DIGITAL INDUSTRIES SOFTWARE

Accelerating process design optimization

Dow uses HEEDS in conjunction with Aspen Plus to enhance its processes and meet sustainability goals

Executive summary
In the chemical industry, multivariate analysis involves simultaneous analysis of complex data sets that include multiple interdependent variables, such as temperature, flow rate and chemical composition. By analyzing data on multiple variables, engineers can identify the most sensitive factors affecting energy efficiency and performance and select a design or operating condition that meets the process or product requirements. Traditional methods, such as parametric studies, can be too time-consuming or fraught with computational limitations. This white paper examines how Dow Inc. uses smart multivariate analysis and optimization coupled with process flow sheet simulation to quickly optimize a polymerization process while achieving sustainability goals.

Authors:
Reza Haghpanah and David Vickery (retired), Dow Inc.
Shawn Baggerley, Ernesto Lopez and Nathan Chase, Siemens Digital Industries Software

Contents

Introduction

Distillation is a widely used technique for separating and purifying a wide range of substances, from simple liquids to complex mixtures.

The U.S. Department of Energy estimates that there are more than 40,000 distillation columns in North America, and they consume about 40 percent of the total energy used to operate plants in the refining and bulk chemical industries.[1] If applied to the U.S. petroleum, chemical and paper manufacturing sectors alone, using separation technologies to purify chemicals that are more energy efficient could save 100 million tons of carbon dioxide (CO_2) emissions and $4 billion in energy costs annually.[2] Distillation is more economical than the alternatives, but it is still costly in energy and capital. To get the column positioned for the lowest economic investment for the life of the asset, new designs require a significant amount of time and effort to optimize trade-offs between capital and long-term energy costs. We continue to make empirical adjustments to further improve columns in existing processes to reduce costs and help the company improve the bottom line.

In general, when seeking to perfect any operation, the engineers and operators who manage process units are limited to seeking relationships between a small number of variables, often in two or possibly three dimensions. Although it can be useful, this is often inadequate for finding optimal global operating conditions. Furthermore, it is often difficult to ascertain whether the conclusions drawn from these correlations are causative or merely coincidental. The distillation process can range from simple to highly complex operations involving many steps. The variables associated with the process are numerous; thus, defining optimal conditions based on limited dimensionality can be a time-consuming task.

Historically, designing and operating the distillation assets associated with producing these materials has largely been characterized by parametric studies or using gradient-based optimization algorithms, where a limited number of process conditions have been examined to find a "good enough" solution or a local optimum. Exploring these areas was limited by the time and optimization techniques available to the process modeler. Not being able to identify and target operations at the global optimum results in missed opportunities to conserve upfront capital expenditures or additional annual expense in the form of less-than-optimal operational conditions, possibly for many years.

Chapter 1
An increasingly complex competitive environment

Success in process optimization is being defined in a different context today than it was a few years ago. For example, it is rare to engage with any professional closely associated with an operation involving large quantities of heat being generated or raw materials being consumed who is also not being tasked with new methods to achieve stipulated sustainability targets. This added goal converts the typical cost-performance equation to a cost-performance-sustainability equation. Entirely new dimensions, which may have originated at the same time as the process itself, are being considered. They may have profound impacts on traditional production methodologies.

Many of these industrial processes, while profitable when producing large quantities of materials, operate on thin margins on a per-unit basis. The economics of the installation as well as the physical limitations of the equipment, real estate or tolerance of various types of feedstocks may make a facility unable (financially or otherwise) to cope with modifications that would better facilitate achieving these new metrics. To achieve the previously mentioned metrics, it has become necessary to explore all available avenues with as few as possible physical modifications to the existing facility.

The task of perfecting a process on a single target variable can be quite challenging. Today's process engineering professionals are being asked to optimize multiple targets simultaneously while maintaining an understanding of the underlying relationship between these variables and the overall operational profitability of the unit. It is precisely this confluence of business, scientific and environmental concerns that have made it orders of magnitude more challenging to run a successful process operation than ever before. Therefore, tools that are a significant improvement over manual analysis, which can provide benefits above and beyond existing real-time-optimization programs that must be manually reprogrammed and/or are prone to needing frequent updates to perfect the algorithm, are in high demand today.

