REVOLUTIONISING PERFORMANCE

COVER STORY

Richard Caulkin, Tim Michalec and James Esteban, UNICAT Catalyst Technologies LLC, explore how revolutionary scientific modelling allows tailored optimisation of filtration grading and loading profiles to deliver 50% improvements in catalyst bed life.

Hydroprocessing is a crucial process in the refining and petrochemical industries, essential for producing high-quality fuels and meeting environmental standards. Included in the family of hydroprocessing applications are hydrotreating, hydrocracking, and hydroisomerisation, all of which play a key role in producing renewable fuels. During hydrotreating, raw feed streams react with hydrogen in fixed bed reactors that perform hydrodesulfurisation (HDS) – sulfur removal, hydrodenitrification (HDN) – nitrogen removal, hydrodemetallisation (HDM) – contaminant metals removal, and/or hydrodeoxygenation (HDO) – oxygen removal. Hydrocracking and hydroisomerisation processes also use fixed catalyst bed reactors that reconfigure hydrocarbon molecules through cracking and isomerisation reaction mechanisms. These catalyst beds operate at around 225 - 425°C and 30 - 150 bar, depending on the feed quality and processing conditions. These processes increase the efficiency of fuels and reduce harmful environmental contaminants in final products. Since these reactor systems have fixed catalyst beds, pressure drop across hydroprocessing reactors can be a challenge to maximising the overall life cycle of the catalyst materials.

High pressure drop in hydroprocessing reactors can lead to suboptimal catalyst performance, decreased reactor efficiency, feed maldistribution, shorter operating cycles, and increased operational, catalyst and maintenance costs. This article explores the use of UNICAT's Advanced Filtration System (AFS) as a solution to mitigate pressure drop and enhance overall reactor performance.

In addition to commercial data, a computational modelling case study of a generic hydroprocessing reactor is presented, highlighting comparative differences between reticulated ceramic and AFS filtration medias discussed.

Pressure drop discussion

High pressure drop in hydroprocessing reactors can negatively impact performance due to maldistribution of reactant streams, decreased conversion rates, shorter run cycles, and increased energy consumption. These issues not only impact the economic viability of hydroprocessing units, but also have negative environmental and regulatory impacts. Shorter operating cycles lead to increased spent catalyst disposal costs, lost revenue, and higher maintenance costs.

In hydroprocessing applications, the development of catalyst bed pressure drop is associated with catalyst bed fouling from a variety of potential causes including, but not limited to: feed stream contaminants, deposition of foulants, formation of coke, adverse side reaction products, and the deposition of feed poisons. These foulant materials can be deposited steadily throughout the operating cycle or during sudden unplanned events of adverse operating conditions, e.g. emergency shutdowns. Reactor pressure drop increases as the available void space in the catalyst bed is packed with foulant materials. New catalysts used in hydroprocessing applications have an available void space of approximately 35 - 40%. This available void space provides suitable volume for reactant vapour and liquid streams to evenly distribute across the catalyst bed, as well as provide longevity of performance and some tolerance for fouling over the cycle. As the available void space is decreased, pressure drop across the reactor increases and distribution of the reactant streams can be disrupted. This is where pressure drop mitigation grading plays a crucial role in catalyst bed protection. UNICAT's AFS catalyst bed grading offers filtration that has nearly twice the available void space of fresh catalyst and is designed to evenly distribute foulants throughout the graded filtration media, as well as provide continuous flow channels to prevent the disruption of evenly distributed reactant streams.

It is especially important to highlight that the distribution of reactant gas and liquid streams in mixed-phase applications is set by the reactor internal components. There are several case studies that highlight the importance of proper distribution achieved by modern reactor internals and the value associated with subsequent catalyst utilisation from upgrades in the mechanical components installed in these reactor systems. To maintain proper distribution, it is important that flow paths be maintained and not disrupted by either catalyst materials and/or foulants as they deposit in the reactor voids (Figure 1). UNICAT's AFS is designed to provide high available void space to capture foulants, but also with uniform flow channels to allow for the retention of flow distribution to avoid poor catalyst utilisation (Figure 2). This results in greater catalyst utilisation over the entire lifecycle of the catalyst and a retention of even distribution.

Graded bed design

Implementing a well-designed grading system is one of the most effective ways to avoid long-term pressure drop increases. Initially, catalyst companies developed top bed grading systems to filter out fouling contaminants with varying degrees of success. These initial designs contained smaller spherical support balls, 'wagon wheels', and rings layered at the top of the bed. The rings sat directly on top of the catalyst bed, which consists of cylinder or lobed catalyst particles. Using wagon wheels and rings was fairly successful, but it was limited due to internal void space in rings which are too large to filter the smallest contaminants. Particulates subsequently become trapped at the interface between graded ring layers – primarily between the final ring layer and the top of the catalyst bed. This area often has the only void spaces small enough to capture the smallest particulates. As these transition regions become packed, the overall cross-sectional open space is compromised, resulting in an increase in pressure drop, which can ultimately lead to premature shutdowns. Improvements in pressure drop protection from reticulated ceramics resulted in additional pressure drop protection.

