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Optimize terephthaldehyde reactor operations

Korea's largest chemical company uses innovative modeling techniques to design high-performance reactors

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Research teams applied a hybrid modeling approach when simulating the numerous chemical reactions to manufacture terephthaldehyde (TPAL). This case history explores how computational fluid dynamic (CFD) and advanced process modeling (APM) methods are used in combination to optimize the multitubular fixed-bed catalytic reactor at the heart of the TPAL process.

Background. LG Chem, Ltd., Korea's largest chemical company, needed to design two high-performance multitubular reactors for two different petrochemical processes. At the heart of the processes was a multitubular fixed-bed catalytic reactor. This unit is complex and involves many different phenomena that must be considered simultaneously during engineering design.

The only way to do this rigorously and reproducibly is to execute a detailed predictive model of the unit. CFD models of both reactors were available, but the design team recognized that the combination of catalytic chemical reactions on the tube side with complex shell-side fluid dynamics is a problem that cannot be addressed by CFD techniques alone.

LG Chem used a hybrid modeling approach for the designs. This involved coupling a commercial CFD package to model the fluid dynamics on the shell side, and an advanced process modeling tool to model the catalytic chemical reactions and related phenomena on the tube side. These models were executed simultaneously; each model calculating key input information for the other program.

The detailed predictive hybrid model allowed the design team to rigorously quantify the effects of changes to key design variables on critical performance indicators such as the shell-side temperature profile. For example, it was possible to investigate the effects of changes to the baffle geometry on aspects such as the temperature profile at the center of various tube centers, tube wall heat transfer coefficients, temperature rise in the cooling medium, pressure drop in both shell and tube side, concentration profile of each chemical species along the tube and final conversion in each tube.

Both reaction processes were commercially important. Case 1 involved enhancing a very complex existing design to obtain optimized operation in a new plant. The resulting advanced high-performance reactor design achieves significant improvements in uniformity of operation across the tube bundle, leading to improved conversion, better controllability and longer catalyst life. Case 2, the main focus of this article, involved development of a similar but less complex high-performance reactor for a low-cost production TPAL.

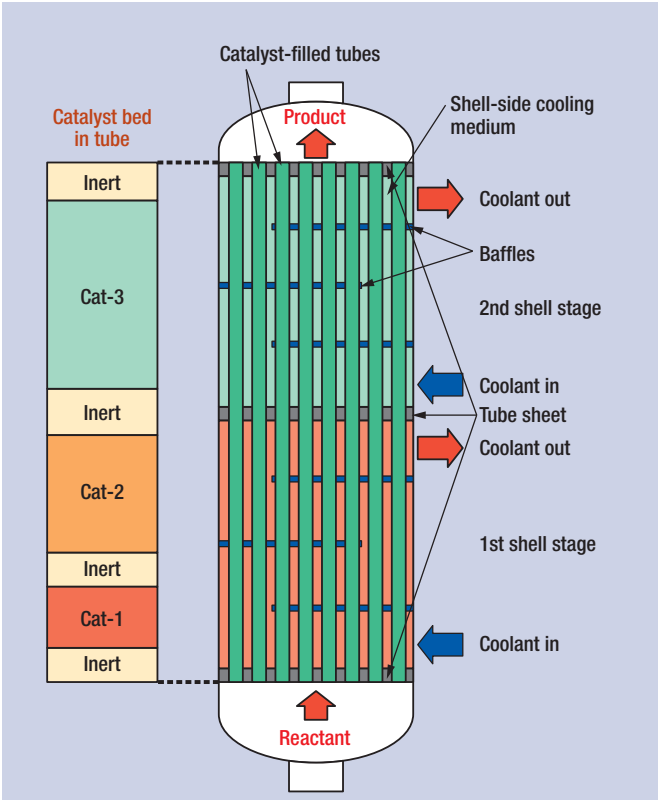

FIG. 1 Typical multitubular configuration showing multiple shell compartments and catalyst packing sections.

TPAL process. TPAL is a promising intermediate for various polymers, such as liquid-crystal, electron conductive polymer and specialty polymer fibers. It also serves as the starting material for fine chemical derivatives including cyclohexanedimethanol and

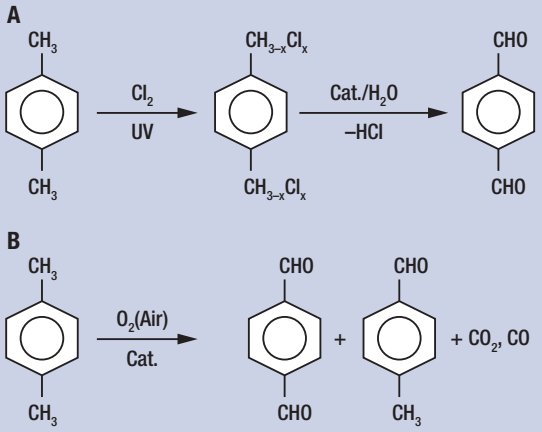

FIG. 2 a. The current commercial process for TPAL production (x = 1 or 2).
b. The process of selective oxidation of p-xylene to TPAL and PTAL.

p-hydroxymethylbenzoic acid and is the primary raw material in production of fluorescent whitening agents. However, despite the extensive possibilities for TPAL applications, its range of use is limited by high production costs.

