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New method to analyze the throughput-pressure behavior with the corrected twin screw channel geometry and the induced drag flow of screw elements by using 3D FEM simulation

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New Method to Analyze the Throughput-Pressure Behavior with the Corrected Twin Screw Channel Geometry and the Induced Drag Flow of Screw Elements by Using 3D FEM Simulation

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Abstract. The mathematical modeling of the throughput-pressure behavior of the co-rotating twin screw extrusion process was subject of a variety of publications. Due to limited options within the area of numerical simulations, most of the modeling was based on analytical simplifications and adaptions. For that reason, commonly known models for describing the throughput behavior of co-rotating twin screws are based on the concept of the kinematical inversion principle. Within this concept, in comparison to the real kinematic behavior supposing the screws are rotating with a rotational velocity, the barrel is inducing the drag flow with an approximated translational velocity in the system. Further, the channel geometry is transferred to a rectangular shape with a constant channel height and is set in two-dimensional level for a simplified calculation. However, with regards to the geometrical diversity of the co-rotating systems with varying ratios of outer to inner diameter of the screws, the resulting channel geometry indicates different heights which have a significant influence on the inducing drag flow within the process. The model for the melt throughput-pressure behavior allows a variation of general screw and barrel geometry ratios but neglects the significance of the induced drag flow depending on the varying channel height. For that reason, a new method to measure the influence of the non-inverted drag flow by using 3D FEM simulations are presented in this paper. With the presented data, it is possible to extend the conventional model by considering the varying channel height and the correct induction of the drag flow with different screw ratios. The results indicate a systematical deviation between the analytical model and the data of this study. Overall, the consideration of the varying channel height increase the accuracy of the induced drag flow within the calculation of the throughput-pressure gradient.

Keywords: Co-rotating twin screw extrusion, finite element method, throughput-pressure behavior, drag flow.
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INTRODUCTION

Due to the high standards of quality requirements for compounding products alongside of increasing the throughput of self-wiping co-rotating twin screw extruders the analysis of the throughput-pressure behavior is an essential part of various models for describing the co rotating twin screw process [1]. In contrast to screw extruders which are flood fed, the twin screw extruders are starved fed and the screw speed will change in levels of fill in screw elements but not the throughput which is determined by the input of the material in the feeding zone. As a result the throughput-pressure behavior is strongly influenced by the geometry of the screw elements within the extruder [2]. The most important screw elements regarding this context are the conveying self-wiping elements described by Erdmenger [3] and were used in this investigation. The resulting polymer melt flow of the conveying elements consists of the superimposition of pressure flow due to local differences within the pressure gradient and the induced drag flow of the rotating screw flank [4]. In analytical models [4-7] the channel geometry was transferred to a rectangular shape with a constant channel height and is set in two-dimensional level for a simplified calculation. With the channel model of a single screw extruder, the screw is considered as fixed while the barrel as rotating around the screw [8]. This kinematic model, which is used for the throughput-pressure behavior neglects the significance of the induced drag flow depended on the varying channel height. In order to improve the approximation and analytical calculation of the throughput behavior of co-rotating twin screw extruders a new method to compare the different inductions of the drag flow by using 3D FEM simulations was developed and the results will be compared to the results of the analytical models presented in this investigation.

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METHOD TO ANALYZE THE INDUCED DRAG FLOW OF A CONVEYING TWIN SCREW ELEMENT BY USING THE FINITE-ELEMENT-METHOD

For the numerical investigations, the CFD-Solver Extrud3D was used. Extrud3D is an extension of the subroutine Featflow which was developed to calculate incompressible Navier-Stokes equations of fluid dynamics in the two and three dimensional area with the use of the FE-method [9]. It is developed in collaboration between the TU Dortmund, the IANUS Simulation GmbH and the Paderborn University. Within the FE simulations, the kinematical behavior is the same as in real processes. The screw induces the drag flow with the rotational speed (w) and the velocity of the barrel is nonexistent in comparison to the inverted model which is used in the analytical calculations. For further investigations, it was necessary to extract the unwound twin screw channel geometry of the 3D model. The post-processing evaluation was done with the open source, multi-platform data analysis and visualization application ParaView [10]. An overview about the evaluation method is shown in figure 1.