Collecting process data from many potential sources, deciding how to interpret it, using the data in a predictive model to gain insights into the process and applying those insights to dynamically optimize the same process simultaneously is commonly referred to as multivariate analysis.

Chapter 2
Challenges with multivariate analysis

Challenges with multivariate analysis

Multivariate analysis involves analyzing multiple variables simultaneously to understand the relationships among them, and to find which variables are most important in explaining variations in the data. There are many types of multivariate analysis techniques, each with its own strengths and weaknesses. The choice of technique will depend on the specific question being posed, the nature of the data available and the goals of the analysis. Often, it requires a person trained in data science who may or may not be familiar with the process to assist with the analysis.

Although multivariate analysis is a powerful tool for understanding the dynamics of complex systems, it is impractical to use it without tools that enable you to understand these complexities.

Dimensionality

Generally, the more complex the process, the more variables, or dimensions, associated with it. The number of dimensions, the relationship of these dimensions to the others in the analysis as well as the relative frequency these dimensions change all directly influence the feasibility of using the data to manually optimize the process to the desired target variable.

Datasets that have many variables are referred to as having “high dimensionality.” High dimensionality can lead to several challenges, including the curse of dimensionality, which refers to the phenomenon where the complexity of the solution increases exponentially as the number of variables rises. This can lead to difficulties in modeling, visualization, interpretation and manual process optimization.

Interpreting the results

Single versus multiple objective analysis:
Virtually all process environments are complex and dynamic. It is necessary to understand the underlying physics occurring inside of the process to select the proper target variables for an optimization task. The question becomes whether the goal of the analysis is to find a best solution that optimizes a single objective function, or if it can be better obtained via a multi-objective multivariate optimization where multiple objectives are considered simultaneously.

For example, in the context of process optimization, the objective function may be to maximize the yield of a product or minimize the cost of production. In contrast, multi-objective, multivariate analysis considers many objectives simultaneously and is used to name a set of solutions that are optimal or near optimal for all objectives. Multi-objective optimization techniques are commonly used in engineering and scientific research to explore the trade-offs between objectives and identify the best settings of process variables that satisfy multiple objectives.

If the goal is well defined and the problem is relatively simple, single-objective multivariate analysis may be sufficient. However, if the aims are conflicting or multiple goals need to be considered, it may be necessary to use multi-objective, multivariate analysis to find optimal solutions that satisfy all objectives.

Identifying local versus global optima:
In optimization problems, the goal is to find the best solution that minimizes or maximizes an objective function. The best solution can be a global or local optimum.

A global optimum is the best possible solution in the entire feasible region of the problem. It is the solution that yields the best objective function value among all possibilities. Finding the global optimum can be challenging and requires exploring a large search space of possibilities.

In contrast, a local optimum is the best solution in a particular region of the feasible space. Local optima are typically easier to find than global optima, but they may not be the best possible solution. For example, a local optimum may be found using gradient-based methods that only explore the immediate neighborhood of the current solution.

Algorithms are used to run search strategies to show local and global optima. Gradient-based methods are efficient in finding local optima but can get trapped in them and fail to find the global optimum. Additionally, they are highly dependent on the selected starting point. In contrast, evolutionary algorithms and other global optimization methods are used to explore a larger search space and have a better chance of finding the global optimum but may require more computational resources while being less dependent on the starting solution.

Optimization

Once the model has been validated and the best process variables identified, the model can be used to perfect the process by predicting the best possible conditions for achieving a desired outcome. The model can be used to show the input variables that will maximize the output variables or to find the optimal balance among multiple output variables.

Chapter 3
Introduction to HEEDS software

Today's design and operation environments require more intelligent search strategies that automatically adapt to the prevailing constrained landscape based on search goals. In many instances, there is no single ideal response indicative of a single objective function, but instead a family of solutions that satisfy the prevailing constraints and the governing goals. These families of solutions are not easily determined and/or computed and, hence, require search strategies that are able to simultaneously address the optimization of multiple objectives. Additionally, in a highly multivariate environment, many combinations of solutions can exist that satisfy an applicable set of goals. Several series of minima or maxima may exist that satisfy the constraints of a given design or operation schedule.