The selective oxidation of p-xylene to TPAL has been one of the key recent challenges in selective-oxidation catalysis. The commercial process for TPAL production (Fig. 2a) involves two steps: chlorination of p-xylene and hydrolysis of chlorinated xylenes. This method inevitably involves chlorine (Cl_2) and hydrochloric acid (HCl)—both have toxic and corrosive properties and are undesirable from a process safety and environmental standpoint. These compounds add to the complexity of the process and are dominant factors on the high price of TPAL.

For these reasons, significant efforts were made to develop a selective oxidation process using heterogeneous catalysts, with p-xylene and air as reactants (Fig. 2b). However, the yield of TPAL was too low, and the thermal stability of metal oxide catalysts—required for high selectivity of the TPAL reaction—was not sufficient for viable commercialization.

Following extensive catalyst screening, coupled with molecular modeling, new tungsten oxide-based binary and tertiary catalysts can provide high performance in the selective oxidation of p-xylene to TPAL.[1–3] Fig. 3 is an abridged reaction set for TPAL.

This new catalyst can provide excellent thermal stability, and can possibly facilitate potential continuous mass production of high-purity TPAL at low manufacturing cost.

With the new catalyst system, process development projects began investigating a multitubular reactor (MTR) and separation and purification steps for TPAL production. The reactor design developed uses a state-of-the-art hybrid modeling approach.

Multitubular reactors. MTRs are widely used throughout the petrochemical/chemical and refining industries for fixed-bed catalytic reactions. However, their operation is highly complex and difficult to achieve. An MTR can contain numerous—sometimes 20,000 or more—catalyst-filled tubes within a shell. Typically, each tube is packed with several grades of catalyst and inert to control the reaction, or different types of catalyst to promote different reactions in different sections of the tube. The shell can be divided into multiple compartments, each maintained at a different average temperature to maintain the correct temperatures within the corresponding section of the tube. Fig. 1 shows a typical MTR configuration.

KEY REACTIONS

1. $C_6H_4(CH_3)_2 + O_2 \rightarrow C_6H_4CH_3CHO + H_2O$
2. $C_6H_4(CH_3)_2 + 2O_2 \rightarrow C_6H_4CHOCHO + 2H_2O$
3. $C_6H_4CH_3CHO + O_2 \rightarrow C_6H_4CHOCHO + H_2O$
4. $C_6H_4CH_3CHO + {}^{11}\!/_{2}O_2 \rightarrow 8CO + 4H_2O$
5. $C_6H_4CH_3CHO + {}^{19}\!/_{2}O_2 \rightarrow 8CO_2 + 4H_2O$
6. $C_6H_4CHOCHO + {}^{9}\!/_{2}O_2 \rightarrow 8CO + 3H_2O$
7. $C_6H_4CHOCHO + {}^{17}\!/_{2}O_2 \rightarrow 8CO_2 + 3H_2O$
8. $C_6H_4(CH_3)_2 + 2O_2 \rightarrow C_6H_5CHO + 2H_2O + CO$
9. $C_6H_4(CH_3)_2 + {}^{5}\!/_{2}O_2 \rightarrow C_6H_5CHO + 2H_2O + CO_2$
10. $C_6H_4(CH_3)_2 + {}^{5}\!/_{2}O_2 \rightarrow C_6H_4CHOOH + 2H_2O + CO$
11. $C_6H_4(CH_3)_2 + 3O_2 \rightarrow C_6H_4CHOOH + 2H_2O + CO_2$
12. $C_6H_4(CH_3)_2 + {}^{13}\!/_{2}O_2 \rightarrow 8CO + 5H_2O$
13. $C_6H_4(CH_3)_2 + {}^{21}\!/_{2}O_2 \rightarrow 8CO_2 + 5H_2O$
14. $C_6H_5CHO + {}^{9}\!/_{2}O_2 \rightarrow 7CO + 3H_2O$
15. $C_6H_5CHO + 8O_2 \rightarrow 7CO_2 + 3H_2O$
16. $C_6H_4CHOOH + 4O_2 \rightarrow 7CO + 3H_2O$
17. $C_6H_4CHOOH + {}^{15}\!/_{2}O_2 \rightarrow 7CO_2 + 3H_2O$

KEY COMPONENTS

$C_6H_4(CH_3)_2$	: p-Xylene
C_6H_5CHO	: Benzaldehyde
$C_6H_4CH_3CHO$	: p-Hydroxybenzaldehyde
C_6H_4CHOOH	: p-Tolualdehyde
$C_6H_4CHOCHO$	: Terephthaldehyde

FIG. 3 Abridged reaction set for p-xylene → TPAL.

