Three Essential Operations in a Plant: Simulation Models Turn Innovative Ideas Into Reality

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White Paper

Introduction

Whether it's a pilot plant or a complex petrochemical plant, these facilities rarely run like a well-oiled machine. There are always unknown variable dependencies that are difficult to understand, and there's substantial room for improvement. In many situations, optimization is not the focus for plants because there are issues with reliability and safety that take precedence. Does this sound familiar? The ability to simplify job tasks and boost efficiency will greatly enhance plant performance but also, make your job easier.

In particular, building simulation models to resolve issues of reliability and safety from the three key areas of your plant will enable you to discover value-added, easy-to-implement process improvements. The three areas of a plant discussed in this white paper are at the heart of many chemical processes: reactors, distillation columns and heat exchangers. Each of these types of equipment has unique characteristics that bring equally unique challenges.

It is common practice to create simulation models during the conceptual design phase of a greenfield project. For columns, a rigorous rate-based column model can predict performance under different operating conditions. Using equilibrium models with efficiency factors is less reliable because efficiency may be lower at higher operating rates, which will lead to building a column with poor efficiency. With the prevalence of heat exchangers and the constant pressure to improve energy efficiency to meet company-wide initiatives, designing them appropriately is important to identify operational issues such as vibrations, erosion, fouling up front and optimal heat transfer.

A New Way of Looking at Process Simulation Models

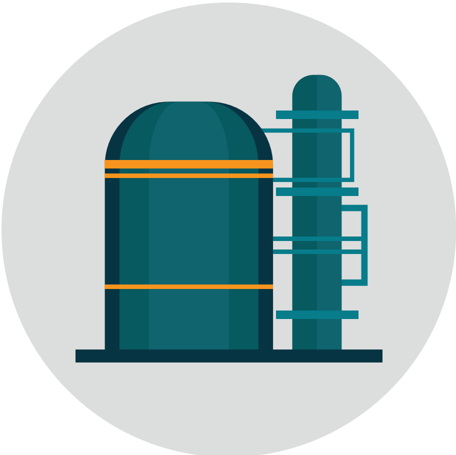
Process models can help guide better operating decisions in the plant, but operating engineers might not be comfortable developing and using models. On the other hand, a good user interface in Microsoft® Excel can make powerful models easy for any operating engineer to understand and use. Models provide increased value when used for plant production support during troubleshooting, changing operating conditions and justifying innovative ideas for continuous improvements. This model-based approach to decision-making brings all the knowledge stored in powerful models to the surface so that any engineer or operator can make more effective day-to-day operational decisions in the plant.

Spreadsheets are commonly used across all teams to look at historical plant data, determine profit and loss and calculate mass and energy balances. Bringing a process simulation model into Excel can provide better insight for teams, and can easily be built on top of an existing model.

This white paper will focus on why modeling reactors, distillation columns and heat exchangers will increase confidence in the way you run your plants. The models you build will empower plant manufacturing and operations teams by giving them a tool that increases collaboration and encourages innovative ideas without compromising on safety or plant uptime.

Why Model Your Existing Reactors?

A reactor is critical for yield conversion and quality, where lower-value raw materials A and B might react to make a higher-value product C (A+B→C), so that it's central to the economics of the plant. It is possible to model your reactor stoichiometrically; this is a non-predictive model as you dictate the amount of A that is converted to B. However, it would be more useful to build a predictive model to help optimize your process, either based on equilibrium or kinetics.



Many ethylene plants use predictive models of their existing reactors or furnaces to understand best operational parameters. The SPYRO® model, a rigorous kinetic-based ethylene model, is predictive and able to anticipate species coming out of the steam cracker based on geometry, feed composition and operating conditions. A predictive batch reactor model, such as those used in many specialty chemicals companies, enables optimization around batch times and raw material utilization. It also enables you to run more batches in a day and use expensive raw materials more efficiently. These batch models also apply to polymer processes, which are typically challenging to model because of the multi-step and solids processing but can be modeled out of the box with Aspen Polymers™.

