# **Computational Modeling Solving Real-Time Industrial Problems**

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# Abstract

Recent advances in computational fluid dynamic (CFD) techniques and computing power have opened opportunities to use this tool for design developments and troubleshooting operational problems. This article discusses a recent development to improve spent catalyst distribution in a Fluid Catalytic Cracking (FCC) regenerator. Uniform spent catalyst distribution is key to achieving even coke combustion and bed temperatures resulting in more complete coke burn and improved catalyst activity retention. This paper highlights how CFD tools were used in the development of TechnipFMC's latest "compound angle wye bathtub" distributor. Data from several commercial regenerators show uniform temperature profiles with the new spent catalyst distributor, validating the use of CFD to develop and design FCC equipment and resolve operational issues.

**Keywords:** Fluid catalytic cracking (FCC), FCC regenerator, spent catalyst regeneration, computational fluid dynamics (CFD)

# Introduction

The FCC process is well established with over 300 refineries using FCC units to upgrade low value feedstocks to valuable products such as gasoline and propylene. As the FCC environment evolves, refiners are often challenged to operate their FCC units to meet the optimum economic point. TechnipFMC's suite of FCC technologies are licensed in over 60 grassroot units and more than 250 revamps. To support this position TechnipFMC, along with its FCC Alliance partners, Axens, IFPen and Total, make considerable efforts to optimize existing designs and develop new designs to meet the operating objectives set by operators.

TechnipFMC's recent FCC technology improvements include a riser termination device to quickly separate FCC catalyst from the product vapors to avoid post riser cracking reactions, catalyst distributors to uniformly distribute spent catalyst in the regenerators, air distributors for uniform gas distribution and fluidization, high efficiency oil injectors, and many others. These developments have, to some extent, benefitted from the use of computational fluid dynamic (CFD) modeling. CFD provides unique insight into how existing designs perform and understanding of how design changes will perform in the real world. CFD is currently playing a major role in the FCC industry allowing innovative solutions to enter the market faster and more cost effectively. As CFD capabilities and computing power improve, the use of this tool will continue to increase.

For over a decade, TechnipFMC has actively used CFD for design optimization and to troubleshoot FCC operation. CFD provides information required to understand and determine how hardware modifications and operational changes will impact gas-particle flow behavior and

overall performance of the unit. TechnipFMC generally uses Barracuda VR® software, which is specifically designed to model gas-particle fluidized bed reactors. VR or Virtual Reactor® is able to model industrial-scale, thermal, chemically reacting, fluid-particle systems in a computationally efficient manner. It is parallelized using the latest graphics processing units and transient simulations of full-scale FCC regenerator systems, such as those presented in this paper, and can be run to completion quickly enough to allow for evaluation of multiple design alternatives. VR considers the full particle size distribution (PSD) of catalyst within the reactor, which is important for achieving a realistic representation of the particle-fluid dynamics within a fluidized bed. The software features and capabilities have been well validated with both large-scale experimental data and with commercial operating reactors across the broad industry. Additionally, Fluent and FEA simulations are used as necessary, to address specific problems.

This paper discusses development by TechnipFMC of the FCC Alliance's spent catalyst distributor from a simple "hockey stick" distributor to most recent "compound angle wye bathtub" distributor. The goal behind this development was to improve spent catalyst distribution in the regenerator bed to promote uniform coke combustion. CFD modeling was used to predict the catalyst distribution for various design options and guide the development of the mechanical design.

### **Catalyst regeneration**

Regeneration of catalyst is a fundamental step of the FCC process. Catalyst is regenerated by burning coke deposited on the catalyst during the catalytic conversion of oil to regain its activity. During regeneration, the catalyst absorbs heat which it transfers to the riser in order to provide heat for oil vaporization and endothermic cracking reactions. Traditional FCC regenerators operate in either partial or full burn combustion mode. In the early 1980's Total developed a Resid FCC processing scheme, with two stages of regeneration, known as R2R™. This RFCC technology is exclusively licensed by TechnipFMC and Axens and is under continual improvement by the FCC Alliance partners.

A key differentiating design feature of R2R technology, illustrated in Figure 1, is that catalyst regeneration is achieved in two stages in series, where the first stage operates in partial combustion mode followed by complete combustion mode in the second stage. The first regenerator typically burns 60 to 80 percent of the coke on the catalyst and any hydrocarbons entrained from the stripper. The resulting low first stage regenerator temperature minimizes hydrothermal deactivation of the catalyst. Partially regenerated catalyst is then transferred to the second stage regenerator where it is completely regenerated. The configuration rejects a portion of the heat of combustion as carbon monoxide (CO) enriched flue gas from the first stage regenerator temperature increases catalyst-to-oil ratio maximizing unit conversion. Additionally, it reduces catalyst deactivation, resulting in low catalyst make up rate.