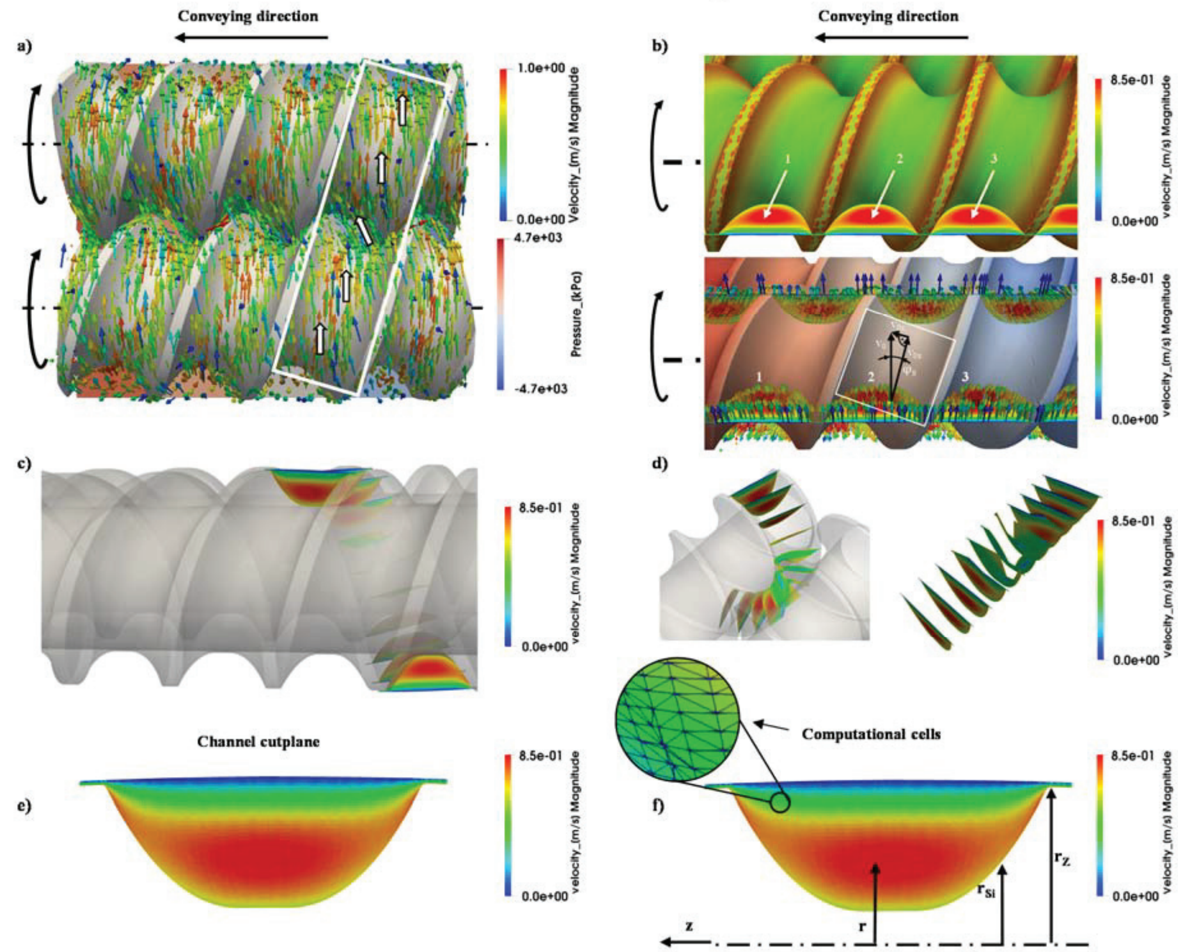

FIGURE 1. Overview about the Evaluation Method a)- f) Used for the FE-Simulations to Calculate the Induced Drag Flow for the Twin Screw Channel Geometry

