Case history: Optimization of FCCU with multivariate statistical modeling

Process models and simulation methods can be used to simulate the fluidized-bed catalytic cracking unit (FCCU) process.\textsuperscript{a,b} Likewise, kinetic or multivariate statistical models have been used. Rigorous non-linear reactor kinetic models have typically been applied to develop project design, support refinery planning, etc. However, kinetic models have had limited applications in maintaining FCCU operations and in optimization projects for many reasons. Kinetic models tend to be time-consuming and expensive to build and run. They are also difficult for the refinery engineers to maintain due to their complexity.

**Solutions.** Multivariate statistical models based on operating data and using standard software can provide a suitable alternative to support process optimization. These models can be readily and cost-effectively developed. Such models can be used for FCCU troubleshooting, along with optimization and training purposes. They are also suitable for real-time process monitoring and are suitable for evaluating changes in feed and operating variables.

Several generic examples will demonstrate the power of multivariate statistical process models. For example, a case history will illustrate the development of accurate models for the Lukoil’s Nizhgorodnefteorgsintez (NNOS) refinery: The Lukoil NNOS models can accurately estimate online FCCU product yields, gasoline research octane number (RON) and regenerator bed temperature (RBT). With this information, Lukoil was very successful in meeting the new market demand for premium gasoline by optimizing the catalyst, feed and FCC operating conditions.\textsuperscript{1}

**Background.** In August 2005, Lukoil announced a major investment to upgrade the NNOS refinery: This investment was in response to increased gasoline demand by passenger vehicles.\textsuperscript{2} For Russia and the CIS, demand for regular gasoline was replaced in favor of premium gasoline with the migration to Euro 5 standards.\textsuperscript{3}

In 2005, a licensor was selected to provide the design for a new FCCU. The new unit was successfully commissioned and operational in 2011.\textsuperscript{4} The unit is a modern, short contact time riser design FCCU.\textsuperscript{4,1} The FCC catalyst uses a distributed matrix structures (DMS) technology platform.\textsuperscript{4} DMS technology enables high bottoms conversion with low coke make; all contributing to higher yields of gasoline and light olefin products.\textsuperscript{5} In addition to catalyst, a technical service team assisted the NNOS refinery and was requested to build accurate FCC process models and provide simulation capability.\textsuperscript{6} Application of multivariate statistical modeling was selected as the best approach to meet the refiner’s needs.

**Benefits from statistically modeling an FCCU.** Rigorous non-linear reactor kinetic models have been used to develop project design yields and to support refinery planning, especially in defining linear programming sub-models and evaluating new FCC feeds. However, applications of kinetic models to support FCCU operations and optimization projects are less common due to the significant effort to produce accurate results for each operating scenario.\textsuperscript{6} Kinetic models, even if more accurate, require more specialized knowledge to build and calibrate. **Result:** Kinetic models are time-consuming and costly to run; in addition, they are difficult for the refinery engineers to maintain.

An attractive alternative to kinetic models is using multivariate statistical models based on unit operating data. These models can be readily and cost-effectively developed by refinery engineers with the support of their catalyst supplier. Benefits of multivariate statistical models include:

- **Easy to build using standard software**
- **Does not require a detailed knowledge of the FCC hardware design to develop**
- **Easy to maintain and update, e.g., by updating models if conditions change**

**FIG. 1.** Time series of coke yield (Customer A).
- Enables a detailed understanding of the impact of process variables on unit operations in a transparent and user-friendly way; they can be used for unit troubleshooting, optimization and training purposes.
- Suitable for real-time process monitoring to detect deviation from expected base operation behavior.
- Easy to use in the prediction mode; they can be used to examine the impact of different feed qualities, change in reactor temperature, etc.

**POWER OF STATISTICAL MODELS**

There are many good reasons why a refiner should consider application of statistical modeling to an FCCU, as illustrated in several examples.

**Example 1: Real-time monitoring of catalyst and SO\(_2\).** In this example, an FCCU was experiencing coke-yield limit issues. Following the change to a new catalyst, initially the operating data trended as the previous condition, as shown in **FIG. 1.**

![FIG. 1. Time series of coke yield (Customer A).](image)

Later, coke yield began to increase (**FIG. 2**). At this point, the operations and management team became concerned. The issue was explaining why the coke yield was increasing and how to reverse the trend.

