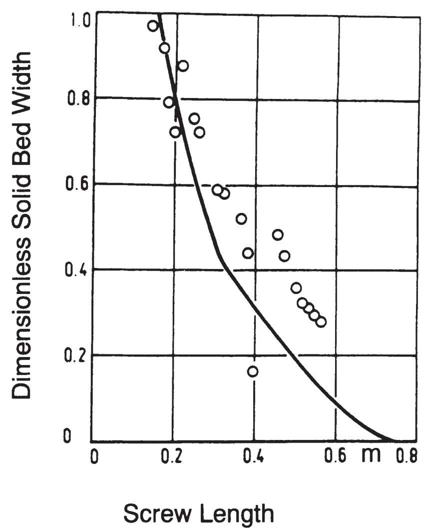

Fig. 4. Melting curve for PC ($D = 63.5\,mm$, $\dot{m} = 19\,kg/h$)

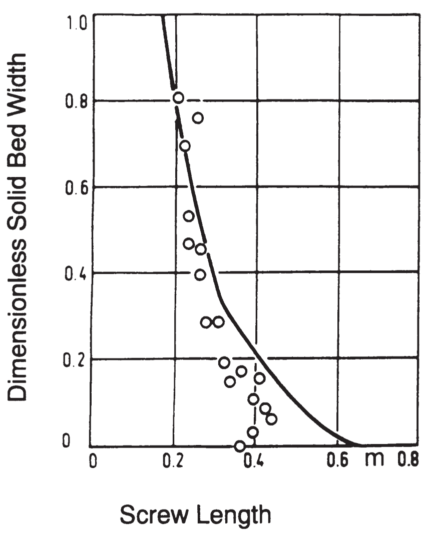

Fig. 3. Melting curve for PC ($D = 63.5\,mm$, $\dot{m} = 32\,kg/h$)

software can be used in the design and shaping of new extruder screws that are needed for specific applications. On the other hand, however, errors in running processes can be discovered through simulation of the operating point in question, since the calculation results provide information on the conveying and plasticisation behaviour of the extruder. Over and above this, it is also possible to determine the most appropriate combination of existing extrusion plant components (barrel, screws, shear and mixing sections) by means of simulation calculations.

3.1 Designing a barrier screw for a grooved bush extruder

By way of an example of screw design with the aid of simulation, a 90-mm screw is to be designed for processing polystyrene. A grooved bush is to be employed in order to achieve a high melt throughput, and the defined melting necessitates the application of a barrier screw.

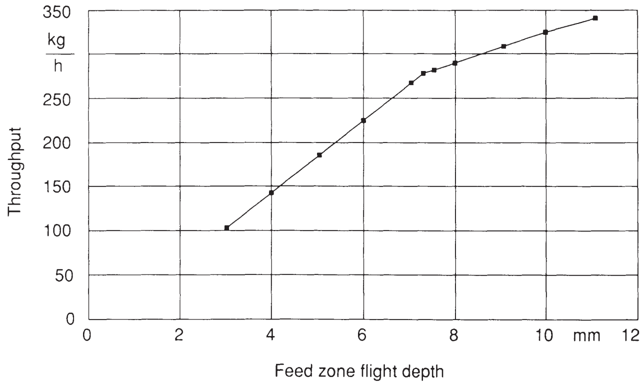

Fig. 5. Throughput as a function of the feed zone flight depth
material: polystyrene, screw diameter 90 mm screw speed 75 min $^{-1}$

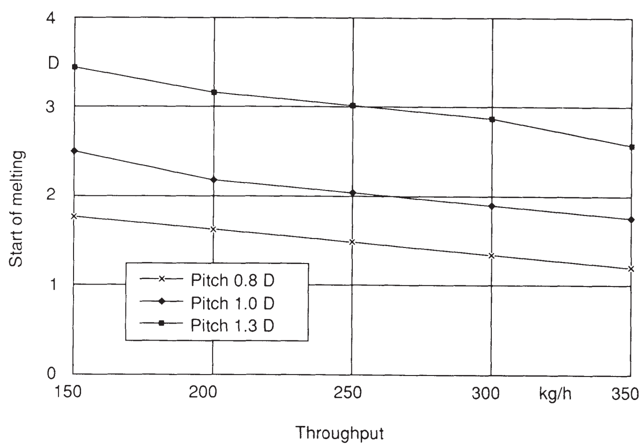

Fig. 6. Start of melting as a function of throughput and pitch
material: polystyrene, screw diameter 90 mm, screw speed 75 min $^{-1}$