The reactions within the tube catalyst beds are strongly exothermic throughout. To guarantee stable operation and high productivity on a commercial-scale plant, detailed modeling is highly recommended to define the interactions between the shell and tube sides early in the detailed design stage.

High-accuracy hybrid modeling can bring significant design and operational benefits. For example, it can help ensure an appropriate axial temperature profile that favors the reactions occurring at the corresponding tube locations, and maintain a uniform temperature profile across the tube bundle; thus, all tube-side reactants "see" similar temperatures.

Good temperature distribution enables higher overall operating temperatures, greater conversion and throughput, and longer catalyst life. It also reduces the likelihood of hot-spot formation and consequent progressive catalyst burnout that results in poor conversion and controllability, and early catalyst replacement.

A good design is thus achieved by adjusting key aspects of the shell-and-tube bundle geometry to provide *optimal heat control* within the shell-side fluid. The goal is to eliminate danger areas where hot spots (areas of significantly higher temperature than their surroundings) can occur.

To achieve this operating mode, it is necessary to accurately

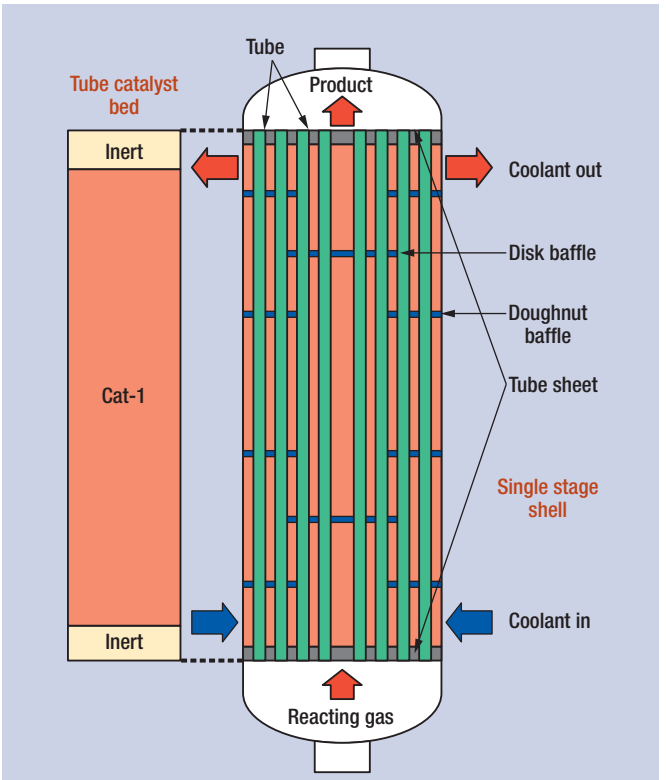

FIG. 4 TPAL multitubular reactor configuration.

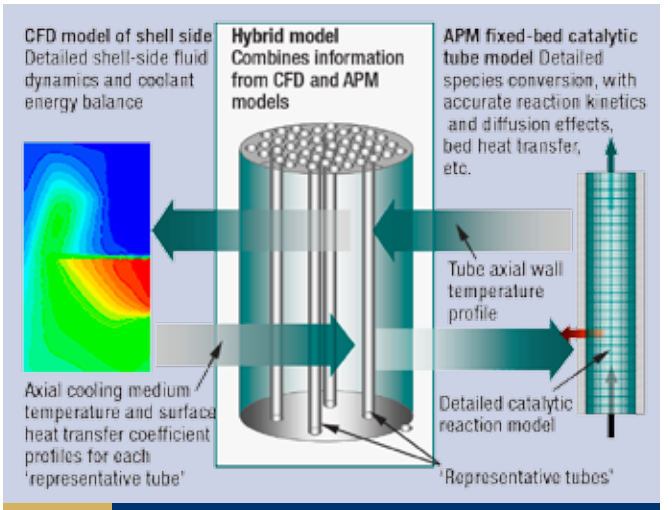

FIG. 5 Schematic of the hybrid modeling architecture applied to multitubular reactors.

