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DIGITAL TECHNOLOGIES

How digitalization is turning data into value in the heart of the refinery: FCC catalysts

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Digitalization has impacted the world of refining for the past several decades. From the rather humble beginning of the conversion of analog to digital instrumentation, industry now enjoys advanced control and optimization systems to maximize profitability and reliability. Today, one could easily envision monitoring and adjusting refinery operations remotely using only a smartphone! Acting as the heart of the refinery, fluid catalytic cracking units (FCCUs) are tightly connected with many key processes in a refinery, and, because of this, FCCUs can reap the most benefits from digitalization.

While FCCU operating conditions are continuously fine-tuned using advanced controls, one optimization area that has remained relatively untouched by digitalization is catalyst design. Just as process conditions can be analyzed to dial in desired product yields, the same analyses can be used to identify opportunities to improve catalytic performance. Catalyst optimization carries an extra complication in that changing catalytic selectivity can take weeks or months. Even fast-acting additives can take days to baseload into an FCCU. Therefore, managing uncertainty is critical for optimizing FCCU catalysts to truly maximize value capture.

This article details digital techniques and tools for analyzing market dynamics alongside unit operations toward the goal of developing high-value-generating catalyst formulations. These digital techniques enable the authors' company and operators to effectively manage large changes in relative product value [C_3= vs. C_4= vs. gasoline vs. light cycle oil (LCO)] by identifying catalyst formulation strategies that maximize value delivery over a broad range of market scenarios.

Changing market conditions necessitate embracing digitalization. No other unit operation in U.S. refineries has faced greater uncertainties than FCCUs during the pandemic and subsequent recovery (**FIG. 1**). As gasoline consumption came to a halt during COVID-19 lockdowns, FCCUs were operated at the lowest recorded feed rates since the 1980s. Market impacts during the height of COVID and subsequent rebounds were swift and unpredictable. FCCU utilization and feed qualities responded to abnormal market demand. Unusual operating conditions were often required to keep units running. As a result, many traditional constraints were no longer present.

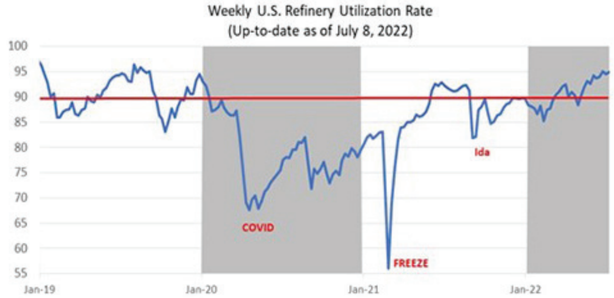


FIG. 1. U.S. refinery utilization as a percentage of rated capacity. Source: U.S. EIA.

All these changes were in response to product slate pricings becoming very volatile, with a heavy emphasis on petrochemicals and bottoms elimination. **FIG. 2** highlights the recent extreme volatility of propylene, butylene and gasoline. Even with significant changes in FCCU operating strategies, catalyst reformulation—except for using ZSM-5 to convert excess gasoline—has been infrequent. Refineries resorted to supplementing fresh catalyst with purchased equilibrium catalyst (Ecat) to save costs, often with a negative impact on overall profitability.

With peak gasoline demand already looming on the horizon, COVID has accelerated the timeline. To stay relevant, the traditional paradigm of the FCCU as the classic "gasoline machine" in a refinery must adapt to a new reality. As the hydrocarbon processing industry (HPI) enters a new era for refining, digitalization will play a growing role in the transformation to a new FCCU.

Traditional hurdles to catalyst optimization. It is widely recognized that the appropriate choice of FCCU catalysts can enable the highest margin capture; however, it is also all too common to see relatively infrequent catalyst optimization and change requests (**FIG. 3**). This mismatch between opportunity and behavior could be driven by many factors, such as:

- Uncertainty in market outlook: What if the market takes a dramatic turn as a catalyst change is being implemented?
- Concerns about how catalyst changes might adversely impact FCCU operability: What if uncontrolled risks outweigh potential benefits from a catalyst change?
- Time and resources required to execute a catalyst evaluation process (**FIG. 4**): What other priorities do team members have?

