

Process simulation gets real

Patrick McGrath and Suresh Sundaram show how off-line process models can help the bottom line



PROCESS simulation practice has evolved rapidly over the last 20 years. In the engineering domain, the role of simulation has changed from simply “automating design calculations” to being the centre of “integrated engineering workflows” that support a variety of decision-making tasks from conceptual design to process design to plant troubleshooting. Process companies use a variety of synergistic engineering technologies (in-house and commercial) in conjunction with steady-state process simulation, such as process synthesis, economic evaluation, dynamic modelling and equipment modelling.

In the plant, modelling technologies playing a critical role in the plant operations, planning and supply chain domains. Empirical modelling technologies in advanced process control (APC) are now a standard in the continuous process industry. First-principles simulation models have a proven track record in real-time optimisation (RTO) in many process industry segments and linear programme (LP) modelling in planning, scheduling and supply chain management activities is the norm. In addition, companies are utilising a variety of in-house and third-party models to support decision-making across enterprise operations.

Engineers in the chemical process industries (CPI) build models for a variety of applications, including process design, troubleshooting, yield accounting, scheduling and planning, process optimisation and operator training. These models come in a variety of forms, including steady-state/dynamic, off-line/on-line, calculators, parameter estimators and data reconcilers. Historically, it has generally been necessary to build these various applications with different tools. As a result, it is not unusual for chemical manufacturers to have developed, or purchased, several models that represent the same physical system, with such models having been constructed at different times by different engineering staff. The inherent inefficiency of this circumstance can be further exacerbated if an organisation does not possess and utilise an effective knowledge management system. In worst cases, the cost of projects which might otherwise be economised by leveraging previous work may approach those of a grass-roots effort.

Today, advances in simulation software

and IT infrastructure are making it possible to build multiple applications for a given physical system in a single modelling environment. The model may represent a single equipment unit operation (constructed using a single simulation tool) or an entire asset (constructed by aggregating models built with one or more simulation tools). The model may be modified for various applications, but the essential data structure is re-used. The model has seamless connectivity to plant data, databases and other applications. Models are archived in a central knowledge management system, enabling re-use of the intellectual property embedded within the models. The model can be deployed via configurable user interfaces, either to single desktops or to the wider enterprise. These advances deliver the promise of “model-centricity,” enabling the interdisciplinary collaboration necessary for engineering, operations and business management organisations to effectively deploy capital expenditure (Capex) and operation expenditure (Opex) investments in an optimal manner.

This article presents a real-world example where a legacy first-principles process design model was used to optimise real-time operations at a chemical facility.

the company

Lyondell Chemical Company, headquartered in Houston, Texas, is North America’s third-largest independent, publicly-traded chemical company. Lyondell is a major global manufacturer of basic chemicals and derivatives including ethylene, propylene, titanium dioxide, styrene, polyethylene, propylene oxide (PO) and acetyls. It also is a significant producer of automotive fuel blending components. The company has a 58.75% interest in Lyondell-Citgo Refining, a refiner of heavy, high-sulphur crude oil. Lyondell is a global company operating on five continents and employs approximately 10,000 people worldwide.

Lyondell operates eight world-scale PO plants, three of which manufacture styrene monomer as a co-product via proprietary Lyondell process technology referred to as POSM (propylene oxide/styrene monomer). Lyondell operates two POSM plants in Channelview, Texas, and in autumn 2003 started up a third plant in Maasvlakte, the Netherlands.

business challenges

The nature of the PO market has changed dramatically over the last several years as the business has matured to that of almost a pure commodity chemical, which caused Lyondell to adjust its operational focus. Specifically, in commodity businesses, value is realised through volumes, margins and on-stream factor. As such, Lyondell PO manufacturing plants have sought to improve energy efficiency and yield in a bid to reduce costs while maintaining operational reliability.

POSM plants are characterised by large-scale equipment, a large equipment count, several billion lb/year hydrocarbon throughput, a high degree of mass and energy integration, and intensive energy use. As such, postulating and solving the facility-wide process optimisation problem is not trivial, necessitating the use of sophisticated real-time optimisation technology. It was therefore decided to develop such a system incrementally, beginning with the energy-intensive PO refining train at the POSM 1 plant in Channelview, Texas.

Optimisation of the PO refining train would address the following business objectives:

- Reduce energy costs.
- Increase yields.
- Improve operability.
- Increase process understanding for higher fidelity engineering studies for de-bottlenecks and grass-roots designs.

solution

The primary scope of the project was to minimise the amount of energy used to refine PO. POSM plant PO refining train distillation columns are very large, and because the PO refining technology makes use of an extracting solvent, they are highly integrated.

Over the years, a number of improvements to the POSM 1 PO refining train have been made to increase capacity and reduce variable costs. Hence, the project team recognised that a significant incremental improvement in energy efficiency could likely only be made by improving the process technology. However, all the legacy process improvements had been based on single-unit operation or sub-system calculations, ie a holistic analysis of the entire refining train had never been attempted. As such,

the project team was reasonably confident that the process technology could be further advanced, allowing for new cost savings to be identified and implemented. The team decided that the best way to achieve this objective would be to provide real-time guidance to the operations staff with a rigorous (process model based) on-line optimiser.

