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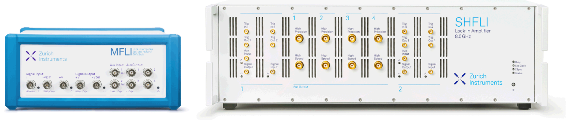

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Analytical and Numerical Methods for Optimizing Screw Geometries of an Injection Molding Plasticizing Unit with Focus on Standard Three-Section Screws

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Abstract. At present, there are only few established simulation programs for the estimation of processes in an injection molding plasticizing unit. Their results are quite often inaccurate and troubleshooting has proved to be difficult. Therefore, a new simulation software was developed to predict the optimum screw geometries and process parameters for the respective applications. This work focuses on standard three-section screws, which are the most common. At first, extensive material characterization and appropriate material models are the basis for high quality process simulations. Hence, several observations with different measurement devices were conducted for determining thermodynamic and rheological material parameters. Secondly, the three-dimensional helix shape of the screw channel consisting of feed, compression and metering section can be approximated via an unrolled screw channel. Afterwards, a 2D grid generator is used to divide the unrolled channel in numerous small grid cells. The screw pitch, channel height and flight number as well as further geometric parameters can be variable along the axial screw length. Finally, the simulation can be examined by using a clear separation of the melt and solid fraction, several mathematical and physical models, especially the finite difference method, the melting model based on *Tadmor* and *Gogos*, *White* and *Potente* and a numerical temperature calculation based on *Miethlinger* and *Aigner*. The axial screw motion during the plasticizing process and the idle time due to the cooling cycle are considered as well. The simulation output includes the pressure/throughput behavior, melting profile, temperature development and power consumption. In addition, by the use of different optimization methods and a special correction factor relating to the solid-bed velocity, the obtained results have been compared and verified with suitable experiments.

INTRODUCTION

The plasticizing process in general and the single screw plasticizing process in particular is the most important polymer processing technique. In injection molding and extrusion, calculating the solid conveying capacity, the melting capacity, the pressure throughput behavior and temperature development is a subject of international research. Hence, the development of new physical and mathematical approaches is essential for low energy plasticizing units at high output rates in association with good melt quality and low polymer degradation. The approximations used in existing simulation are based on the melt only, therefore a clear separation of the melt and solid fraction is essential. Basic research has already been conducted by *White* and *Potente* [1], *Tadmor* [2], *Tadmor* and *Klein* [3], *Tadmor* and *Gogos* [4], which provides a good understanding of the fundamentals of the melting behavior in single screw plasticizing process. Extended research in general and in terms of numerical temperature calculation can be found in the literature provided by *Aigner* et al. [5][6].

A special focus of this work is the consideration of the lateral drag flow in presence of a moving solid-bed. In the melting section, the polymer melt is not only surrounded by the screw bed, screw flight and barrel surface, but also in contact with unmelted material. In a first approximation, this compacted solid-bed is moving with a certain velocity. Moreover, the melt flow is described by a one dimensional pressure-/drag flow in direction of the unrolled screw channel. In order to improve this one dimensional estimation, several correction factors can be found in literature, which consider influences of screw flight and leakage flow. The lateral drag flow due to a moving solid-bed is often not taken into consideration. Hence, the aim is to find a correction factor, which is dependent on geometric definitions

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and the solid-bed velocity. Therefore, numerical solutions are evaluated for a pure pressure flow on the one hand, and compared with a pressure flow including a lateral drag flow on the other hand.

MATERIAL AND TESTING

The technical polymer PA6 B30S provided by Lanxess (Köln, Germany) was used to compare the simulation results with the experimental analysis. This material is suitable for injection molding processing. Details are listed in Table 1.

