Molecular management for refinery-petrochemical complexes

Designing a digital twin for process simulation of an integrated complex enables enhanced molecular management to deliver higher margin

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The future comprises a world of fuels refineries, refinery-integrated petrochemical complexes and crude oil to chemicals. Through the energy transition, the latter two will no doubt be more resilient toward future demand- and/or supply-side dynamics.

The potential for incremental improvement with increased conversion capabilities of a fuels refinery with added petrochemical integration is $1.5-2/bbl of crude processed. The value gained from effective molecular management is significant. Key objectives of molecular management for the overall complex are:

- Improvement in gross product worth by maximising high value products
- Reduced cost of feedstock by replacing expensive imports with low value streams

However, with the increase in complexity of refinery-integrated petrochemical complexes, a gap has developed in the tools needed to effectively drill down to the stream carbon number level on a continuous basis. Traditional tools used for refinery optimisation rely on bulk properties such as cut point for stream optimisation. Such methods have been found to have limitations in fully achieving the objectives of molecular management. The latest process simulation tools address this by enabling detailed carbon number breakdown from crude assays through to blending and petrochemical units, for the whole integrated complex. These enhanced capabilities enable identification of site-wide optimisation opportunities across the integrated complex, as well as ongoing sustainment of benefits through real-time monitoring and re-optimisation.

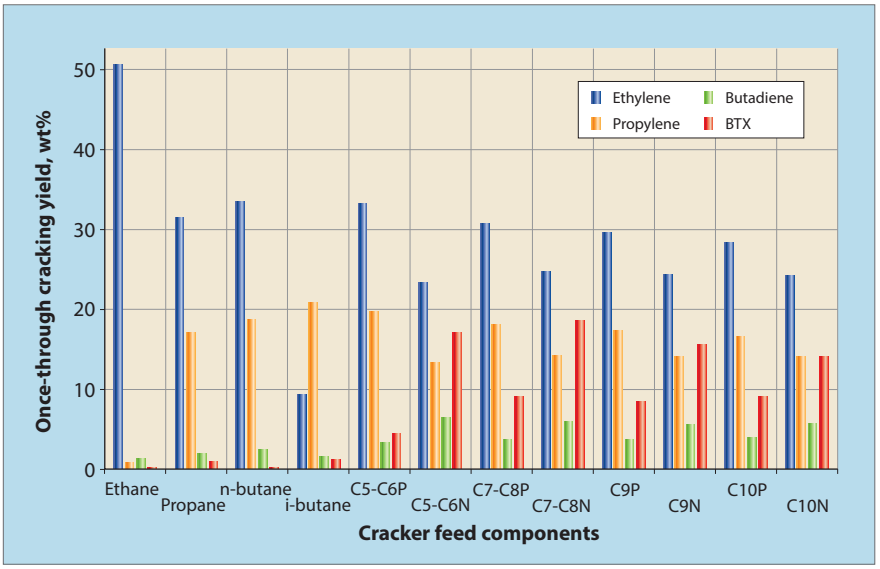

Figure 1 Once-through steam cracking yield for feed components

Why manage molecules?

To recognise the need for molecular management and carbon number level simulation, it is important to understand the difference in nature of refining and petrochemical processes. The purpose of refinery naphtha processing units is to maximise octane barrels which can be blended into gasoline. Isomerisation and dehydrocyclisation reactions improve octane, with thermal cracking a side reaction that is minimised to prevent yield loss. However, for steam cracking in petrochemicals, thermal cracking of naphtha is optimised to produce olefins.

Due to differences in the units' reactions, selection of molecules to be processed is extremely important. Replacing molecules from one process unit to another can improve yields from both the specific units as well as reducing operating expenses such as energy consumption, other utilities, catalyst, and chemicals.

The yields from a steam cracker can vary extensively depending on the feedstock carbon number and different isomers (see **Figure 1**).

