Tools for Modelling Single-screw Systems

Part 1: The Possibilities of Computational Methods. Simulation of the plastication process covers the most important issues of process optimisation. The software helps the user to understand and analyse the relationships, and to optimise the plastication unit of the extruder or injection moulding machine.

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The Institute for Plastics Technology (KTP) at the University of Paderborn has spent the last 25 years focusing on modelling the process behaviour of single-screw plastication units. The results are continuously translated into simulation tools. The two software programs REX (German for computer-aided extruder design) and PSI (German for Paderborn injection moulding simulation) have already shown their mettle in industrial use.

The basic idea behind the modelling is to use dimensionless characteristics to describe the process behaviour of single-screw plastication units as simply as possible with the greatest accuracy [1]. The results of this work are translated into handy software tools as part of two-year joint research projects. The use of such tools makes it possible to optimise existing and new processes cost effectively, because they enable the user to interpret the changes in screw geometry without the need for cost-intensive experiments.

Translated from Kunststoffe 6/2006, pp. 109–113

Modelling and Simulation Capabilities

The basic principle behind the use of PSI and REX to simulate the process behaviour of screw geometries is an axial division of the screw into small intervals for which simplifications can be assumed. This simplification is necessary in order that analytical models may be formed from the descriptive differential equations. However, since screw geometries are becoming increasingly complex, process behaviour can no longer be described just by analytical models. For this reason, resort is being made more and more to numerical methods. The finite element (FE) or finite difference (FD) methods form the basis of a numerical model. The use of FEM to simulate a complex experimental design returns an analysis of the factors (e.g. geometrical variables) that affect the process variables (e.g. pressure-throughput behaviour). The results serve as the basic data for approximation equations aimed at increasing simulation speed (Fig. 1).

After all the equations for the various intervals have been derived, coupled solving of the entire system is performed. This approach enables complex screw geometries to be simulated highly accurately in a few seconds [3].

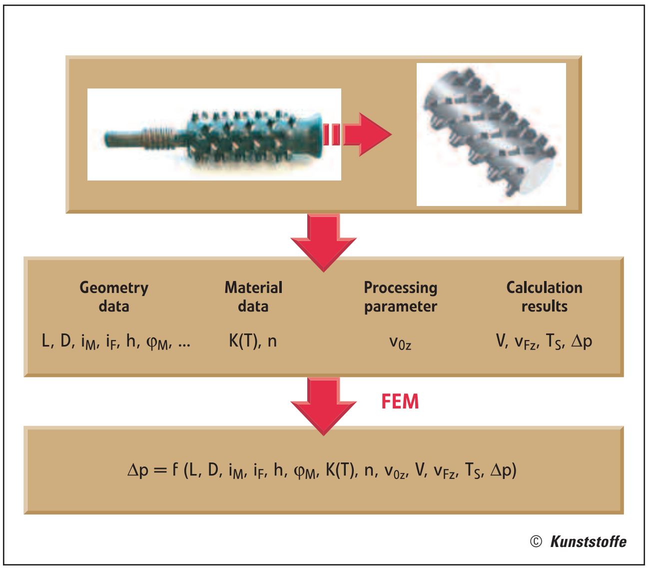

Fig. 1. Forming the process model with the aid of FEM for the rhomboidal mixing section (Figs.: KTP)

Figure 2 shows how computer-aided screw optimisation works. From a series of input parameters, and with the aid of the mathematical equations, different parameters for evaluating the process behaviour are computed. Of the input parameters, the material data require special care because a complete description of the rheological, thermodynamic and technical characteristics is required. These values need to have been determined to high levels of accuracy because every deviation can falsify the computational results. A good way to manage material data of this kind is afforded by the Paderborn Material data base, PaM [4]. Aside from material data, the geometrical dimensions of the screw and the cylinder, along with the process parameters, are required.

