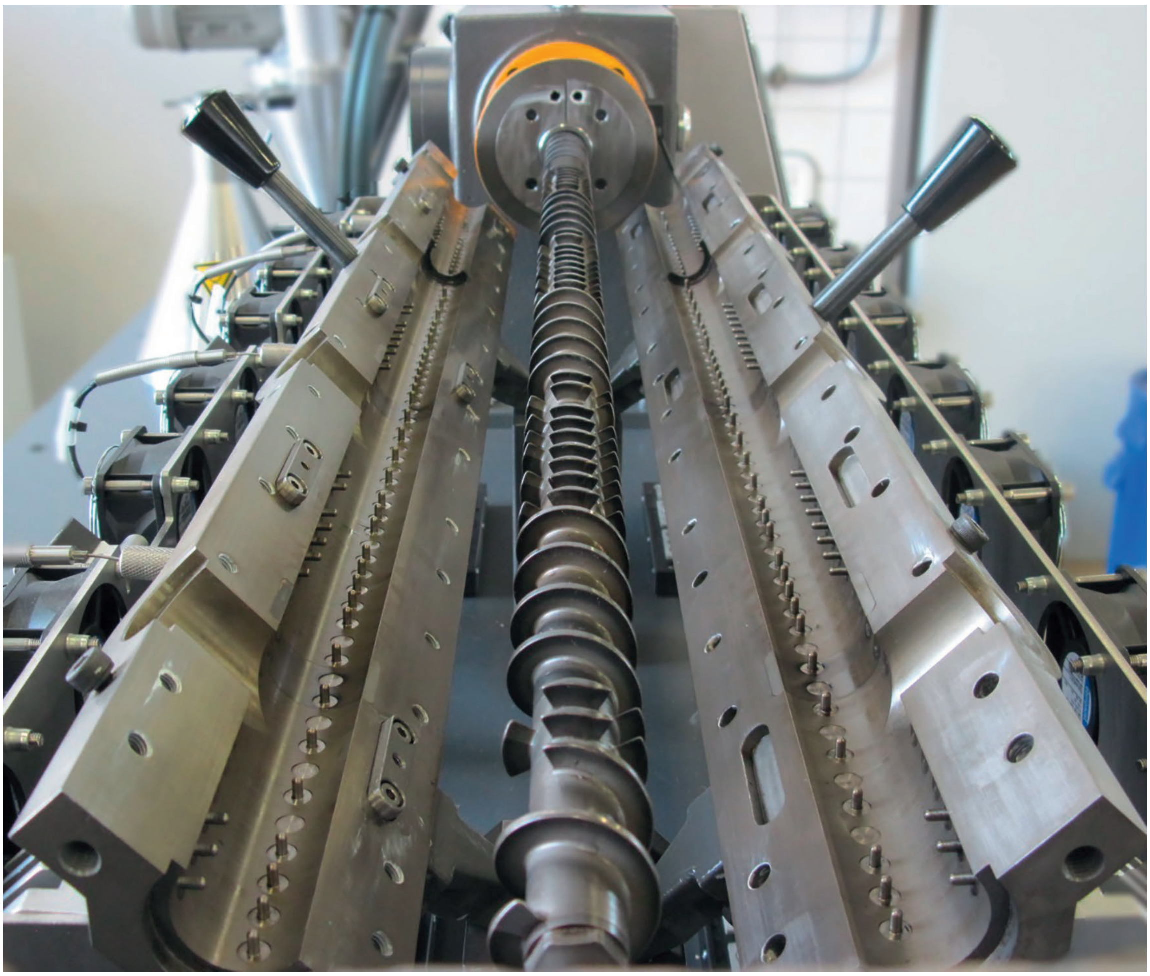
Understanding Kneading Holistically

Predict Co-Kneader Behavior Efficiently with Procedural Understanding

Thanks to its special working principle, the co-kneader fulfills top mixing requirements. Until now, however, its design could not be based on simulation, because processing knowledge and modeling approaches were lacking. Systematic investigation together with analytical and numerical models overcome this hurdle and provide the basis for computer-aided optimization.