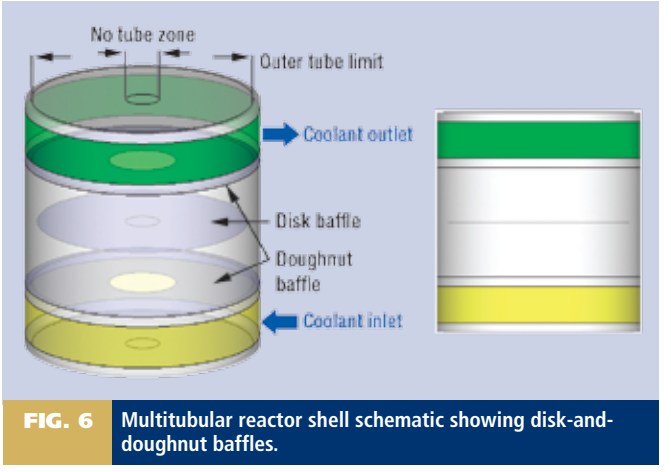

FIG. 6 Multitubular reactor shell schematic showing disk-and-doughnut baffles.

quantify heat transfer at all points throughout the reactor. This requires performing fluid dynamics analyses on the shell side to accurately calculate heat transfer coefficients. The reactions occurring in the tubes (which are affected by fluid temperature) are also investigated to calculate the correct tube-wall temperatures for the unit heat-transfer calculation. The two effects must be considered simultaneously.

MTR for the novel TPAL process. The geometry of the multitubular fixed-bed catalytic reactor for the new TPAL process is simple. It comprises a single shell compartment with 5,000 tubes filled with a single catalyst, suitable for a reaction with low heat release and small production target. Overall reactor geometry is similar to that of conventional shell-and-tube type heat exchangers, but with no tube zone in the center of the reactor. The reacting gas enters at the bottom of the unit.

The shell structure and coolant conditions are designed to ensure the optimal temperature conditions for the main chemical reactions in the tube-side catalyst bed. Coolant flow in the shell is channeled by doughnut-and-disk type baffles located alternatively along the length of the reactor. The size and positioning of these internal structures are critical. Incorrect decisions can lead to poor reactor performance. Indeed, this study showed that reactor performance was very sensitive to certain changes in the internal dimensions, a fact that could not have been recognized by using conventional design methodologies.

Quantification of the detailed effects of internal geometry changes on MTR performance is usually extremely difficult, if not impossible. However by using the hybrid modeling method approach, the design team was able to determine the effects of even the smallest changes to the reactor internals.

Hybrid modeling method approach. Both projects involved creation of a high-fidelity model that coupled a commercial CFD package with a commercial advanced process modeling (APM) and simulation tool. The high-accuracy predictive models required for successful MTR design can result in a numerical solution involving simultaneous solutions of hundreds of thousands or even millions of equations. It is essential that modeling tools are used in imaginative and innovative ways that make the most of their respective computational strengths. The ability to obtain high-accuracy predictive results in a manageable timeframe is the key justification for the hybrid modeling approach.

The hybrid CFD-APM approach makes it possible to consider various micro-scale phenomena in the tube side, such as chemical reaction, adsorption, mass and heat transfer in the catalytic beds (including intra-particle diffusion and reaction), heat transfer resistance at the bed-wall boundary, and macro-scale fluid mechanics in the shell side, such as coolant flow distribution and heat transfer in complicated geometries *at the same time*.

Models that do not consider all of these effects cannot be fully predictive, and thus run the risk of resulting in erroneous analysis and nonoptimal or even unsafe designs. Examples of this approach used APM hybrid simulation to troubleshoot runaway reaction in an existing multitubular catalytic reactor.[4,5] The approach has

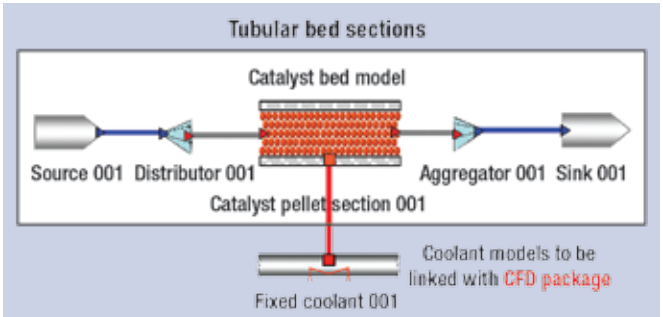

FIG. 7 Tubular bed model for Case 2; in Case 1, many such sections were linked together, each containing a different catalyst or inert.