As an example, a large chemical company was changing their Nylon 6 (polycaprolactam) recipe to use a different type of modifier. The molecular weight was expected to increase but the model predicted that it would decrease. The outcome was that the molecular weight decreased as predicted.

Stoichiometric Model: A non-predictive model where you define the stoichiometry (e.g. A turns into B).

Equilibrium Model: A predictive model where you define the equilibrium constant(s) using thermodynamics to calculate yield.

Rate-Based Kinetic Model: A predictive model (CSTR, batch, plug flow, fluid bed) based on kinetics that are used when reactions are relatively slow.

An Aspen Plus® process flow diagram was built, taking into account reaction kinetics in the column reactor to optimize polymer production in a Nylon 6 (polycaprolactam) plant.

The reaction rate parameters were tuned against experimental data from Tai and Tagawa[1]. The model reliably predicts monomer conversion over a wide range of conditions.

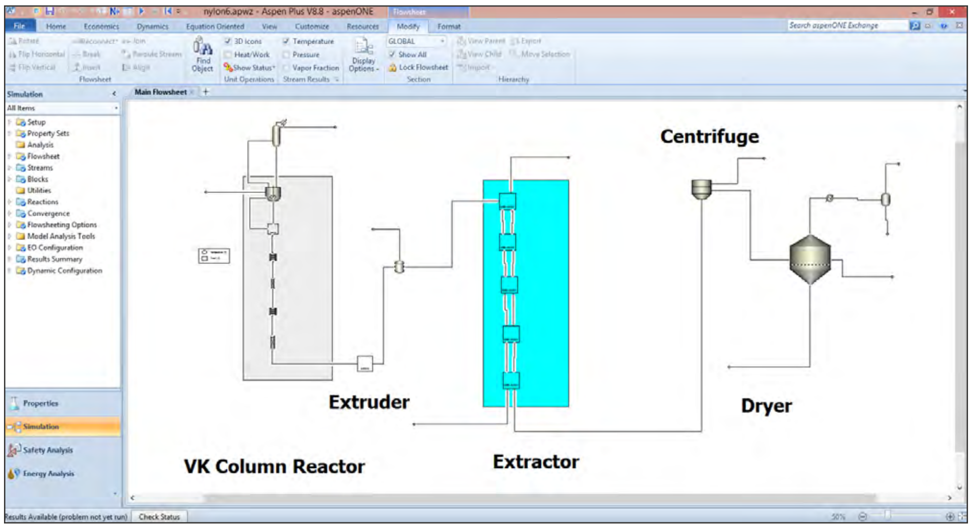


Figure 1a: Process flow diagram of Nylon 6 in Aspen Plus

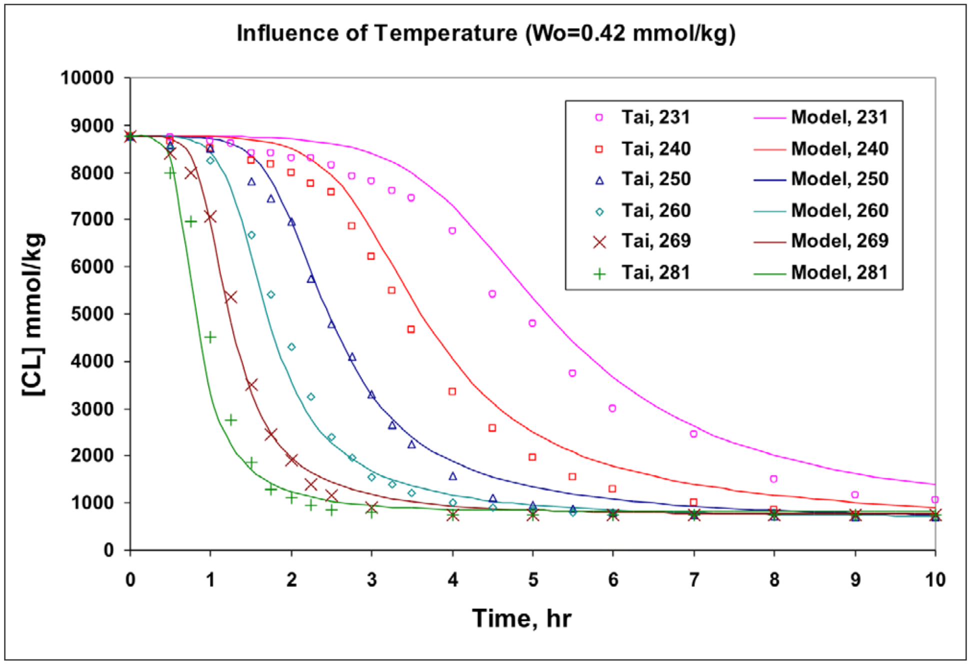


Figure 1b: Caprolactam concentration vs. temperature

1 K. Tai, T. Tagawa, J. Appl. Polym. Sci. 27 (1982) 2791

See an Aspen Plus example model for a LDPE process from the **AspenTech Support Center**.

Revamps

Borealis, a global polymer company, needed to increase the capacity of their lowdensity polyethylene (LDPE) plant. Their tubular reactors were frequently fouled by undesired high molecular weight polymers that built up on the walls over many months of operations. The operators needed to compensate for slower heat transfer rates by adjusting the operating conditions, including cooling water flow rates and initiator injection rates. The operators used the model to tune current performance against the plant and then ran case studies to identify new operating conditions to meet product specifications (molecular weight and density).

A model can help visualize performance, avoid unsafe operations (there is potential for thermal runaway) and meet quality and production targets. Borealis built an Excel front end on top of the reactor model for operator decision support so that operators could easily run the simulation models themselves.

On the other hand, if you're in a tough market and you're trying to make less product, you could find the optimal operating conditions to turn back the reactor while staying within the product specifications.

