Huntsman Polyurethanes
smartLite simulation software

Process optimization by simulation

Understanding material behavior is fundamental to the design of new products. For non-linear materials such as molding plastics, whose properties can vary significantly with temperature, rate and other processing conditions, predictions are particularly complex. Computer assisted engineering (CAE) and simulation software are gaining in importance because they avoid or drastically reduce the traditional trial-and-error phase on the machine, which can be time-consuming and expensive.

Huntsman Polyurethanes is actively pursuing modelling and simulation work for product development. For smartLite®, a range of blown thermoplastic soling materials, the company initially offered an in-house simulation service to customers. Underlining its commitment to the footwear industry, a user-friendly software package was made available as part of the comprehensive smartLite offer, enabling sole designers and molders to do their own simulation work. The new tool is the result of a collaboration between Huntsman and Simcon, a German company specializing in software for injection molding, cost calculation and CAE services.

New material, new process technology

smartLite is an innovative soling technology that combines the performance benefits of thermoplastics with the comfort and reduced weight of a microcellular structure. The pelletized smartLite materials contain a mix of dissolved blowing agents which is released during the injection molding process. “It’s a proprietary combination of blowing technologies which is neither of the classical physical nor the classical chemical type,” says Jan Vandenbroeck, of Huntsman’s Modelling and Simulation Department at Everberg, Belgium.

.../

During processing, the injection mold cavity is filled only partially with the material. After the gate is closed, the gas diffuses out and expands the melt to fill the remainder of the space. This thermoplastic blowing
mechanism creates spherical bubbles and leads to a microcellular structure which is quite different from flexible or rigid polyurethane foams. The open or closed cell matrix of such two-component systems is characterized by “struts” and “windows” influenced by the reaction and polymerization process.

**Bubble growth**

With smart\textit{Lite}, the growth of the gas bubbles is influenced by the pressure, temperature and viscosity of the melt. Other parameters such as injection speed and the amount injected can also be varied. It is obvious that different filling amounts will influence the final result, because bubble size and gas pressure inside the bubbles will be different.

Bubble growth is of major importance for achieving lower densities to minimize the use of raw materials while preserving excellent physical properties. Density distribution and bubble size are important for the quality of the molded part, as is the pattern of mold filling.

Huntsman's innovation and knowledge around smart\textit{Lite} centers on taking advantage of this bubble growth and controlling it with the help of computational fluid dynamics (CDF). Injection molding with the additional factor of expansion, however, makes it much more complicated to calculate the flow dynamics.

**Pioneering development**

While mold filling analysis is an established optimization aid for compact injection materials, so far no commercial software was available for simulating the processing of thermoplastic foams.

So the simulation tool for smart\textit{Lite} required new developments in mold flow analysis based on detailed research into how the melt flows while expanding and how the bubbles influence the flow of the material. A whole new model for this type of blown soling material had to be developed.

In its research project focusing on this preliminary scientific work Huntsman co-operated with the renowned Institute for Plastics Processing (IKV) at the Technical University of Aachen, Germany.

.../

**New model needed**
Modelling the behavior for novel materials entails mathematics, physics and chemistry. It starts by asking about the laws applying to this type of material, the type of equations that could be used for the assumptions to predict, in this case, the bubble growth and melt flow, and the kind of material data and process interactions that need to be measured to make this model work. It is the accuracy of the assumptions and the practical data measured that will determine the quality of the simulations.

The theory and equations that make the simulation run and predict the flow correctly for this type of material then need to be written into code (programming language), so that it can be tested and evaluated.

Finally, in order to provide customers with a tool they can easily work with, the translated, process-oriented module had to be linked to a user-friendly visual interface. “As our core competencies are polyurethane chemistry and materials, we turned to Simcon for implementing the smartLite module,” says Vandenbroeck.

Founded in 1988, Simcon is one of the pioneers of simulation software for injection molding and has a long experience in this field with compact thermoplastics. The company also sells cost calculation software for parts and molds and offers rheological, thermal and structural mold and part optimization as a service. Based in Herzogenrath near Aachen, Simcon’s team of plastics engineers, mathematicians and software developers is also collaborating closely with the IKV.

Modelling details
smartLite modelling consisted of three elements: a model for bubble growth, a model for flow simulation and the linking of both. The bubble growth model is described by two differential equations: one for the growth of the bubbles in the molten polymer for a given bubble gas pressure and one for the diffusion of the gas out of the melt into the bubble.