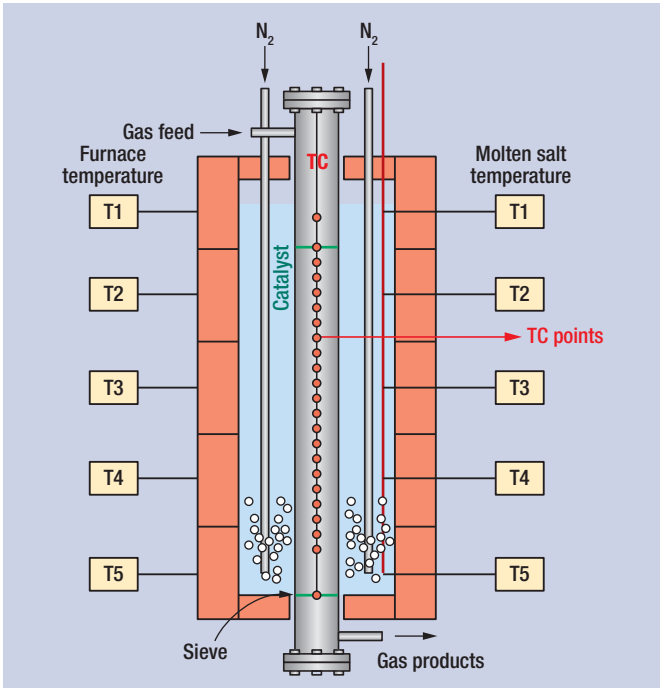

FIG. 8 Single-tube experiment setup for collecting accurate temperature profile and concentration information prior to parameter estimation.

subsequently been applied to numerous partial oxidation reactor designs, as well as Fischer-Tropsch gas-to-liquid production. A similar approach was also adopted for the modeling of an industrial crystallization process and for modeling of aerobic bioreactors to consider close interaction between fluid flow and the biological reactions.[5,6] The hybrid model architecture approach is shown in Fig. 5. A commercially available interface communicates information between the CFD and APM models.

CFD model. The TPAL design project applied a three-dimensional CFD reactor model for the shell compartment with doughnut-and-disk type baffles as shown in Fig. 6. To decrease computation load and time, the geometry is simplified by excluding ducts and slits for providing coolant during the initial screening exercise. These were applied later to the most promising design candidates.

The tube bundle is represented as a porous medium, and the entire zone of the tube bank is declared as a single thread of cells. The meshed geometry for the TPAL reactor contained about 500,000 quadrilateral cells.

Advanced process model. For the tube-side calculations, the configuration of a two-dimensional single-tube model was constructed as illustrated in Fig. 7. It used customized versions of library models for fixed-bed catalytic reactors.[7] The library models contain first-principles models of the fundamental chemical phenomena including diffusion of reactants and products between bulk fluid and catalyst and intra-particle diffusion. They also contain accurate relationships for internal-bed heat transfer and bed-to-wall heat transfer. The distributor and aggregator models convert scalar component compositions and flow into radially distributed values and vice versa. The library models were extended to include thermal oxidation reactions occurring simultaneously with standard catalytic reactions.

Typically, multiple tube sections are used to model the different sections of catalyst and inerts along the length of a single tube. The effect of different catalyst profiles can be studied simply by varying the dimensions of the tube section models. However, this was not required in the TPAL reactor case, which uses a single catalyst throughout.

Model validation. Before connecting the process and CFD models, it is important to determine the most accurate possible values for all key parameters in the reaction model by applying formal model-based parameter estimation techniques to experimental data. This is known as *model validation*.

For MTRs, model validation typically involves mathematical optimization of the kinetic model for catalytic reactions occurring in a single tube and to determine the parameters that most closely match the observed steady-state or dynamic experimental data. Experiments must be conducted under closely controlled, preferably isothermal conditions, thus ensuring that the effects of most interest are isolated. If correctly done, the parameters determined in this way will be valid for all scales of operation in a way that can never be achieved through similar experiments on a more complex commercial operating unit.

With the appropriate level of information in the experimental measurements, rate constants (i.e., the activation energy and pre-exponential factor in the Arrhenius equation) and adsorption equilibrium constants (heat of adsorption and pre-exponential factor in van't Hoff equation) can be fitted with high accuracy. This approach provides accurate information for the model during subsequent simulation and optimization; in addition, it also captures valuable knowledge about the reaction set for use in other studies and analyses. The more accurate the parameter values determined from experimental data, the better the predictive capability of the model to ensure it is capable of quantifying the effects of small but potentially significant changes through design.

For the TPAL case, a number of pilot-plant experiments were done in a single-tube fixed-bed reactor. Process variables, such as temperature profile along the tube center and concentration of each chemical species at two positions in the bed, were measured.