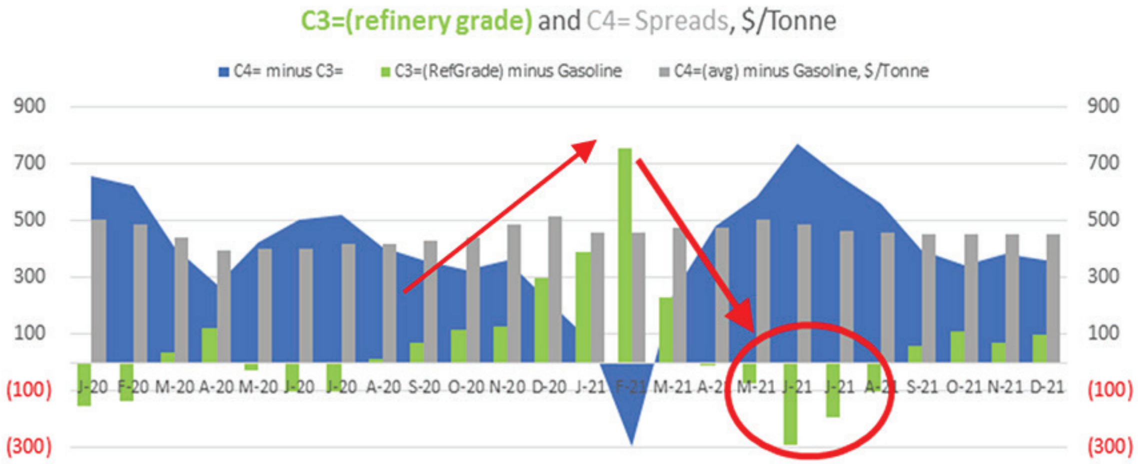


FIG. 2. Evolution of relative values of propylene, butylene and gasoline on a mass basis ($/t).

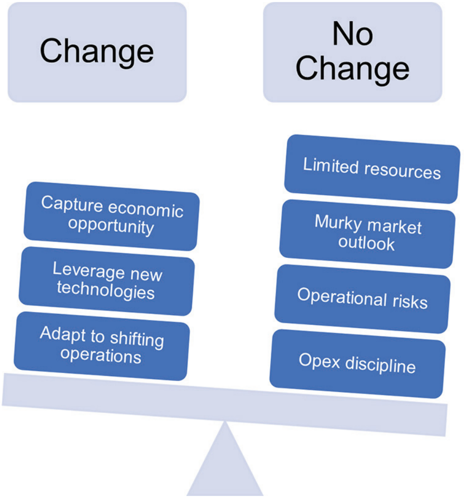


FIG. 3. Encumbered change process limits' ability to capture opportunity.

While catalyst optimization may not be at the top of an FCCU operator's priority list, catalyst optimization can be quite profitable for a refiner. FCCU operating data is often shared with catalyst suppliers (sometimes even with real-time connectivity), enabling catalyst suppliers to anticipate and lead catalyst optimization discussions rather than just respond to change requests. In addition, catalyst suppliers regularly analyze Ecat samples from refineries and have access to their database of standardized testing results on catalyst performance in that unit over time, including earlier catalyst changes.

Rather than waiting for a customer to request an updated FCCU catalyst, the authors' company analyzes market and operating data, proactively proposes and implements catalyst changes, and monitors trials—all on a continuous basis as part of the technical services offered by catalyst suppliers. This scenario can be realized today by lowering the barriers for starting catalyst optimizations, thus tipping the balance in favor of change. Once the hurdle to change is removed, refiners can respond to market changes even faster.

Digitalization tips the scale toward making changes to capture maximum value. Historically, technology providers have employed time-tested processes for designing catalysts based on customers' performance needs, and subsequently implementing a catalyst trial with the promise of improving operations by using new formulations. These conventional processes relied heavily on customer analysis and input to define catalyst optimization targets. With the rapid evolution of the refining market, refiners may find that they have less time to evaluate FCCU catalysts than in the past. To compound the situation, today's highly dynamic market requires quicker and more proactive action to meet rapidly changing refined product demands. The inherent latency of the process makes it very challenging to react to market changes faster than 3 mos–6 mos on a continuous basis.