A look inside the co-kneader whose behavior when processing polyethylene and polystyrene was simulated © SKZ

The properties of engineering plastics are decisively influenced by the additives mixed into them [1]. The co-kneader (**s. Title figure**) is a single-screw extruder for compounding and modifying polymers and other substances. Although co-kneaders are specialists for the processing of highly filled plastics, rubbers, and TPE (thermoplastic elastomers), they keep expanding into one new application after another. They are particularly in demand wherever mixing specifications are high, or where temperature and shear sensitive plastics are to be compounded.

The process design of screw-compounders continues to be based on trial-and-error methods that have produced a number of empirically optimized series and configurations. This kind of process optimization is, of course, very time and labor intensive and cannot offer companies any sort of efficient support. Simulations, on the other hand, enable an economical way to vary all kinds of processing conditions. A deeper understanding can be gained this way that is hard to obtain experimentally.

The numerous investigations of single- and multi-screw compounding systems cannot be easily transferred to the co-kneader due to its geometrical conditions and the working principle. The oscillating motion of the screw, the interruptions of the screw flights, plus interactions with the kneading pins make it difficult to represent and model a co-kneader. This is why a good technical understanding of the processes within the kneader has to be established, and new models have to be developed on this basis.

The Co-Kneader

The co-kneader is a single-screw extruder which, in addition to rotating, performs an oscillating motion in the screw axis [2]. This working principle effects longitudinal mixing processes in addition to the radial ones and fulfills top mixing specifications. The processing unit consists of an axially separable screw housing and a modular screw (**Title figure**). Various feeder and mixer elements with different kneading flight lengths are used here. Thanks to its modular construction, the screw can be adapted for various requirements. Four rows of kneading pins protrude into the screw channel along the axis on the cylinder wall.

In order to prevent the kneading pins from contacting the screw during movement sequences, the screw flights are not continuous, but separated into the kneading flights. Together with the motion, this construction results in easily manageable shear forces, large relative shifts in the mass layers, and ultimately in a high mixing effect. This is why the co-kneader is used for compounding temperature and shear sensitive plastics, rubbers, and in the food industry [3]. To ensure continuous melt discharge despite its oscillating motion, the co-kneader can be combined with a single-screw melt extruder [4]. The investigations presented here focus on the co-kneader processing unit, since existing studies can be consulted regarding the melt compounders [5, 6].

Experimental Investigation

A laboratory co-kneader (type: MX 30–22 F40–6, year of construction 2014, manufacturer: Buss AG, Pratteln, Switzerland) with a 30 mm screw diameter, 22 L/D ratio, and 5.5 mm stroke was used for the experiments. Three screw configurations were investigated in all: screw configuration 1 mainly utilizes KL kneader elements with shortened kneading flights in the melt feeding zones. In screw configuration 2, KN kneader elements with longer kneading flights than on KL elements were used, whereby a stronger shear effect ought to result, since the material is sheared over a longer time period between flank and kneading pin. Moreover, polymer mass back flow is reduced, so that KN elements exhibit higher feed effects which in turn lead to shorter dwell times for the plastic [2]. In screw configuration 3, mainly conveying elements are used after the first mixing zone in order to enable investigation of processing behavior with reduced shears. For the screw configurations, various working parameters were investigated, such as the number of pins, speed, and throughput, as well as their influences on the processing of both polyethylene (PE) and polystyrene (PS).

Generally speaking, for mixed-feed screws the power required for PE is always higher than for PS, as shown in **Figure 1 left**. This difference can be explained by the higher viscosity (MFR = 0.3 g/10 min) and higher melting enthalpy (approx. 500 J/g) of semi-crystalline PE compared to lower viscosity amorphous PS (MFR = 3.7 g/10 min, melt- »

