Twin screw extruder · Simulation · Modelling · Optimisation

The process behaviour of compounding extruders at given boundary conditions is primarily determined by the selection and arrangement of the screw elements. Until today, the screw configuration is usually selected by experience or by applying the trial-and-error method. Apart from that theoretical models for the estimation of the process behaviour can be found in literature. As these models are usually quite complicated and various models show interdependencies, only a simulation program make these models available in a user friendly way.

Within this paper a software for the simulation of co-rotating twin screw extruders will be presented. By applying this software it becomes possible not only to optimise existing extrusion lines but also to support engineers in early stages of the design of new compounding lines.

**Computer Aided Simulation of Co-Rotating Twin Screw Extruders**

Polymers need to be modified, as the properties of the raw material right after the synthesis in polymer reactors usually do not fulfil the demands of the customers. The compounding step includes all processes needed to adapt the properties of the raw polymer to the customer requirements. Possible process steps are the addition of fillers as calcium carbonate and talc, the addition of additives and the blending of different polymers.

The machine that is most important from both the economical and the technical point of view is the co-rotating, tightly intermeshing twin screw extruder. One of the main characteristics of this machine is the modular setup which makes it possible to adapt the screw- and the barrel-configuration to a given process task. The process behaviour of this kind of machines is essentially defined by the raw material, the process parameters and the screw configuration.

Engineers assigned to design or to optimise such an extruder have different options to perform this task (cf. Fig. 1). The most common way is to run trials on a lab scale extruder. The experiences collected during these trials are then transferred to the production scale machine using scale-up rules. The problem applying this approach is that there are currently no comprehensive scale-up rules that are applicable for any kind of problem. On the other hand extensive lab trials are very time and cost intensive.

Another approach would be to apply theoretical models. As most theoretical models are quite complex and there are interdependencies between different process models the most comfortable way to use theoretical models is to use simulation software. Currently we know of five different simulation programs capable of solving the problem [1–5]. In the further course of this presentation we will focus on the program SIGMA developed in the Polymer Engineering Department of the University of Paderborn [4].

**Underlying principles and scope of the calculation**

The results of a calculation run in the SIGMA simulation program can be obtained either in the form of profiles over the length of the screw configuration or in the form of scalar variables which characterize the melt as it is discharged out of extruder. The first type of result takes in the:

- pressure profile,
- filling degree profile,
- melting profile,
- axial melt temperature,
- local power consumption,
- minimum and mean residence time,
- local axial mixing coefficient and
- degree of dispersion of mineral fillers

while the scalar variables are the following:

- integral filling degree,
- maximum conveying capacity in the solids conveying section,
- melt temperature,
- power requirement and torque,
- mean axial mixing coefficient and
- longitudinal degree of mixing.

Some of the process models mentioned above are described briefly in the following sections of the paper. More detailed descriptions can be found in the literature [e.g. 4, 6, 7].

**Pressure Profile** The basis of all simulations is the calculation of the pressure profile. To...
develop the corresponding model the flow profiles in the screw elements was investigated using three dimensional finite element simulations. In Fig. 2 the flow profiles in a conveying element is shown. One can see that in the intermeshing region of the screws a completely different flow profile is present compared to the remaining regions. 

Knowing these results it appears reasonable to model the intermeshing region independently from the other section. The flow rate in the intermeshing region can be described with a satisfying degree of accuracy using the following equation:

\[ V_{\text{int}} = A_{\text{int}} \cdot t \cdot n_0 \]  

To model the other sections we use a channel model (cf. Fig. 3). The flow rate in the screw channels and in the radial clearances are coupled using a balance of flow rates using a triangular control area. The flow rates in the channel and the radial clearance are modelled by the description of the results of 2 1/2 dimensional finite element simulations. The commonly used pure analytical approaches can not describe experimental results with the desired accuracy. The accuracy obtained by the models used in Sigma is shown in Fig. 4. The symbols characterise the results of the finite element simulations while the lines represent the profiles calculated with the models implemented in Sigma. For both conveying and reconveying elements, a good description was generated.
Power Consumption

To calculate the power consumption one has to sum up the power consumption in:

- the solids conveying section,
- the melting section,
- the melt conveying section,
- the radial clearance between screw and barrel and
- in the nip region.

Compared to the power consumption in the other sections, the power requirements in the solids conveying section can be neglected. The model to describe the power consumption is based on the following simplifying assumptions:

- The melt is assumed to be wall adhering.
- We assume a laminar and creeping flow of an incompressible fluid.
- All material data – except the viscosity – are thought to be independent of the temperature. For the calculation average values are used.