TABLE 1. Material data for simulation - PA6 B30S

Description	Abbrevation	Value	Unit
Melting temperature (peak)	T_m	222.0	°C
Enthalpy of fusion	h_m	255050.0	J/kg
Specific heat capacity (liquid)	c_{p_l}	2250.0	$J/(kg.K)$
Heat conductivity (liquid)	λ_l	0.22	$W/(m.K)$
Bird-Carreau-Yasuda / Arrhenius			
Zero shear viscosity	η_0	139.94	$Pa.s$
Time constant	k	0.0011	s
Power law index	n	0.4258	–
Yasuda parameter	a	2.9750	kg/m^3
Reference temperature	T_r	260	°C
Activation energy	E_A	86110.87	J/mol

SIMULATION SETUP METHODS

The basic setup of the used screw simulation software is illustrated in Figure 1. First of all, detailed definition of process, material and geometry data is a precondition. The three dimensional geometry of the screw channel consisting of several sections is approximated via an unrolled screw channel. A special grid generator is used for subdividing the unrolled channel geometry in numerous small grid cells in channel direction (z-direction) and in direction of the channel height (y-direction). Secondly, an initial melt flow rate is calculated considering a fully developed melt flow in the metering section. Afterwards, the axial screw motion due to the injection molding plasticizing process and a new total volume flow rate including drag flow, pressure flow and back flow (Equation 1) can be calculated in a first approximation.

$$\dot{V}_{total,1} = \dot{V}_D + \dot{V}_P$$

$$\dot{V}_{total,1} = i\left[\frac{b^* h v_{1z}}{2}\mathtt{CFD}_{\mathtt{SF}}(1-\mathtt{CFD}_{\mathtt{LF}}) - \frac{b^* h^3}{12\eta}\frac{dp}{dz}\mathtt{CFP}_{\mathtt{SF}}(1+\mathtt{CFP}_{\mathtt{LF}})\right] - \underbrace{\frac{b^* h}{\sin\varphi_m}}_{back\ flow}\dot{s} \qquad (1)$$

The melting model by *Tadmor* and *Gogos* [4] is the basis determining the melting behavior in the simulation program. It is a drag induced melting model with a focus on crystalline materials, because of the abrupt change from the solid to the liquid phase. With the finite difference method, it is possible to calculate the temperature distribution and in further consequence the associated viscosity, which is necessary for the pressure calculation.

Finally, using a numerical procedure, the calculation of the total pressure differential in direction of the unrolled channel is repeated with a modified mass flow rate, until the pre-defined back pressure is reached at the end of metering section. According to *Rauwendaal* [7] the power consumption can be estimated as well.

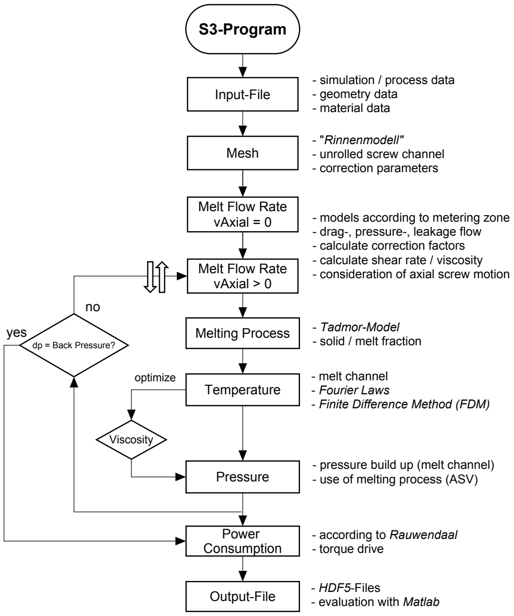

FIGURE 1. Flow chart of the simulation program

Correction Factor - Moving Solid-Bed

The **C**orrection **F**actor **P**ressure flow considers the influence of moving **s**olid **b**ed relating to pressure flow (in the melt channel) in direction of the unrolled screw channel (z-direction). The basic equation for this two dimensional pressure flow is:

$$\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} = \frac{1}{\eta}\frac{dp}{dz} \tag{2}$$