The solution was to implement the AspenONE Performance Management for Chemicals software. This would allow the team to:

- Re-use existing Aspen Plus process models developed when the plant was designed.
- Tune the process models to match current operating conditions using real-time process data and parameter estimation techniques.
- Deploy the process models on-line to calculate optimal operating conditions, and providing these results as guidance to the operations staff in the form of an electronic shift report. Operating targets included selected purges, reflux flows, steam flows and solvent flows.
- Store selected on-line process model predictions in the plant data historian.

The solution leveraged existing plant infrastructure including a modern distributed control system (DCS), process data historian, laboratory information management system and IT network. Information stored in Lyondell's model library, including process design models and a significant body of physical properties work served as building blocks for the application.

The POSM 1 PO refining RTO application was developed in about three months by a joint team of Lyondell and Aspentech engineers working closely with the operations staff. Plant implementation required about ten days. The transition of the units went quite smoothly. Product quality was held constant, and as the roll-out progressed the operations and technical staff gained increasing confidence in the fidelity and robustness of the application.

A rigorous process model is now running on-line, tracking the POSM 1 PO refining section. The application generates optimum operating targets that the plant operator can use as guidance for maintaining the plant at optimum efficiency, ie lost opportunity costs are held at or near zero. All major process variables predicted by the model are stored in the Aspentech solution, so that they can be used for trending and analysis. On-line model results can be re-created offline, for process support work, de-bottlenecking studies, or grass-roots design.

The application is robust and generates highly accurate heat and material balances, including high fidelity predictions of product trace component compositions. The application has been permanently commissioned in POSM 1 and has been generally well-accepted by operations staff.

business benefits

The project significantly exceeded expectations with respect to improving energy efficiency. Since commissioning the system, energy consumption in the POSM 1 PO refining train has been reduced by more than 11%. *Ad-hoc* technology transfer to the POSM 2 plant in Channelview resulted in a 5% decrease in energy consumption. A similar technology transfer to Lyondell's third POSM plant in Maasvlakte resulted in an 18% decrease in energy consumption. Because PO refining is energy intensive, these achievements significantly reduced variable operating costs, translating to well over \$1 m in energy savings per year across the three plants. Note that these achievements were realised with no significant capital expenditures.

In addition to real-time process optimisation, a number of off-line modelling studies provided significant additional economic benefits, including:

- Several minor physical process changes and regulatory control improvements that have greatly improved operability.
- It was possible to shut down several large unit operations in the equipment configuration, which has reduced operating and maintenance costs, improved reliability, and will provide significant capital savings for future plant designs.
- A POSM 1 PO refining tower design retrofit project will be constructed in an upcoming turnaround, which is projected to provide a very attractive return on capital via improved refining yields.

lessons learned

Several lessons were learned during the development and implementation of this project:

- Plan the work. When undertaking a project of this scope, it is important to resist the temptation to immediately start developing simulations. It is always preferable to first develop a detailed plan, elements of which should include a defined project scope, schedule, contracting strategy, work breakdown structure, milestones (stage gates), and roles and responsibilities matrix.
- Validate the model off-line. Off-line model validation efforts can significantly expedite on-line application development. Define "steady-state" and carefully select the process data. Model validation process data should be very different from model development process data, spanning a

broad operating

range. Also, define when un-reconciled model results are "close enough." The model reconciliation strategy must be carefully rationalised: the calculated model variables defined with constant (zero) off-sets should generally be process variables that are routinely and accurately measured, and the off-set between a measured plant variable and its corresponding parameterised model variable should be reasonable.

- Optimise the model off-line. Objective function design and testing is best accomplished off-line. The specification of constraints must be carefully considered; if the application is being used as an advisory tool, the bounds should be opened up. For closed loop control, it is better to highly constrain the optimisation. It is also important to consider how to value energy. This means getting a thorough understanding of energy contracts, incremental costs and steam balances.
- Maximise the value of the data historian. Historise all tags that could possibly be of interest, which should include compositions, temperatures, pressures, and flows, and be disciplined in configuring tags by using meaningful naming conventions.

conclusions

Companies have historically used process models exclusively for design and incidental troubleshooting. But as this example shows, significant value can be obtained by using these same process models for real-time optimisation and real-time modelling. Similarly, high-fidelity real-time models can find valuable application as tools for conducting traditional off-line engineering studies. Thus, a single application can provide economical and powerful capabilities for a multiplicity of purposes, including improving plant performance, determining the optimum set of operating conditions to take advantage of fluctuating market conditions, reducing plant variable operating costs, and identifying safety concerns. **tce**

POSM 1 PO refining train at Lyondell's Channelview Chemical Complex

Patrick McGrath (Patrick. McGrath@lyondell.com) is a business solution leader at Lyondell; Suresh Sundaram is director of product marketing at Aspentech