PSI and REX return the results in the form of scalar variables and as a change in function along the screw length. In detail, these are

- throughput,
- feeding throughput at the hopper,
- change in pressure,
- change in melting (Fig. 3),
- change in temperature,
- change in minimum and medium residence times,
- change in wall shear stress,
- distribution of residence time,
- heat flows of the individual heating bands,

- drive power,
- torque,
- degree of shear deformation and shear rate.

Coupling of Solid and Melt Transport

For the modelling, the simulation initially assumes that melt-dominated transport occurs. This assumption agrees well with experimental data for large screw diameters. The values can deviate in the case of small diameters because solids transport becomes the limiting factor due to the smaller channel cross-section. In that event, throughput can be simulated with coupled solid-melting transport. In this variant, a check is made as to whether the feed zone is capable of delivering the melt-dominated throughput. If not, the throughput is calculated from the material data and the geometry of the feed zone.

Two further options arise when grooved feed bushes are used. Pressure-resistant throughput is computed as a function of the frictional conditions in the vicinity of the grooved bush, while the threshold-speed-dependent throughput, is computed as a function of the sum of the heat flows in the grooved bush. This means that the crossover point from solids to melt-film friction is taken into account.

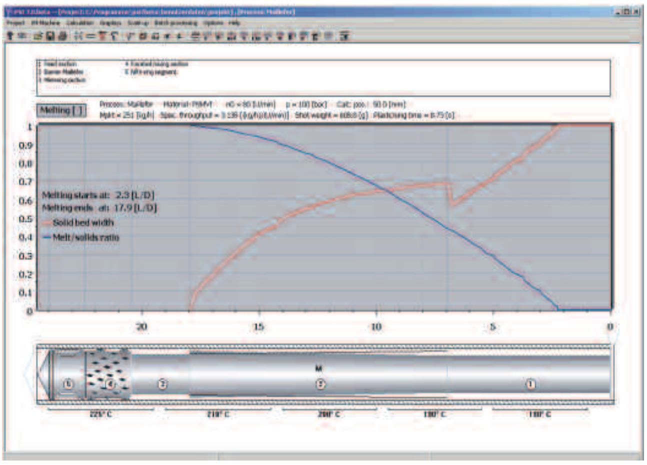

Fig. 3. Simulation of change in melting behaviour along the screw length in PSI

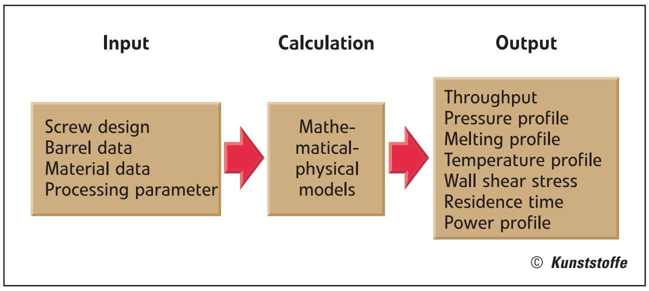

Fig. 2. The approach underlying computer-aided screw design

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Table 1. List of participants in the PSI/REX joint project

Implementation of Two-Dimensional Computations

Screw geometry has so far been simulated with one-dimensional models which simulate the change in process conditions in the channel direction. Influences at right angles to the direction of principal flow are allowed for by correction factors. Flow in new screw designs, such as wave, pin and barrier screws, is characterised by a strong level of interaction between two or more channels. For one-dimensional simulations of barrier screws, the assumption has to be made that the same pressure gradients obtain in the melt and the solids channels. Only this assumption allows the equation to be solved for the barrier screw. Two-dimensional simulations eliminate this assumption. To this end, separate intervals are formed for each channel and flight interval (Fig. 4), an aggregate equation is derived for each channel and flight interval, and all equations for one screw zone (here, for example, the barrier zone) are converted into a system of equations. The result is a matrix equation of the following form:

