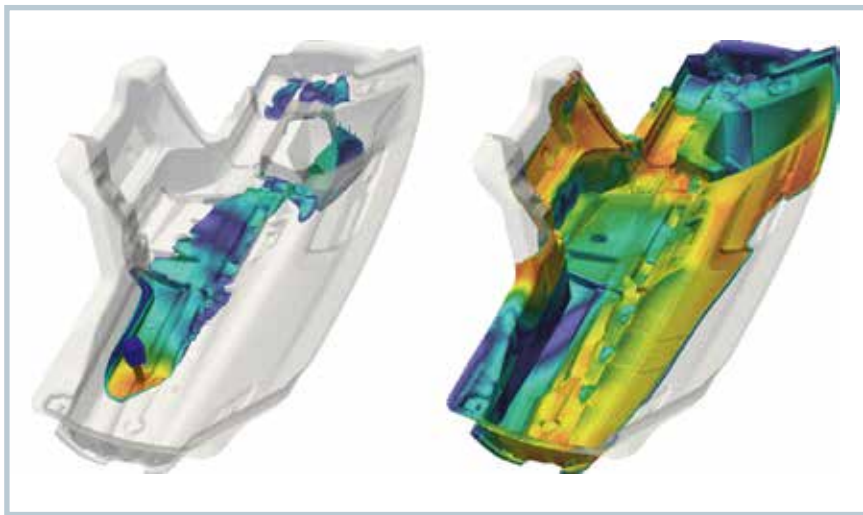


From Virtual Foam Cell to Finished Component

Ultrasim Software Simulates Processing of Polyurethane Systems

The properties of foams are primarily determined by their reactive processing. New simulation methods with wide-ranging material models are designed both to calculate the foaming process and predict the resulting foam properties. Specific examples already show extensive correlations between simulation and practice.



Foaming simulation: injection of a BASF Elastoflex E foam into an open mold (left) and the resulting filling pattern 20 s later (right). Based on CAD data for the finished component, the foaming simulation (red: areas of high material stress) helps to find the best possible injection path, improve the foaming position or evaluate the venting concept (© BASF)

Polyurethanes (PU) are extremely versatile plastics. Not only their chemical composition but also their processing determines the properties of the end product: from flexible to rigid, low density to virtually solid, thermoplastic to thermosetting. To meet the demands of the intended application, material developers must focus on the requirements of the user. The latter want to achieve the best possible result by correct processing. Considerable experience and technical knowledge are needed on both sides to continually improve the foaming process as well as the product properties. Simulation of the foaming process of a polyurethane system in the mold can be helpful here.

The wide variety of PU foams, dependence of their end properties on the processing method, and transformation of the material from a liquid polyol-isocyanate mixture to an expanded, fully reacted foam pose a challenge for both simulation models and the necessary material characterization. For example, the material measurements in the laboratory required for foaming simulation can often not be conducted under the same conditions as in later production. Therefore, another aim of simulation models is to predict the properties of the foam based on its initial composition. These models can be used, for example, to adapt material properties measured under laboratory conditions to real production processes.

To achieve this, it is, however, not enough to describe the foam macroscopically. Rather, simulation models must be calculated on different scales, particularly at cell level, and suitably coupled [1–7]. The following article explains how foam properties such as viscosity, elastic modulus or thermal conductivity can be predicted. It also discusses the role these properties play in component simulation.

Simulation of Mold Filling during the Foaming Process

The key material data for simulation of the foaming process are the density/time curve and the build-up of viscosity and elasticity from the mixing stage to complete foaming of the component. If these time curves are known, it is possible, for example, to adjust gate positions when foaming in a closed mold or injection paths (**Title figure**) in the case of open mold injection. If the air phase is simulated as well as the foam phase, potential air voids can be predicted and counter measures taken. If gravity is taken into account, the influence of the mold orientation or even its change during the foaming process can be analyzed. The special form of fluid mechanics equations is known [8–10]. Thanks to ever faster computer hardware and the latest mathematical methods, it is possible to calculate these equations and use them in practice, even for complex components such as dashboards [11] or steering wheels [12].

The **Title figure** shows how, with the aid of Ultrasim simulation software from BASF SE, Ludwigshafen, Germany, foam

injection into the open mold (left) and the subsequent foaming process (right) are predictable. This is based on special density and viscosity measurements and a model that applies these to the production process.

Chemical Reaction and Foam Expansion

The crucial density curve for foam expansion directly depends on the release of physical and chemical blowing agents. Local differences in release rates, e.g. because of the temperature distribution in the mold, lead to density gradients such as can be seen in **Figure 1**. In the following, purely water-blown foams with CO₂ as the blowing agent are described. To calculate the CO₂ release rates, simple kinetics as per Baser [13] are frequently used. These equations calculate the actual concentration of OH groups, water conversion and the remaining isocyanate groups. They assume that the foaming reaction can essentially be described by a gelling and blowing reaction as shown in **Figure 2**.