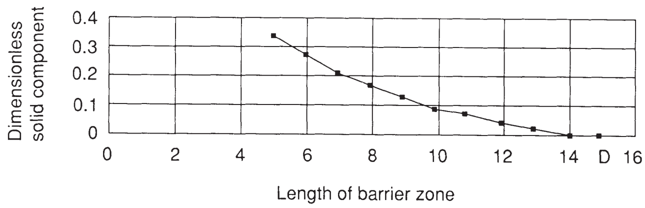

Fig. 7. Residual solid component as a function of the barrier zone length
material: polystrene, screw diameter 90 mm, screw speed 75 min $^{-1}$

First of all, it is necessary to specify the depth of the feed zone which will give the requisite throughput of 280 kg/h at medium speeds. Fig. 5 shows the calculated correlation. The flight depth in the feed zone is thus selected at 7.5 mm. Following this, the length and the start of the barrier screw are to be established by means of simulation calculations. A total length of 25 D is available for this. In our opinion, meltpool formation should have already commenced at the start of the barrier section so that the melt can overflow at the start of the barrier thread already. Fig. 6 shows the point of meltpool formation, calculated from the start of the first band heater, as a function of the machine throughput and the screw pitch in this zone, which has a channel depth of 10.5 mm. For the throughput required here and a pitch of 1 D, the zone up to the point of meltpool formation has a total length of 2.5 D.The barrier zone should thus start at 3 D after the first band heater.

The melting capacity of the screw is of decisive importance when it comes to determining the length of the barrier zone. To ensure that the process can be operated reliably, the material should be completely melted at the end of the barrier zone. Fig. 7 shows the percentage of residual solid material content at the end of the barrier zone as a function of the length of this zone. In our case, this leads to a barrier zone length of 13 D. Fig 8 shows the corresponding REX graph. The end of melting is attained.

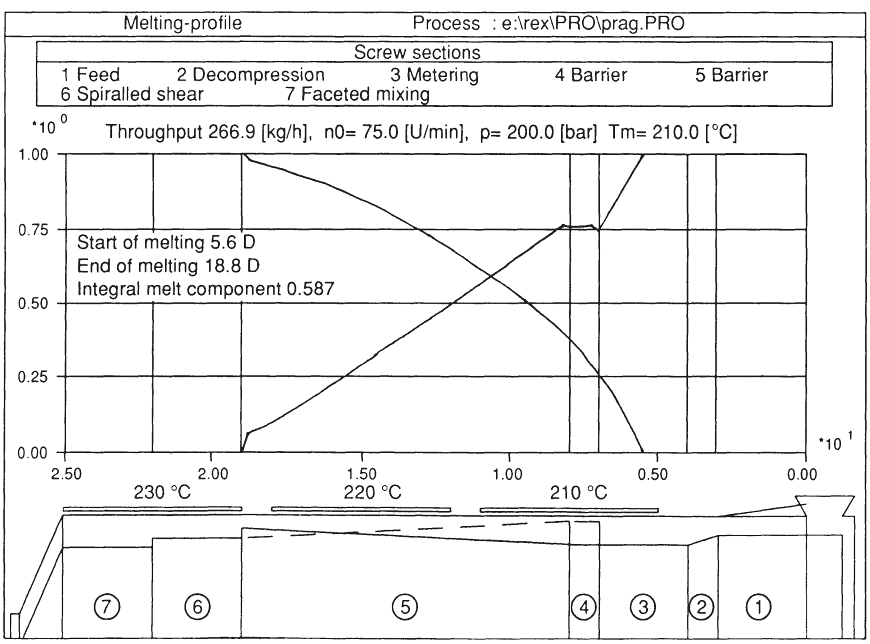

Fig. 8. REX-graphics (melting curve)

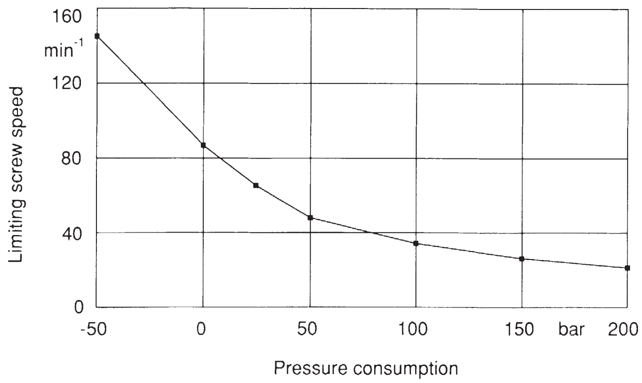

Fig. 9. Limiting screw speed as a function of the pressure consumption in the shearing and mixing sections
material: polystyrene, screw diameter 90 mm