Recent advances in digital tools and analysis techniques enable the authors' company to deliver proactive FCCU catalyst solutions and to keep refining partners updated on the evolving market. As the catalyst optimization challenge has become more complicated, the authors' company has developed novel approaches for simplifying and attacking this problem (**FIG. 5**). Starting from customer operating and Ecat data, the authors' company's digital solutions build comprehensive understanding of refinery targets, and then tailor a catalyst solution (or even a suite of catalyst solutions) for the individual needs of each FCCU. By proactively generating a customer's Request for Proposal (RFP) document, the authors' company removes latency from the process, resulting in less lag time from market adjustments to reformulation results in improved value capture. For example, capturing a \$0.50/bbl opportunity 6 mos earlier is worth ~\$5 MM/yr for a 50,000-bpd FCCU.

This digital tool suite allows the FCC optimization problem to be solved step by step, starting with an in-depth analysis of operating/yields data and Ecat data. The catalyst optimization starts with an analysis of FCCU product pricing, which could reflect regional market outlooks or refinery-specific values. Understanding relative product pricing (e.g., naphtha > LCO, or C_4= > C_3=) enables a focus on value-generation strategies. Next, operating data are analyzed using data visualization dashboards, along with automated data processing techniques, to identify specific constraints or limitations that are preventing the FCCU from achieving higher perfor-

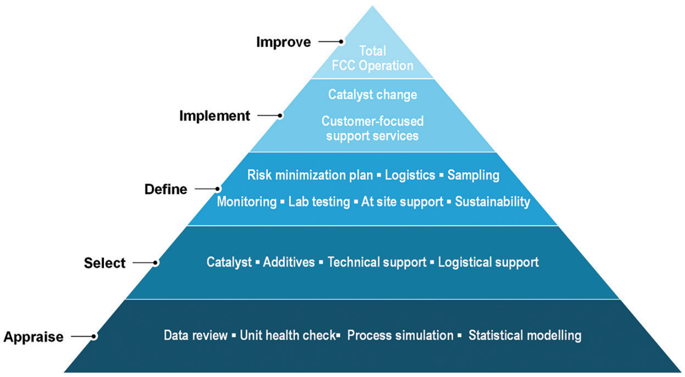


FIG. 4. FCC catalyst optimization process.

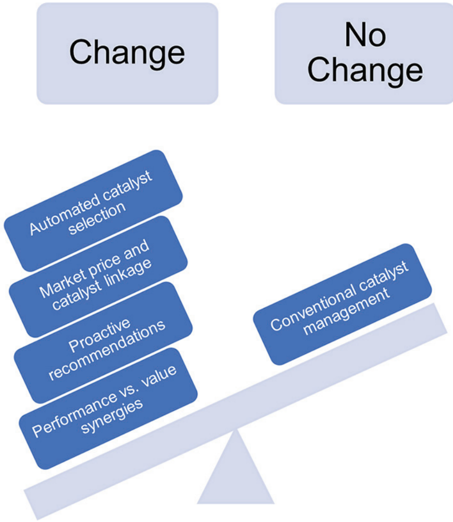


FIG. 5. A streamlined digital work process enables improved value capture.

mance. The analysis of Ecat data is used to benchmark the incumbent catalyst against historic performance profiles, along with other comparable units with similar constraints and objectives, to identify any opportunity to improve specific performance dimensions.

Once value-generation strategies and constraints are combined with an Ecat analysis, it is straightforward to design a catalyst formulation strategy to meet a refinery's needs. This catalyst design process translates a formulation strategy into a custom catalyst by automatically searching through the authors' company's technology space for a "recipe" with the required performance characteristics. The final catalyst formulation is tested against different economics and operating conditions to ensure that the catalyst design is robust and will deliver value over a variety of scenarios.