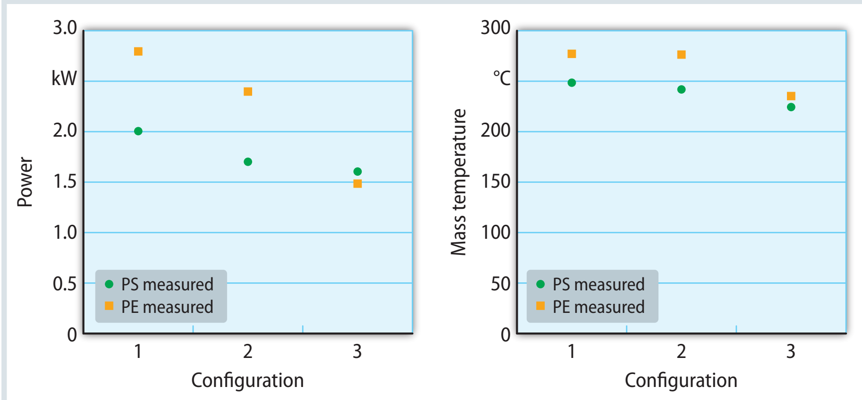


Fig. 1. Power introduced (left) and melt temperatures (right) at the end of the extruder shown with various screw configurations at 8 kg/h throughput and 400 rpm Source: SKZ, graphic: © Hanser

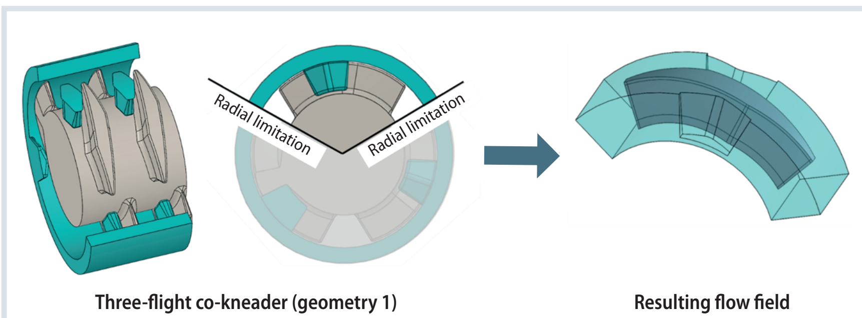


Fig. 2. Simplification of the calculation geometry with axial and radial boundaries using the example of a three-flight co-kneader (geometry 1) Source: IKT, graphic: © Hanser

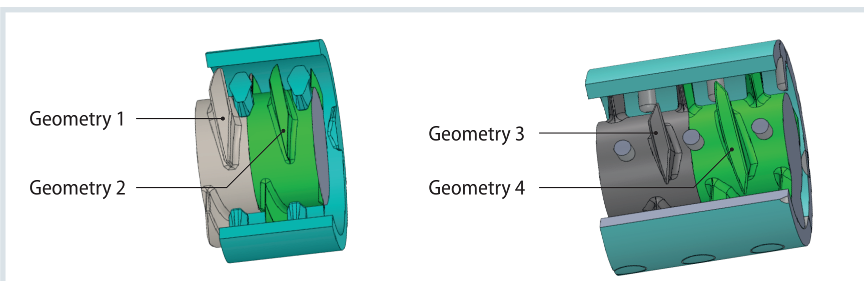


Fig. 3. Simulated geometry variations: geometries 1 and 2 are three-flight co-kneaders, geometry 3 and 4 have 4 flights. The difference between geometry 1 and 2 is between flight width. Geometry 3 and 4 differ in respect to flight width and length Source: IKT, graphic: © Hanser

The Authors

Jochen Kettemann, M. Sc., has been a research assistant in the field of processing technology at the IKT (Institut für Kunststofftechnik) at the University of Stuttgart, Germany, since 2016; jochen.kettemann@ikt.uni-stuttgart.de

Univ. Prof. Dr.-Ing. Christian Bonten has been the Director of the IKT since 2010.

Rebecca Wolff, M. Sc., has been a research assistant in the section for compounding and extrusion at the Kunststoff-Zentrum (SKZ), Würzburg, Germany, since 2019.

Dipl.-Ing. Johannes Rudloff has directed the section for compounding and extrusion at the SKZ since 2016.

Dr.-Ing. Marieluise Lang has directed the section for materials, compounding, extrusion at the SKZ since 2015.

Dr. rer. nat. Thomas Hochrein has been the Managing Director of Research and Continuing Education at the SKZ since 2017.