$$\underline{A} \times \underline{p} + \underline{b} = \underline{\dot{m}}$$

where p is the pressure vector, A is the throughput of

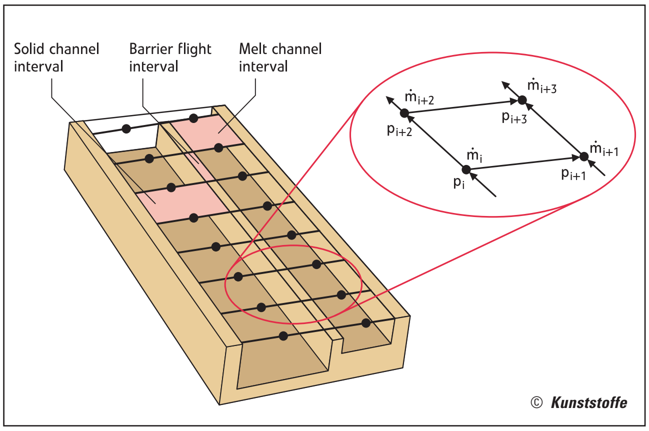

Fig. 4. Plan of interval subdivision for deriving the system of equations for the barrier zone

matrix, b is the throughput vector and $\underline{\dot{m}}$ is the vector for the mass balance. Aside from a higher simulation speed, new simulation possibilities have been created since the system equations can be solved with different fundamentals (Fig. 5). In addition to the variants illustrated, a variable shear gap height across the barrier section can be allowed for. This systematic simulation also has to be applied to the simulation of the wave, pin and energy transfer screws.

the simulation models for the standard geometries apply here. To actively support this trend, the simulation possibilities were extended with the aforementioned screw designs for selective breaking up of the solids bed. The use of such concepts permits a reduction in melt temperature, combined with high screw speeds. For this reason, new models had to be devised and implemented for simulating the pressure-throughput behaviour, the temperature progression and the melting of the

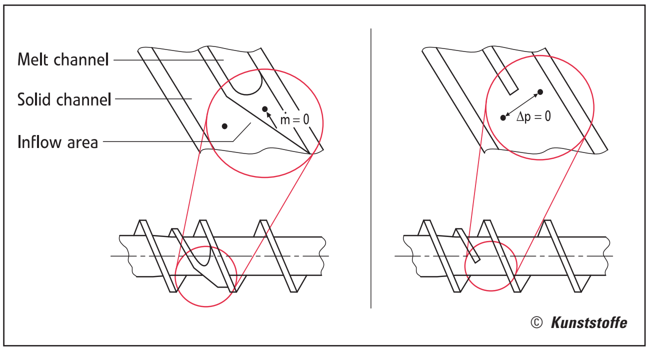

Fig. 5. Illustration of the open and closed barrier zone with the assumed fundamentals for reducing the system of equations

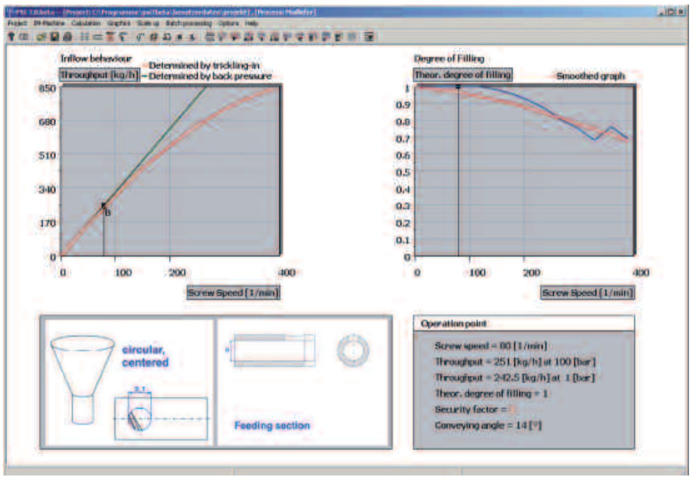

Fig. 6. Illustration of the result of simulated granule feeding from the hopper to the screw flight

Simulation of High-speed Machines

Currently, machine manufacturers are working on the use of faster screws to increase throughput. It transpires that polymer along the length of the screw. This means that nowadays simulations can be performed either with the conventional model, which simulates the melting of an existing solids bed, or with the disperse melting model, which describes continuous melting of individual particles in the melt.