Case Studies

SABIC increased profits by an estimated 17 percent by optimizing ethylene oxide selectivity in the reactor at their petrochemical plant. They optimized the methanol conversion by determining ideal CO_2 injection rates, bed lengths and bed feed temperatures through their reactor model.

Oxiteno, the largest surfactant producer in Latin America, needed to react quickly to fluctuating feedstock and energy prices to capitalize on the most profitable assets. They simulated an entire ethanolamines plant, including the reactors, using Aspen Plus and Aspen Simulation Workbook™ to support capacity increase, resulting in an unexpected 15 percent less steam consumption. The model was placed in a simple Excel interface for operational decision-making, eliminating the guesswork around the feasibility of running the plant at different capacities and conditions.

Best Practices

Build a predictive model with the appropriate level of detail and tune it against known conditions in the plant. Then use an optimizer in the simulation to find the optimal conditions. Run sensitivity studies to understand how the reactor behaves and how the operating conditions affect the yield and conversion. Finally, tune the reaction kinetics, mass transfer coefficient or heat transfer coefficients if needed. Once you have the reactor model, building a plantwide model of your process is useful for plant-wide optimization.

In order to have a more accurate prediction, use **Aspen Custom Modeler® (ACM)** for a more rigorous model. ACM considers spatial variations inside complex reactors.

Summary

Reactor performance involves complex phase equilibria and reaction kinetics. It is difficult to grasp the complex interactions among feed recipe, operating conditions, yield, conversion and production rates. Use predictive, rate-based reaction models to provide insight and understanding which helps operate your reactors more effectively, and receive higher yields and better product quality. Building a predictive model of your reactor will result in better process insight and improve the economics of your chemical plant.

"We can simulate very fast and have good operational parameters to keep our plants producing market needs in terms of product distribution, product quality and minimizing energy consumption."

- Engineering Technology Manager, Oxiteno

Why Model Your Existing Distillation Columns?