Prof. Dr.-Ing. Martin Bastian has been the Director of the SKZ Institute since 2006.

Acknowledgments

IGF project 18650 N of the FSKZ e.V. research association was funded from 1 August 2016 to 31 January 2019 by the Federal Ministry for Economic Affairs and Energy (BMWi) through the AiF as part of a program for the promotion of industrial community research and development (IGF) based on a decision of the German Bundestag. We would like to express our thanks for this financial support. We also wish to thank the Buss AG of Pratteln, Switzerland, and the X-Compound GmbH of Kaisten, Switzerland, for their assistance and generation of geometries.

Service

References & Digital Version

- You can find the list of references and a PDF file of the article at *www.kunststoffe-international.com/2020-6*

German Version

- Read the German version of the article in our magazine *Kunststoffe* or at *www.kunststoffe.de*

ing enthalpy approx. 150 J/g). As for screw configuration, it turns out that the elements with wide kneading flights (KN) bring less energy into the material than the elements with narrow kneading flights (KL). This is surprising, since it can be expected that wide flights mean a higher average shear rate. Conveying capacity is, of course, better, due to the wider blades, so the filling level is lower, and this effect predominates among the materials investigated.

The mass temperatures at the end of the extruder (**Fig. 1 right**) reflect different power inputs; screw configuration 3 thereby shows that, given a suitable configuration, the materials exhibit lower mass temperatures, and PE can be processed at temperatures similar to those for PS despite its higher viscosity.

To understand the sequences within the machine, it is therefore essential to evaluate melt transport, full fillings, backflow lengths, and dwell times. The local filling level of the extruder was determined via dead-stop tests. In such tests, the extruder is stopped quickly, and the cylinder is opened so that the sequences in the machine can be analyzed. It turned out that filling levels increased with increasing throughput and decreasing speed (rpm). KL-type kneader elements generally exhibit the highest filling level. This ultimately influences both dwell time and extruder power. To verify the models developed, dwell times were determined using a titanium dioxide tracer and a melt color sensor at the end of the extruder (s. below).

Modeling

The following text presents the analytical and numerical calculation models developed for co-kneaders. Flow variables that could not be detected experimentally can be resolved using numerical flow simulations. Among these are flow direction and shear rate. An extruder can also be investigated in detail in a three-dimensional view [7]. Analytical calculation models provide important processing variables such as power and temperature along the extruder that can be used to design it efficiently and optimize its application [7]. Both approaches are summarily explained in the following. For a more precise derivation of the models, please refer to Lang et al. [8].

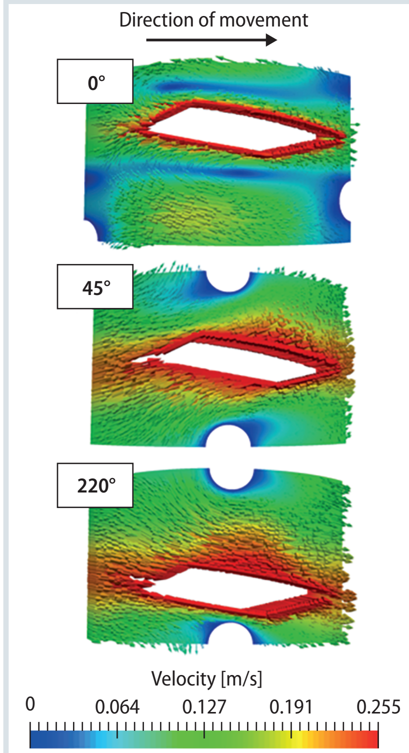


Fig. 4. Velocity profiles of characteristic flight positions of a four-flight co-kneader (geometry 3, KL element). The flow field was cut radially, a color scale shows the different velocities, arrows their direction Source: IKT, graphic: © Hanser

Numerical Modeling

Model assumptions were made to enable modeling of the kneader by conventional simulation methods [9]. **Figure 2** shows the simplified flow domain of a kneader blade position. Since stationary models are calculated first, characteristic kneader blade positions have to be set and simulated. To take the overlaid movement also into account, the overlaid oscillating screw motion in axial direction must be considered for every blade position in addition to constant rotary speed. In order to consider an extruder configuration across the board, the calculated flow quantities were averaged over the individual sections and evaluated.