Performance of a regenerator is generally determined by parameters such as uniform bed densities, stable and even combustion / temperature profile. These parameters depend on effective distribution and mixing of spent catalyst and combustion air. Maldistribution can lead to temperature variation in the bed, afterburn, catalyst losses and inadequate regeneration, which can impact catalyst circulation, activity and the product yields. Ensuring even distribution of

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combustion air is relatively easy, however, the uniformity of the spent catalyst into the regenerator bed depends on the distributor design. The progression of FCC Alliance's spent catalyst distributor technology from a simple "hockey stick" with open slots at the bottom for catalyst outflow to a "compound angle wye bathtub" distributor is shown in Figure 2. The main driving force behind this development has been to improve the spent catalyst coverage in the regenerator, especially for large size regenerators.



Fig. 1 RFCC technology with two stage regeneration, R2R™



Fig. 2 Evolution of TechnipFMC spent catalyst distributors

FCC regenerator catalyst beds are essentially turbulent "back mixed" beds where the inherent mixing of gas and catalyst is reasonably good and strongly influenced by the bed geometry and in-flow/out-flow of catalyst. The vertical / axial mixing is generally better compared to radial, and radial mixing generally suffers with an increase in regenerator diameter. If spent catalyst is not well-distributed across the vessel, then variations in the catalyst bed temperatures are seen. Earlier, smaller regenerators had acceptable temperature variations, but as units increased in size, the dense bed temperature variation also increased as shown in Figure 3. These regenerators include either the "hockey stick" or short "single arm bathtub distributor", which are generally extended from the regenerator wall towards the vessel centerline, providing limited coverage and distribution of spent catalyst into the catalyst bed. The limited distribution of spent catalyst across the regenerator results in an uneven coke burn-off from the catalyst, impacting unit performance, such as reduced catalyst activity leading to increased catalyst addition, as well as potential for afterburn, even in partial burn units.



Fig. 3 Industrial data of Partial Burn 1<sup>st</sup> stage Regenerator - Dense bed temperature variation vs. regenerator size

The data in Figure 3 is from 1<sup>st</sup> stage regenerators of R2R units, which operate in partial burn, removing the majority of hydrogen from coke, and thereby reducing the potential for high temperature hydrothermal deactivation in the second stage. The impact of uneven coke burn-off in the first stage does not greatly influence catalyst activity in two-stage regeneration. However, it can result in localized afterburn in the first stage and can impact the performance of the second stage regenerator. In single-stage full burn regenerators, where the temperatures are higher, the impact on the catalyst is more severe. The uneven coke burn-off may result in excessively coked particles flowing to the riser and poor catalytic performance, poor yields and increased dry gas formation. Bed and dilute phase temperature variation and afterburn can impact the mechanical reliability of the internals and may often require a capacity reduction to control the dilute phase temperatures. These issues have driven the improvement of the spent catalyst distributors for use in all types of regenerator designs, especially for large regenerators.

#### **Compound Angle Wye Bathtub Distributor Development**

TechnipFMC's "compound angle wye bathtub" spent catalyst distributor has been developed to address catalyst maldistribution which is observed as non-uniform bed temperatures in the regenerator. The compound angle wye bathtub distributor design, which is an improvement to an original concept of slanted wye bathtub distributor design, was optimized using extensive CFD modeling and has been validated through commercial results. Multiple simulation cases were performed to understand the significance of parameters such as wall height, bathtub inclination angle, slot width by height ratio, wye angle, catalyst flux, aeration and many others. Several different configurations were modeled prior to finalizing the compound angle concept. CFD was instrumental in studying different configurations with a wide range of parameters, which would not be possible with physical testing and investing a significant amount of time and money.

The original slanted wye bathtub concept was based on having multiple arms extending into the regenerator so that incoming spent catalyst travels along the length of the arm and distributes through the slots. Compared to the original slanted wye bathtub, the optimized design is initially inclined at a steep angle to ensure catalyst flows into and down the arms, followed by a shallower angle to reduce the catalyst velocity and prevent it from overflowing at the end of the bathtub arms. Where catalyst flows into the distributor arms a baffle is positioned to prevent catalyst overflowing and direct it into the two branches. Open slots in the upper section of the arms are eliminated to prevent premature distribution.

A comparison of CFD modeling results from the original slanted wye and the optimized compound angle wye bathtub is shown in Figure 4. The catalyst flow in the bathtub is presented as density distribution in a plan view, as well as along the length of the arms. Modeling of the original design shows a large portion of catalyst from the standpipe accumulates and overflows at the split into the two bathtub sections with a relatively small amount of catalyst flowing down the arms and through the slots. A plan view of the density profile indicates that catalyst coverage is concentrated at the split section only. The catalyst density profile along the side view indicates the flow in the initial section of the wye arms is more active compared to the latter half.