Yield of ethylene and propylene is expected to reduce while yield of heavier products is expected to increase with an increase in the feed carbon number. Even for feeds with the same carbon number, cracking yields change with changes in C/H ratio, for instance paraffinic feeds have higher ethylene yield. Different feeds can be cracked separately or co-cracked, all having an impact on the cracking yields and furnace run length. Aromatics components in the feed rarely crack to produce ethylene and propylene, but these may be too costly to separate prior to processing.

The profitability of the aromatics

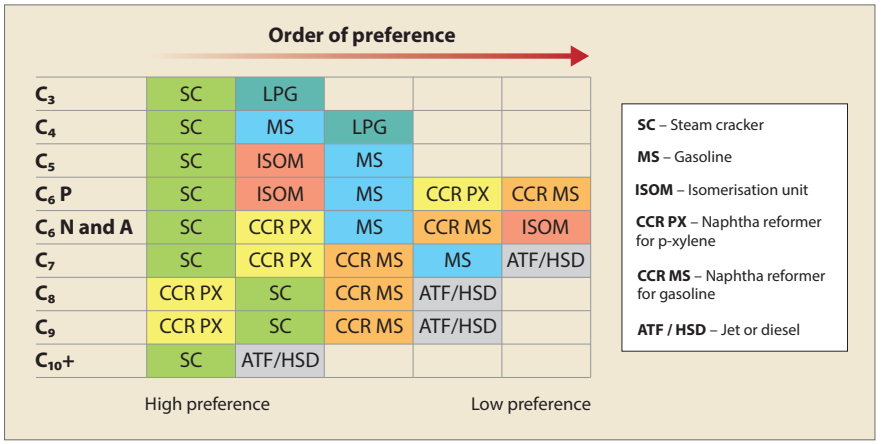

Figure 2 Feed selection criteria

is driven by the reformate yield and distribution of components in the reformate. Higher yield of xylenes over benzene is preferred from the aromatics, which could be achieved by selecting the right feed for the naphtha reformer.

Selection criteria for different feeds in refinery process units depends on the predicted octane barrels produced by feed components.

Figure 2 explains typical preferences which can be used to select feeds for different process units and product blending:

- Lighter hydrocarbons like C_2 components in off-gas and LPG are preferred feedstock for a steam cracking unit as these molecules provide higher yield of lighter olefins.
- First preference for routing C_5/C_6 molecules should be the steam cracker due to the significant premium for light olefins over gasoline. C_6 naphthenes and benzene in the reformer feed will contribute to benzene product for an aromatics reformer and can produce off-spec product for a gasoline reformer.
- C_7s tend to crack more in the ISOM unit compared to C_5/C_6 and therefore should be minimised. Routing of C_7 molecules to the aromatics reformer is preferred over the gasoline reformer. This routing leads to a reduction in the A7/A9 ratio in a transalkylation unit and improves octane barrels of gasoline pool.
- C_7+ components in heavy and medium naphtha can also be used for middle distillate blending. If C_7+ components cannot be processed in any of the process units, they can be blended in middle distillates diesel rather than selling them as open grade naphtha.
- C_8s are preferred feedstock for an aromatics reformer as they reduce the throughput of most of the process units in the aromatics and recycles as well. This reduces cracking to light ends and the opex of the units, and improves p-xylene yield.
- C_9s in aromatics reformer feed reduce the A7/A9 ratio of a transalkylation unit which improves the yield of xylenes and reduces benzene yield.
- C_{10}+ components are generally not preferred in aromatics, but these can be processed in a steam cracker.

The latest process simulation tools are critical for estimating optimum steam or molecule routing based on stream composition

Apart from the reactions and yields, feed selection criteria strongly depend on opex and the relative prices of fuels compared with petrochemicals. The latest process simulation tools are critical for estimating optimum steam or molecule routing based on stream composition. Molecular management is not limited to optimisation of refinery naphtha only, as the optimised routings are applicable for streams from the petrochemical complex as well.