Thermal and catalytic oxidation should be considered simultaneously. To fit accurate parameters, LG Chem performed two different sets of experiments: one for thermal oxidation only, with inert packing, and the other for the "real case" involving both thermal oxidation and catalytic oxidation occurring within catalyst packing. First, the parameters for the thermal oxidation reactions were fitted using thermal oxidation experimental data. Parameters for the catalytic oxidation reactions were then determined using the "real

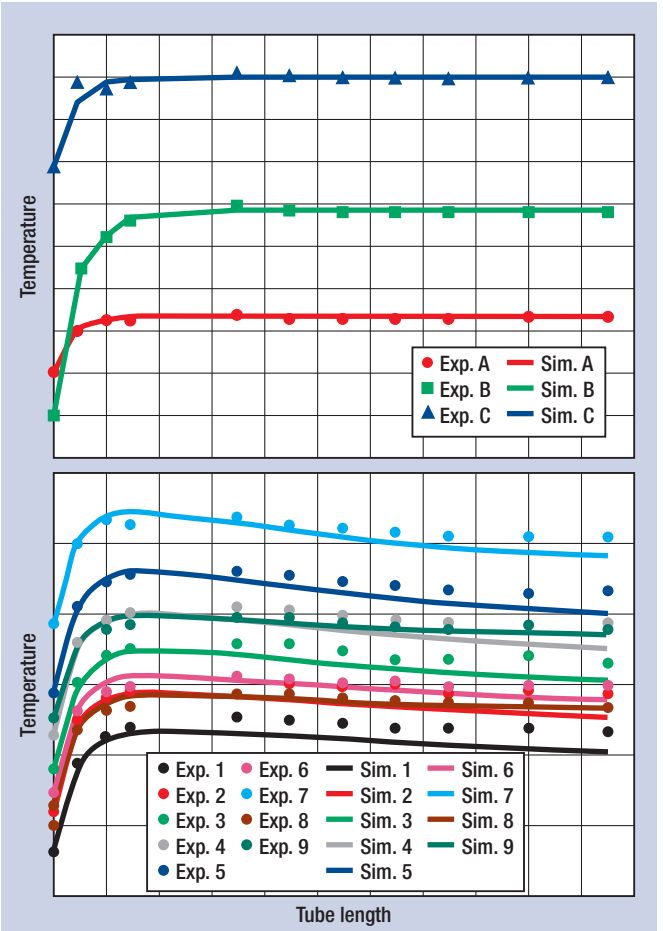

FIG. 9 Comparison of experimental data and model predictions following parameter estimation for (top) thermal oxidation and (bottom) catalytic oxidation.

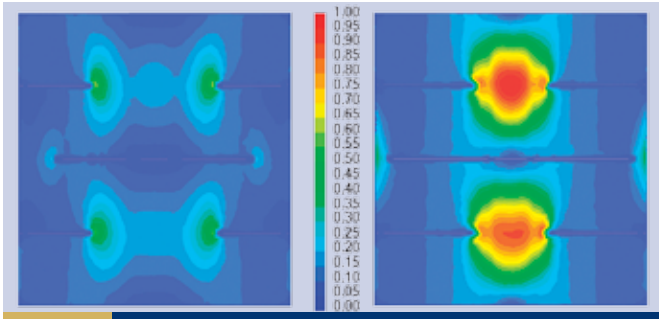

FIG. 10 Velocity distribution through the shell for poor (left) and optimal (right) design.

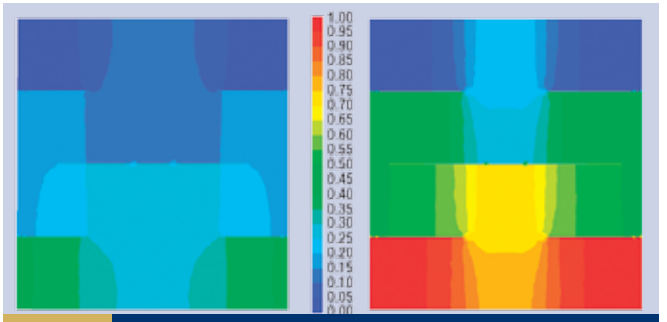

FIG. 11 Pressure distribution through the shell for poor (left) and optimal (right) design.

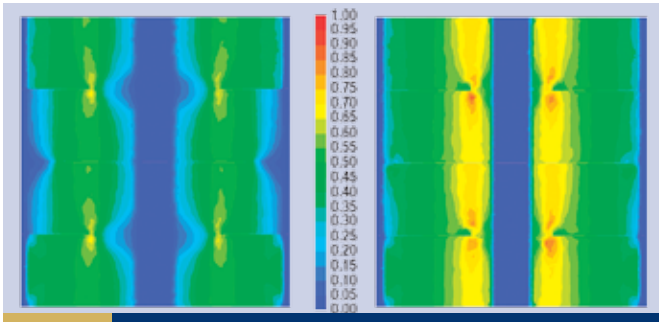

FIG. 12 Heat transfer coefficient through the shell for poor (left) and optimal (right) design.

case" data, taking into account the parameters already fitted for the thermal oxidation reaction. All of the reactions listed in Fig. 3 were used for the catalytic oxidation reaction; nine of them (1 to 7, 12 and 13) were used for the thermal oxidation reaction.