Many processes produce multiple co-products. Changing market conditions may make some products more attractive than others. A rigorous process model can help guide operating decisions to optimize the product blend. For example, the methylamines process shown in Figure 2 converts ammonia and methanol into three products that include MMA, DMA and TMA. The DMA is much more valuable than TMA, so a fraction of the TMA is recycled back to the reactor to be reformed. The process model can identify optimal operating conditions to meet production targets, and it can verify the operability of the columns and other equipment under proposed scenarios.

Root cause analysis for the various operational issues in a column is not straightforward, and these issues are frequent process bottlenecks. You might notice something is wrong when there is a loss in product, a spike in a pressure measurement or lack of control in an area of the column. It takes an experienced operator to know the cause behind what is happening and how to manage it when an issue arises, and sometimes they might not know.

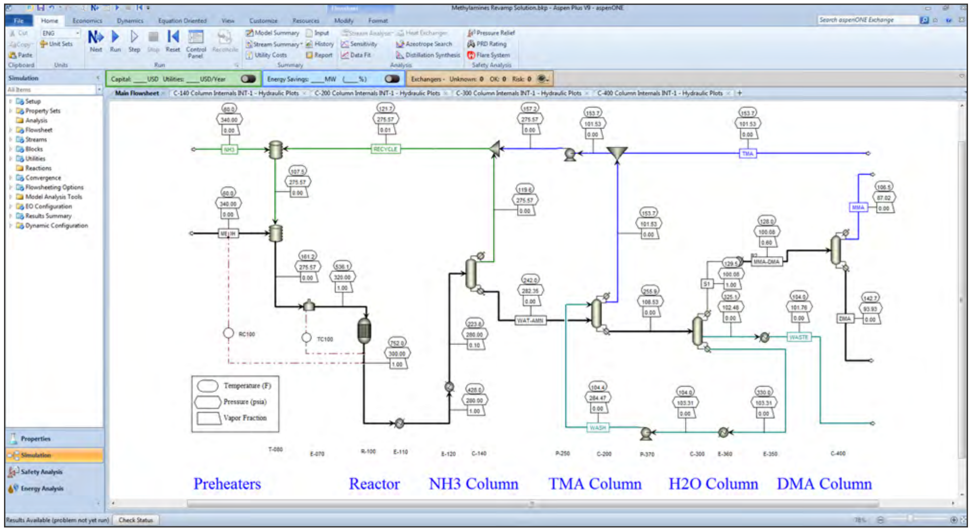
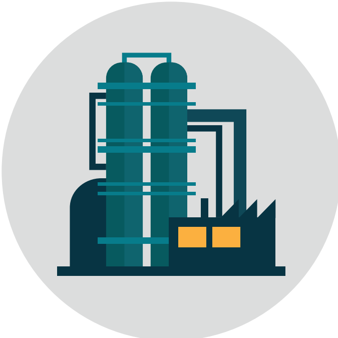


Figure 2: Methylamines process

The column is an integral part of the process, so shutdowns may affect the throughput and quality of product slates. Even if you are one of the lucky few with a back-up column, you'll find that modeling a column early to understand process impact will be valuable. In today's changing market conditions, knowing if your column can handle a turn-up or turn-down would be a huge advantage.



Whether you are concerned about impurities within the off-product or if there are certain government regulations to adhere to operationally, modeling gives you the flexibility to understand the cost trade-offs in column operations. It can help you answer questions like, "How far can I push my tower without violating regulations?" Cost effectiveness can also be considered depending upon the severity and duration of an incident. If a column requires a turn-up, you will need to weigh the trade-offs between preheating the feed or increasing condenser pressure. The optimal solution will be different for every plant.