The authors' company has developed and implemented innovative digitized internal processes and external tools in recent years that make use of advances in digitalization and data connectivity. This digital transformation enables an unprecedented level of partnership between the authors' company and its customers, which facilitates maximum mutual value capture through efficient use of respective assets. Systematically applying a custom-engineered digital tool suite can break down a highly complex problem into a few manageable pieces. The next section illustrates how these tools are used to tip the balance in favor of change, thus capturing refinery value (compare **FIGS. 4** and **5**).

Digital transformation of catalyst optimization processes. Catalyst optimization must start with assessing customer needs and understanding how to design a catalyst to meet them. One tool to accomplish this assessment is an FCCU dashboard that organizes large operating datasets into a simple visual. The FCCU dashboard enables users to conduct a quick and thorough analysis—making it straightforward, with minimal work—to understand an FCCU's operating strategies and needs. To illustrate an example, **FIG. 6** shows dashboard charts for an FCCU that is staying within C_3 + C_3= constraints by limiting riser temperature and feed rate. As a result, bottoms rates are significantly higher than demonstrated minimum values.

Based on the demonstrated catalyst performance, liquefied petroleum gas (LPG) is quite valuable (also confirmed by an FCCU product price-set analysis). Simultaneously, bottoms production is higher than minimum rates, showing an opportunity to improve bottoms cracking. Looking at a few key operating variables (such as regenerator dense bed temperature, air rate, catalyst circulation rate and catalyst activity), this unit has some operating flexibility that can be coupled with a catalyst change to improve yields (**FIG. 7**). This example illustrates that by examining just a few data charts, it is straightforward to analyze an FCCU's operations enough to identify clear opportunities for improvement.

Once operators understand what factors may be limiting an FCCU's ability to generate increased value, it is a straightforward process to assess "shadow value" for overcoming constraints. Analyzing market pricing or refinery-specific pricing can highlight key value drivers for an FCCU. In the example price set in **TABLE 1,** LPG=s carries high value, but it may be less obvious than the value of low bottoms. **TABLE 1** shows typical volume-based pricing ($/bbl) for FCCU products, but also tabulates mass-based

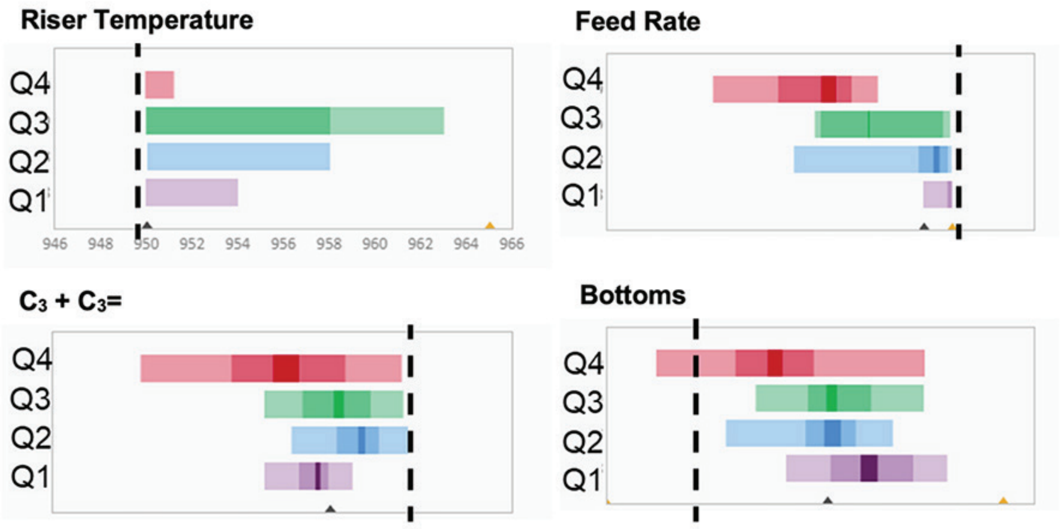


FIG. 6. FCCU operating data dashboard reveals bottoms cracking improvement opportunity due to operation against LPG constraint.

pricing ($/mT) and relative mass-based pricing, using light cat naphtha (LCN) as the standard. By examining mass-based pricing, it becomes clear that bottoms products have only half the value of gasoline, and that these products are only valuable when converted to LPG saturates and fuel gas.