For flow simulation, the 2.5D midplane modelling for compressive flow behavior from Simcon’s Cadmould program was used. The 2.5D method is well suited for thin-shell parts such as soles that require relatively short analysis times. It avoids the need to apply massive computer power to complex 3D simulations.
The molded part is described by shell elements for this numerical analysis of filling, and calculation is performed on a layer-by-layer basis. The pressure equation is solved by the finite-element method (FEM), and the volume flows are calculated from the pressure gradient. Different viscosity models can be used.

To couple both models, the change in density due to bubble growth is entered into the continuity equation. Changes in the specific heat conductivity, the specific heat transfer and the rheological properties of the material are taken into account.

**Validation**

The accuracy of the smartLite modelling and software was verified by a series of tests and experiments. They have shown that the simulation tool accurately predicts the filling behavior and the density/bubble size distribution of these blown thermoplastic materials during injection molding.

The influence of variations in processing conditions (melt temperature, injection time), design or rheological parameters (concentration of blowing agent) can be readily analyzed with the simulation.

**Easy-to-use software**

The new modelling tool, devised and owned by Huntsman and “powered” by Simcon’s Cadmould program, has a user-friendly visual interface. The customer’s geometry data can be imported from almost any CAD system. The software automatically creates a finite-element mesh and runs on standard PCs under Windows®.

**Advantages**

Simulation allows for quick and cost-saving assessments early in part and mold development. In the past, designing a mold meant trial-and-error. With computer modelling customers can focus their trials and save considerable time on optimization.
With the software you can deduct the best filling pattern and injection points. You can also check in advance the potential maximum pressure of the system and devise the optimum filling degree without any or too much overpacking. It also allows to determine the best locations for venting, an important aspect, as air compression in the cavity can cause burner marks or so-called “dieseling.” With two injection points, critical locations of the welding line (i.e. where the flow fronts meet) can easily be prevented. It also helps to reduce scrap and optimize production cycles by assuring worry-free processing.

Simulation gives customers a clear idea of the variation possibilities before cutting in metal. By allowing molders to test a number of critical factors and make adjustments to the tooling or part it will facilitate new developments and reduce time to production and market.

-ENDS-

Jan Vandenbroeck, Modelling and Simulation Department
Huntsman Polyurethanes, Belgium;
Phone +32 2 758 9551 Fax +32 2 758 9062
jan_vandenbroeck@huntsman.com

Dr. Paul F. Filz, Managing Director,
Simcon kunststofftechnische Software GmbH, Germany;
Phone +49 2407 908580 Fax +49 2407 9085858
pfilz@simcon-worldwide.com

For further information, please contact:
Huntsman Polyurethanes
smartLite® team
Everslaan 45
B-3078 Everberg
Belgium
Fao : Bart Van Edom
E-mail : bart_van_edom@huntsman.com
Tel: + 32 2 758 9601
Fax: + 32 2 758 7601

Editors’ notes
Huntsman is a global manufacturer and marketer of commodity and differentiated chemicals. Its operating companies manufacture basic products for a variety of global industries including chemicals, plastics, automotive, aviation, footwear, paints and coatings, construction, technology, agriculture, health care,
textiles, detergent, personal care, furniture, appliances and packaging.

Originally known for pioneering innovations in packaging, and later, rapid and integrated growth in petrochemicals, Huntsman today has revenues of $11.5 billion, 11,300 employees and 62 operations in 22 countries. The world's most significant and essential industries rely on Huntsman businesses to manufacture basic products for a variety of end-use applications.

Statements in this release that are not historical are forward-looking statements. These statements are based on management's current beliefs and expectations. The forward-looking statements in this release are subject to uncertainty and changes in circumstances and involve risks and uncertainties that may affect the company's operations, markets, products, services, prices and other factors as discussed in the Huntsman companies' filings with the Securities and Exchange Commission. Significant risks and uncertainties may relate to, but are not limited to, financial, economic, competitive, environmental, political, legal, regulatory and technological factors. Accordingly, there can be no assurance that the company's expectations will be realized. The company assumes no obligation to provide revisions to any forward-looking statements should circumstances change, except as otherwise required by securities and other applicable laws.

smartLite® is a registered trademark of Huntsman International LLC in one or more, but not all, countries.