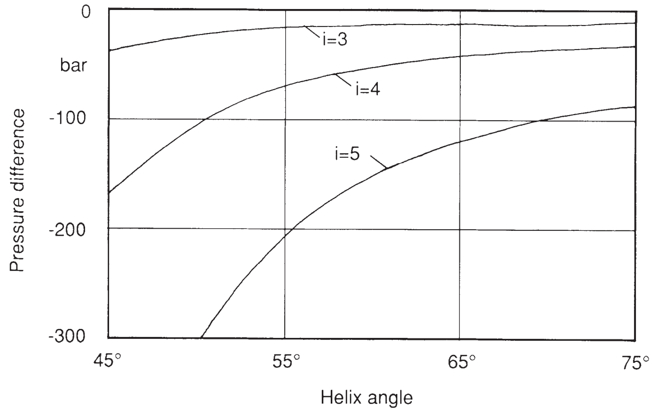

Fig. 10. Pressure difference in the spiralled shearing section as a function of the helix angle

The remaining 5 D of screw length are to be used for homogenisation in a shear and mixing section. Apart from the equally important influence that this has on the quality of the plastic melt, minimisation of the pressure consumption is also necessary so as not to endanger the throughput. Fig. 9 shows the influence of the pressure consumption of the shearing/mixing section combination in the screw that has been made up on the limiting speed of the extruder. The limiting speed here characterises the transition from solid material friction to melt film formation in the feed zone of the screw and hence both the upper limit of the linear correlation between throughput and speed and the end of pressure-independent conveyance. In order to ensure that this limiting speed is sufficiently high, the shearing and mixing sections should be designed to be neutral in pressure terms as far as possible. In order to make allowance for this correlation, the use of spiralled Maddock shearing sections has been increasingly propagated over the past few years. These display improved conveying behaviour compared with the standard shearing elements. In the same way, the use of faceted mixing sections has advantages over toothed disc mixing elements. Fig. 10 illustrates the way in which the conveying behaviour can be designed to be neutral in pressure terms through the careful selection of the pitch on a spiralled shearing section [12].

Further simulation calculations with the screw geometry determined in this way will naturally permit further improvements to detail. Fig. 11 shows the REX diagram of the screw optimised in this way.

3.2 Designing the second section of a degassing screw

In this example, the pitch of the metering section of a degassing zone is to be designed in such a way that an optimum partially-filled region develops beneath the degassing hole. Fig. 12 shows the underlying screw geometry

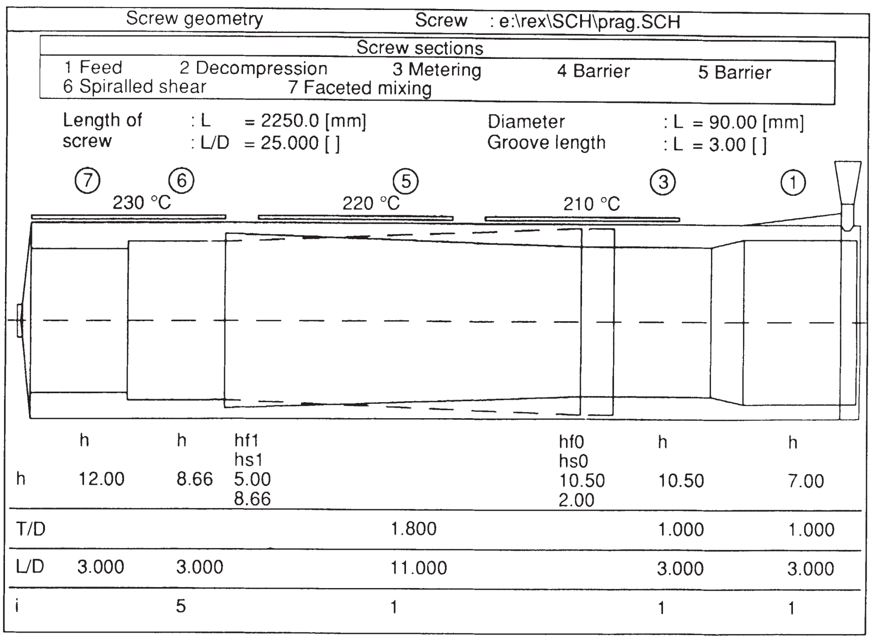

Fig. 11. REX-graphics (screw diagram)