The mathematical approximation from differential to difference quotient is applied to Equation 2 and the discretization of the momentum equation is examined. The correction factors for different h/b^*-ratios and solid-bed velocities v_{sz} can be calculated. It should be mentioned that b^{**} is the width of melt (across the channel, x-direction) in the melting section, which is defined as the corrected channel width b^* minus the solid-bed width at the corresponding z-position. The following equation shows a mathematical approximation in order to describe this correction factor:

$$\mathtt{CFP}_{\mathtt{SB}} = \frac{\Delta p_{num}}{\Delta p_{analyt.}} \tag{3}$$

$$\mathtt{CFP}_{\mathtt{SB}} \approx 0 \quad ... \quad v_{sz} > \frac{2b^{**}}{17h}, \qquad \mathtt{CFP}_{\mathtt{SB}} \approx 1 \quad ... \quad \frac{h}{2b^{**}} < 0.1, \qquad \mathtt{CFP}_{\mathtt{SB}} \approx 1 - \frac{17}{2} \cdot v_{sz} \cdot \frac{h}{b^{**}} \quad ... \quad \textit{any other} \tag{4}$$

Equation 5 describes the pressure profile along the unrolled screw channel, starting at a certain length Z_0 (start melting). This length depends on the drag induced melting model, considering several boundary conditions and process parameters. Nevertheless, based on Equation 1 the pressure difference can be calculated gradually in z-direction:

$$\Delta p_j = 0 \qquad ... \quad z_j < Z_0$$

$$\Delta p_j = \Delta p_{j-1} + \left[\tfrac{b_j^{**} h_j v_{1z}}{2}\mathtt{CFD}_{\mathtt{SF}}(1 - \mathtt{CFD}_{\mathtt{LF}}) - \tfrac{\dot{V}_j}{i} - \tfrac{b_j^{*} h_j}{\sin\varphi_m}\dot{s}\right] \cdot \tfrac{12\eta_{eq,rep_j}\Delta z_j}{b_j^{**} h_j^3 \mathtt{CFP}_{\mathtt{SF}(1+\mathtt{CFP}_{\mathtt{LF}})}} \cdot \mathtt{CFP}_{\mathtt{SB}} \quad ... \quad z_j \geq Z_0 \tag{5}$$

$$\Delta p_{analyt.} = \textstyle\sum_{j=nodeZ(Z_0)}^{j=nodeZ(Z_{end})} \Delta p_j \qquad j = 1, 2, 3...$$

RESULTS AND DISCUSSION

In order to validate the simulation results of the melting behavior we conducted experiments on an injection molding machine (e-motion 310/100T) by the company ENGEL (Schwertberg, Austria). The used plasticizing unit has the following setup and geometric data: standard three-section single screw with a diameter of D_s = 40 mm, L/D ratio of 20, pitch t = 40 mm, flight width e = 4.8, channel height of the feed section h_F = 6.125 mm, channel height of the metering section h_M = 2.675 mm, length of the feed section l_F = 9D, length of the compression section l_c = 6D, length of the metering section l_c = 5D and a screw clearance δ = 0.125 mm. On the bottom side of the barrel there are at least 10 bores for mounting the pressure sensors. In sum we have used seven pressure sensors.

The used process settings with the PA6-B30S material, explained in the chapter Material and Methods, are screw speed of 143.2 U/min, back pressure of 150 bar, metering stroke of 2.0 D and a cooling time of 20 seconds. In Figure 2 and 3 are respectively four diagrams in order to illustrate the simulation results (red curves). At the top left side the solid-bed fraction (melting curve) over the axial screw length (L/D-ratio) is located, whereas the mean temperature of the melt is located at the top right position. Furthermore, on the bottom side one can see the pressure build up (left position) and driving torque (right position) again applied over the axial screw length. Additionally, the blue circle markers indicates the experimentally determined pressure signals. All simulation results and pressure signals are evaluated at half metering stroke. If we compare these two figures, one can see that the pressure profile of Figure 3, which considers the lateral drag flow in presence of a moving solid-bed, matches the experimentally determined pressure signals much better. This is the expected result and can already be seen using FDM (Finite Difference Method), because the overall pressure build up should be reduced, if the h/b^{**}-ratio is between 0.1 and 1 and the solid-bed velocity is in the range of 0 up to 0.1 m/s. Moreover, the melting curve and the driving torque is reduced as well, which is also more realistic compared to the experiments.

