11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

MULTISCALE SIMULATION OF SEMI-CRYSTALLINE THERMOPLASTICS IN THE INJECTION MOULDING PROCESS

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Key Words: *Polymer processing, multiscale simulation, crystallisation, integrative simulation.*

Semi-crystalline materials are one of the most important material groups in polymer processing. In contrast to the amorphous materials the macromolecules of the semi-crystalline polymers can arrange in periodic patterns and form crystalline superstructures. Because of several limiting factors such as entanglements or variations in the molecular weight crystals are usually not perfect but consist of amorphous and crystalline domains with different physical properties. The mechanical properties depend on the morphology, the degree of crystallinity and the molecular orientation of the formed microstructure.

To take locally variable thermo-elastic properties of injection moulded plastic components into account, an original integrative and multi-scale simulation model is proposed here. This approach starts with a 3D injection moulding simulation, involving mould filling, heat transfer between melt and mould, and melt cooling. This simulation is performed by using the CFD and heat transfer (HT) modules of COMSOL Multiphysics [1] to compute the filling and cooling process at the macro-scale for an isotactic polypropylene (PP). From this analysis, result fields, written in the VTK format, are transferred to the 3-D SphaeroSim program, developed at IKV, for the simulation of the solidification process. Based on the concept of cellular automata, this program calculates the free energy function and converts it to a nucleation probability. This probability is used to determine the distribution of spherulite germs. By integrating the line integral from the germ to the crystal growth front the expansion of the spherulites is specified and the resulting microstructure calculated [2]. We take temperature and flow fields from the injection moulding simulation into account to consider cooling and flow induced effects on the microstructure.

The predicted crystalline microstructures, at different locations in the thickness of a PP plate, are transferred to the homogenisation tool HOMAT. HOMAT uses the method of asymptotic homogenization [3] to evaluate the effective thermo-elastic properties of each semi-crystalline microstructure. A special two level

homogenization scheme [3] has been developed to take into account the radial distribution of amorphous and crystalline lamellas. The predicted effective local mechanical properties are finally used in a structural analysis of the PP plate at the macro-scale. The presented multi-scale simulation model takes account of the inhomogeneous material properties during injection moulding processes and offers a wide range of new simulation possibilities, such as the prediction of residual stresses, shrinkage and warpage of semi-crystalline plastics parts.

Acknowledgments: The depicted research has been funded by the Deutsche Forschungsgemeinschaft (DFG) as part of the program Cluster of Excellence "Integrative Production Technology for High-wage Countries". We would like to extend our thanks to the DFG.

REFERENCES

[1] COMSOL Multiphysics Reference Manual, Version 4.3b.

[2] R. Spina, M. Spekowius, C. Hopmann: „Multiscale Modeling of Polymer Crystallization“, Proceedings of the 2013 COMSOL Conference, Rotterdam, 23rd-25th October, 2013 (http://www.comsol.com/2013-user-presentations/).

[3] G. Laschet, T. Kashko, S. Benke, M. Öte, K. Bobzin: „Prediction of effective properties“, in „Integrative Computational Materials Engineering”, Ed. G.J. Schmitz and U. Prahl, Wiley VCH, Weinheim, chapter 5, pp. 81-115, 2012.