FLUID DYNAMICS

Achieving the Perfect Flow

Thanks to a new process, Bayer MaterialScience now consumes 60 percent less energy for the synthesis of toluene diisocyanate (TDI). Fluid dynamics engineers from Bayer Technology Services helped with the modeling of the new reactor.

On the yellow sign attached to the lattice fence it says “Sprudelstand” in German, which indicates an air-water bubble test facility. After entering the gate next to the sign, you will suddenly find yourself at the foot of a massive transparent plastic pipe, which juts vertically some 10 meters into the air. Bubble tests have clearly not taken place here for quite a long time. Most recently Bayer Technology Services mainly used this apparatus at the Chempark Leverkusen for mixing tests with gases.

Dr. Volker Michele is one of the people who is responsible for performing such bubble tests. The fluid dynamics engineer works in Reaction Engineering & Catalysis at Bayer Technology Services. His expertise comes into play when, for example, someone in the Bayer Group wants to know how two reaction components will mix with each other in a reactor.

Michele points to the upper end of the facility structure. “Up there, we have two inlets through which air is fed into the pipe. We then observe how the two streams of air mix together along the pipe.” The fluid dynamics engineers make use of a trick to allow the two streams of air to become viewable: mist is mixed into one air stream so that it is easily visible to the naked eye. With a camera Michele and his team then record the trails of mist left in the pipe. However, that is not all they can see. The short white wool threads attached to the inside wall of the pipe also provide important information. During the experiment their free ends flutter with the airflow. If the threads do not angle downwards properly, it is a sure sign that something has to be changed in the mixing configuration.

These tests, performed with simple air as a substitute for other components in normal ambient temperatures, are called cold-flow experiments. For fluid dynamics engineers like Michele such an experiment is an important tool in his work. The plastic pipe represents a reactor, and the airflow will show him how the two gaseous reaction partners will later behave in the reactor.

Something similar was the very assignment of a project with Bayer MaterialScience. They had the idea to change the final reaction step of the multistage TDI synthesis, which until now had been performed in a liquid solvent. The plan was to have the reaction partners come together in gaseous state instead. The advantage is clear: since the solvent does not have to be distilled off after the process is completed, one can save a lot of energy compared with the previous method – as it turned out, up to 60 percent. With a savings of this magnitude, weighing the pros and cons is clearly unnecessary! However, implementing the plan was

Material for Foam

The Bayer MaterialScience plant in Shanghai will have the capacity to produce 250,000 metric tons of toluene diisocyanate (TDI) per annum. Adding this to the capacities of its TDI plants at other sites around the globe, the company is among the world’s biggest producers of this important starting material for the production of polyurethane foams. Among the areas of applications are mattresses and upholstered furniture, shoe manufacturing as well as the textile and automotive industries. TDI production capacities worldwide are currently more than two million metric tons per annum.

For modeling on his computer, fluid dynamics engineer Dr. Volker Michele also relies on a practical experiment: the air-water bubble test performed here in Leverkusen.

"We consider what individual chemical reactions can take place, what materials can form and then disappear again and, above all, what kind of influence this can have on the respective situation in the reactor."