The power introduced by the screw can be distinguished into a part due to viscous dissipation and into a part due to the pressure build-up. The part due to kinetic energy can be neglected.

\[ P = P_{\text{Diss}} + P_{\text{Pump}} = P_{\text{Diss}} + \Delta p \cdot V \]

The calculation of the pressure build-up power is based on the model developed to describe the pressure throughput behaviour. Using this model it is possible to calculate the pressure gradient in dependence of the flow rate imposed to the system, the geometrical data and the material data. The dissipated power is calculated using finite element simulations as a data basis. The results of these simulations were described using approximation equations.

\[ K(T) = K_0 \cdot e^{-\beta T} \]

(3)

Applying these assumptions we get a simplified energy equation:

\[ \frac{\partial T}{\partial z} = -\frac{1}{p \cdot c \cdot \nu_0} \left( \frac{1}{2} \frac{\partial q}{\partial y} + \frac{(\tau - \gamma)}{p \cdot c \cdot \nu_0} \right) \]

\[-e^{\beta(T-T_1)} \]

(4)

To describe the heat flow \( \dot{q}_y \) we use Fourier’s law:

\[ \dot{q}_y = -\lambda \frac{\partial T}{\partial y} \]

(5)

The solution of the differential equation gives the temperature change in a section of constant geometry and constant material data (with the exception of the viscosity). Fig. 6 shows a comparison of the calculated and measured temperatures in a ZSK 30 co-rotating twin screw extruder. A sufficient degree of accuracy can be found.

Mixing

A comprehensive modelling is complicated as several mixing mechanisms have to be distinguished. One very common approach is to distinguish between distributive and dispersive mixing.

The task of distributive mixing is to smooth fluctuations in product properties. If the smoothing is mainly concentrated in the direction of the main product flow we talk about longitudinal mixing, while mixing in the direction perpendicular to the main product flow is usually called cross-sectional mixing.

The former effect can be described easily by means of residence time distributions as shown in Fig. 7.

The values to characterise this kind of mixing are:

- the minimum residence time \( t_1 \),
- the average residence time \( t \) and
- the variance of the residence time distribution \( \sigma^2 \):

\[ \sigma^2 = \int_{t_1}^{\infty} (t - \bar{t})^2 \cdot f(t) \cdot dt \]

(6)

The cross-sectional mixing can be described in a simplified way using the results of the pressure calculation as the ratio of the flow rate in the radial clearance to the flow rate in channel direction.
The model of the dispersive mixing is somewhat more complicated. In numerous investigations three different mechanisms were identified in the dispersive mixing of mineral fillers:

- rupture of agglomerates in a small number of fragments,
- erosion of primary particles from the surface of agglomerates and
- (re-) clustering of agglomerates.

Within Sigma models were developed to describe each mechanism individually. The models were superimposed afterwards. The model is able to describe experimental results with a sufficient degree of accuracy as shown in Fig. 8.

**Simulation example**

As an example for a SIGMA simulation we will use a direct film extrusion process. During this process a Polypropylene is melted, a Filler Masterbatch is added in the molten polymer and finally the edge cut of the film production line is added. The trials this example is based on were run on a Coperion Werner & Pfleiderer ZSK30 co-rotating twin screw extruder. The actual trials were motivated by a production problem running screw 1 in Fig. 9. There was a severe problem related to the feeding of the masterbatch. We found the problem related to the quite soft melting section of screw 1. Modifying the melting section (screw 2) we could improve the melting process (cf. Fig. 10). The changes resulted in a comparable melt temperature at the exit and a comparable power consumption of the extruder. Thus the changes in the extruder improved the process and did not result in higher costs directly related to the process. On the other hand higher pressures in the melting section occurred that will most probably cause more wear in this section.

**Conclusion**

In this paper we described briefly some of the models implemented in the simulation program SIGMA. The software is a tool that aides engineers to design and optimise co-rotating twin screw extruders. Current results show that the release state of the software is in a way that the software is able to predict actual processes with a satisfying degree of accuracy. This degree of accuracy can only be achieved with a set of accurate material data.
Although these data are crucial for a good simulation, it is sometimes difficult to determine and sometimes even more difficult to evaluate data.

One has to face these difficulties and make sure that the software is used by an experienced engineer that is able to question the results.

Keeping this in mind simulation software is a very good tool that aids engineers assigned to optimise or design extruders.

References


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