Fig. 8 shows the laboratory experimental setup used. A single catalyst-filled tube is immersed in a well-controlled bath of coolant under conditions that are as far as possible isothermal. Temperature measurements are taken along the center of the tube and in the jacket walls.

Fig. 9 compares the temperature profiles (y-axis) along the tube center (x-axis) at different experimental conditions with the values predicted by the catalytic-tube model. The first graph is for the thermal oxidation only case, and the second graph is for the thermal and catalytic oxidation case. As illustrated, there is a good agreement between experimental and predicted values for all cases. **Result:** The postulated reaction sets describe the observed data well, and the experiments performed were appropriate, yielding accurate parameter values.

Execution of the combined simulation. Once key parameter values had been determined from the experimental data, the hybrid TPAL reactor model was assembled and executed to simulate and optimize the commercial-scale reactor design. The CFD and reaction models were linked via a proprietary interface, which took care of execution control, data transfer and mapping of data between the CFD and corresponding "representative tube" surface points in the reaction model. It also calculated the heat sources for the CFD model and the body forces acting on the shell-heat transfer medium. Interface configuration information was provided via a simple text file listing the number of representative tubes, x and y coordinates of representative tubes within a horizontal cross-section of the shell, tube length, tube diameter, tube pitch and flow configuration (co-current or counter-current).

In this work,144 representative tubes were used, each representing a much larger number of neighboring tubes within the tube bundle.

The combined model was executed from the CFD user interface, with the tube-reaction models executing in the background. With this approach, it was possible for the design team to easily make changes to the reactor geometry and to quantify the effects.

On iteration between the two models, the CFD model provided accurate shell-side fluid temperatures based on detailed hydrodynamics. These were passed to the tube models, allowing them to

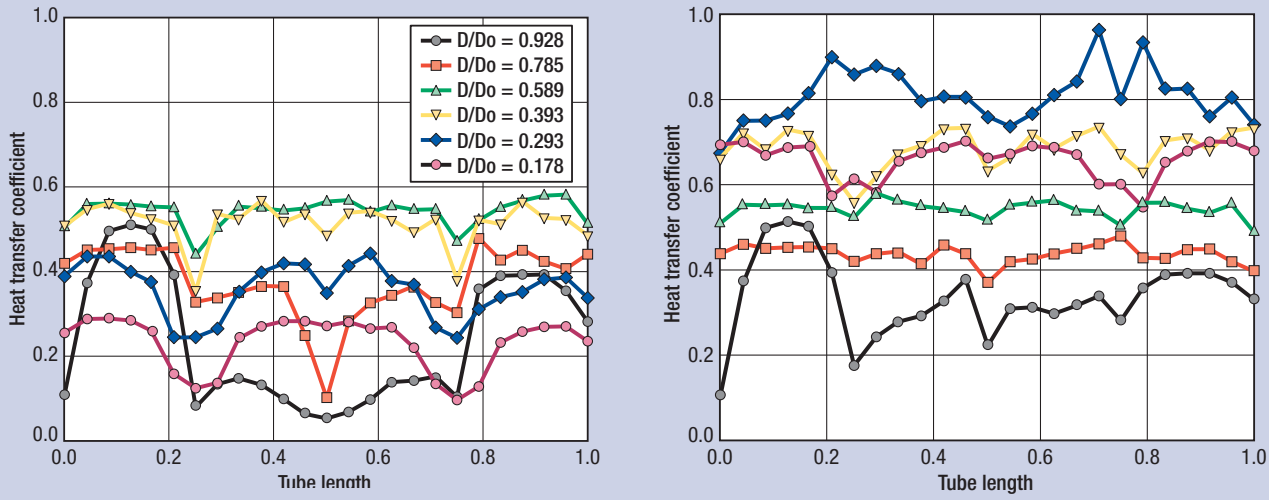

FIG. 13 Heat transfer coefficient distribution for selected tubes for poor (left) and optimal (right) design.

calculate the exothermic reactions and bed-heat transfer through the bed and tube wall with high accuracy. This information was used to provide heat-source terms back to the CFD model.

Design variables considered included reactor diameter, baffle window size, baffle span, inner and outer tube limit, coolant flowrate and temperature, tube size, tube arrangement and pitch, and so on.

Results. A number of cases were studied using the hybrid model. First, the effect of catalyst layer height and the feedrate was studied to determine the optimal reactor height. Then the model was used to check whether there was any advantage in using a multistage shell structure. It was found that a single stage was sufficient for the required performance. Finally, the detailed geometry of the 3D tube bank and baffle structure was determined by investigating many alternatives. For the purposes of this article, results from a "poor" case and an "optimal case" are presented based on the reactor length and shell configuration determined in the first two studies. Values in results are normalized to preserve confidentiality.