Multi-objective optimization strategies enable the discovery of suitable solutions for this schema. When there is a trade-off amongst the objectives, a resulting family (suitable solutions) of designs or potential operating points is referred to as the Pareto front. This is a set of non-dominated solutions where none of the objectives can be improved without diminishing the performance of at least one of the other goals.

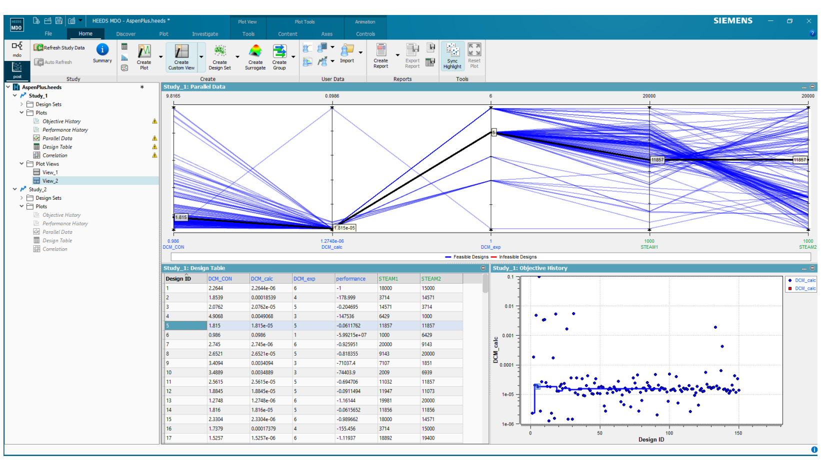

Figure 1: A view of the HEEDS software being used to conduct simultaneous searches to find the best possible solution within the allotted timeframe.

These challenging problems are best explored by leveraging the strengths of both global and local optimization techniques. HEEDS™ software, which is part of the Siemens Xcelerator business platform of software, hardware, and services, is a highly efficient optimization search framework that is used to deploy global and local techniques simultaneously. HEEDS is a multidisciplinary design analysis and optimization (MDAO) software that is used to leverage key design space exploration strategies (integration, automation and exploration) to accelerate data-driven methods for improved decision-making.

Using HEEDS enables a user to leverage a proprietary hybrid-adaptive search framework (SHERPA) that combines local and global techniques in a unique way whereas various search strategies are deployed simultaneously to solve the problem (hybrid). With an adaptive nature, HEEDS can be used to alter its solving techniques in real time to find a timely schema to solve the optimization problem.

HEEDS can be used to integrate and automate your digital twin models to support data-driven methods for improved decision-making. This approach allows solutions free of any human preconceptions or biases, and can generate surprising solutions that are comparable to, or better than, the best human-generated efforts.

Designers, engineers and operators use HEEDS to find innovative solutions to their everyday design and operational challenges of sustainability. In its simplest form, how do we as designers, engineers and operators fulfill the needs of the current generations without compromising the needs of future generations, all while ensuring a balance between social well-being, environmental care and economic growth?

Chapter 4
Integrating HEEDS with Aspen Plus – a novel approach

As one of the world's largest chemical companies, Dow Inc. recognizes the importance of staying agile and innovative to remain relevant in this digital-first economy. Faced with a growing global business and the need to be sustainable while remaining profitable, the company researchers were looking for ways to perfect their design optimization process.

The Dow team found a unique approach to streamline its entire chemical process design and optimization by integrating Aspen Plus® software, a process modeling platform, with HEEDS, using its powerful SHERPA optimization search framework.

The result: A well-aligned chemical design process that is optimized for energy consumption.

By leveraging the HEEDS with Aspen Plus, the Dow team was able to develop a novel approach it called high-throughput modeling (HTM). It offers the same benefits of high-throughput research and can be used for perfecting existing processes and developing new designs. One potential use of this new capability is related to optimizing existing operations or new designs. Traditional techniques involve a parametric study manipulating one variable at a time on a platform such as Aspen Plus to find the optimal conditions or using derivative-based optimization techniques. There are challenges and shortcomings associated with this approach. As processes get more complex, there are more variables to manipulate to arrive at the best solution. More variables require more time to perfect, so the greater the chance a good enough answer will be accepted rather than finding the true optimum. By not reaching the global optimum, the company spends added capital or annual expense.

