The role of process simulation in petroleum refining has evolved significantly over the past 20 years. While simulation technologies have long been an established tool in process engineering, additional capabilities are now available which promise to significantly expand the range of typical applications. In particular, there is a strong trend for simulation models to move into the world of operations, where they can be used to provide new insights for operational decision making.

Meanwhile, petroleum refiners are enjoying very good business, with high capacity utilisation and strong margins. Still, there are significant opportunities for forward thinking organisations to improve operational performance and maintain their competitive advantage for times when margins may thin out. Process simulation has an important role to play in supporting these initiatives to drive efficiency and reduce costs, especially now that models can make a significant impact beyond the traditional focus of process design.

Applying models in operations and planning support
One of the most significant developments is the increasing application of engineering models in refinery operations. While most companies have used rigorous process simulation models for engineering and design, very few were using these models to optimise plant operations. Recent innovations in petroleum simulation technologies, such as the ability to link to and utilise more detailed crude analysis, and the propagation and availability of assay properties across the flowsheet, have made it both possible and attractive for refiners to leverage their investments in models to improve operational decision making.

Another major development in refining has been the availability of simulation technologies to model multiple units, including the main refinery reactors. This allows refiners to study the complex interactions between units for a more comprehensive assessment of the impact of operational changes, instead of analysing each unit in isolation. This avoids suboptimal decision making, and delivers measurable improvements from feedstock and operational optionality.

Simulations can now be expanded in scope to include most or all of the main refinery units. However, refinery wide optimisation is an area where rigorous process simulators may still be limited in their performance. Linear programming (LP) optimisation tools such as Aspen PIMS™ dominate the refinery wide optimisation applications, but simulation tools have a valuable role to play in maintaining and improving the accuracy of the LP planning models. More accurate planning models enable refiners to make more confident feedstock selections and develop achievable operating plans, as well as making it easier to apply those plans in the actual operations.

In short, advanced refinery simulation technologies are helping refiners bridge the gap between process modelling and planning, thus delivering benefits to operations and to planning functions.

<table>
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<th>Table 1. CEPSA refineries in Spain</th>
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<td>Refinery</td>
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Rigorous multi-unit refinery modelling

CEPSA selected the Aspen RefSYS™ refinery simulation product. Aspen RefSYS is based on the Aspen HYSYS® process simulation product foundation, combined with significant improvements to predict and display petroleum stream properties based on crude assays, to quickly configure multi-unit simulations, and to model key refinery reactor units rigorously.

Aspen RefSYS allows the user to predict the behaviour of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. Given reliable assays information, thermodynamic data, realistic operating conditions and the rigorous Aspen RefSYS equipment models, actual plant behaviour, including stream refinery properties such as cold properties, octane numbers, RVP, sulfur, nitrogen, metals contents, etc., can be accurately calculated.

Rigorous kinetic models from AspenTech are featured for the most important reactors of an oil refinery such as FCC, naphtha reforming, hydrocracking and hydrotreating. These models have been successfully used to predict unit operations in both online and offline applications. The reactor models can be tuned to match real operations using specialised calibration interfaces.

CEPSA's distillation model applications

The first models created by CEPSA using Aspen RefSYS were the two distillation trains in the Algeciras refinery, including crude, vacuum, naphtha stabilisation and naphtha splitter units. These were built by the planning group using the same rigorous tray by tray column models as used in Aspen HYSYS for engineering studies. These models were updated to the specifications required by the planning application. These include distillation points, gasoil cloud point and other operating variables such as temperatures, pressures, stripping steam flows, etc. Figure 1 shows the PFD of the Aspen RefSYS model and Figure 2 the properties stream view.

CEPSA has found that simulation models are better suited for LP data generation than the traditional assay cutting models tuned with empirical data. Firstly, traditional models require large sets of test run data, generated by feeding the actual units with a single crude. This makes it difficult to obtain high quality and consistent data, is very expensive, and can compromise actual production.

Secondly, traditional models do not represent the impact of many operating variables or do it in a linear fashion, and therefore do not provide representative data in a wide range of operating conditions.

Although the representation of a particular plant data set can be superior with empirical models due to the large number of parameters that can be tuned (in the rigorous distillation models, once the internal liquid and vapour traffic has been set, only tray efficiencies can be tuned), empirical models do not extrapolate well to other operating conditions and result in large deviations.

