Computer Simulation Helps Solve Difficult Flow Problem in Fixed Bed Catalytic Reactor

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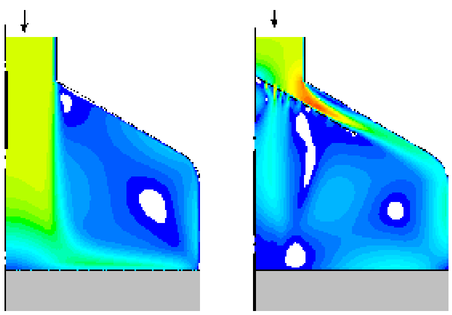

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Computer simulation helped solve a difficult flow problem in a fixed bed catalytic reactor in two days. The reactor performance was considerably below expectations and studies had revealed that catalytic particles had been dispersed to the outer edges of the reactor, presumably by a strong eddy located above the fixed bed surface. Engineers tentatively planned to install a deflector to lower the velocities parallel to the surface of the fixed bed. But they hedged their bets by simultaneously commissioning a computational fluid dynamics simulation of the reactor. The simulation showed that the planned deflector would actually reverse the problem by pushing the particles into the center of the bed instead of pushing it to the outer edges. After several iterations of analysis, a new design for the deflector was developed that evened out the flow distribution and solved the problem.

Degussa has its origins in the refining of precious metals. Today, the focal point of the company's activities is in the chemicals sector, and Degussa is one of the leading chemical companies worldwide. Degussa's products are mainly specialities and occupy leading positions in their respective markets. The products are grouped into the three segments of Chemical Products, Health and Nutrition and Precious Metals and Banking. Among the products in the Chemical Products segment are hydrogen peroxide, rubber chemicals and pigments, silicas and chemical catalysts and the polymers. The Health and Nutrition segment holds the dental products, pharmaceutical products and additives for animal feed.

Horizontal velocity

The reactor mentioned above is 4 meters in diameter and has a gas inlet located centered above a fixed particle catalyst bed. Engineers were fairly certain, even prior to performing the CFD analysis, that the problem was caused by gas entering the inlet, moving directly to the center of the bed, and, when deflected by the bed, generating horizontal velocities that forced the particles to the sides of the bed. Installing a flow deflector between the gas inlet and the particle bed seemed a promising idea but engineers recognized the potential pitfalls. They had no way of knowing, besides guessing, what the existing flow patterns were inside the bed, nor what impact the deflector would have on these patterns.

They were concerned that the problem might remain even after installing the deflector. They needed quick answers because each day of non- performance would cost money.

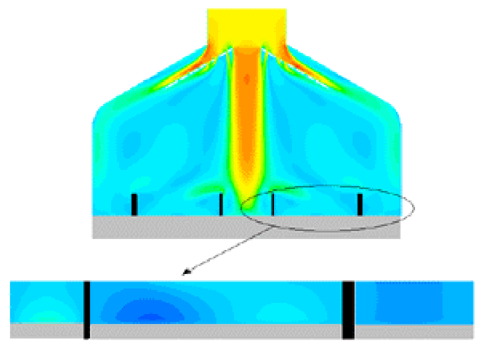
Engineers decided to approach the simulations center, which offered an evaluation between the different design alternatives by using computational fluid dynamics (CFD). CFD produces solutions for problems with complex geometries and boundary conditions. A CFD analysis provides fluid velocity, fluid temperature and fluid concentration values throughout the solution domain.

The results of the analysis allow an engineer to optimize fluid flow patterns or temperature distributions by adjusting either the geometry of the system or the boundary conditions such as the inlet velocity/temperature, wall heat flux, etc. CFD also can provide detailed parametric studies that can significantly reduce the amount of hardware experimentation necessary to develop a prototype and thus reduce design cycle times and costs.

CFD software selection

The company currently uses FLUENT CFD software (Fluent Inc., Lebanon, New Hampshire) after a selection process that involved careful consideration of the leading products available. One reason was the ease of use of Fluent. The program offers a graphical user interface that simplifies model building and definition of boundary conditions. All modules of the program are integrated into the interface, reducing learning time and making it possible to switch to any module with a single mouse click. The other reason for selecting FLUENT is its good combustion models which, although they were not used in this problem, are frequently used in other applications at Degussa. A very useful feature of the software is the modeling of diffusion flames by probability density functions (PDF). As a result, the concentration of all major flame components like oxygen, carbon dioxide and water are determined but in addition any type of radical byproduct can be calculated. When we compared FLUENT against the other leading CFD vendor on a reference case, we found that the FLUENT software predicted temperatures quite accurately while the competitor, also using a pdf-model, was about 1000K too high.

We analyzed the fixed bed reactor using this software on a Digital Equipment Alpha workstation with 512 MB RAM and began by analyzing the existing reactor configuration. The particle bed was modeled with the use of porous cells that provide a specified resistance for a fluid flowing through them. The analysis results confirmed that the high velocity gas entering the reactor established eddy currents that moved the catalyst to the sides of the reactor. Next, we added the proposed deflector design to the model. The proposed deflector is shaped like a Chinese hat with an angle of 135 degrees and placed close below the gas inlet. The analysis showed that the deflector reversed the direction of the eddy current and didn't



Engineers chose a deflector configuration with a 40 cm hole. After2 weeks of running the reactor, visual proof showed that the bed hadn't moved.

improve the problem. The fixed bed particles would have been pushed to the center of the reactor.

Design alternatives

Following this, we considered a number of alternative deflector designs. An obvious solution was an opening in the central region of the deflector in order to split the incoming gas stream into two parts: one entering the reactor in the center as before and the other part coming from the outer edges and equilibrating the eddy current from the center stream. It all concentrated on one question: How big should the hole be? The target was the minimization of the velocities parallel to the fixed bed surface in order to immobilize the pellets of the fixed bed.

The time required to perform this part of the analysis was greatly reduced by a FLUENT feature that allows cells to be toggled between obstructions or clear areas simply by clicking on them with a mouse. This made it possible for us to quickly alter the size and shape of the opening in the deflector and re-run the analysis. After about 10 iterations, we found a deflector configuration with a 40 cm hole that provided optimum results. In addition to that measure two cylindrical rings were put into the bed with approx. 0.1 m sticking out of the bed. The diameter of the rings was also optimized. The optimized design was used for the reactor and after 2 weeks of running the reactor visual proof was given that the bed hadn't moved.

The success of this and other applications has deepened the trust in CFD at Degussa. We use CFD on a wide range of chemical applications. In many of these applications, FLUENT/UNS is used, a version of the software that creates an unstructured mesh, making it possible to model complicated geometries in considerably less time. While the company's researchers are capable of handling problems of great complexity, manpower limitations lead us to concentrate on problems with shorter project times. The success of these applications, which have had an economic impact orders of magnitude higher than the cost involved in the analysis, convinced management to recently approve a plan to increase staffing for CFD analysis.