The AFS has fixed triangular openings that provide enhanced particulate and contaminant trapping benefits. It offers high available void, high crush strength, optimised packing efficiency, low pressure drop and high particulate pick-up capacity. This deep bed filtration technology leads to longer cycles and improves unit profitability (Table 1).

UNICAT has combined commercial experience with detailed dynamic simulation technology to develop a new model for graded bed design. While AFS provides high capacity for particulate removal, it remains important that a complex model to complement this technology will provide optimal bed designs. Modelling applications demonstrate an increase in capacity for similarly sized graded beds with only traditional rings to AFS of up to 200%, and from reticulated ceramics to AFS of up to 150%. Due to the open design of AFS, effective capture volume is greater, which provides increases in catalyst cycle life by 1.5x to 2x respectively. Modelling enables bed grading designs to be optimised with cycle life targets and maximum catalyst activity without customers needing to wait multiple cycles before changing layer volumes. Historically, the primary method for graded bed design optimisation was to react in response to spent catalyst samples. The reality is that changes in design take one to two change out cycles before the collected evidence can be used to make improvements to the loading scheme. UNICAT combines historical performance with computational fluid dynamics (CFD) modelling to provide instant optimisation. This is important as processing objectives can change, and the company can respond to new operating targets for each operating cycle.

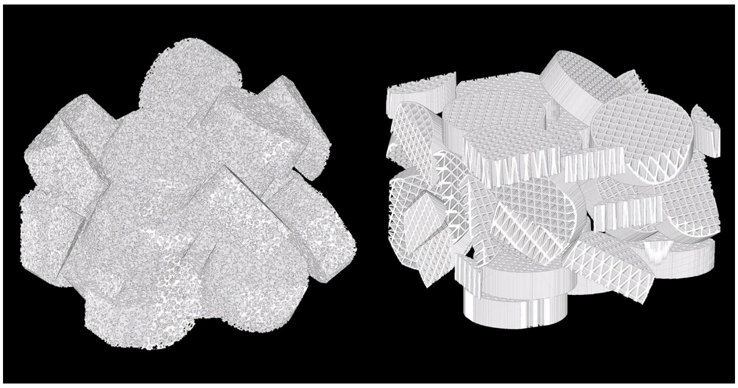

Figure 1. Cut-away images of (right) AFS 4510 and (left) reticulated ceramic filter media generated from UNICAT's Revolutionary Computer Modelling Software.

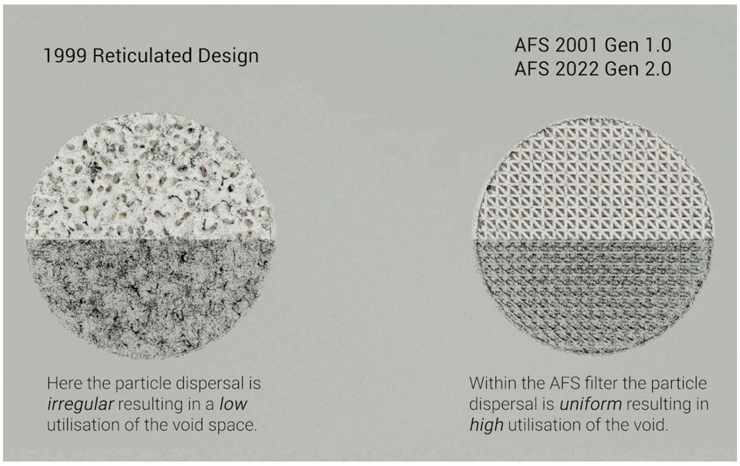

Figure 2. Showing the particle dispersal in Reticulated Design as irregular vs AFS being uniform.

Case studies

The model used to generate data referenced within this case study is a packing prediction simulation tool, to which CFD can be applied to simulate fluid movement within the generated packing structures.

Within the model, both objects and the packing space are represented as collections of 3D pixels (voxels), with objects able to move independently of each other. As such, shapes of any complexity can be simulated, provided the resolution is sufficient to characterise the objects accurately.

In the case study reported, the external dimensions of AFS and reticulated pieces were roughly equal; there is a 6% difference in total free void space between the graded AFS and the reticulated filter beds. However, internal capture volume differs by 33% in favour of AFS (Table 2).

CFD simulations performed on the respective packings elucidated start of run pressure drops for the filter beds at different flow rates (Figure 3).