Dr. Volker Michele, Bayer Technology Services

Checking the Flow

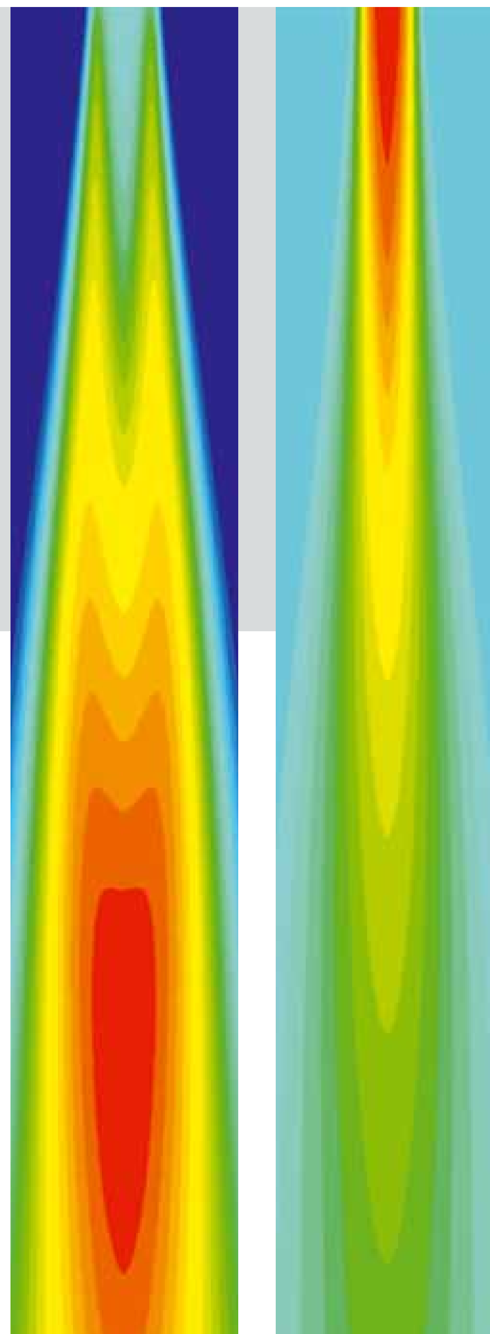
The Fluid Dynamics team at Bayer Technology Services is concerned with everything that goes into reactors – regardless of whether it is gaseous, liquid or solid. Using a computer and the appropriate data, the fluid dynamics engineers can simulate, for example, at what point in the course of a reactor it comes to what chemical reactions, as well as how temperature and pressure change in the process. The computer simulation produces pictures like the two adjacent illustrations that depict the joining together of reaction partners. The color gradients show the different speeds (right) and temperatures (left) in the mixing zone.

The work of fluid dynamics engineers involves not only new plants, such as the TDI project in Shanghai or the carbon nanotube production unit that began operations in 2010. The continuous improvement of existing facilities is also among their responsibilities. Depending on the particular case, the focus may be optimizing mixing processes, or it can often be a matter of improving separating and refining processes.

far from easy. It took more than 10 years for the general idea of a gas-phase reaction to culminate in the construction of an actual facility. This summer Bayer MaterialScience will commission its first TDI plant in Shanghai based on this new technology (*see also technology solutions 1/2010, page 30*).

Although Michele has never been in Shanghai, he definitely put his mark on the new production plant. The reactor geometry and process control are largely the result of his work. In addition to the cold-flow experiments, he needed the computer in his Leverkusen office – and the right data for computer calculations.

There are several critical issues to be considered if you want to produce TDI in the gas phase. One important aspect is that the two reaction partners do not react immediately to form TDI. An intermediate stage forms at first, after which TDI then develops in a second step. Consequently, the length of the reactor should not be too short, because otherwise the reaction time will not be sufficient to proceed beyond the intermediate stage. On the other hand, if the reactor should be too long, byproducts can develop, which would then have to be separated painstakingly from the desired main product.



Complex proceedings inside the reactor: each color stands for a different temperature (left) or a specific speed (right).