Using the OpenFoam simulation environment, two different kneader elements were simulated for each of two machine types (**Fig. 3**). The stationary, isothermal simulations were compared with regard to the resulting velocity fields, and the averaged shear rates were compared for each machine type and configuration.

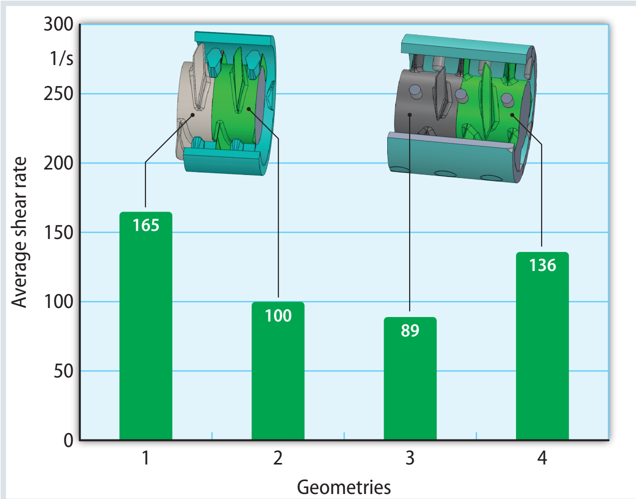


Fig. 5. Comparison of the average shear rates for geometries 1 to 4 Source: IKT, graphic: © Hanser

Analytical Modeling

For analytical modeling of the co-kneader, a proven procedure for single and twin-screw extruders, as well as for planetary roller extruder was applied [6, 7, 10, 11]. To do so, the geometry is split up into short sections of the same geometry that are then described by approximately ten geometrical parameters such as screw channel number, height and width, number of pins, and width of the interruption between the kneading flights. The geometry parameters can be used together with materials data to calculate processing variables. Individual process steps, such as melt conveying and temperature development, are first considered separately and then coupled in a calculation program via an iterative calculation process. Then it was assumed that dimensionless characteristic numbers can be used to describe melt conveying, for example, by superimposing drag and pressure flow. Then a balance of energy, mass, and power flows of the extruder is done for energy considerations.

Results and Evaluation of the Calculation Models

The most important results within the analytical and numerical calculation models are presented and evaluated in the following. The numerical simulations focus on a comparison of shear rates in the melt dominated, fully filled zone of the co-kneader. By contrast, the analytical model considers several design relevant variables, such as dwell time, mass temperature, filling level, power input, and pressure over the entire length of the extruder.

The numerical simulations were evaluated both qualitatively based on the velocity field and quantitatively by calculating the average shear rate. The velocity profiles of three characteristic blade »