The simulations represent only completely filled screw channels with melt within a twin screw process. The flow field, or velocity profile which is represented with the velocity vectors in a) was analysed via cutplanes b). The results of the cutplanes and the flow field of the melt, excluding the screw, are marked with 1, 2 and 3. These are the channel cutplanes and were placed within the screw channel with a specifically developed evaluation routine in ParaView. With regards to the channel windings and the threat angle, the channel cutplanes represent the exact 2D approximation of the twin screw channel geometry c) (including the gap between barrel and screw). Further the channel cutplanes containing the information about the flow field within the channel. Because of the wound geometry the flow field was adapted to the normal direction of the channel d) and was conducted with a transformation of the vector flow field to achieve a corrected flow field in the direction of the channel. After the transformation of the flow field, the channel cutplane e) and its computational mesh were assigned to cylindrical coordinates f). The calculation of the induced drag flow in the numerical simulation is achieved with a Taylor-Couette-system with isothermal and shear thinning material behavior with following functional relationships (1-2) [11]. The variable ω_Z describes the angular velocity of the barrel.

$$v_z(r) = r_Z * \omega_Z * \cos(\varphi_S) * \left[\frac{r}{r_Z} * \frac{1-\left(\frac{r_{Si}}{r}\right)^{\frac{2}{n}}}{1-\left(\frac{r_Z}{r_{Si}}\right)^{-\frac{2}{n}}} \right] \tag{1}$$

$$\dot{V}_{Drag,3D} = \sum_{k=1}^{\text{Number of cells}} v_{z,k} * A_{cell,k} \tag{2}$$

The radius for each individual computation cell r_{Si} was determined and assigned to each cell (figure 1 f)). In addition to that the surface area was taken into account and further assigned to each cell information. The related velocities v_z were multiplied with its surface area and summed up for the overall drag flow within the channel cutplane.

ANALYTICAL CALCULATION OF THE DRAG FLOW WITHIN THE TWIN SCREW CHANNEL

The principle of the kinematical inversion was developed for single screw extruders and the rectangular shape of the channel geometry within the screw and was consequently transferred to the twin screw channel geometry. For the calculation of the throughput-pressure behavior the real channel geometry a) is transferred to a rectangular shape with a constant channel height "$\bar{h}$" and is set in two-dimensional level for a simplified calculation b). This model is commonly used to calculate the throughput-pressure behavior of twin screw extruders in analytical models and simulation software for twin screw processes (figure 2) [5-7].

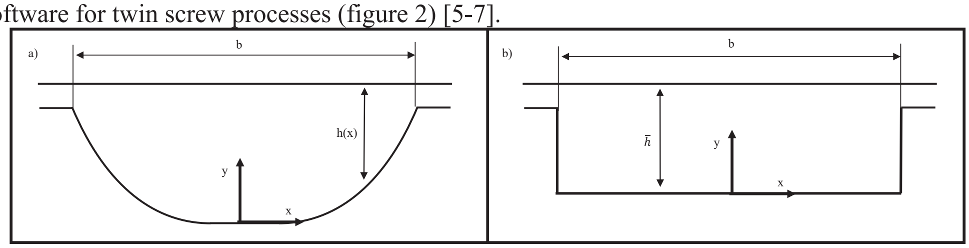

FIGURE 2. Height Approximation h(x) of the Real Twin Screw Channel Geometry a) with a Rectangular Screw Channel b) which is commonly used in Throughput-Pressure Models

To determine the drag flow, a Couette-flow-system was used. The drag flow was calculated with the following equations (3-5). Within this equations v_{0z} is the peripheral speed of the screw and D_b the barrel diameter.

$$\dot{V}_{Drag,TS} = \int_{-\frac{b}{2}}^{\frac{b}{2}} \int_{0}^{h(x)} v_{0z}(y,x)\, dy\, dx \tag{3}$$