Challenges

Quality parameters measured and analysed by the refinery engineers are usually based on bulk properties. Distillation and density are considered the most important properties for refining units. Though gas chromatography is performed for selected streams in naphtha processing units, components routed to refinery products are seldom analysed. The molecules lost in jet from the crude unit and the composition of hydrocracker naphtha are occasionally analysed in the refinery. On the other hand, the focus for petrochemicals is usually on pure components rather than bulk properties. Some of these components can be lumped together for monitoring purposes but detail to the level of isomers is required for a few units. For example, N+2A is used as a feed quality indicator for a gasoline reformer, however C_7/C_9 distribution is important for an aromatics reformer.

Simulation tools for refinery and petrochemical units are developed based on the information available – bulk properties for a refinery and composition for petrochemicals. Integrating these tools to create a complex-wide process model has been a challenge for process engineers in the past.

Tools based on linear programming (LP) are a solution for bigger optimisation problems such as crude selection, however they are rarely configured for molecular management. Even when they are used, LPs have their own limitations. Organisations focused on refining operations use comparatively simplistic techniques to simulate petrochemical units in LPs; petrochemical operators typically start optimisation at the naphtha feed and do not simulate component based assays and the fractionation efficiency of refinery optimisation.

Although LP tools allow some flexibility to simulate refinery-petrochemical integration, utilising simplified LP models can give

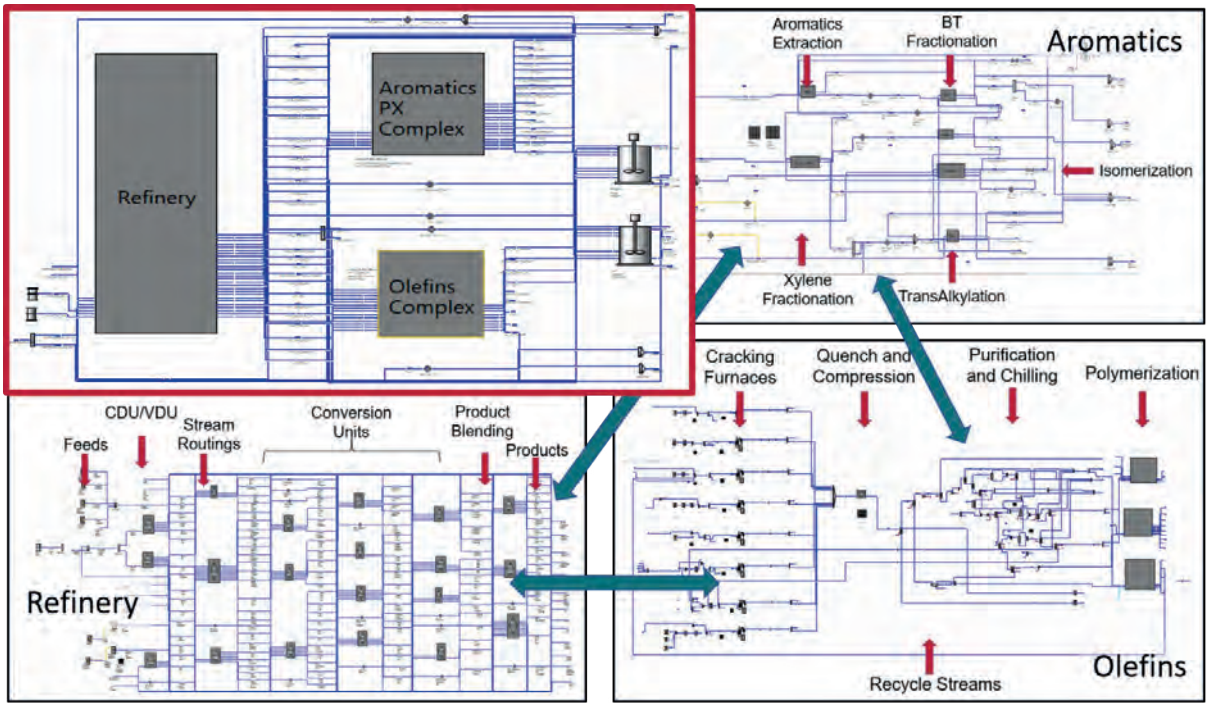

Figure 3 Petro-SIM model of an integrated refinery-petrochemical complex

erroneous results, for instance feed quality parameters in the form of bulk PNA, which do not capture the effect of carbon numbers in the steam cracking operating parameters. Also, a significant fraction of components are continuously recycled in aromatics units, which has an impact on unit opex and the maximum feed that can be processed. Very few refiners simulate these recycles in an LP based model.