Fig. 10 shows the velocity distribution of coolant through the shell in a vertical cross-section of the reactor. Note that the velocity approaches a maximum around the edge of the doughnut baffle. In the poor design, the high resistance to the cross-flow passing through the narrow tube pitch limits flow velocities in the center of the reactor, causing performance problems in the reacting tubes in this region. To improve performance while maintaining a reasonable coolant pump size, optimal values were determined for the size of doughnut baffle window and the inner tube limit. The optimal design shows a narrower window, forcing fluid through at higher velocity, thus improving heat transfer.

Fig. 11 shows the pressure distribution of coolant through the shell. The pressure drop across the optimal design is higher than that of the poor design because of the larger flow resistance caused by the narrower baffle window. From a capital and operating cost perspective, pressure drop usually needs to be minimized within an appropriate reactor performance range. However, the optimal design was accepted in this case despite the high pressure drop, because the reactor performance is much more important and—fortunately—the corresponding cost increase was estimated as negligible. This clearly illustrates the benefit of accurate quantification. It also demonstrates that this type of analysis can be used to immediately exclude designs that require unnecessarily large initial investment and operational cost for coolant pumps.

Fig. 12 shows the distribution of heat transfer coefficient calculated from the flow direction and velocity of fluid at local positions. In the poor case, areas of low heat transfer coefficient can be clearly seen near the center and along the walls of the reactor. In the optimal case, these are eliminated; the reacting tubes near the center have the highest coefficients. Fig. 13 shows the same data in a different representation. Six representative tubes were selected along the radial position of the tube bank, and the tube wall heat transfer coefficients were plotted along the length of the tube. Note that the three lowest lines (pink, blue and black, representing the two innermost and one outermost measure tubes, respectively) have moved significantly upward relative to the others, indicating a higher heat transfer coefficient.

Fig. 14 illustrates the effects of the above adjustments on the key design objective—the temperature distribution along the center of each catalyst-filled tube. The poor case has marked temperature gradients across the tube bundle for tubes in the same axial position. As a result of the considered adjustments to the internal geometry, the optimal case shows virtually uniform radial temperature profiles. Thus, the reactants in all tubes are subject to the same or very similar external conditions at any cross-section of the reactor, with no discrepancy of performance arising from the radial position of the tube within the tube bundle. Also, the reactions occurring within the tubes—and conversion—are very similar for all the tubes across the bundle.

A potential risk of not optimizing the design is the formation of hot spots, particularly near the center and wall at the reactor inlet. This would decrease the total performance of the reactor and accelerate catalyst degradation and deactivation, eventually leading to the shifting of reactions away from their optimal regions in the bed, further loss of performance and possible early shutdown.

The detailed understanding of performance that can be gained from the results raises the possibility of running the reactor at higher temperature, if this is desirable to increase conversion. This is a decision that can be taken as required by operational staff, based on detailed quantitative information provided by the design team.

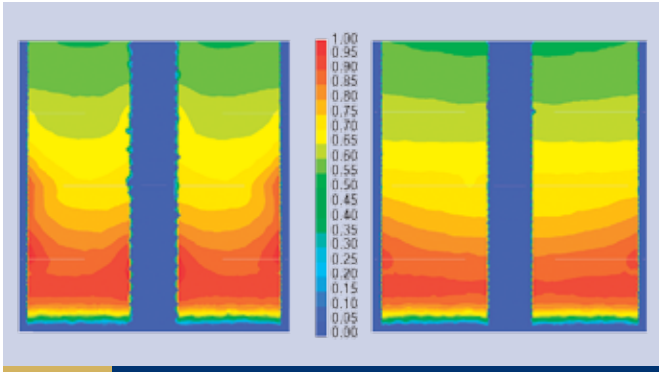

FIG. 14 Tube center temperature distribution through the shell for poor (left) and optimal (right) design.

Final options. The hybrid model made it possible to explore many different design options for the TPAL reactor in a short space of time and to base design decisions on *high-accuracy quantitative data.* The information from these cases was used to determine the final design geometry with high-performance characteristics as well as to provide design information such as the capacity for the coolant circulation pump.

The optimal reactor design assures improved heat transfer efficiency leading to uniform performance over all tubes in the reactor, providing greater controllability, operational flexibility and extended catalyst life. It is also the most cost-effective in terms of initial capital investment and operating cost.

Subsequent to the main design work, it was found that performance could be raised further by improving coolant and feed distribution before entering into the reactor. The studies on distributors were initially performed using 3D CFD simulation, and then the full effects were evaluated by using hybrid simulation. The hybrid modeling approach can and has been successfully used to design new high-performance multitubular reactors and, at a more general level, to explore and prove innovative technology approaches. **HP**

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