In this example, upgrading 1,000 bpd of bottoms to LCO would increase its value by 50% ($31/bbl gain), which could be worth $0.60/bbl ($31/bbl × 1,000 bbl/d/50,000 bpd) or $11 MM/yr. Of course, some of the bottoms will be converted to less-valuable products, but the gain from conversion to higher-value products outweighs the loss from the less-valuable products.

Considering operations and economic analyses, a catalyst that can maintain current LPG= and reduce bottoms yield can be valuable for the refinery. The question becomes: How can we distribute incremental conversion products without losing LPG=? Better yet, how can we optimize the C_3=/C_4= ratio? The authors' company has developed mathematical algorithms that compare catalyst performance characteristics with unit constraints and economics to optimize performance. By systematically exploring the full catalyst design space, a mathematical algorithm can identify a catalyst design, which is a true game changer under all expected conditions and not just incrementally better than the incumbent catalyst.

In the FCCU example, it is easy to conclude that the best catalyst for the unit is a catalyst that has the highest LPG= yield. Only by analyzing operations and economic data in tandem does it become clear that a viable path toward maximizing value may be through de-emphasizing LPG yield. In this case, the FCCU has room to increase reactor overhead temperature, but currently cannot

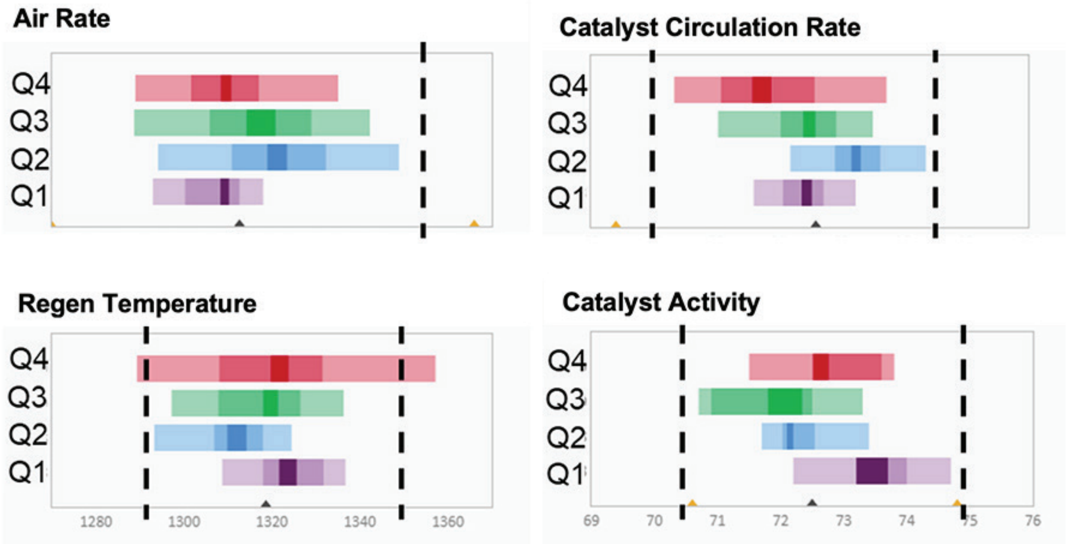


FIG. 7. Additional key operating variables highlight unit flexibility available to capture performance enhnacements.