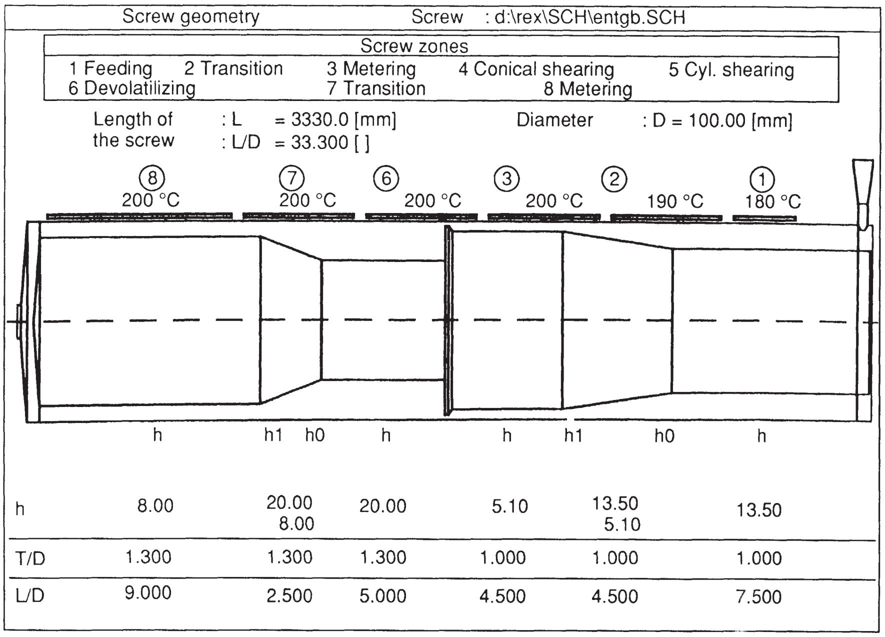

Fig. 12. REX-graphics (degassing screw)

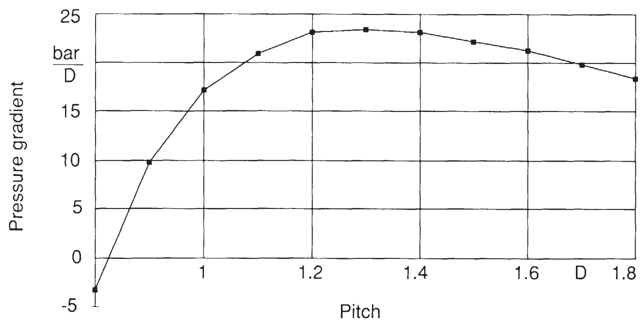

Fig. 13. Pressure gradient in the axial direction as a function of pitch materal: ABS, screw diameter 100 mm, screw speed 65 min

for an ABS screw. It is the pressure gradient in the final screw section that has the decisive influence on the length of the partially filled section. Fig. 13 shows this parameter as a function of the pitch. A peak can be seen for the pitch $t = 1.3 \times D$. Fig. 14 shows the corresponding pressure curves. With other pitches, the pressureless section is too short, and hence there is a danger of flooding in the event of fluctuations in the die back pressure.

3.3 Screw selection for conventional extruders

Simulation calculations can be employed not only to recalculate real extrusion processes and to design new ge-

