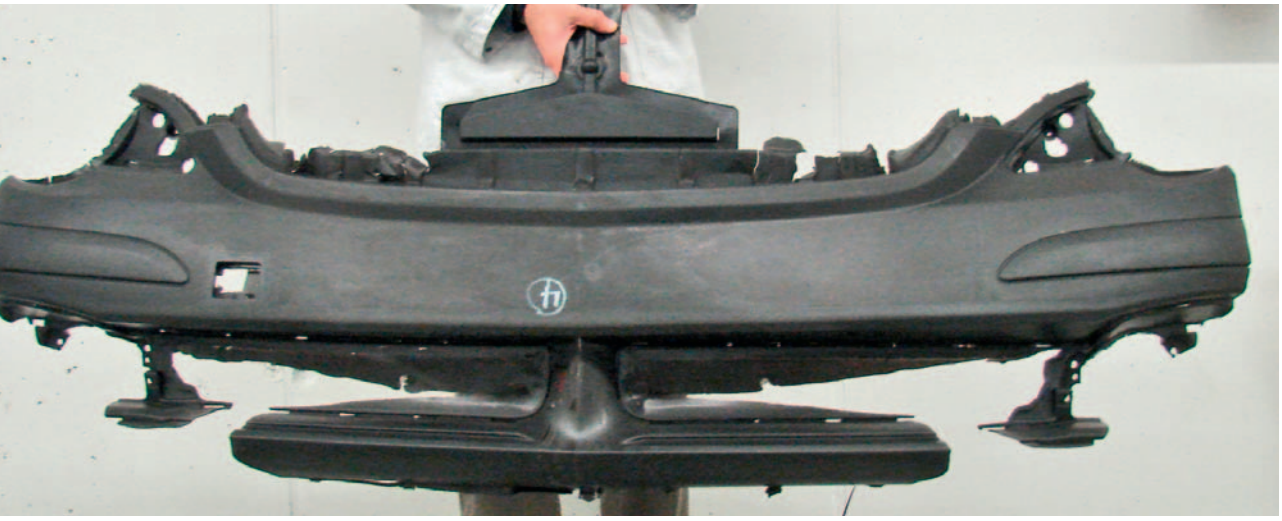

The 75 % filling of an injection molded front spoiler corresponds well with the result of a simulation (see bottom) (figures: SimpaTec, BASF Polyurethanes)

Simulating Reaction Injection Molding Processes

RIM Simulation. So far, there has been a lack of simulation tools suited to routine polyurethane RIM processes. This could be about to change: the tool presented here has cleared the first test hurdles.

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Many problems that can occur in injection molding can be avoided by simulating mold filling in advance. Current commercial software tools are mainly designed to simulate thermoplastic materials. Simulating reaction-injection molding processes (RIM), though, is much more complicated, which is probably why there are as yet no satisfactory solutions for this on the market. In view of this, BASF Polyurethanes GmbH, Lemförde, Germany, and SimpaTec GmbH, Aachen, Germany, decided to collaborate on developing a simulation tool for polyurethane (PU) RIM systems.

The objective was to be able to predict the filling behavior, including the fiber orientation, the shrinkage and the warpage of the finished part, while allowing for the chemical cross-linking reaction. The focus lay mainly on simulating fast-curing, quasi-compact materials. The development work was based on Moldex3D (manufacturer: CoreTech System Co., Ltd), a commercial software package for computational fluid dynamics.

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Description of the Simulation Method

The simulations are performed on a field part and two other "test-plate molds." Simulation comprises stages of filling, hardening of the material and