Equation represents the real twin screw channel geometry. This equation is simplified for the rectangular channel model with (4) and (5). The variable "n" respresents the RPM of the system.

$$v_{0z} = 2 * \pi * n * D_b \tag{4}$$

$$\dot{V}_{Drag,RE} = \frac{1}{2} * v_{0z} * b * \bar{h} \tag{5}$$

In addition to that, a new analytical description for the channel height h(x) was developed in these investigations. In contrast to the rectangular model, an, approximation of the real channel height h(x) was defined (figure 3).

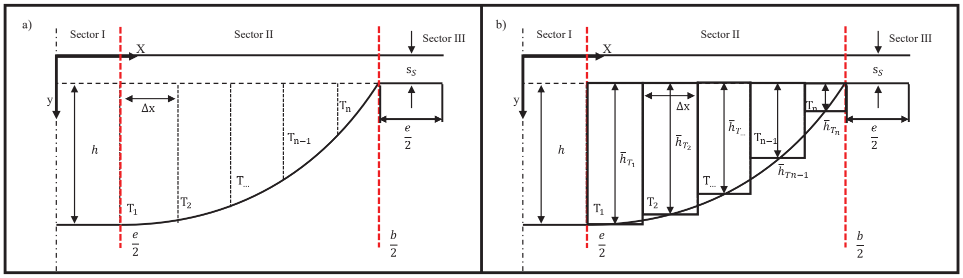

FIGURE 3. Approximation of the Twin Screw Channel by Dividing the Area with a Finite Number of Rectangular channels a) with Sectoral Channel Heights b)

The general idea was to divide the twin screw channel in smaller rectangular channels and include the area by using the primitive of h(x) which is approximated by H(x) via Taylor series (6).

$$H(x) = D_i * x - a * x + \frac{1}{3} * a_1 * \left(x - \frac{1}{2} * e\right)^3 + \frac{1}{5} * a_2 * \left(x - \frac{1}{2} * e\right)^5 \tag{6}$$

For each sector the area A_{T_n} (T_n – T_{n+1}) was calculated and expanded with the radial clearance of the screw and the barrel S_S (7).

$$\bar{h}_{T_n} = \frac{A_{T_n}}{\Delta x} + s_S \tag{7}$$

Therefore the drag flow was calculated in each sector for a Taylor-Couette-system (8).

$$\dot{V}_{Drag,T_n} = \frac{\omega * \Delta x}{2 * \left(1 - \left(\frac{r_{ST_n}}{r_Z}\right)^{\frac{2}{n}}\right)} * \left[\left(r_Z^2 - r_{ST_n}^2\right) - \frac{n * r_{ST_n}^2}{n-1} * \left(\left(\frac{r_Z}{r_{ST_n}}\right)^{\frac{2*(n-1)}{n}} - 1\right)\right] \tag{8}$$

The total drag flow is the sum of the drag flow of each sector (9).

$$\dot{V}_{Drag,AH} = \sum_{n=1}^{n} \dot{V}_{Drag,T_n} \tag{9}$$

COMPARISON BETWEEN NUMERICAL AND ANALYTICAL RESULTS

The geometry and process data (table 1 and table 2) are based on the conveying elements of a Coperion ZSK25 twin screw extruder and a Barmag 45 compounder. All calculations and simulations were realized with isothermal circumstances. The material data which were used is based on Polyethylen (PE) material data.

