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MODELING THE POLYMER CONVERSION DEPENDENT VISCOSITY CHANGE IN THE PRODUCTION OF THERMOPLASTIC MATERIALS

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Simulation in Liquid Composite Molding (LCM) is an intrinsic part of predicting and optimizing issues in the polymer composite material production. It gives insight into process phenomena, which are not easily accessible experimentally, and especially valuable opportunities for novel process design. For example, thermoplastic composites offer advantages (e.g. easier recycling etc.) over their thermoset counterparts, however, also introduce challenges into to the production procedure (different mixing performance, turbulence, etc.). For that reason it is of paramount importance to investigate and understand the key phenomena via computational fluid dynamics (CFD).

For the simulations the open source CFD tool OpenFOAM® was used in order to easily implement the required models into the already existing fluid dynamic framework.

In the ongoing project the production process of polyamide 6 via anionic polymerization of ϵ-caprolactam is investigated. The low viscosity of the starting material poses the major difference compared to conventional resin fluids in reactive processing. The increased viscosity of the polymer creates a change of viscosity in the flow regime over multiple magnitudes. In order to describe the flow one has to correctly model the polymerization process [1, 2] and the dependence of viscosity on the polymer conversion as well as the temperature. With these models local phenomena on the flow domain can be observed, which significantly contribute to the entire process (see figure 1).

On the one hand filling experiments were conducted in the first step at constant temperature in order to guarantee the comparabilty between experiments and simulation with constant viscosity (see figure 1). On the other hand experiments were performed in order to describe the change of viscosity during the polymerization process itself. Additionally the polymerization simulations were validated by the means of kinetic constants obtained from literature [1]. In all investigations good agreement between simulations and experiments were found.

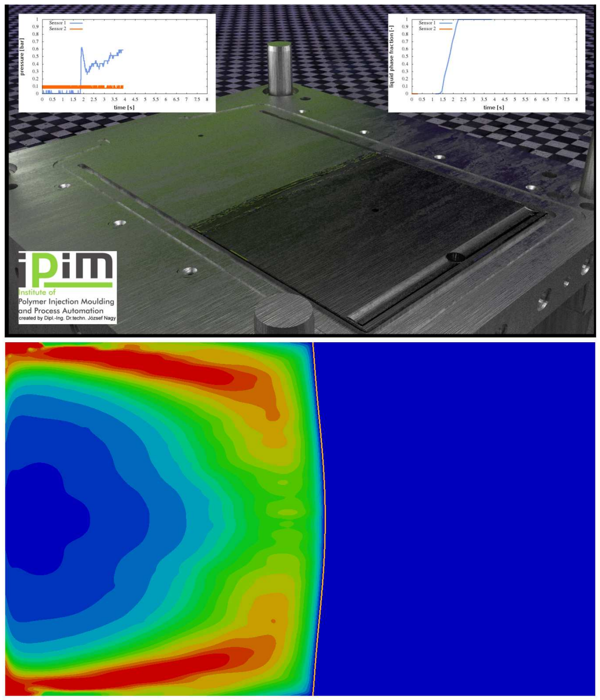

Figure 1: Mold filling simulation and polymer conversion of a flat plate geometry

With these results further work will focus on the implementation of the overall production chain (plastification, mixing of components, filling, polymerization and subsequent crystallization) within a single investigation in the OpenFOAM® framework. Such a modell would faciliate both process and mold geometry design as well as on site process optimization on industrial scale.

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