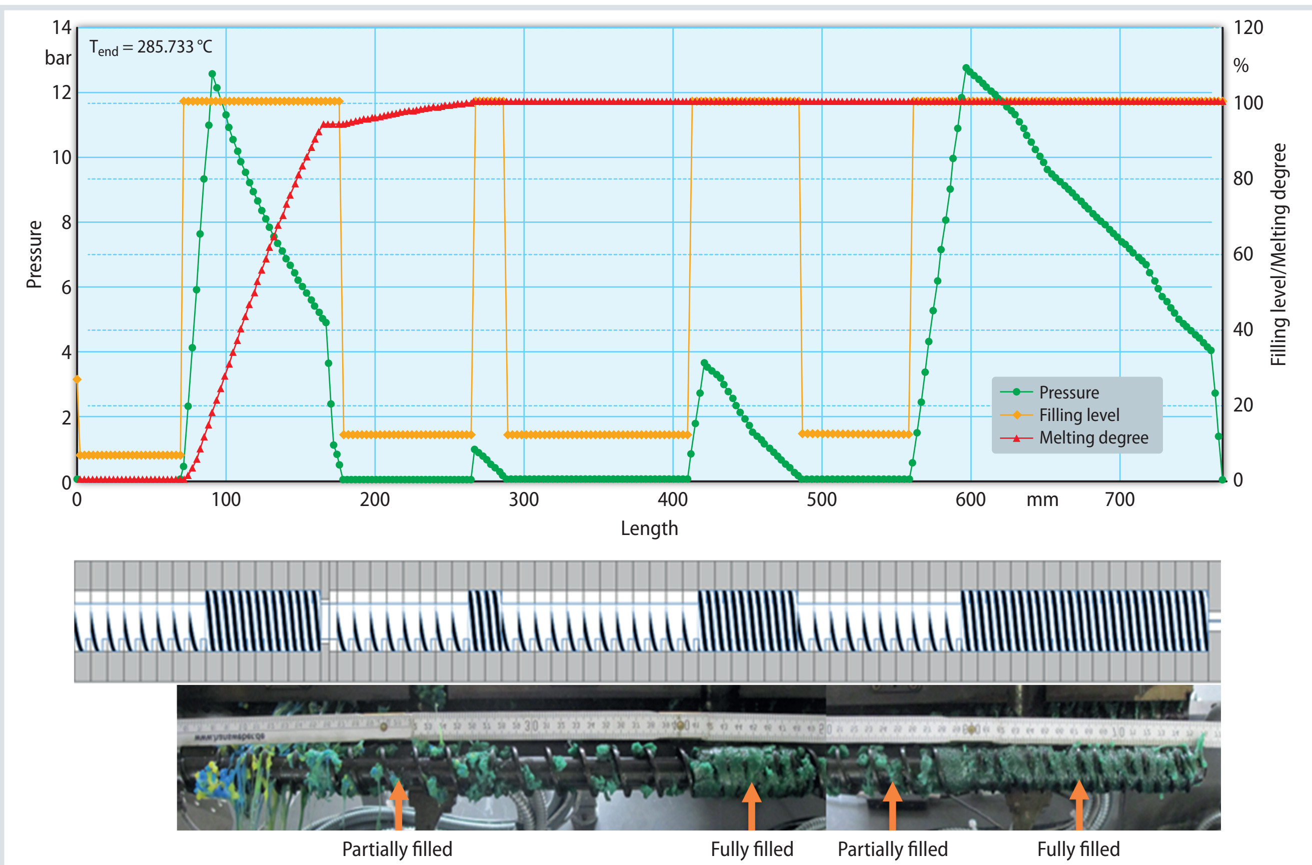


Fig. 6. Comparison of simulated pressures, filling levels, and melting degrees of PE: conveying elements are interrupted in the screw drawing, and kneading elements are shown fully Source: SKZ, graphic: © Hanser

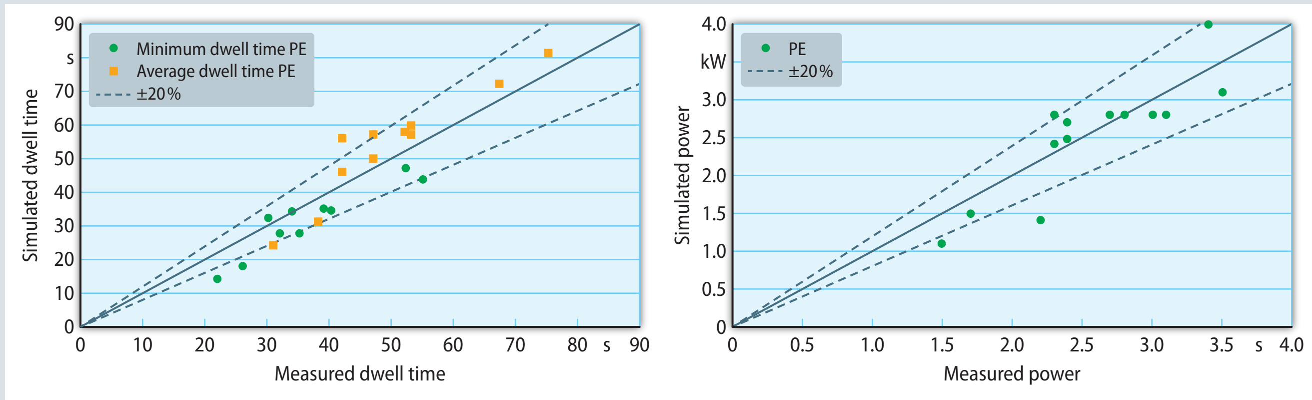


Fig. 7. Comparison of simulated and measured values: on the left the accumulated minimum or average dwell times, on the right the powers, each for different operating points with PE as the matrix material Source: SKZ, graphic: © Hanser