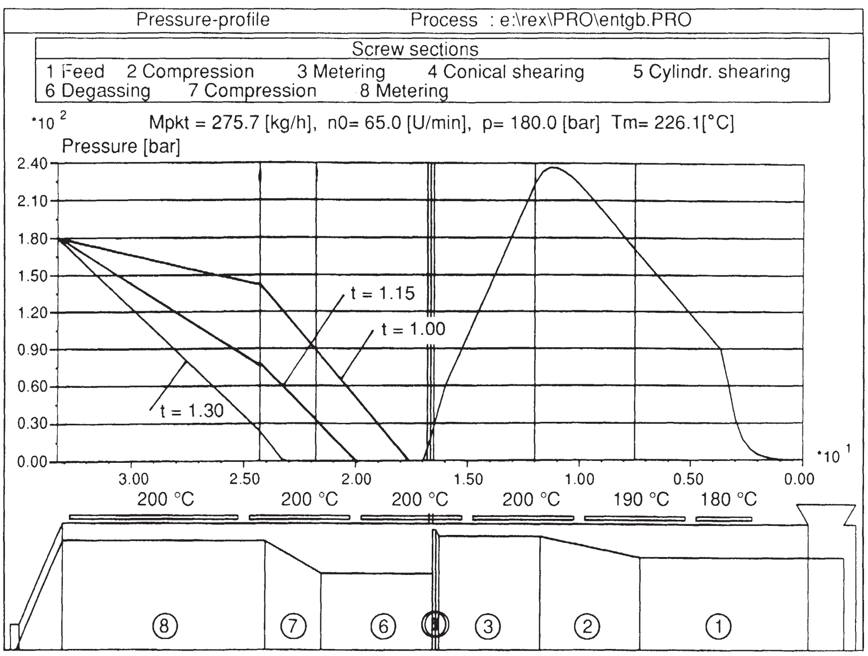

Fig. 14. Pressure profile of the degassing screw as a function of the pitch at the second stage

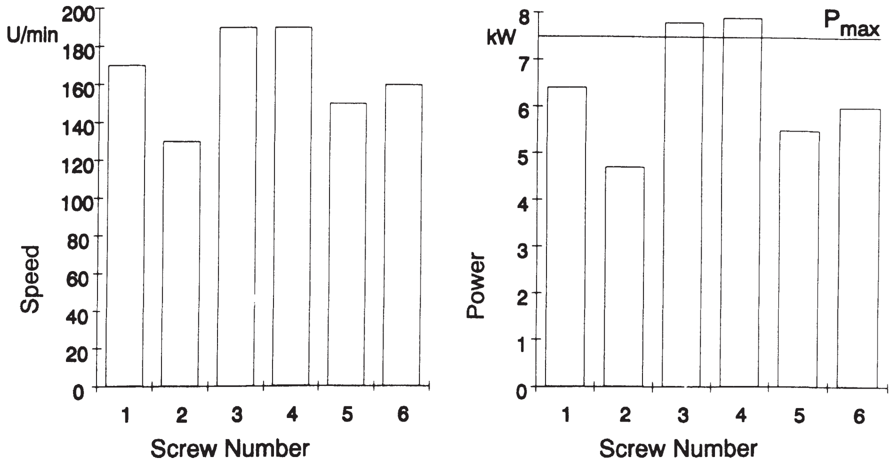

Fig. 15. Speed and drive power of different screws

ometries but can also be used for component selection when an extrusion line is set up. The REX software package is confined to the plasticising unit here and, in particular, to the screw. The type of problem that can be solved with REX is explained below, taking a fictitious example.

A 45 mm smooth pipe extruder with a drive power of 9.3 kW is available for the extrusion of a profile in polypropylene (Hostalen PPH 1050). The melt throughput is to be 40 kg/h to ensure correct alignment with the downstream units and the melt temperature is to be between 250 and 260 °C. Good melt homogeneity is naturally assumed as well.

Since the extrusion line will only be running for a limited period of time, one of the screws already available is to be used on this machine. The choice is between four three-zone screws, 20 D in length, each of which has different channel depths and zone lengths. Two of these screws can be optionally equipped with a mixing section in the metering zone. Table 5 gives an overview of the geometries.

In order to calculate the desired operating points in advance using the simulation software, the speed required for the specified throughput is established as the first step. These results and the drive power required in each case are shown in Fig. 15. All the screws are capable of conveying the requisite melt throughput at appropriate speeds. The two screws with the shearing section display the lowest specific throughputs and thus require the highest speeds. This also leads to the highest drive powers. If the machine is to be run at no more than 80 % of its maximum power in "steady-state" operation, so as to leave sufficient reserve for torque peaks, then the shearing section cannot be used for the application described. Fig. 16 shows the pressure curve

Table 5. Screw geometries

	Pitch	Channel flight depth	Zone length
Screw 1	1 D	8.3 mm > 2.6 mm	3 D-6 D-10 D
Screw 2	1 D	6.6 mm > 3.1 mm	6 D-8 D-5 D
Screw 3		Nr. 5 with shear zone	
Screw 4		Nr. 6 with shear zone	
Screw 5	1 D	8.1 mm > 2.8 mm	7 D-4 D-8 D
Screw 6	1 D	6.2 mm > 2.7 mm	3 D-6 D-10 D