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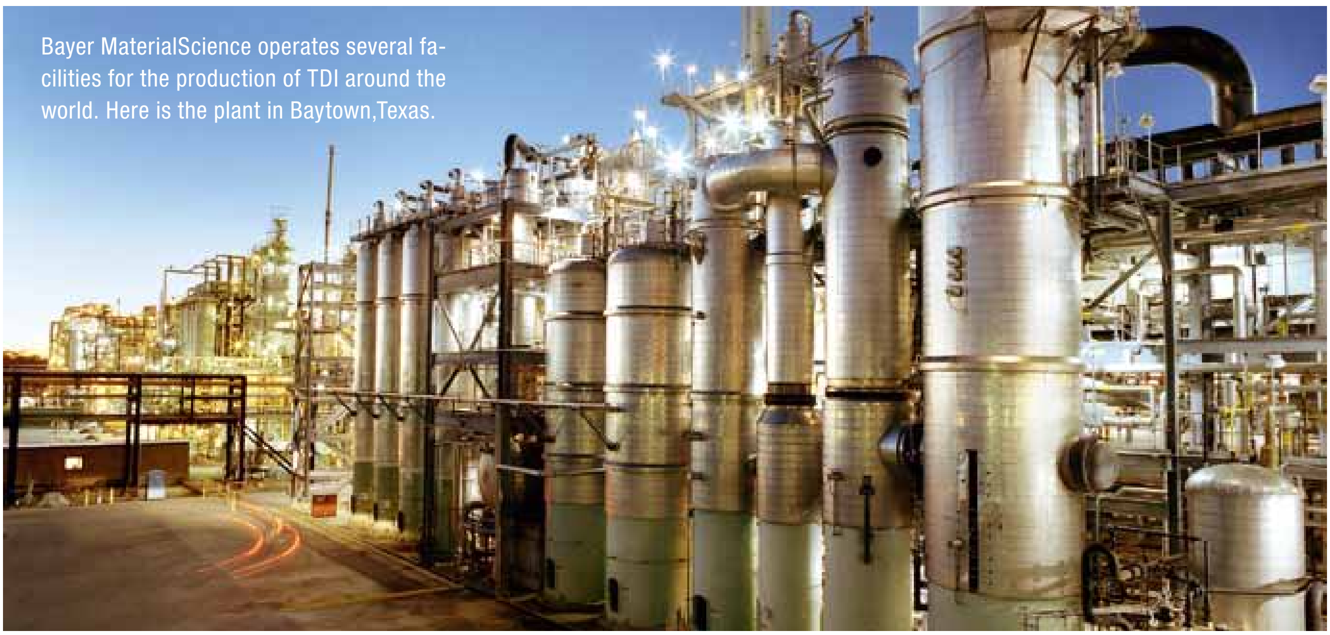
Dr. Steffen Kühling, Bayer MaterialScience



Bayer MaterialScience operates several facilities for the production of TDI around the world. Here is the plant in Baytown,Texas.

The idea is to design a reactor and its process conditions, such as temperature, pressure and mixing intensity, so that as much TDI as possible is ultimately produced at the end of the reaction route.

Considering all this complexity, Volker Michele cannot rely alone on cold-flow experiments. All sorts of computations are also necessary in order to realistically simulate the processes in the reactor. “In such cases we carefully consider what individual chemical reactions can take place, what materials can form and then disappear again and, above all, what kind of influence this can have on the respective situation in the reactor.” After all, some of these reactions are accompanied by volume expansion and can also release a lot of heat. Both these factors will change the conditions in the reactor.

From his colleagues working in Kinetics, Properties & Modeling, Michele received the kinetic data covering all conceivable reactions and substances intermittently occurring in the reactor. He fed these data into his Computational Fluid Dynamics model and let the computer make the calculations. He specified reactor geometry and varied, for example, the temperatures and flow rates for the starting materials. The software then delivered copious data sets on, for example, the distribution of temperature in the reactor or the concentration fields of the individual components. In this way, he was eventually able to deduce the optimal conditions.

Dr. Steffen Kühling, Head of Production & Technology Isocyanates at Bayer MaterialScience, is particularly pleased with the work done by Volker Michele and his colleagues. “You do not very often find this combined know-how in both cold-flow experiments and computational fluid dynamics,” says Kühling. “As a consequence, Bayer Technology Services was a particularly helpful partner in this project.”

Friedhelm Steffens agrees. At the Isocyanate Technology Center of Bayer MaterialScience he shares responsibility for implementing innovation in TDI production processes. Although the gas-phase reaction had never been realized in a plant of such dimensions, Steffens was absolutely convinced it was going to be a success even before the start-up in Shanghai. So, his department has long been thinking ahead and is striving to introduce the new process at other TDI production sites because of the enormous energy savings. “As the next step, we are planning a similar facility in Dormagen,” Steffens said.