The high-throughput modeling approach allowed us to perform mixed-integer nonlinear optimization. An objective function is defined and then the program can run thousands of iterations, adjusting parameters simultaneously to arrive at a globally optimized solution. All of this is done without having the human resource run through the simulations manually one at a time.

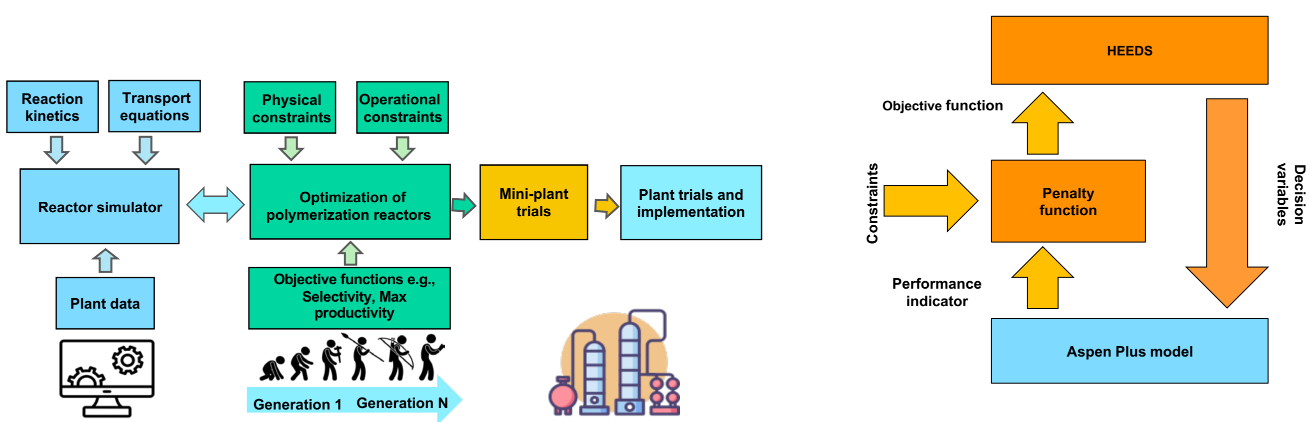

Figure 2: A design optimization process flowchart showing the high-throughput modeling approach using HEEDS and Aspen Plus.

The team also developed a platform to use cloud computing for the HTM approach. Cloud computing enabled Dow process modeling experts to use the HTM approach without dedicating their workstations as a full-time modeling computer, or purchase and manage a costly tower computer. In addition, parallelization is a secondary benefit of running HTM on cloud computing resources. Leveraging cloud computing for HTM simulations allows for dynamic scaling of cloud resources. This enables us to deliver the optimal amount of cloud resources to satisfy the demand of all researchers while minimizing cost by only keeping cloud resources online while in use.

Using this novel approach provides a tremendous new capability in industry. This new approach has been used to optimize existing operations and develop new designs to help Dow meet its 2025 sustainability goals via energy minimization and reducing CO_2 emissions.

For instance, in 2021, this method was used to help optimize condensation polymerization reactors that produce polydimethylsiloxanes (PDMS) for sealants, adhesives, coatings and emulsions. In the condensation polymerization reactor, cyclic siloxane byproducts (commonly referred to as Dx with 3<x<12) are generated.

In recent years, there has been an increasing demand from customers to produce siloxanes with lower cyclic concentrations to reduce environmental impact. Using the high-throughput modeling approach, the team was able to show new operating conditions that reduced the cyclic generated in the process by 45 percent. Since the Dow siloxanes are used in a wide array of consumer products, customers and hence the wider society benefitted significantly from this work as well.

In addition, the solution helped maximize the reactor efficiency, increasing the yield by 2 percent without any added capital, thereby greatly reducing the overall costs and carbon footprint of the plant.