Proven basis of the digital twin

KBC has developed and improved Petro-SIM models for refinery-petrochemical integration over many years, working on design configuration and optimisation engagement with clients. Petro-SIM has a seamless transition from bulk properties to component based simulation and vice versa. Information for components available in crude assays, as well as generated from the refinery reactor models, is carried through to petrochemical models using Petro-SIM's infrastructure. Reactor models are calibrated based on the performance of the operating unit, which allows process engineers to track information at a molecular level that is rarely available at the operating unit.

The main function and value of the complex-wide process simulation model is understanding the interaction between different process units and product yield. This can be quickly and easily done, as the equilibrium and kinetic based models for all the refinery, steam cracker, and aromatics units are in a single Petro-SIM simulation flowsheet (see **Figure 3**).

This combination holistically and seamlessly captures the effect of feed molecules. The integrated process model carries detailed composition and non-linear kinetics and can be used to augment the LP model to boost profitability through effective molecular management. LP models are still required for bigger optimisation problems, however an integrated process model is needed to routinely validate the optimised solution estimated by an LP. The optimised solution analysed through the integrated process model should be used to validate various constraints and to estimate operating targets.

Various process streams are exchanged between refinery and petrochemical units in the complex-wide model. Apart from feeds to cracker and aromatics, many other streams are also mapped, for instance off-gases and propylene from a refinery, integration of the hydrogen network, and so on.

KBC has deep experience of using integrated models for refinery-petrochemical complexes for identifying and implementing opportunities for profit improvement for the parties involved: re-routing of streams, changing unit severities, and modifying the degree of fractionation. In joint venture projects, a single integrated model is valuable for transfer pricing of intermediate streams between respective parties, based on stream quality. After all, it is the streams' molecular nature which ultimately determines its value in use. The use of the integrated model extends to the cost side too, with integrated modelling of utilities.

The integrated model can be used to estimate transfer pricing, as well as optimise the overall complex for the mutual benefit of all parties involved.

Case study

A KBC client was planning to build a grassroots refinery-petrochemical complex. According to the design of the integrated complex, C_5 from a cracked gasoline hydrotreater was to be routed as a feed to the steam cracker. The C_5 material was highly olefinic and therefore would give poor cracking yields unless it was hydrogenated to saturate the ole-

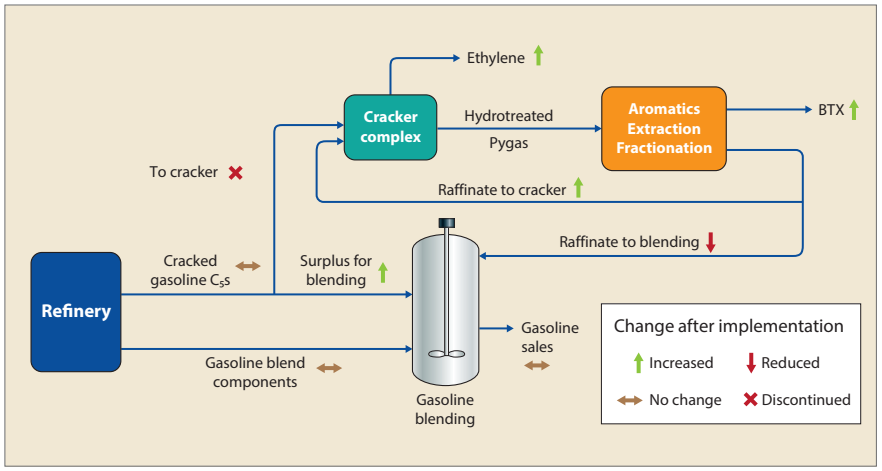

Figure 4 Case study for refinery and cracker complex integration

fins. Based on the relatively small quantity of C_5, a dedicated hydrogenation system was not economically justified. The next best option was to blend C_5 into the gasoline pool as it had relatively high RON and would boost gasoline production owing to its lower specific gravity. However, routing this stream to the gasoline pool without any other change would have reduced petrochemical yield and would therefore have given lower overall margins. The other potential constraint was the high RVP of C_5 which would have caused issues with the RVP and VLI of gasoline.