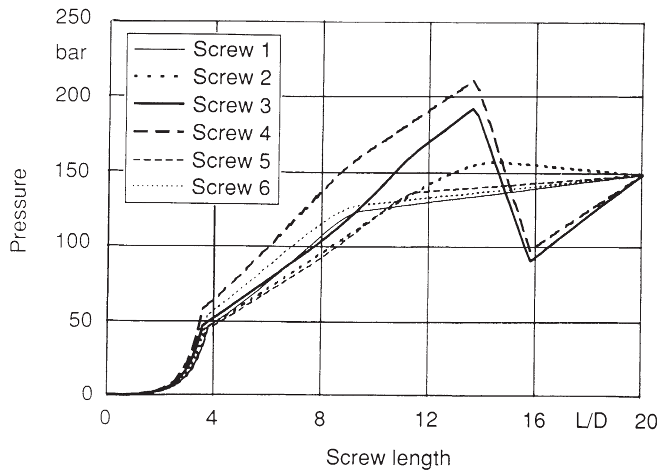

Fig. 16. Pressure profile over a the screw length for the six screws

over the screw length. The four screws without a shearing section do not display any major differences in their pressure curve. The shearing section entails a pressure loss of approximately 100 bar for this throughput and forces the pressure level up in the preceding section.

A decision can thus only be made from the qualitative angle. The calculated melt temperatures are employed for this on the one hand and, on the other hand, the point at which the material is completely plasticised is established during the melt curve calculation. The earlier that is the case, the better the homogeneity and quality of the melt. These two process variables and their correlation are shown in Fig. 17. If the material melts rapidly, this leads to relatively high melt temperatures on account of the long, melt-filled residual screw length. Screws 1 and 5 lead to quite high melt temperatures and are thus not used. Screws 3 and 4, which are equipped with the shearing section, also turn out to be unfavourable. Screw 2 displays what is probably the poorest homogeneity on account of the weak melting rate and is thus not used either. Screw 5 offers the best chance of success in this case.

The ideal way to select the right screw would, of course, be to conduct tests with all six screws. This means that the machine will be unavailable for production for a number of

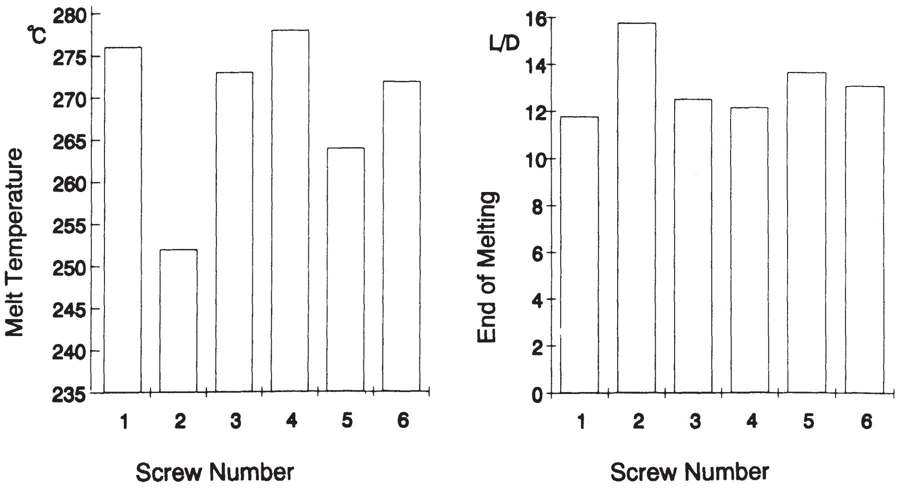

Fig. 17. Melt temperature and end of melting for a different screws

days and would also lead to high personnel costs. The simulation results show clear differences for the different screws in this case and thus certainly provide decision criteria. The outlay is considerably lower with this method. Providing that both the requisite material data and the geometries are known, a skilled program user will not need more than an hour or so for the calculations.

