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4. Figure and Table legends should be in 10 pt BOLD. References should be indicated by superscripted numbers in the text and listed in 10 pt plain in the format: number. surname(s) initial(s), Title of paper, *Journal name*, year, volume, pages.
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   - Physical Characterization (Structures)
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   - Basic Improvements in Screw, Mold and Die Design
   - Function Integration with Injection Molding Technologies
   - Extrusion and Compounding
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   - Multi Scale Characterization and Simulation
4. Polymers & Sustainability
   - Bio based Polymers
   - Polymers for Energy Applications
   - Polymers and Environment
   - LCA of Polymers

Simulation Aided Twin Screw Optimization for Polymer Nanoclay Composites

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Introduction

The aim of this project[1] was the improvement of the screw configuration of a co-rotating twin screw extruder, which was used for processing of polymer nanoclay composites (PNC). A complete design of experiment would mean a vast number of experimental runs on the compounder. Therefore computational fluid dynamics (CFD) were chosen to simulate different processing conditions on various screw elements and whole sections of the screws. The computational results where compared with selected experiments on the injection moulding compounder.

Experimental

Different conveying and kneading elements[2], as well as a mixing element were chosen to build up the screws. In pre-studies the throughput, the screw speed and the pressure limits where determined, to verify the experimental setups of the simulation. The verifiable results of the experiments were the pressure at the tip of the screw and the starved regions. In the simulation the pressure build up, the dissipative energy input and the mixing index[3] were calculated. The simulation was done with the program Polyflow from Ansys Inc. (Cecil Township, Pennsylvania, USA). The setup was isothermal and the used materials were a PP Bormed DM55 pharm and a PP BB 412 E, both from Borealis, with and without filler. The compounds consisted of 5 wt% compatibilizer (BYK Scona TPPP 2112GA), 5 wt% layered silicate (Rockwood Nanofil®5) and 90 wt% polymer. The viscosity was measured with a cone/plate rheometer as well as with a capillary rheometer. By calculating single screw element pairs and adding the pressure gradients along the screw, it was possible to get results of whole screw segments. By using the method of dimensionless pressure gradient[2, 4], changes of viscosity and processing conditions could be calculated without new simulations.

The mechanical properties of the produced materials where determined using a universal testing machine (Zwick Z250) and the morphological investigations were done using an SAXS measuring system (Nanostar).

Results and Discussion

The simulation of whole sections of the screws showed that the pressure build-up was independent of the boundary conditions. It can be demonstrated that the setup of the CFD was in good agreement with the measured pressure at the screw tip and the predicted starved regions.

The optimized screw consisted of mixing and kneading elements in the place of the backwards conveying elements. With this configuration it was possible to avoid the high pressure peaks and to decrease the dissipative energy input by simultaneously increasing the residence time. The desired effect of compensating the lower dissipative energy input by a longer residence time couldn't be confirmed by mechanical as well as morphological investigations.

References

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