KBC reviewed all available streams that can be used to replace C_5 as a cracker feed. Raffinate from the aromatics extraction unit was partially returned to the cracker as feed, with the balance sent to the gasoline pool to meet volume demand for gasoline. The raffinate was rich in paraffins with C_6-C_8 components, an ideal feedstock for steam cracking. KBC proposed to replace the C_5 feed to the steam cracker with raffinate, routing the C_5s to the gasoline pool.

A complex-wide model was used to capture the impact on the cracker yield for both feeds and changes in gasoline RVP/VLI. Due to differences in the product specifications, summer and winter operations were analysed and it was found that all of the C_5 could be absorbed in the gasoline pool. There was an overall increase in petrochemical yield due to better cracking from raffinate while maintaining gasoline target volume production. This resulted in an economic benefit of almost 7c/bbl of crude. An overview of this case study is shown in **Figure 4**.

A digital twin for unit monitoring

Extending the availability of real-time unit operations data to refinery and petrochemical process engineers can transform their situational awareness of unit performance. With a greater understanding of the factors affecting unit performance, in real-time, deeper unit optimisation can be achieved.

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Utilising the complex-wide Petro-SIM model, with detailed embedded reactor representations calibrated using operating data, allows the integrated model to represent true unit operations over a wide range. To constitute an integrated process digital twin for evaluating unit operations in real-time, the complex-wide process simulation model can be put into operation with real-time operations data from sites' DCS, historian (OSIsoft, PI or other), and laboratory information systems (LIMS) to deliver real-time, high-fidelity virtual representations of hydrocarbon molecule transformation and associated operating conditions. This involves activating the in-built capabilities of the process simulation model without middleware being required.

To track unit performance, well-defined KPIs are used for ongoing scrutiny by unit operations engineers. For each KPI identified, actionable recommendations and procedures for correcting the poor or inefficient performance are developed. One of the key KPI measures is the comparison of reconciled data, with results from process simulation and the LP model used to validate the performance of these tools.

Petro-SIM's data reconciliation utility assesses the health of raw data available through the historian and LIMS. This includes raw mass balancing of sulphur and nitrogen for naphtha processing and petrochemical units, as well as carbon and hydrogen.

The digital twin can estimate parameters which require complex calculations such as cyclone velocity in a RFCC, chemical hydrogen consumption in each reactor, and remaining catalyst life in hydroprocessing units. Margin improvement indicators (MII) configured in the digital twin indicate the loss of margin or gap that needs to be closed to improve the profitability of the complex. The impact of MIIs on margin is estimated using complex-wide digital twin calculations and is configured in the digital twin of a process unit. Monitoring of MIIs ensures that the process engineers and operators continue to optimise the unit. Deviations from target and loss associated with this can then be reported on a continuous basis and acted on, thereby developing a culture of profitability in the organisation.

Case study

KBC worked with a refinery which was designed to produce light and

middle distillates for the domestic market. A new aromatics complex was commissioned near to the refinery which was operated and managed by a different organisation. Most of the feed for the aromatics unit was imported naphtha.

Although a part of the naphtha stream from the refinery was transferred to the aromatics plant, both the refinery and the aromatics plant maintained their own production accounting and reported financial performance using a naphtha transfer price. The refinery was using naphtha as low flash blendstock for middle distillates with the surplus sold to the aromatics plant. As the transfer price of naphtha to the aromatics plant was lower, blending in middle distillate was profitable for the refinery.