Modelling was undertaken to better understand how foulant of a specified particle size distribution and feed rate behaves when introduced to both filtration units over a typical cycle (Figure 4). Solids were introduced in the reactor at a uniform rate of 5 mg/m^3 over the life span, with the feed consisting of scales and flakes (> 1000 µm), coke (100 - 800 µm), iron sulfide fines (10 - 100 µm) and solid silica (10 - 50 µm). Particle size distribution was skewed to the fine size and was identical for both examples.

Pressure drop was measured incrementally at 6 month equivalent intervals over both filter beds. Both beds had a foulant removal efficiency of >98%.

Modelling demonstrated the differences between AFS and reticulated beds in terms of pressure drop stability vs onstream time. The highly tortuous internal paths within the reticulated pieces mean that foulants can block the void spaces relatively quickly, and do not fill each piece uniformly. Loading in each piece tends to occur quite high within the individual reticulated pieces, preventing effective filling of lower regions and preventing the full utilisation of the capture volume. Therefore, effective reticulated capture volume is around 50% of that of AFS (as opposed to the 33% measured), leading to increased pressure drop and greater feed maldistribution over a shorter cycle.

In the real-world data provided above, pressure drop begins to increase notably after 18 months for reticulated ceramics, compared to 36 months for the same feed conditions with AFS.

In order to provide a robust sense check for the CFD model, over the last two years UNICAT has had several optimised commercial applications which have validated the modelling software prediction tools within a 3% predictability range.

Table 1. AFS vs reticulated ceramic

	Reticulated ceramic	AFS
Loading	Reticulated ceramic various sizes	AFS with silica-uptake rings
Lifetime	Standard run	50% + run length for AFS

Note: both the loadings had equal grading volumes

Table 2. Comparison of internal capture volume, AFS vs reticulated disc

	Bed height (in.)	Reactor volume (ft^3)	Internal capture volume (ft^3)
AFS	211	999	194
Reticulated	211	999	139

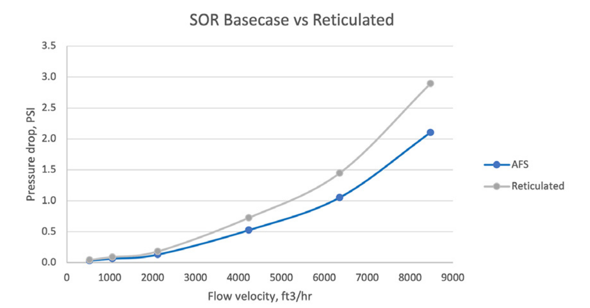

Figure 3. AFS pressure drop vs reticulated over differing feed rates, start of run (SOR) for reactor Rx.

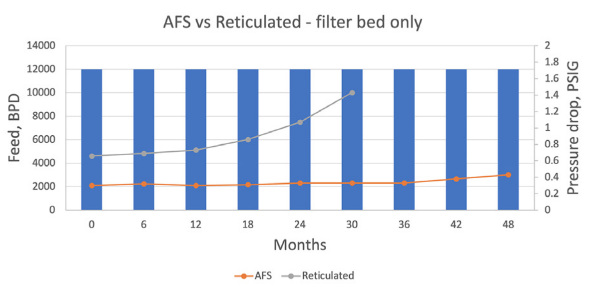

Figure 4. Predicted pressure drop vs time for an average feed rate of 12 000 bpd (2800 ft^3/h or 80m^3/hr).

Conclusions

There is a clear correlation between the maximisation of catalyst bed lifecycle in hydroprocessing services and the application of pressure drop protection technologies for optimisation of overall process unit performance. In fixed bed reactor applications, AFS demonstrates several advantages leading to excellent performance regarding pressure drop protection and mitigation. AFS provides improvements in overall capture volume and initial pressure drop, which result in both lower SOR pressure drop, as well as sustained lower pressure drop. This results in a 150 - 200% lifecycle improvement.

AFS incorporates continuous uniform flow channels which are designed to improve both the even distribution of foulants as deposition occurs, as well as preserve the flow distribution set by the reactor internals. Preservation of flow channels provides maximisation of catalyst usage by supporting the even distribution of reaction components. The even distribution of foulants permits higher overall loading, optimal graded bed sizing, and reduction of catalyst change out cycles. This performance advantage is highlighted in the case study provided, demonstrating an overall longer operating cycle, as well as sustained lower pressure drop throughout the extended cycle.

Coupled with the experience of many commercial applications, UNICAT has developed a complex packing model for the simulation of performance and to develop predictive modelling capabilities. Scientific modelling allows tailored optimisation of graded bed requirements and loading profiles based on current reactor feed conditions. This provides a high level of confidence in the optimisation of process unit operating cycle life, as well as a real time method for performance predictions.