Process simulation has been widely used in refineries for more than 30 years. Steady state and dynamic simulations are established tools for the design of new process units and optimisation (off and online) of existing facilities. While mathematical models of separation systems and other unit operations are available in most commercial process simulators, refinery reactors are very specialised models and, in most cases, are simulated as standalone units. As a consequence, the interactions between different processing units are not fully explored and the true operating window is never captured.

Many refiners have recognised the potential benefits of extending rigorous modelling to refinery wide simulations that model all of the process units as an integrated system. This approach would provide a powerful tool to help optimise refinery operations, and would be an important element in sustaining a competitive advantage in light of new regulations, growing competition and decreasing margins. However, such refinery wide models were expensive and time consuming to create.

In response to this need, AspenTech and UOP have developed a new simulation tool called Aspen RefSYS, which enables refiners to create rigorous refinery wide models using a standard, easy to use solution. This product combines AspenTech’s refining industry process simulation flowsheet technologies and the refinery reactor models developed by UOP and AspenTech.

This article illustrates a typical example of how rigorous refinery wide modelling can be used to help companies make more informed operational and investment decisions. This article analyses different strategies for benzene control in gasoline: an important issue facing many refiners because of its significant health and environmental implications.

**Refinery wide simulation**

Refineries are very complex processing plants and each one is unique with respect to its capacity, its processing units and...
its feedstocks. Understanding the true economic potential of a refinery is a complex challenge, due to the intricate interdependency of its processing units. Linear programming (LP) models have been successfully used in the decision making process for many years; however, refiners should be aware of the limitations of this approach. The LP model is an excellent economic evaluation tool, but because the model itself is built with parameters that are not always kept up-to-date to truly reflect the refinery capabilities, or is kept up-to-date with simplifying assumptions, it does not deliver the optimum economic answer and cannot adequately resolve questions related to operating constraints and new paradigms. Due to these limitations, the incorporation of rigorous models into existing work processes can help to ensure that daily operational decision making is based on more complete and accurate information.

A refinery wide simulation tool can therefore provide a range of important benefits, including the ability to:

- Understand the impact of changes in unit operations.
- Find the best set of operating conditions.
- Quickly test the LP model accuracy.
- Update the LP vectors in a timely manner.
- Respond quickly to operational changes/upsets and new regulations.
- Identify process bottlenecks.
- Evaluate different process configurations.
- Maximise the efficiency of existing equipment.

### Components of a refinery wide simulation tool

To provide companies with an effective and easy to use application, a refinery wide simulation tool based on rigorous models needs to incorporate a number of key components; these include:

- Thermodynamic engine: phase equilibria and the calculation of thermodynamic properties are necessary to any rigorous simulation.
- Assay management system: the access to assay libraries and to assay characterisation tools are necessary to represent the crude oils.
- Calculation of petroleum properties based on assay information: petroleum properties such as octave number, pour point, cloud point, flash point must be calculated at any point of the flowsheet. Special property blending calculations are essential.
- Library of standard unit operations: the user must be able to build a simulation model using pre-defined unit operations as distillation columns, heat exchangers, etc.
- Refinery reactors: first principle models for refinery reactors must be available for the user. These models must be ‘tuneable’ using plant data. Kinetic models must be developed from real pilot/plant data.
- Flowsheeting environment: unit operations and reactors can be linked together in a flowsheeting environment. The flowsheeting environment holds the model topology and invokes all model calculations.

### Analysis of benzene control strategies

To demonstrate how refinery wide modelling can help companies optimise their operational performance, a typical scenario in which a refinery needs to identify the optimum benzene control strategy for a particular set of operating conditions has been examined. The details of the refinery and its operational status are outlined below.

Figure 1 is a simplified process flow diagram for the refinery model. Crude oil is fed to the crude distillation unit that was modelled as a rigorous column with four side-strippers and four pump-arounds. The atmospheric residue is sent to the vacuum distillation unit (VDU), where VGO is obtained and used as the feedstock to the FCC unit. The FCC unit was rigorously modelled including the reactor (riser, stripping and regeneration), the FCC main fractionator and the gas plant. The HF alkylation unit was also part of the simulation.

Naphtha is drawn from the top of the CDU and sent to the naphtha stabiliser where light components are removed. Stabilised naphtha is hydrotreated (not rigorously modelled in this work) and sent to the naphtha complex (Figure 2). The naphtha complex comprises the reforming and the isomerisation units.

These two units play an important role in the benzene contents and final quality of gasoline. The reformer is a CCR platforming unit operating at 500 kPa (72.5 psia) and all four reactors at 510 °C (950 °F). The use of a refinery wide simulation tool allows the study of the interdependency of those two units, the interactions with the different crude blending options, the influence of the operation of the CDU and the connection with the other units that produce gasoline.

Two different crude oils are blended before being fed to the CDU. Table 1 shows some properties of crude oils ‘A’ and ‘B’.

### Base case

On the base case, crude oils ‘A’ and ‘B’ are blended using a 1:1 ratio on volume basis. Table 2 shows the properties of the feed stream to the reformer unit and Table 3 shows the gasoline pool composition.

### Influence of pre-fractionation

One of the strategies employed to control benzene in gasoline is the prefractionation of naphtha so that benzene and benzene precursors are removed from the reformer feed. Once those components are removed, they are sent to the Isomerisation unit, where benzene is saturated. Choosing the right benzene reduction strategy requires an understanding of the impact that each strategy has on such factors as overall gasoline production, refinery balance and economics. The rigorous simulation model of the refinery makes it possible to analyse different alternatives and process conditions and identify the optimum approach.

Benzene concentrations in the reformate depend on the amount of benzene and benzene precursors in the feed to the reformer. Benzene formation occurs by conversion of cyclohexane and methylecyclopentane to benzene and through the dealkylation of heavy aromatics to benzene.
Using the simulation model, the influence of the initial boiling point of the reformer feed on some key properties was analysed. Since all operations (distillation columns, reactors, heat exchangers and others) are part of the same simulation model, this study can be performed in a straightforward way. Figures 3, 4, 5, and 6 depict the influence of the D86 IBP of the reformer feed on the reformate research octane number, benzene concentration, hydrogen yield, and reformate, isomerate and gasoline yields, respectively.

It can be concluded that the benzene concentration on reformate, and therefore on gasoline, can be significantly reduced if the initial boiling point of the reformer feed is increased. The decrease in the hydrogen and reformate yields must be analysed in the context of the overall refinery, taking into account the hydrogen demand in other processing units. The increase in the reformate octane number suggests that the severity of the reformer could be reduced.

Further opportunities

Whilst this analysis has identified the potential for significant performance improvements by making minor alterations to the operating strategy, the refinery wide simulation model also makes it possible to evaluate the impact of a broader range of potential changes to explore whether they could offer greater benefits.

This could include using model to examine the detailed impact of different feedstocks on the downstream units, including the reactor units. For instance, the blending ratios of crudes ‘A’ and ‘B’ can easily be changed and those changes are automatically propagated through the flowsheet. The optimum reforming temperature and initial boiling point of the reformer feed stream can thus be determined for a different blending ratio. In this way, it is possible to view the model as a desktop virtual refinery that allows refiners to gain a much better understanding of their complex operations. This greater understanding can help to identify improvement opportunities, and can ultimately lead to more efficient and profitable refinery operations.

References

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