When production rates increase or feed conditions change, columns may experience operability issues such as flooding and high pressure drops. Most engineers and operators cannot immediately identify whether or not a column is operating within the optimal operating window; typically, the operating window itself is unclear. Models can identify operating limits, and engineers can apply models to find compensatory changes to operating conditions to get around hydraulic limits. Operating pressures can be increased to reduce vapor traffic and reflux, or pump-around rates can be adjusted. Other variables can also be manipulated to stay within the desired operating window.

See an Aspen Plus example model for a methylamines reaction and distillation from the **AspenTech Support Center**.

Revamps

Engineers can use models to evaluate options for re-traying or re-packing existing columns and evaluate the capital and operating cost trade-offs involved in such changes. A model can also help you determine when a physical modification is unnecessary and that other modifications, such as preheating the feed to alleviate a high liquid rate or changing reflux ratios, may improve column operations.

Case Studies

CanSOLV was able to choose the most economical and efficient design for the scale-up of their CO_2 capture process from three possible options. DuPont achieved a 10 percent increase in column capacity for their existing bioethanol separation process. Reliance saved $2.4M USD from their column revamp in a benzene/toluene separation process by solving a poor separation efficiency issue.

Best Practices

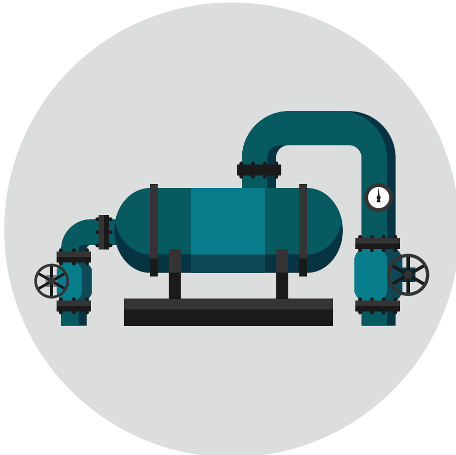
Model not only your column, but also the auxiliary equipment, including the reboiler and condenser, with fully specified utilities so that more accurate data can be fed into other parts of your process model, bringing your model closer to reality. A more accurate pressure drop across each piece of equipment will improve your overall mass and energy balance.

Summary

Conduct a hydraulic, thermal and emissions analysis as needed in your column model. Determine the column operating envelope to see when you are drifting away and identify potential issues before they happen. Use the model for changing operating conditions and easier troubleshooting.

Why Model Your Existing Heat Exchangers?

In any process, managing heat is one of the biggest challenges. Heat exchanger equipment is designed for certain operating conditions, but surfaces foul over time, feed conditions may change, and tubes may plug throughout its service life. Exchanger maintenance is critical. You need to decide when to shut down and clean an exchanger. When an exchanger is down, other exchangers in the process need to take up the slack. Heat exchanger models can be put online applications to monitor heat exchanger fouling, predict and optimize maintenance schedules and evaluate alternate operating procedures when an exchanger is down for maintenance.



So why model your heat exchanger? A model provides detailed thermal and hydraulic performance of the exchanger under various operating conditions. It will let you know of operational issues like fouling, vibration and erosion and their underlying sources. These capabilities give you a holistic way to understand system performance and help you make the right economic decisions.

Revamps

For example, a case of turn-down operations could look possible from a thermal performance point of view; however, it could still translate into unsafe operating conditions if you're not considering structural issues. Knowing this information up front enables you to explore different solutions, such as adding an impingement plate or deresonating baffles to address tube vibration issues.

Case Studies

Westlake Chemical was able to eliminate a predicted vibration problem when designing a heat exchanger for a steam cost-reduction project before the design was finalized.

Perstorp discovered that one of their heat exchangers in the polyalcohol process was performing at reduced efficiency, which related to the specification provided by Alpha Laval, the manufacturer. They modeled the plate heat exchanger and found that it was overdesigned by 100 percent due to excessive safety margins built into the design which caused excessive fouling on the cold side. This resulted in an estimated savings of $25,000-$45,000 USD per year from reduced utility and maintenance costs.