3.4 Fault detection in running processes

The REX simulation software can be employed for detecting faults in running processes if the shortcomings can be established through the analysis of a process variable which can be calculated by REX. The following examples can be given by way of an explanation:

Fig. 18 shows the simulation result of an operating point at which the melt temperature is too high. A sharp increase is seen in the region of the torpedo and this is obviously the

Nomenclature

A,B,C	coefficient of the Carreau function
a(T)	temperature-dependent factor
c	heat capacity
k	coefficient of power law
n	power law exponent
p	power consumption
T	temperature
v	velocity
x	width-coordinate of the screw channel
y	height-coordinate of the screw channel
z	length-coordinate of the screw channel
β	temperature coefficient
γ	shear rate
λ	thermal conductivity
η	viscosity
ϱ	density
τ	shear stress

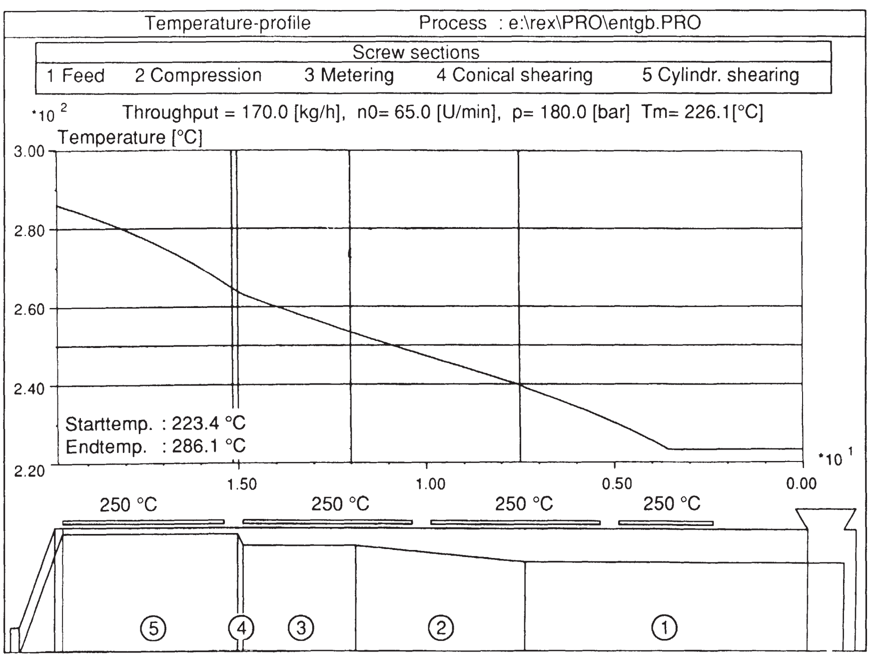

Fig. 18. REX-graphics (melt temperature curve)