CEPSA applies the distillation models in support of its planning and scheduling activities in three different ways, as illustrated in Figure 3.

Crude fractionation database

The first application of the Aspen RefSYS distillation models is to create CEPSA’s crude database. This now reflects actual distillation column performance with accurate prediction of product properties, including distillation overlaps, instead of straight cut properties.

The models are run for all crudes in the CEPSA basket (more than 50) in several modes of operation for each distillation train. Basic crude assay information is obtained through
the commercial ChevronTexaco database in Spiralsoft’s Crude Manager combined with CEPSA’s own laboratory analysis.

The crude fractionation database is published and available in CEPSA’s Intranet and is updated every six months. This frequent update is possible only because Aspen RefSYS is able to generate consistent crude distillation data with minimal effort. This data is then used to feed both the corporate LP model for crude evaluation and the refinery crude tanks scheduler.

Monthly refinery operating plan
The next application of the Aspen RefSYS distillation models is in support of the monthly operating plan for the already committed crude diet. The refinery LP tool is used to develop operating strategies for the maximum monthly operating profit, considering the available marketing information.

The LP tables that represent distillation column yields and properties are updated from the results of the simulation model each time a new feed blend is evaluated. Where possible, blending and distillation calculations are done inside the simulator model rather than blending product fractions from individual crudes inside the LP, since this provides more accurate results and avoids the complexity of LP pooling calculations. This is a somewhat recursive process between the simulation of a given crude blend and LP optimisation.

This approach ensures the LP representation of the units is always closer to the actual unit behaviour as the rigorous model can be easily updated for any unit equipment modification or temporary operational change.

Column product yields and properties are also used to feed conversion unit proprietary calculations to produce the complete set of information the LP requires for its conversion submodels.

The rigorous distillation model is run by planners directly through a Microsoft Excel interface linked to the Aspen RefSYS model. This automates the collection of key simulation input and output variables in a single environment and eases the use of the simulation by economic planners.

Daily unit target setting
The third application of the distillation models is for setting daily unit targets by the schedulers in the distillation units.

For each feed tank composition (a tank may last between one and three days), the distillation model is run with the planned set of specifications and the expected yields and additional properties are obtained. Any other variable impacted by the feed blend change (such as furnace outlet temperature) is adjusted to reflect the new feed requirements. The high fidelity Aspen RefSYS distillation model accounts for all variables and constraints, and provides realisable targets without depending on isolated and often outdated spreadsheets.

This model data provides an accurate operating reference guide for the new feed blend, and operators adjust to the new operating targets by changing set points in the control application. Its use is particularly beneficial in the few hours when the tank switch operation takes place until a new steady state is reached, as operators can make proactive adjustments to quickly and simultaneously achieve the new operating mode and its steady state.

Actual unit performance is also compared with the model predicted performance and this information is used for unit monitoring. When any significant deviation between the model and actual performance is found, further analysis is performed by the engineering department to identify the cause, such as column flooding, fouling or any other operating problem.

Operational benefits
Simulation models built in Aspen RefSYS are able to represent refinery unit behaviour over a wide range of operating conditions. The confidence in the model results, and consequently in the data used to create the operating plans within the LP, encourages the operations teams to actually execute the plans and to monitor their implementation. This planning/monitoring cycle between planning and operations cannot be implemented without consistent models that both groups use and trust over a wide operating range.

The empirical models that were used previously in the distillation units typically generated more optimistic plans from the LP system. When operations implemented these plans and found them to be unrealistic, it caused friction between the planning and operations groups. Having a common model, validated by engineering, now sets the right basis for collaboration in developing optimal and achievable operating plans, and for any team discussion and problem resolution. Aspen RefSYS plays an important role in each of these workflows by saving time, improving consistency, and minimising errors.

Conclusion
The implementation of Aspen RefSYS models in CEPSA is a successful example of applying rigorous engineering simulation models beyond their traditional use in engineering design projects. The models can be used for refinery business planning with a higher degree of confidence than simple models tuned with empirical data.

CEPSA model results are used to feed its internal LP tool in the support of its corporate long term planning activities through the fractionated crude database, monthly operating plans, and planning, execution and scheduling.

Going forward, based on the experience with distillation models, the application will be extended to include conversion models as well.

References