

Numerical Solutions of a Coupled CFD-Enthalpy Model for Partly Molten Polymer Processes in Complex Geometries

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ABSTRACT

Many processes in the field of chemical process engineering involve multi-phase and/or even multimerial problems. In the recent past there is a significant progress in the field of computational treatment of such processes. Our work is motivated by a particular polymer compounding process in twin screw extruders. The CFD based simulation of fully filled parts in such extruders is already possible even though the large aspect ratios (sub millimeter gaps and diameters or screw length in the range of several centimeter), rotating domains (for twin screws there is no possibility of coordinate transformation) and complex rheology (nonlinear shear dependent and temperature dependent viscosities) lead to a rather challenging setup. Our ingredients in the code Extrud3d are higher order finite elements (Q2P1), parallelization with domain decomposition, dynamic mesh deformation based on monitor functions and Newton-multigrid solvers. Extrud3D is an adaption of FeatFlow, further developments on Extrud3D are necessary when the simulation also include a secondary disperse polymer phase fed to the process. Polymer engineers make use of an intrinsic cooling behavior by these secondary feed strategies. From an engineering point of view there are several questions which should be answered by using numerical simulations. How do particles interact and distribute downstream? What are the local and integral thermodynamic impacts on the flow due to the phase change in the melting process? How does the morphology of particles change in the combined melting/compounding process? In our approach, we have used an adapted version of the so called enthalpy model. Whenever possible, we compare our results with experiments which are conducted at our partner institute KTP (Kunststofftechnik Paderborn).

References

- [1] G. Karrenberg and J. Wortberg, “Development of a Custom Material Model for 3D-CFD-Simulation of Melting Processes in Polymer Processing”, *In Society of Plastics Engineering Annual Technical Conference (SPE Antec), Las Vegas, Nevada (USA)*, April 28-30, pp. 10391044, 2014.
- [2] Mierka O., Theis T., Herken T., Turek S., Schrippner V. and Platte F., “Mesh Deformation Based Finite Element - Fictitious Boundary Method (FEM-FBM) for the Simulation of Twin-screw Extruders”, *Ergebnisberichte des Instituts fr Angewandte Mathematik Nummer 509, Fakultt fr Mathematik, TU Dortmund*, No. 509, 2014.
- [3] D. M. Stefanescu, “Science and Engineering of Casting Solidification”, *Springer*, 2009.