In the optimized compound angle wye bathtub design, catalyst build-up and overflow at the split section is eliminated via increased angle of inclination and installation of a baffle. The initial angle of inclination ensures sufficient catalyst momentum to move it down the bathtub, represented by the active catalyst zone. In the latter half of the bathtub arms, the lower angle slows the catalyst down allowing it to flow uniformly through the slots. The improved catalyst discharge density along the bathtub length, resulting from the two-angle design, is shown in the plan view. It indicates that the design achieves uniform flow of catalyst along the span of the arms, which improves spent catalyst coverage across the regenerator.

A quantitative comparison of percent mass flow deviation from ideal uniform catalyst distribution along the bathtub length for original and optimized configuration is shown in Figure 5. The results indicate that the compound angle wye design is closer to the ideal "even" catalyst distribution than the original concept. This is achieved by incorporating features such as a raised baffle section at the split, compound angle of inclination and optimized slot distribution. The use of the CFD modeling technique was key in optimizing the wye bathtub design parameters. The CFD results

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were promising enough that TechnipFMC adopted the "compound angle wye bathtub" for subsequent regenerator designs.



Fig. 4 Wye bathtub performance comparison (original vs. optimized design)

### **Industrial Example**

The original and compound angle wye bathtub distributor designs have been applied to several commercial FCC regenerators and resulted in improved performance. Two commercial regenerators, one with original slanted wye bathtub (Unit A), and other with compound angle wye bathtub (Unit B), are shown in Figure 6. Both the regenerators are single stage and operate in complete combustion mode. They are large regenerators with reduced catalyst bed section diameters in the range of 35 to 40 feet. Unit A regenerator with original wye bathtub did use a baffle at the split to ensure catalyst flowing down the standpipe would not end up overflowing above the crotch area.



Fig. 5 CFD results Comparison - Max standard deviation from ideal uniform distribution



Fig. 6 Commercial regenerators with original and compound angle wye bathtub distributor

The performance of both regenerators is compared in Figure 7. Unit A has an average dense bed temperature variation of 7°C, whereas Unit B is experiencing an average of 2°C dense bed temperature variation across the bed. The dilute phase temperature variation for Unit A and B is 35°C and 12°C respectively. The Unit B regenerator is running with minimal temperature variation in both dense and dilute phase and low afterburn in the range of 15°C. The improved temperature profiles in Unit B with the compound angle wye bathtub present greater unit flexibility to operate at high throughputs or provide more flexibility on feed selection. The commercial results shown here and results of CFD analysis indicate that the compound angle concept is superior to the original wye design. This distributor is now offered as a standard design for the first stage regenerator in R2R technology as well as for single-stage regenerators. Even with the successful implementation of the compound angle wye bathtub design, we continue to explore ways to further improve the design.



Fig. 7 Industrial data - Dense bed and dilute phase temperature variation (Slanted vs compound angle wye bathtub distributor)

TechnipFMC has recently introduced a "submerged compound angle wye" bathtub as an improved version of the compound angle wye design, where the major portion of the distributor arm(s) is submerged in the catalyst bed. The main driving force behind this modification is to enhance spent catalyst mixing in the catalyst bed, promote bed combustion and reduce afterburn. This concept was, again, extensively modeled to gain confidence prior to commercial application. The design has now been in operation for more than two years and has shown significant improvement in unit performance with respect to reduced afterburn and temperature variation in dense and dilute phase. The pre- and post-turn around operation along with some of the CFD results are published in PTQ 2019 Revamp Issue.

A survey of 12 commercial regenerators is presented in Figure 8 and it indicates how they are performing with respect to dense bed temperature variation with different distributors as a function of regenerator vessel diameter. The performance of the new compound angle design shows clear improvement over earlier designs. There is minimal temperature variation in the bed and bed temperatures are not sensitive to vessel diameter.



Fig. 8 Industrial data - Dense bed temperature variation vs. distributor type

# Summary

Computational modeling is playing an increasingly important role in understanding gas and particle flow dynamics in the FCC process, enabling designers to offer low-risk, high value improvements to clients. Occasionally cold flow models were built, which are expensive and time consuming, and they do provide both qualitative and quantitative results to some extent. The latest generation of CFD modelling tools enables rapid exploration of different configurations and homing in on the best solution. Compared to cold flow testing, these tools allow a deeper

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understanding of what is happening at all points in the system. Existing designs were modeled, and changes were made to achieve the desired catalyst flow patterns. This design, optimized solely using CFD, has been verified in several large commercial regenerators.

# Acknowledgement

The authors would like to acknowledge the TechnipFMC FCC Alliance members, Axens, IFPEN and Total, for their valuable engagement and efforts to bring innovative solutions and technologies to address the challenges being faced by FCC operators.

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