TABLE 1. Example FCCU price set

	$/bbl	Standard gravity	$/mT	% gasoline
Fuel gas (C_2-), $/MMBtu	15.90	0.508	196	27
Propane, $/bbl	24	0.508	297	41
Propylene, $/bbl	70	0.522	843	116
nC_4, $/bbl	26	0.584	280	39
iC_4, $/bbl	26	0.563	290	40
C_4=, $/bbl	146	0.609	1,508	208
1,3 C_4==	-	-	-	-
LCN, $/bbl	82	0.71	726	100
Heavy cracked naphtha (HCN), $/bbl	89	0.77	727	100
LCO, $/bbl	80	0.93	541	74
Bottoms, $/bbl	61	1.05	365	50
Feed, $/bbl	65	0.9	454	63
Octane, $/bbl	0.5	0.77	4	1

increase conversion because it is operating against a $C_3 + C_3{=}$ limit. Therefore, the straightforward tweak of reducing LPG production tendency can unlock bottoms cracking by allowing the unit to operate at a higher conversion. While this example is relatively simple, it illustrates the complexity that smart algorithms can navigate. These mathematical tools can be used to develop non-intuitive customer solutions that can challenge conventional thinking and generate novel strategies to maximize value capture.

After a solid catalyst formulation strategy derived from detailed operating and economic analysis is identified, catalyst design tools are employed to develop a formulation with the best combination of performance over a wide range of expected conditions and value delivery. These catalyst design tools can search the entire technology formulation space for optimal solutions for a specific application. **FIG. 8** illustrates the systematic identification of optimal catalyst formulations by the optimization algorithm. Viewing these formulations sorted by performance (in this case, \$/bbl) easily shows how different approaches compare and, more importantly, how performance rankings change with market economics and physical constraints of individual FCCUs.

By using a multidimensional analysis to attack catalyst formulation problems, it is possible to produce a catalyst that maximizes performance and value over a large operating envelope.

The digital tools highlighted here provide extraordinary depth of analysis to support catalyst optimization; simultaneously, the efficiency with which these tools are applied enables frequent application. These novel digital tools not only enable the authors' company to optimize catalysts for the refineries that it supplies, but they also facilitate conversations with unit engineers, subject matter experts (SMEs) and other techno-commercial decision-makers at refineries to critically explore opportunities together to develop novel strategies that can take on a rapidly evolving marketplace.

Empowering the customer. As the petrochemical industry continues to evolve rapidly, the authors' company also innovates and adapts to enable customers to keep pace with the market. With these digital tools, the authors' company provides recommendations to customers, complete with comprehensive analyses, enabling fast decisions while requiring very few customer resources beyond the FCCU engineer.

Efforts to develop the next-generation digital tools are underway. As the value of catalyst optimization in unit monitoring is demonstrated, customers are sharing data more openly, including across corporate boundaries. The authors' company is actively utilizing platforms to share real-time operations and Ecat data with customers. Mobile deployments for digital dashboards and catalyst analysis tools are now being tested, and advanced data analysis techniques are under development.

Improved connectivity and enhanced digital tools are paving the way for an unprecedented level of shared understanding of refinery objectives and catalyst capabilities. Industry is rapidly moving toward a time when technology providers and refining customers move in lockstep to anticipate and address industry challenges, while maximizing profitability and improving industry sustainability through digital collaboration and idea sharing.

Takeaways. This article highlights how digitalization is used to translate refinery operating data and market analysis into strategies and solutions that can capture value through FCCU catalyst optimization. New digital tools and platforms (**FIG. 9**) bring together key stakeholders at catalyst suppliers and refineries and empower the unified team to respond nimbly to market shifts and