One approach would be to use a valid process model to set the baseline before the catalyst changeover. Then the team could evaluate the process change due to the new catalyst. It would be possible to estimate the expected coke yield for the present operating conditions. By comparing the estimate with the present data for the new catalyst, operations could decide whether the present coke yield is satisfactory (**FIG. 3**). Based on **FIG. 3**, the coke yield for the new catalyst is less than expected for the base catalyst at the present operating conditions. But why? Engineers could use the knowledge captured in the process model to identify which process variables are contributing the most to the higher coke production.

The model in this example is coke yield as a function of feed preheat, feed Conradson carbon residue, riser operating temperature, feed gravity, riser steam rate, equilibrium catalyst nickel content and feed distillation. In this specific example, Ecatalyst activity and feed rate have not been included in the correlation since these variables did not vary significantly during the trial and, therefore, statistically weren’t relevant. However, in general, coke yield is influenced by these variables and would be included in the correlation when Ecatalyst activity and feed rate vary significantly. **FIG. 3** confirms that the new catalyst is more coke selective than the base catalyst for the same processing conditions. Also, the previous model now needs recalibrating to accurately forecast performance with the new catalyst.

In another example, multivariate statistical modeling was used for real-time monitoring of FCCU regenerator flue-gas sulfur dioxide (SO\(_2\)) emissions during a SO\(_2\) reduction additive trial, as shown in **FIG. 4**. In the past, refiners applied a simple relationship between SO\(_2\) and FCCU slurry-oil sulfur to monitor a SO\(_2\) additive trial. Unfortunately, this practice often had poor correlation, i.e., a more sophisticated approach is justified. As shown in **FIG. 4**, the multivariate statistical modeling can provide an accurate estimate of regenerator flue-gas SO\(_2\) emissions. It can be used in real-time monitoring for the performance of a new additive trial. In this specific example, the new SO\(_2\) reduction additive had an improved, higher pick-up factor.

**Example 2: Estimation of flue-gas emissions.** This example shows how real-time monitoring and estimation of coke yield was possible even during a failure of the online...
flue-gas analyzer (FIG. 5). It demonstrates how a multivariate statistical model can be used, with care, for a short period to continue the operation of a unit. Applying the model avoided other consequences that could have caused a unit shutdown, while repairs were made to the analyzer. Furthermore, statistical modeling can be considered for estimating, in real time, FCCU flue-gas emissions—e.g., SO₂, nitrogen oxide and carbon dioxide—to enhance emissions monitoring and reporting to regulators. Even when the flue-gas analyzer is working, many FCCU reports indicate that the analyzer is not always providing reliable measurements. Thus, flue-gas emission models can also be used to highlight issues with the analyzer.

**Procedure for multivariate statistical model.** The main process steps to develop a multivariate statistical model are summarized in FIG. 6. The steps include:

1. Unit operating data is conveniently stored in MS Excel (or similar software).
2. These data are initially screened using basic graphical techniques to identify misleading values. At this stage, it is helpful to plot time series and compare them to known unit operating envelopes and constraints. These same graphs can also be used to identify poorly behaving instrumentation.
3. Once the obvious misleading values are excluded, then unit heat and weight balances are built. This is used to screen out datasets with poor heat and weight balance closure.
4. The good data are transferred to statistical analysis software. The FCCU engineer often has a good feeling for which independent variables impact dependent variables. It is important that the regressions developed have a basis supported by a theoretical understanding of the FCC process. Using standard statistical techniques, the relationship between independent and dependent variables can be confirmed.
5. The next step is step-by-step multiple regressions to build models relating to independent and dependent variables.
6. To validate these models, the results are compared to real operating data. The statistical tests and operating knowledge are used to fine-tune the models.
7. The result is a set of models relating independent to dependent variables that are in a format that can be easily entered into a spreadsheet or the control system. If required, these models can be combined with a graphical user interface (see FIG. 7) and be used in a purely prediction mode to examine new feed, operating scenarios, etc. If this is done, then it is wise to document clearly the limit of validity for each model.