Seamless integration

The high-throughput modeling approach integrates seamlessly with Dow's regular process development workflows, allowing the entire staff to benefit from this revolutionary capability. In addition, the approach can be applied to any process model and implemented across an organization without requiring added capital. For example, any modeled distillation process or reactor can be perfected to achieve a desired objective; whether that is reduced costs, increased capacity or better control. The speed and flexibility of cloud computing has made this solution even more user-friendly. In fact, the Dow process modeling experts used the high-throughput approach without a dedicated computer.

Additionally, HEEDS can be used to interface with a range of modeling tools and computer-aided engineering (CAE) applications, making it an ideal solution for multidisciplinary optimization. Thanks to its proprietary SHERPA optimization search framework, the team was able to run thousands of simulations in a fraction of the time it would take to run all the iterations manually. This freed up resources to work on other efforts while also delivering a more optimized process.

We believe the potential impact of this solution is significant, and Dow, Inc. is already benefitting from this innovative approach compared to previously used gradient-based optimization techniques. Some of the key benefits include simplicity, ease of implementation, robustness and inherent parallelizability.

Siemens Digital Industries Software's HEEDS is a leading design analysis and optimization software package that leverages design space exploration to accelerate product development and reduce overall costs. Designers and engineers in leading organizations across the world rely on HEEDS to find innovative solutions that satisfy all performance requirements.

Instead of starting with a specific design and using a simulation tool to evaluate and perform manual iterations to improve it, engineers can start with their performance goals and use HEEDS to drive the simulation software to identify high-performing designs.

Furthermore, the solution is user-friendly, making it accessible to users with minimal design space exploration experience, enabling them to discover better designs and make informed decisions faster.

Discover better design faster

The solution is built on four guiding pillars:

Process automation: Incorporate process automation technologies to streamline the process and help confirm the quality and consistency of their virtual prototype models.

Distributed execution: Orchestrate simulation tasks across platforms and operating systems. Use a transparent and automatic distributed execution functionality that helps accelerate the process of testing virtual prototypes.

Efficient search: Take advantage of SHERPA, the revolutionary search strategy available only in HEEDS, which is used to simultaneously leverage multiple global and local search strategies and adapt the search as it learns more about the design space.

Insight and discovery: Easily explore performance trade-offs during the virtual prototype design process and effectively facilitate design reviews.

Conclusion

According to the International Energy Agency (IEA), the chemical industry is the largest industrial energy consumer and the third largest industry subsector in terms of direct CO_2 emissions.[3] It reported, "In 2021, the industry recorded 925 million metric tons of CO_2, a 5 percent increase from the previous year." As the chemical industry continues to evolve, the adoption of advanced analytical tools and intelligent search strategies will be crucial to drive efficiency and meet emerging sustainability targets.

The high-throughput modeling approach presented in this paper has proven to be a revolutionary capability that can help chemical companies make informed decisions to improve energy efficiency and overall performance. The use of Siemens' HEEDS software with Aspen Plus is critical to this effort as it enables process automation by seamlessly integrating with existing tools. With its robust and adaptive search functionalities, engineers and designers across disciplines can easily access the user-friendly interface of HEEDS to evaluate various design possibilities and find the optimal solution within the given timeframe and requirements. **Learn more.**

References

1. U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, "Distillation Column Modeling Tools," DOE, Washington, D.C., https://www1.eere.energy.gov/manufacturing/resources/chemicals/pdfs/distillation.pdf

2. Sholl, D., Lively, R.P., "Seven chemical separations to change the world," Nature, 532, 43-437 (2016).

3. International Energy Agency, Chemicals, https://www.iea.org/energy-system/industry/chemicals

Siemens Digital Industries Software

Americas: 1 800 498 5351

EMEA: 00 800 70002222

Asia-Pacific: 001 800 03061910

For additional numbers, click here.

Siemens Digital Industries Software helps organizations of all sizes digitally transform using software, hardware and services from the Siemens Xcelerator business platform. Siemens' software and the comprehensive digital twin enable companies to optimize their design, engineering and manufacturing processes to turn today's ideas into the sustainable products of the future. From chips to entire systems, from product to process, across all industries, Siemens Digital Industries Software – Accelerating transformation.

siemens.com/software

85548-D8 11/23 A