Using a simulation model, a specialty chemicals company optimized the recirculation rate and piping size of their column reboiler to debottleneck their process.

Learn more about the software that makes it easy to switch from **simple to rigorous heat exchanger models**. Use this information to conduct a **pinch analysis**.

Best Practices

Start with a simplified model and then convert to a rigorous heat exchanger model to determine thermal hydraulic performance and mechanical integrity issues. Build a heat exchanger network model of your plant to optimize heat integration via pinch analysis and reduce overall plant energy usage. Size the exchangers for appropriate duties to minimize capital cost; use the models to evaluate off-design cases to ensure the exchangers can operate well over a wide range of conditions. In operations, continue to use these models for troubleshooting and performance monitoring of critical equipment.

Summary

Build a heat exchanger model which provides detailed thermal and hydraulic performance of the exchanger under various operating conditions. During the design or operations phase, evaluate operability under desired conditions to make the right economic decisions.

> "In the past, reactors, columns, strippers and absorbers were simulated separately, and case studies could not be analyzed quickly and accurately. Now the plant-wide model allows Oxiteno to develop new projects and optimization strategies successfully."
>
> - Neide Hori Nagamine, Process Engineer, Oxiteno

Conclusion

Process simulation software goes beyond troubleshooting columns, reducing operating costs or meeting key performance indicators. It can be used to bring a model-based culture to your plant — a shift in mindset from reliance on experiential knowledge to making informed decisions based on reliable and accurate models.

LG Chemical built a model of their existing separation train to gain insight into how they could improve the build of their second separation train, which was needed to accommodate their production capacity that was doubling in size. They designed the new train to use 40 percent less energy than the existing train by testing the feasibility and implementing a double-effect column. They also modeled their heat exchangers to understand changes to the overall unit process. Test results were nearly identical to the simulation results, with the new train design using roughly 40 percent less energy than the existing design.

The best practice is not just creating simulation models of individual pieces of equipment, but also bringing everything together into a plant-wide model, which brings the most value.

Simulation software, therefore, is not only used in design, but it has also become imperative for chemical companies trying to operate their manufacturing plants to stay at the top in this increasingly competitive market. Lean manufacturing and Six Sigma projects to reduce cost and waste are commonplace. Building simulation models of the three key areas of your plant to resolve issues of reliability and safety will enable you to find value-added, easy-to-implement process improvements.

Using process simulation models during all phases of design, operations (including startup, shutdowns and turnaround) and revamps will provide the insight to make the most innovative decisions through collaboration between different teams. The process design group can work closely with the plant operations team to build the designs and provide the models to the production engineers and operators via a familiar Excel interface to share the valuable insight stored in the models.

The largest, integrated petrochemical company in Thailand saved over $1 million USD for a new, optimized plant design, saved $300,000 USD from eliminating plant trials for new polymer grades, and had the added benefit of debottlenecking existing plants using the same model.

SABIC has rolled out existing models to one of their bisphenol A (BPA) plants to empower their production engineers to make model-based decisions. Their experienced plant operators were excited to use these models because they realized they could test their plant improvement ideas in the model without needing to change anything in the plant. Their innovative ideas, which were previously too risky to try, could now be implemented with little risk.

Using a model-based approach makes the difference between using anecdotes versus data to make decisions. There is much to be learned from the former, but much more certainty in the latter. This best practice has been adopted by global leaders in the chemical industry, giving them a competitive edge above others. They believe in innovation, and innovation is at the heart of what we do here at AspenTech.

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AspenTech is a leading software supplier for optimizing asset performance. Our products thrive in complex, industrial environments where it is critical to optimize the asset design, operation and maintenance lifecycle. AspenTech uniquely combines decades of process modeling expertise with machine learning. Our purpose-built software platform automates knowledge work and builds sustainable competitive advantage by delivering high returns over the entire asset lifecycle. As a result, companies in capital-intensive industries can maximize uptime and push the limits of performance, running their assets faster, safer, longer and greener.

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