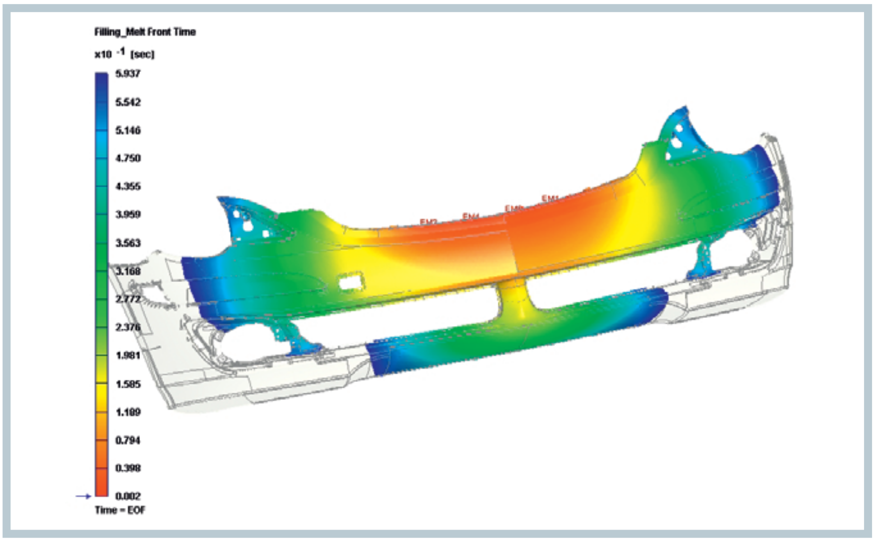

Fig. 1. The Simulation of a 75 % filled front spoiler corresponds well with the real part (see top)

warpage. In order to be able to accurately depict every aspect of what happens in reality, only 3-D simulations are performed.

The movement of the PU system, which becomes more viscous as time passes, can be described mathematically in compliance with the laws of conservation of mass, momentum and energy. It is important in this regard to couple the influences of viscosity and the kinetics of crosslinking to each other so that a more accurate picture of the filling behavior may be obtained.

Discretization of the laws of conservation is effected by means of the finite volume method (FVM), which is now used successfully in all areas of flow simulation. The flow front is calculated by means of the volume-of-fluid method (VOF).

Fig. 2. Partially filled front spoiler obtained by "injecting into cross-linking material" after 1.4 s filling time

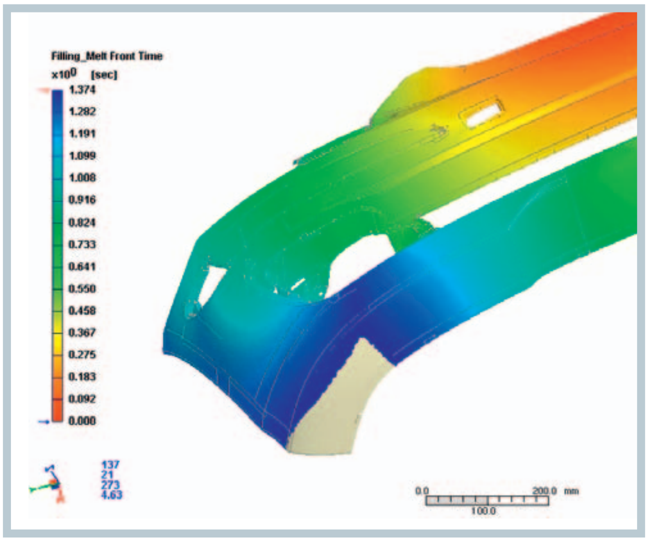

Fig. 3. Simulation of the partly filled front spoiler. After 1.37 s the filling stagnates – a result that is almost identical with the experiment

Time-dependent Filling Study

For a detailed filling simulation, a knowledge of the following material parameters is needed:

- The cross-linking reaction as a function of time and temperature,
- the viscosity,
- the thermal conductivity, and
- the heat capacity,

each as a function of the degree of crosslinking and temperature. Two different, established methods are used to characterize the kinetics of the RIM-PU system. First, a commercial IR spectrometer is used which has been converted for tracking the polyurethane reaction under isothermal conditions. Second, the increase in temperature of the polyurethane system during the reaction is measured as a function of time, and the results are used to determine the parameters of the reaction kinetics under assumed adiabatic conditions. The method of adiabatic temperature increase [1] was used especially for very fast systems. As part of the collaboration, BASF Polyurethanes and SimpaTec managed to develop a cross-linking model and to implement this in the software.

The first experiment consists in simulating Elastolit R 8719/105LT, a polyurethane which cures in about 2 s. For this, an automotive front spoiler filled to 75 % is compared with the results of the corresponding simulation. The real, incompletely filled part and the simulated part match in all important criteria **(Title photo and Fig. 1)**.