In addition, the simulation must factor in the feeding behaviour since, at high circumferential speeds and an unfavourable hopper opening, the filling degree of the screw channel may prove to be < 1. For this, the feeding and filling behaviours beneath the hopper opening were analysed and modelled at the KTP (Fig. 6) [5]. Screw geometries that can be currently simulated are listed in Fig. 7.

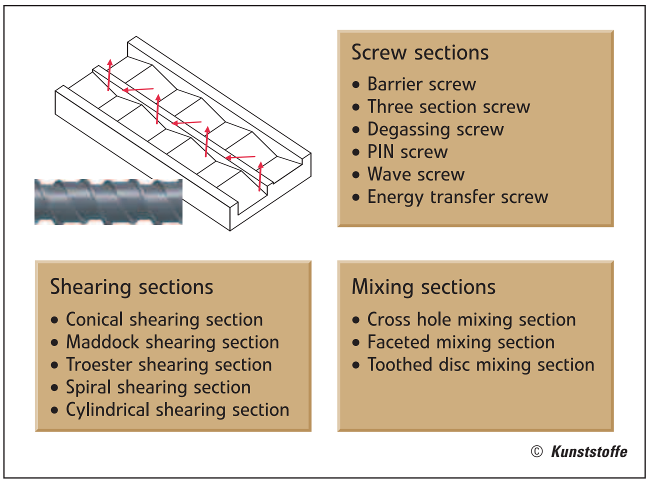

Fig. 7. List of screw geometries that can be simulated with PSI/REX

Additional Modules for Supporting the User

Instead of restricting itself to purely simulating processing, the software must support the user along the path towards the optimum process. For this purpose, there are scale-up and variation modules and, more recently, the possibility of statistical design of experiments (Fig. 8) and the simulation of user-defined functions.

The development of REX 9 and PSI 7 continues. The project plan initially provides for a revision of the models for simulating wall-slipping materials and the drive power. The planned restructuring should facilitate the extension or switchover to FE-like simulation structures and also increase user-friendliness. In this regard, mention should be made of the multigraphics mode, which enables the user to compare several processes in the same chart. By way of a new option, simulation of the non-return valve is being implemented for PSI, which supersedes simulation via substitute switching diagrams and additionally contains simulation of the clamping behaviour. ■

SEQUEL

In part two of this article, we look at how the use of simulations can help plastics processing shops to save on costs. It will appear in the next edition.

ACKNOWLEDGEMENTS

We are indebted to all the project participants (Table 1) for their support and constructive collaboration. This in-depth knowledge transfer enables the KTP to align its research activities with the needs of industry.

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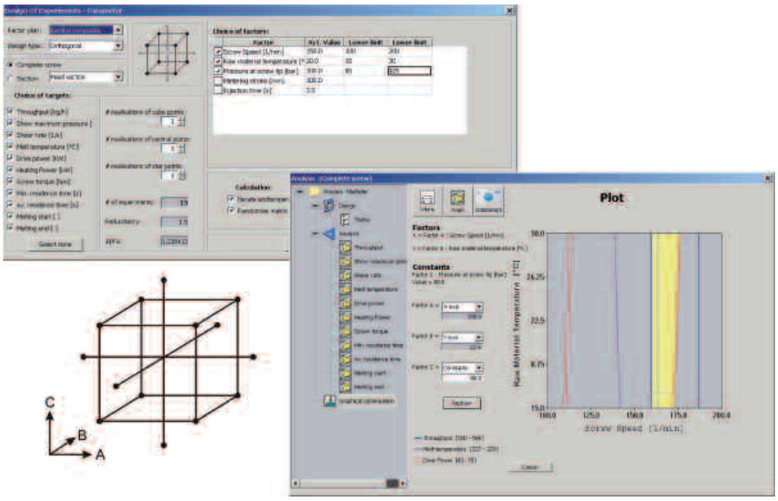

Fig. 8. Simulation of the statistical design of experiments module for devising the optimum operating point (yellow area) of the screw geometry

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