Although this empirical approach supplies the key water conversion data for density development, the kinetic parameters for the effective reactivities must be separately determined for each foam system – a Herculean task given the many different polyurethane systems. When these parameters are known, they have proved particularly useful for simulation of rigid foams, e.g. in foam insulation of refrigerators with BASF Elastocool foams [14, 9].

To facilitate simulation of other foams, particularly the BASF semi-rigid and integral skin foams ElastoflexE and Elastofoam I for automotive interiors, these kinetic models have been expanded and adapted to the relevant products. By using them, it is possible to successfully predict the progress of the reaction and density development according to the local position in the component and the mold and component temperature.

Derivation of Component Properties from Foaming Simulation

From the final density distribution (**Fig. 1**), other properties such as the local stiffness of the material can be derived. For a given material, this primarily depends on

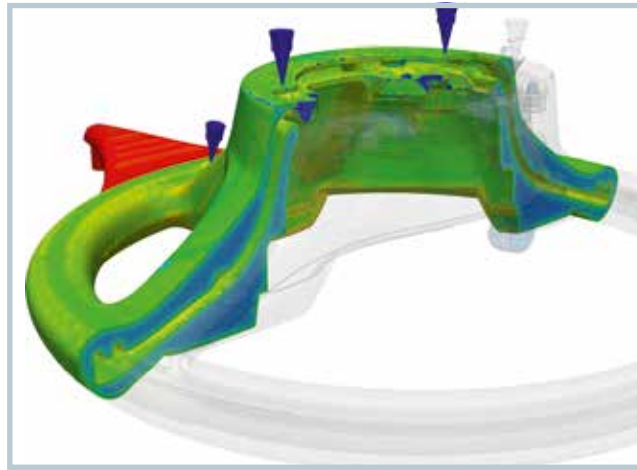


Fig. 1. The calculated density distribution of a BASF Elastofoam I foam shows the typical density gradient for integral skin foams over the component cross section. The spatial density distribution is the decisive factor determining local stiffness and hardness in the steering wheel (© BASF)

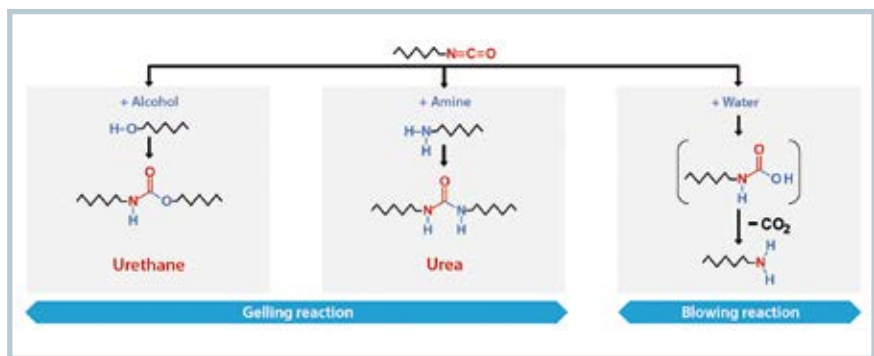


Fig. 2. Representation of the simplified reaction kinetics used to describe polyurethane foaming based on [13] (© BASF)

the density of the foam [15] and can be determined with standard measurements. Alternatively, this correlation can be determined with the aid of micromechanical simulations and the mechanical properties of the foam calculated from the properties of the matrix material and cell morphology (**Fig. 3**) [16]. For this, a detailed kinetic model [6] can supply data on the degree of cure and thus on the elastic modulus of the matrix as well as on the cell gas content in the foam cell.

A more complicated task is the prediction of material properties that depend not only on the cell gas content or density but also on the cell structure of the foam itself. Examples of such properties are the thermal conductivity [2] or acoustic characteristics of foams.

The evolution of cell size distribution during the foaming process can be calculated using so-called population balance methods [17]. The result, however, is highly dependent on the initial gas bubble distribution and other effects that are difficult to quantify, such as bubble coalescence. Nevertheless, such methods can be useful in gaining a better understand-

ing of the qualitative influence of process conditions on cell size distribution and final product properties.

Flow Behavior of the Foam

The second important property during foaming is flow behavior. A characteristic of foamed components is large thickness variation. Here, advantage is taken of the fact that the initially liquid material can flow well through tiny slits and then later reliably foam large volumes. In this process, the foam initially experiences high shear at temperatures close to the mixing and mold temperature. Later, the foam expands due to being heated by its own heat of reaction but may no longer be sheared too much. Areas subject to high material stress at the relevant point in time are shown in red in the **Title figure**. This information can then help process and material experts prevent problem points in critical areas.