To check whether the modeling describes the cross-linking reaction in sufficient accuracy, "injecting into the cross-linking material" is performed, both in the experiment and the simulation. In other words, injection is performed so slowly that the material has cured before the mold has been completely filled. The real part can be removed after a filling time of 1.4 s. With the simulation, mold filling stagnates after 1.37 s due to the cross-linking reaction and the resultant sharp increase in viscosity. The simulation is therefore very adept at reproducing curing of the material during the shot **(Figs. 2 and 3)**.

Fiber Orientation and Warpage

In the simulation, fiber orientation is described by the Folgar-Tucker equation, while the change in orientation to reflect the flow conditions is described by the method of Advani and Tucker.

To be able to validate the simulated fiber orientation, experiments with a perforated plate are carried out. The material used (grade: Elastolit R 4503) has a fiber volume fraction of 15 %. **Figure 4** shows the fiber orientation in the fully reacted perforated plate as measured by ultrasound (across the plate thickness) [2]. The length of the arrows is indica- →

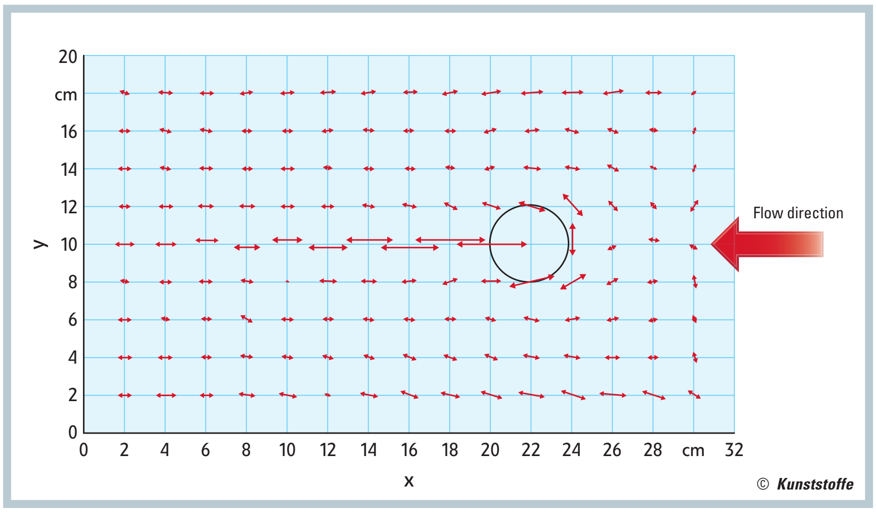

Fig. 4. Experimentally determined fiber orientation of a perforated plate with 15 % fiber by volume

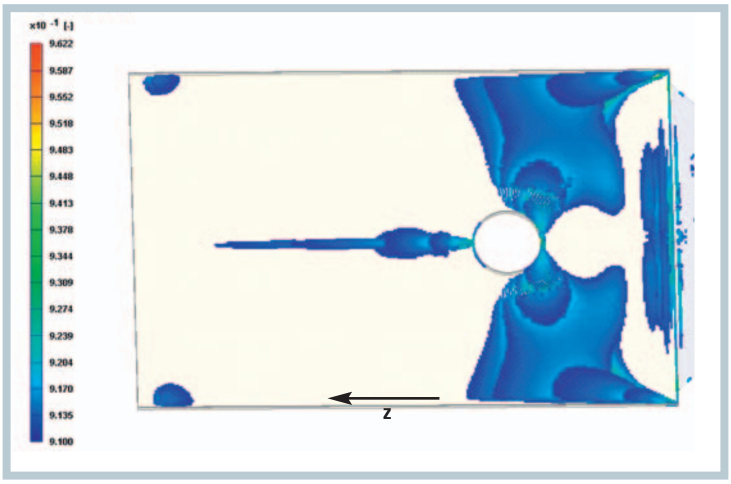

Fig. 5. Simulation of fiber orientation. The fiber alignment >91 % is shown (blue means a high degree of orientation)

tive of the degree of orientation. **Figure 5** shows the simulated fiber orientation of a perforated plate at the end of filling. Only areas of extensive orientation, and degrees of orientation greater than 0.9 (where 1 is optimum orientation), are shown. The comparison reveals good agreement between simulation and experiment.