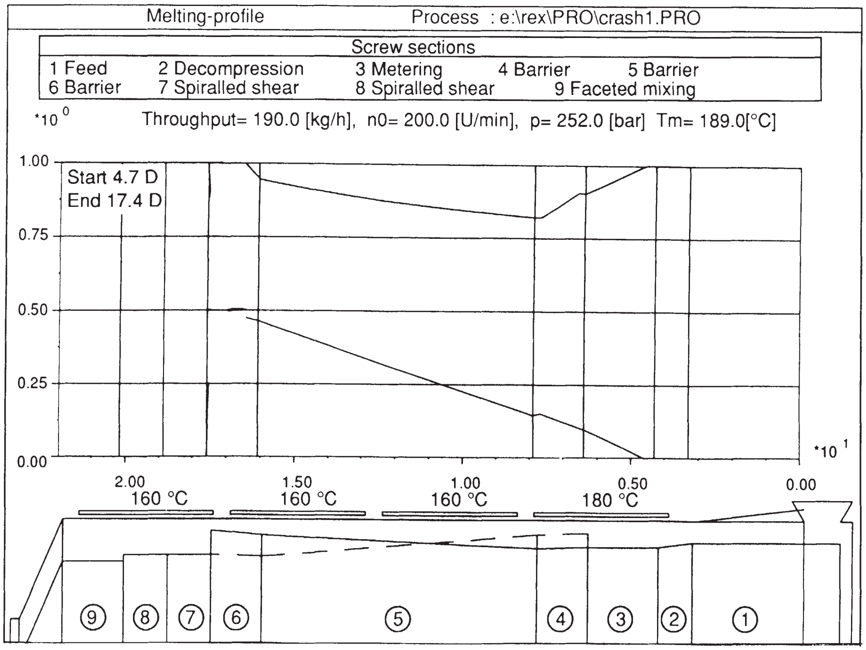

Fig. 19. *REX-graphics (melting curve)*

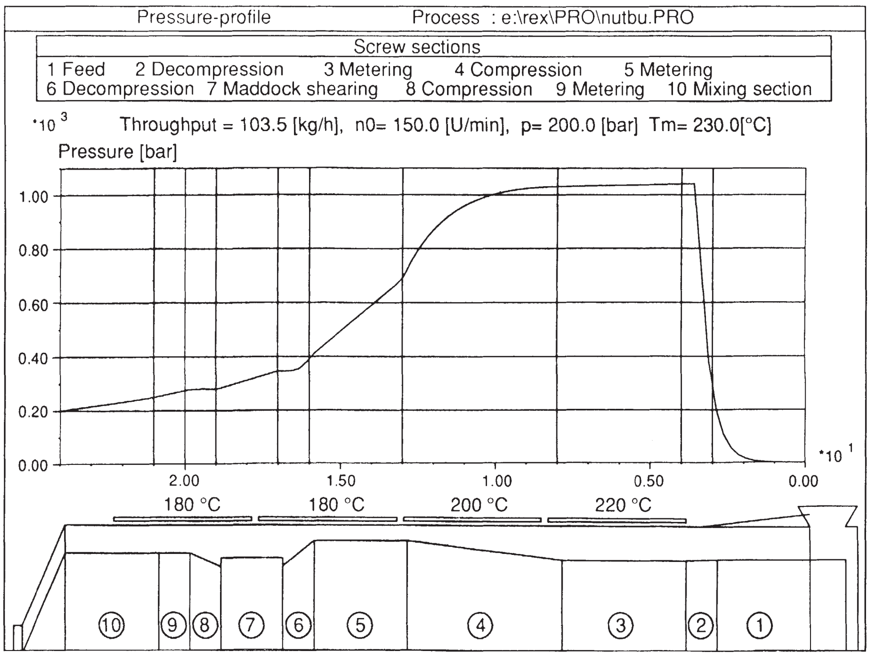

Fig. 20. *REX-graphics (pressure curve)*

cause of the error. The error can be eliminated by modifying the torpedo geometry.

Fig. 19 shows the melting curve in a screw with an insufficient melting capacity which does not attain the requisite throughput due to clogging in the compression zone. The result of the simulation thus reveals the reason behind the reduction in throughput.

Fig. 20 shows the pressure curve of a grooved bush extruder which, on the one hand, displays a very low limiting speed and, on the other hand, has wear problems in the feed zone. Very high pressures are generated on account of the high specific throughput and the poorly coordinated screw. At the end of the groove, these pressures are in excess of 1 000 bar. A different screw design would seem to be necessary in order to provide a solution here.

References

1 *Tadmor, Z., Gogos, G.:* Principles of Polymer Processing. John Wiley & Sons, New York/Brisbane/Chichester/Toronto, 1979

2 *Middleman, S.:* Fundamental of Polymer Processing. McGraw-Hill Book Company, New York, 1977

3 *Vincelette, A. R., Guerrero, C. S., Carreau, P. J., Laffeur, P. G.:* Inter. Polym. Process. 4, p. 232 (1989)
4 *Agur, E. E., Vlachopoulos, J.:* Polym. Eng. Sci. 22, p. 1084, 1982.
5 Extrud-PC. Company brochure, Scientific Process-Research Inc., New Jersey
6 *Potente, H., Hanhart, W., Reski, T.:* Polym. Eng. Sci., p. (1993)
7 *Potente, H., Hanhart, W., Klarholz, B., Schöppner, V.:* Kunststoffe 82, p. 34 (1992)
8 *Klarholz, B., Braun, U.:* Handbuch zum Programm "Rechnergestützte Extruderauslegung 2".
9 *Potente, H.* (Ed.)*:* Rechnergestützte Extruderauslegung. Kunststoffechnolgie Uni-GH Paderborn, 1992
10 *Kessler, H.:* Modell zum stationären und instationären Mischen in konventionellen Einschneckenextrudern. Dissertation Universität-GH Paderborn, 1991
11 *Stenzel, H.:* Grundlagen zur verfahrenstechnischen auslegung von Barriereschnecken in Glattrohr- und Nutbuchsenextrudern. Dissertation Universität-GH Paderborn, 1992
12 *Schulte, H.:* Grundlagen zur verfahrenstechnischen Auslegung von Spritzgießplastifiziereinheiten. Dissertation, Universität-GH Paderborn, 1990
13 *Brüker, J., Balek, G. S.:* Polym. Eng. 29, p. 258 (1989)

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