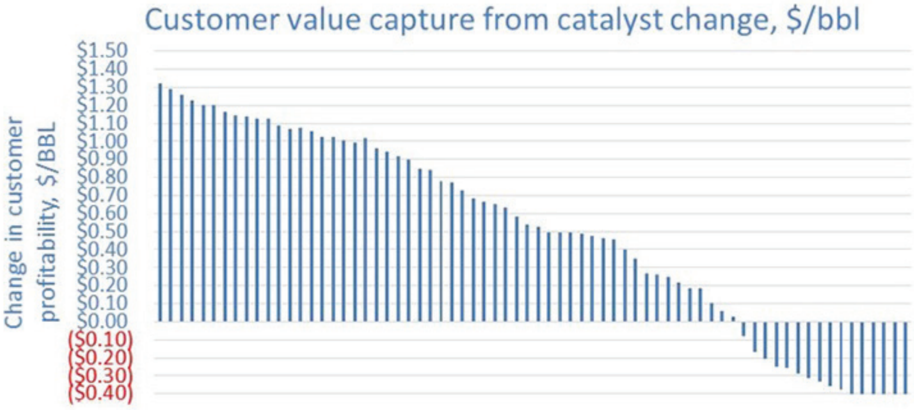
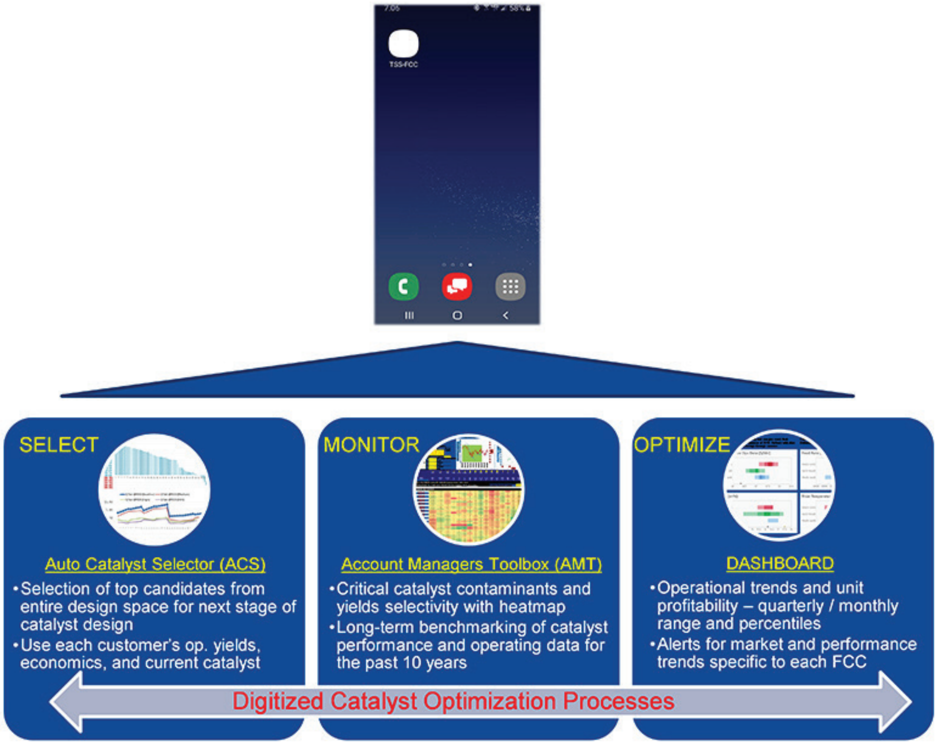


FIG. 8. Predictive model to simultaneously screen catalyst formulations from the universe of available technologies.



Auto Catalyst Selector (ACS)

- Selection of top candidates from entire design space for next stage of catalyst design
- Use each customer's op. yields, economics, and current catalyst

Account Managers Toolbox (AMT)

- Critical catalyst contaminants and yields selectivity with heatmap
- Long-term benchmarking of catalyst performance and operating data for the past 10 years

DASHBOARD

- Operational trends and unit profitability – quarterly / monthly range and percentiles
- Alerts for market and performance trends specific to each FCC

Digitized Catalyst Optimization Processes

FIG. 9. The authors' company's catalyst optimization process is a comprehensive, streamlined, digital workstream that delivers maximum value to refining partners.

challenges. Digitalization also helps to analyze and prepare for future scenarios, enabling refiners to quickly respond to evolving product demands.

It is often said that where there is uncertainty, there is opportunity. This statement may be truer today than ever, given the extremely dynamic state of the HPI. By leading the response to market dynamics, refiners can ride the wave of uncertainty to stay ahead of the competition. This article demonstrates how digitalization is instrumental to uncovering the opportunities that enable refineries to capture value by maximizing the performance of their FCCU assets. The authors look forward to seeing how digitalization will help refiners reach new levels of communication and collaboration never before seen in our industry. **HP**

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