To map this behavior in the simulation, viscosity models are required that take into account the influence of temperature, reaction progress, and local »

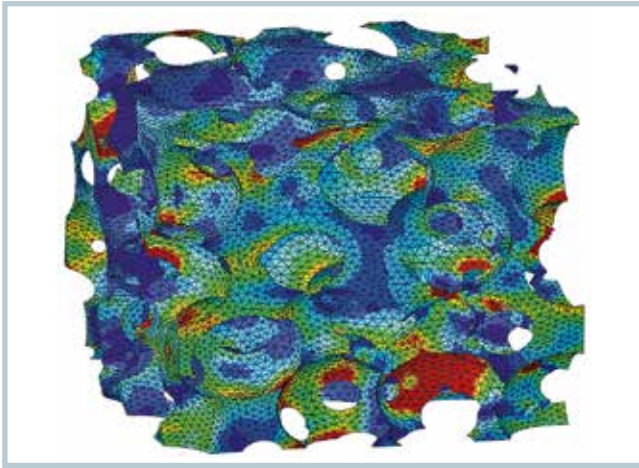


Fig. 3. Local stresses resulting from micromechanical simulation on a foam unit cell. This uses a statistical distribution of gas bubbles for a given density, with the aid of which the elastic modulus of the foam can be predicted (© BASF)

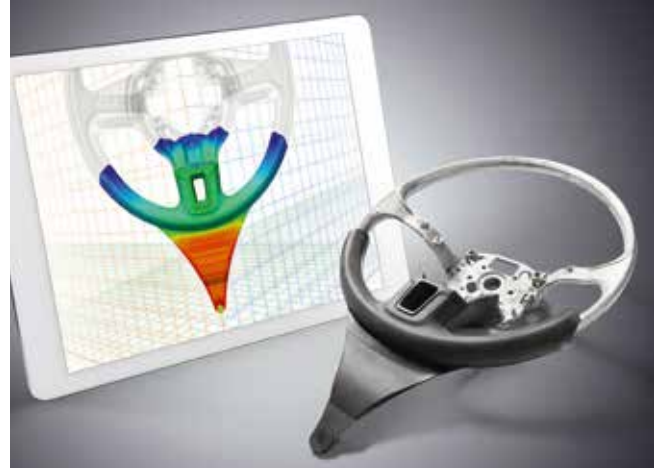


Fig. 4. Filling study to validate the Ultrasim simulation model used for a steering wheel made from an Elastofom I foam. In the simulation and actual trial, both the flow fronts and tiny air inclusions above the center spoke correlate well and confirm the material models and parameters used (© BASF)

shearing. For this purpose, different models are usually combined, e.g. a Carreau equation for shear rate, an Arrhenius equation for temperature dependence, and a Castro-Macosko model for reaction progress. Selection of the appropriate models must be based on the specific behavior of the particular PU foam and the specific requirements of the relevant application. For example, to simulate the foaming of steering wheels, it is essential to know precisely the temperature and shear rate dependence of the liquid material. For dashboards or applications with

low densities and long flow paths, it is usually more important to correctly determine the increasingly elastic behavior of the material at the flow path end.

What all these empirical parameters have in common is a large number of parameters that have either to be determined by measurement [9] or directly fitted so that they can correctly predict flow behavior in a simple component [10]. Another approach is to derive the viscosity of the foam directly from its morphology [7]. This permits, for example, qualitative information to be gained about the influence of shear on foam viscosity in relation to cell structure and the properties of the polyurethane matrix material. As with the micromechanical calculation described above, these rheological analyses must be carried out for a large number of microscopic cell structures in order to parametrize the chosen viscosity model for the component simulation [4].

Simulation of Mold Filling Behavior in the Real Component

If suitable material models are found and reliable material parameters determined, it is possible to adjust the complex foaming behavior in the mold in detail. The filling study in **Figure 4** compares the foam expansion of an Elastofom I foam in a steering wheel geometry as calculated using the BASF Ultrasim simulation tool with filling of a real part. The good cor-

relation of the flow fronts shows that both the reaction kinetics and resulting viscosity increase were modeled accurately. On closer examination, it can be seen that both in the simulation and in the real component filling, tiny air voids occur behind the two lower spokes when the flow fronts unite. These result from the specific combination of component geometry, process parameters, and material properties. The correlation shows that both the process influences and flow behavior of the foam immediately after injection were modeled with sufficient accuracy, including the dependence on processing temperature and material shear.

Conclusion

The models described here show that it is already possible to realistically simulate and predict different properties of polyurethane foams and their processing. This, however, requires deep integration of material models on different scales, efficient numerical methods, and powerful computer resources, as well as continuous further development of simulation methods. The aim with Ultrasim simulation software for polyurethane systems is to offer it as a package to global customers to find new solutions together. This has already proved particularly successful in practical use for the highly complex ElastoflexE and Elastofom I foam systems for automotive interiors. ■

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