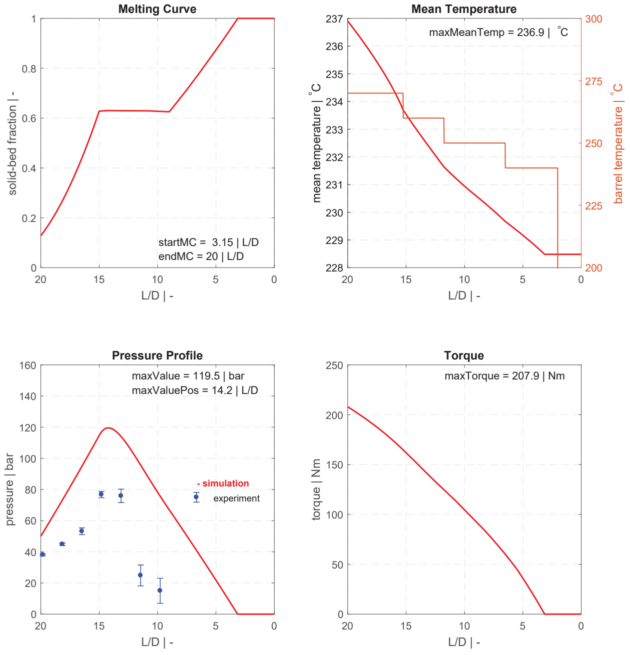

FIGURE 2. Simulation results - without correction factor $\mathtt{CFP}_{\mathtt{SB}}$

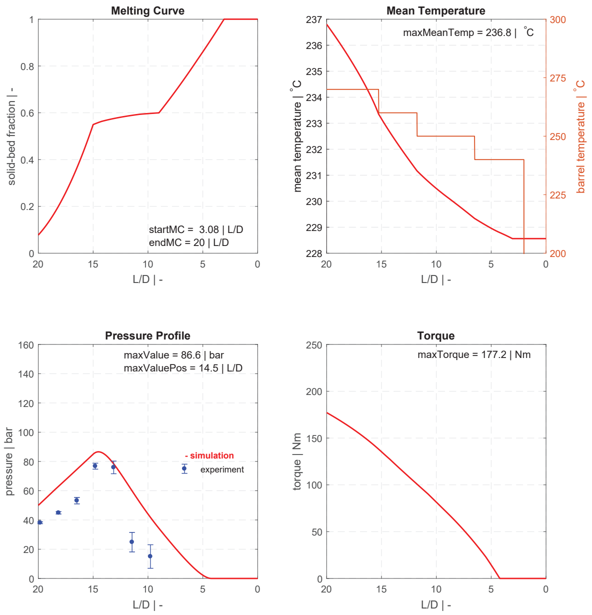

FIGURE 3. Simulation results - considering correction factor $\mathtt{CFP}_{\mathtt{SB}}$

CONCLUSION

To sum up, a new simulation software was developed to predict the optimum screw geometries and process parameters for the respective applications. The three-dimensional helix shape of the screw consisting of several sections with different geometric definitions can be approximated by using a special grid generator (2D). In addition, we have applied and developed a novel correction factor $\mathtt{CFP}_{\mathtt{sb}}$ provided for a one dimensional pressure flow in an unrolled screw channel. This correction factor considers the lateral drag flow due to a moving solid-bed. With this in mind the overall pressure build-up can be reduced to lower values. Furthermore, the driving torque and thus the power consumption can be reduced. Compared to experimentally evaluated data, these facts are very often more accurate, especially in consideration of solid-bed velocities from 0 to 0.1 m/s and .

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