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The warpage behavior of injection molded thermoplastics stems not only from the fiber orientation but also from the volume change of the matrix as a function of pressure and temperature, i.e. pvT behavior. In reactive PU systems, the behavior depends also on the degree of cross-linking c. The pvT model must therefore be expanded by the degree of cross-linking to yield a pvTc model. The assumption here is that the volume decreases with increase in cross-linking.

Corresponding experimental methods are being developed with a view to being able to describe the relevant parameters of the cross-linking-dependent shrinkage regardless of thermal effects. The pVTc model is validated by molding plate samples, both with and without fibers. The measurements are then compared with the simulation results **(Figs. 6 and 7)**. The simulation shows volumetric shrinkage of 0.45 % across the fiber and 0.25 % along the fiber. These values agree well with the measured values of 0.48 % and 0.27 %.

Conclusion

As shown, the new model in the Moldex3D software package is a useful tool for simulating fast-reacting PU-RIM systems. Comparison between simulation and injection molding shows very good agreement. The program can help users to design components which are perfectly matched to the polyurethane system, and can be used for all compact polyurethane systems. It also enables the processor to quickly and inexpensively respond to problems in tool design and parts filling. ■

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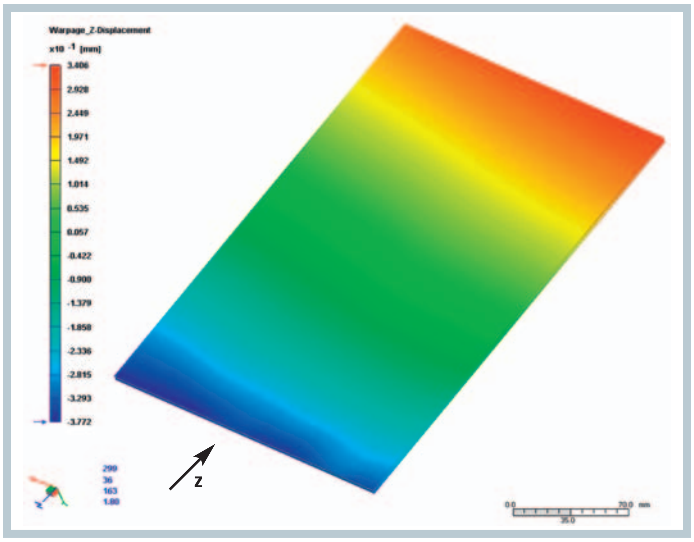

Fig. 6. Simulation of part deformation in flow direction (z)

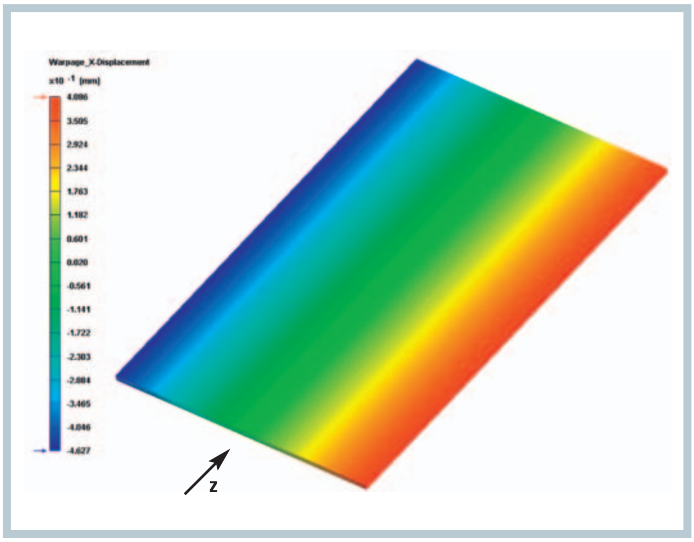

Fig. 7. Simulation of part deformation across the flow direction (z)