TABLE 1. Geometry Data used for the calculations and simulations

Geometry Data	**Unit**	**Coperion ZSK25**			**Barmag45 compounder**	
Ratio D_o/D_i	-	1.45	1.55	1.64	1.61	1.67
Outer diameter screw D_o	[mm]		25		45	
Barrel diameter D_b	[mm]		25.3		45.2	
Inner diameter screw Di	[mm]	17.2	16.1	15.2	27.9	26.9
Axis distance of the screws	[mm]		21.1		36.5	
Clearance between screws Sr	[mm]	0	0.55	1	0	0.5
Element length l	[mm]		24		60	
Threat t	[mm]		24		60	
Clearance between the barrel Ss	[mm]		0.15		0.1	

TABLE 2. Process Parameters used for the Calculations and Simulations

Process Parameters	**Unit**	**Coperion ZSK25**	**Barmag 45 compounder**
RPM	[min^{-1}]	600	200
Throughput $\dot{m}$	[kg/h]	30	50
Barrel temperature Tb	[°C]	215	215
Melt temperature Tm	[°C]	215	215
Power law index n	-	0.58	0.58

To determine the relative deviation ($f_{\dot{V},Drag}$) between the analytical drag flow and the induced drag flow of the 3D simulation the following equation was used for each analytical model.

$$f_{\dot{V},Drag} = \frac{\dot{V}_{\mathrm{Drag,Analytical}} - \dot{V}_{\mathrm{Drag,3D}}}{\dot{V}_{\mathrm{Drag,3D}}} \tag{10}$$

The results of the comparison of the different models are shown in figure 4. The results display that the consideration of the real twin screw geometry based on the height function h(x) and the use of the Taylor-Couette-system in an analytical model will overall improve the calculation of the drag flow for a conveying element. Further, it is visible that the deviation is higher if the ratio D_o/D_i increases for the conveying element. In addition to that, the influence of different geometries for the conveying elements for the twin screw extruder systems (ZSK 25 and Barmag 45) is also ascertainable.

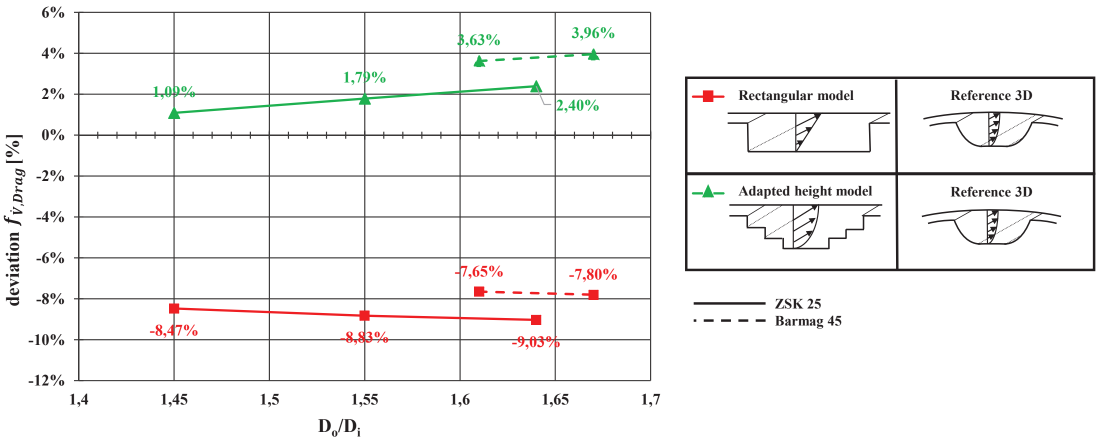

FIGURE 4. Comparison of the Results between the Deviation of the Analytical Calculated Drag Flow within the Rectangular- and Adapted Height Model with the 3D Simulation

SUMMARY AND OUTLOOK

In this paper a new method to analyze the induced drag flow of conveying elements for co-rotating twin screw extruders by using 3D FEM is presented. With this method, it was possible to evaluate different analytical models, which describe the induced drag flow of conveying screw elements, regarding the prediction accuracy of the induced drag flow compared to the 3D results. Based on the investigations it was shown that the consideration of the local channel height h(x) for conveying elements in the analytical descriptions will increase the accuracy of the calculation on average by 7 %. Further investigations are necessary to analyze if the improved calculation of the induced drag flow improves the whole prediction accuracy of the throughput-pressure for co-rotating twin screw processes.

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