KBC compared the quality of imported and refinery naphtha and found that the quality of refinery naphtha was inferior to imported naphtha in terms of carbon number. The paraffin content of refinery naphtha was higher, and it was rich in C_7 whereas imported naphtha had higher C_8/C_9 content. With this comparison it was agreed that the refinery naphtha should be priced at a discount to imported naphtha.

The discount for refinery vs imported naphtha was validated using the integrated process simulation model. In a sensitivity case, a fraction of the imported naphtha was replaced with refinery naphtha. Both the refinery and the aromatics plant were considered as one holistic optimisation for this sensitivity, meaning that a transfer price was not required to estimate the economic impact of this change for the overall complex. This sensitivity case showed benefits of >$5 million/y without any investment.

The model indicated that processing the different quality of refinery naphtha reduced p-xylene production and increased benzene yield. With the higher price of p-xylene compared to benzene, there seemed to be an economic penalty. The middle distillate production was also reduced. Even with all these changes, the sensitivity case indicated improvement in overall profitability. This was due to the significant premium paid by the aromatics plant for imported naphtha.

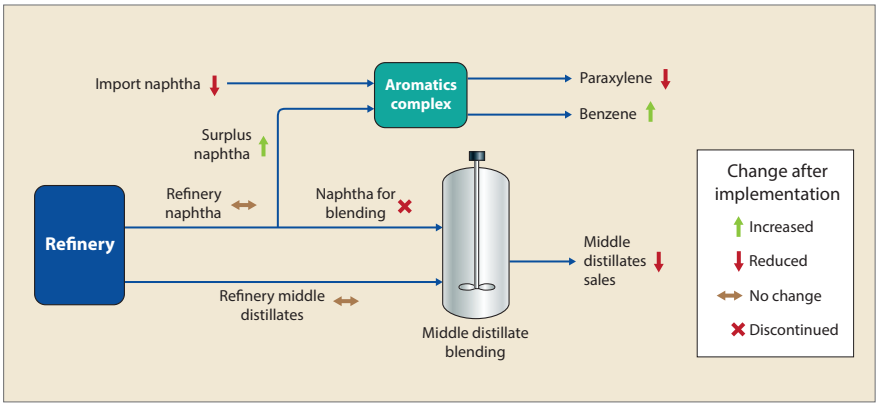

Figure 5 Case study for refinery and aromatics integration

The proposed opportunity was implemented by the refinery and the aromatics plant. The integrated process simulation model for the complex calculated the breakeven price of refinery naphtha. A discount to the breakeven price at which the aromatics plant would purchase naphtha from the refinery was agreed between the two organisations. With a revised transfer price, there was improved profitability of both organisations. With the integrated process model able to monitor the streams for quality changes, an update to the operating strategies of both plants was able to be implemented. An overview of this case study is shown in **Figure 5**.

Conclusion

A digital twin aims to be an accurate representation of an asset over its full range of operation and its full lifecycle. It is ideally created during the initial study to evaluate the feasibility of the asset. It is used and further developed during the design, construction, and commissioning of the asset. It facilitates the optimum design of the asset and the training of the staff who will operate the asset. It works in the present, mirroring the actual plant in simulated mode, but with full knowledge of its historical performance and accurate understanding of its future potential.

KBC's digital twin is built on our rigorous site-wide first principles simulator, Petro-SIM. The plant model inside the simulator synchronises with the plant model inside the enterprise process historian to ensure their separate representations of the plant remain aligned. Data gathered from the plant in real-time is validated and statistically reconciled to ensure that all physical and chemical laws are respected; and electronic noise and dynamic effects are eliminated through filtering, thereby ensuring that data quality issues are identified and mitigated.

Petro-SIM enables identification of opportunities for site-wide improvements in performance, as well as benefit sustainment through real-time monitoring of the entire complex. The potential for improvement of an integrated refinery-petrochemical unit is significant and requires tools that are able to analyse accurately for all of the key optimisation factors. Additional benefits can be achieved through effective molecular management for a refinery and petrochemical complex aided with a detailed carbon number breakdown from crude assays through to blending and petrochemical units.

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