This work process was used to build models for the Lukoil’s NNOS refinery FCCU.⁹

**Example 3: NNOS refinery FCCU models.⁹** In response

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**FIG. 6.** FCC operating data analysis and statistical modeling process.

**FIG. 7.** FCCU process simulator interface.
to the growing demand for premium gasoline, Lukoil’s NNOS refinery choose the DMS catalyst technology. This catalyst technology enables high bottoms conversion with low coke for higher yields of gasoline and light olefin products. In addition to catalyst, accurate process models were built for the Lukoil NNOS refinery. When faced with changing feed and operating objectives, these models, used in real-time, help detect deviations from the production plan. Thus, these models assisted the Lukoil NNOS refinery to maintain operating conditions close to the optimum and to improve profitability.

Figs. 8-10 show the commercial unit operating data and the real-time multivariate statistical model estimate for liquefied petroleum gas (LPG) yield, gasoline yield and gasoline RON, respectively. From these figures, the estimate values provided by the models trended very close to actual conditions. Thus, the models provided good estimates with high accuracy as processing conditions change.

For example, with reference to Fig. 8, the model’s coefficient values and the form of the equation will depend on the specific FCCU design, catalyst and operating conditions. Therefore, the models will be different for each FCCU and, they will require recalibration each time there is a significant equipment or catalyst change.

The Lukoil NNOS refinery FCCU feed is a severely hydrotreated vacuum gasoil. Therefore, it has very low levels of coke precursors. Furthermore, the unit operating objectives are to maximize bottoms conversion with low coke, and to deliver high yields of gasoline and light olefin products. This is achieved using a catalyst that is customized to the unit’s short-contact time design. Combining a low-coke make feed with a coke-selective catalyst leads to a low unit coke production and a low RBT. To manage this low RBT during feed and operating condition changes, an accurate model to estimate the RBT was built, as shown in Fig. 11. The model accurately predicted the RBT for a large range of operating conditions.

In addition to real-time monitoring of product yields, gasoline RON and RBT, Lukoil’s NNOS refinery needed an FCCU simulator to examine new feed and/or operating scenarios. A cost-effective simulator was built in MS Excel by combining the unit-specific models with a graphical user interface. Conditional formatting and comments on specific cells were used to clearly document the validity of the models. Fig. 7 shows an example of the graphical user interface. This interface provides a convenient way to enter user inputs and also summarize the results. This page can be saved or printed to create a record of the case. Alternatively, the results can be archived if a study is being done to estimate the response of the unit to step-wise changes in the feed or operating conditions.

Observations. Multivariate statistical models, based on unit operating data and using standard software, can be successfully used for support of FCC unit operation and optimization. These models can be readily and cost-effectively developed by refinery engineers and catalyst suppliers, as demonstrated by Lukoil at the NNOS refinery. The success of this project, combined with
favorable market conditions, has resulted in Lukoil’s decision to duplicate the design for a second complex.\(^7\)

**NOTES**

\(^1\) The model represents the key characteristics or behaviors of the process.

\(^2\) Simulation uses models to imitate the operation, enabling the examination of new feed and/or operating scenarios.

\(^3\) Lukoil Nizhegorodnefteorgsintez (NNOS) refinery is located in the Nizhny Novgorod area of Russia.

\(^4\) The basic engineering design for the process, technology and equipment is provided by UOP. The unit features side-by-side vessel layout, optimix feed distribution system, vortex separation system riser termination, advanced fluidization reactor stripper technology, RaCat riser technology and combustor style high-efficiency regenerator. The licensor’s process technology and equipment, in combination with the appropriate catalyst, enabled the Lukoil’s NNOS refinery to maximize profitability by achieving best-in-class conversion, total liquid product yields and olefin selectivity.

\(^5\) The catalyst used by the Lukoil NNOS refinery FCC unit is a customized version of BASF’s NaphthaMax catalyst.

\(^6\) Easy to build using standard software such as MS Excel and Statsoft Statistica.

\(^7\) Specific numbers have been removed to protect commercially sensitive data.

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\(^f\) Easy to build using standard software such as MS Excel and Statsoft Statistica.

\(^g\) Specific numbers have been removed to protect commercially sensitive data.

\(^h\) The customer is a refinery in Southern Europe.

**LITERATURE CITED**


7. Lukoil/Honeywell UOP press announcement.

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