positions (e.g. as shown in **Fig. 4**) indicate that a 220° position partially leads to back flow that also affects shear rate. Although the assumptions made strongly simplify the real co-kneading process, the averaged shear rates (**Fig. 5**) reflect the practical experience that a wider flight increases shear rate (cf. geometry 3, KL element and geometry 4, KN element), and a narrow flight reduces it (cf. geometry 1 and 2). Consequently, first tendencies can thus be predicted with reduced effort on the basis of quantitative data. Moreover, it was determined by a simulative parameter study that shear rate depends on rheological properties. Thus, the higher the viscosity of the plastic melt, the higher the resulting average shear rate.

For the analytical calculation, the SimKo simulation tool was developed that is integrated into MS Excel via Visual Basic Applications (VBA). This tool enables 1D simulations to be performed with the compounder models by entering materials, geometry, and processing parameters. The models are validated by comparing the calculated results with the experimental ones. The example in **Figure 6** compares the calculated curves of pressure, filling level, and mixing for a test point with PE with the image recording of a dead-stop test. The kneading elements are fully filled in the calculations, as well as in the experiment. This is also the case for the immediately preceding conveying elements, whereby pressure is being built up to overcome the kneading elements. The start and finish of melting which were not focused on by the work presented here are also reproduced well by the calculation [12; DFG Project: BA 1841/30–1].

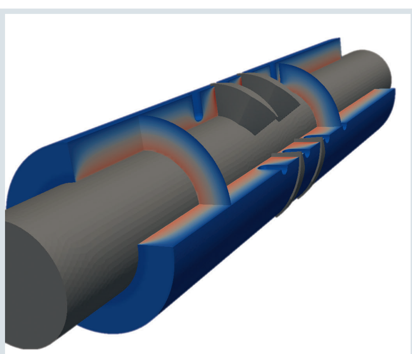


Fig. 8. Velocity field of a three-dimensional co-kneader simulation (four-flight kneader: geometry 3) in OpenFoam with real screw motion using the Immersed Boundary Surface Method © IKT

The modeling precision for a variation of operating parameters and screw configurations is shown in the following using PE as the example. The measured and simulated cumulated dwell times are shown in **Figure 7 left**. Minimum dwell time runs around 20 to 60 s, whereas the calculated average dwell time of 30 to 80 s was approx. 30 % longer. Prediction precision error is less than 20 %.

The comparison of results in **Figure 7 right** also shows errors of the same order in the comparison of results for power and mass temperature at different axial positions. Taking the simplifications made for modeling into consideration, this represents good agreement between calculation and experiment.

Conclusions and Outlook

Systematic experimental and theoretical process investigations contribute to a deeper understanding of the procedural processes within the co-kneader. The experiments make it possible to identify the significant processing parameters, thereby clarifying the interactions taking place between machine configuration, processing parameters, and materials used in the extruder. Within the numerical simulations, assumptions made it possible to reduce complexity far enough for the co-kneader process to be simulated stationarily. The simplified calculation models already provide promising results and can represent first tendencies in variations of geometry and influencing factors. Subsequent studies will have to implement real screw movement using moving simulations. A very promising method for this may be the Immersed Boundary Surface Method which enables any complex screw motion to be simulated. **Figure 8** shows examples of the first results of such a simulation.

For the first time, important processing variables in a co-kneader can be predicted by analytical models implemented in a simulation tool in a few seconds. A wide range of process configurations and materials systems can thus be represented by the model. These studies thereby significantly shorten the gap between the process understanding in state-of-technology in single and twin-screw extruders and the potential for simulations of the co-kneader. Even though only the simulations for the MX30 kneader and material systems used have been validated, the results already enable the accompanying use of simulations for the configuration of screw compounding processes and provide a starting point for further industry-related research and development work in this field. ■