



Hybrid Modeling: AI and Domain Expertise Combine to Optimize Assets

This paper summarizes the business challenges this new technology solves, the three types of hybrid models AspenTech is introducing to the market, several of the immediate areas where they will create value, and AspenTech's unique capability to lead this new wave in technology to help the process industry navigate through a volatile, uncertain period.

Executive Summary

Aspen Technology, Inc. (AspenTech) has invented a method for integrating first principles-based process simulation models and domain expertise with AI and analytics algorithms. The resulting application software is a hybrid modeling system that achieves more than either first principles modeling or AI could alone.

First principles models are well established for their accurate modeling of chemical and hydrocarbon processes. Aspen Plus® and Aspen HYSYS®, the world's premier chemical process simulation systems, have an accuracy and predictive capability validated, relied on, and improved on over four decades of use by industry, researchers, and scientists. Their models and first principles relationships are based on hundreds of years of experience by the world's best process engineers and operators,

Executive Summary



comprising expertise from AspenTech's R&D teams, Aspen Academy's university researchers and customers who have provided inputs and contributions.

To get the final several percentage points of accuracy out of these models, plant data is employed to calibrate these first principles models to observed plant conditions and performance. Effective model calibration requires considerable expertise and experience today, despite the many workflow automation improvements AspenTech has provided.

AI and machine learning are rapidly emerging as tools that can greatly accelerate the ability to employ plant data both to calibrate first principles models and to create data-based models of phenomena and processes quickly. AI has the potential of lowering the expertise bar towards modeling process systems, but it must be combined with domain expertise to create the real-world guard-rails that make it work safely, reliably and intuitively.

Hybrid models combine AI, first principles and domain expertise to deliver a comprehensive, accurate model more quickly without requiring significant expertise. Machine learning is used to create the model, leveraging simulation, plant or pilot plant data, while using domain knowledge including first principles and engineering constraints to build an enriched model without requiring the user to have deep process expertise or be an AI expert. This next generation of solutions democratizes the application of AI within hybrid models to optimally design, operate and maintain assets - deploying them online and at the edge.

AI and machine learning allow us to build a model analyzing a broader set of data while leveraging advanced data science techniques for model prediction. When combined with engineering principles and domain expertise, the models can be built and maintained more quickly than traditional methods without requiring significant user expertise.



With hybrid models, users can model processes and assets that cannot easily be modeled with first principles alone. Examples include:

- batch processes, which can be too varied to systematically model
- fluidized bed processes with complex chemical and fluid behavior
- bio-process reactors and fermenters
- complex refining units

Users get the accuracy of empirical models and the strength of first principles models, leveraging the power of AI paired with domain expertise, to create a more predictive model faster and with less experience required than ever before.

Hybrid models provide a better representation of the plant, which keeps the model more relevant over a longer period of time. This reduces the barrier to entry for using modeling for asset optimization by requiring less effort and expertise. With the models in place, the connected worker becomes free to perform higher value-added and strategic work.

AspenTech will be deploying hybrid modeling capabilities across its existing software suite through a model alliance approach, which synchronizes fit for purpose models in different functional areas needed to safely, reliably, sustainably and profitably operate an asset. An example of the model alliance is the use of reduced order unit models in planning, dynamic optimization and online equipment monitoring, all derived from the same root refining unit operating data set and simulation model, achieving closed-loop production optimization.





The process industry faces unprecedented uncertainties and macro-economic threats. Process industry leaders face unparalleled volatility in all phases of their business. External factors including hydrocarbon price turbulence, changes in remote working needs and supply chain interruptions are making change inevitable for process manufacturers, from the smallest to the most global. Addressing challenges ranging from changes in feedstock price and demand to society's drive towards sustainability, organizations must weigh complex trade-offs. Software technology, and in particular AI, is widely viewed as one of the primary tools available to equip organization to thrive amid these challenges.

Market Volatility and Energy Transition

A trio of external forces are forcing continued volatility and turbulence on energy and chemical companies globally. The global market supply and demand shock and economic recovery we are entering, the societal drive for energy transition and carbon zero industry, and the social contract driving for zero casualties and environmental incidents all have a massive impact on industry executive teams' thinking.

Process industry companies are fixated on flexibility, strategies for resilience in producing at unpredictable utilization factors and with extended maintenance intervals, yields and operating margins. Faster models, solving key economic units or entire sites rapidly, tuned better to plant operating conditions, answer the crucial questions needed to achieve those goals. Hybrid modeling makes it possible to model and deploy quickly — even remotely — to address dynamic market forces and asset conditions. These models become key ingredients to transform operations through the future self-optimizing plant.

The Disappearing Expert

As a generation of experts retires, process organizations face a gap in essential knowledge and a new generation of workers without the longevity to develop that critical expertise. Hybrid models, embedded with AI, address those gaps, creating immediate value for organizations and assets. All but those enterprises with the deepest pockets need the ability to build and deploy these models without scarce and expensive experts.



Sustainability Pressures

Formidable decarbonization goals across industry will not disappear after the current economic cycle. The pressure to move towards a circular economy also creates many innovation challenges. Hybrid models provide the ability to optimize and evaluate optionality across a wide asset scope, to select the best strategies to meet these goals. Companies are challenged today to contend with the complexity that sustainability pressure imposes on their operating and strategy decisions.



AspenTech's Vision of Hybrid Modeling in the Process Industry



Democratizing access to powerful and accurate models, across all sized assets and companies, is a crucial step in understanding how a specific process will behave or respond to unexpected change. As plants and their systems have increased in complexity, these models have become essential to operations.

Hybrid models combine AI and first principles to deliver a comprehensive, accurate model more quickly without requiring significant expertise. Machine learning is used to create the model leveraging simulation or plant data, while using domain knowledge including first principles and engineering constraints to build an enriched model - without requiring the user to have deep process expertise or become an AI expert.

With hybrid models, users can model processes and assets that cannot easily be modeled with first principles alone. The accuracy of empirical models and the strength of first principles models, leveraging the power of AI along with domain expertise, creates a more predictive model.

AspenTech is uniquely positioned to leverage over 40 years' domain expertise to make AI applicable to process industries, delivering industrial AI. AspenTech brings three fundamental capabilities together:

- strong and deep domain expertise in process industries
- strong capabilities to capture and analyze the quantities of data available through the proliferation of connected sensors
- innovative leadership in turning machine learning and AI into industrial solutions.

A Simple Example

One simple example demonstrating a polymer reaction process shows the dramatic difference between simple machine learning and the AspenTech hybrid modeling approach (see figure below).

The left chart shows the correlation achieved by applying machine learning to plant data from a polymer reactor to develop a model. The right chart displays the significantly better results achieved by adding first principles guidance for a hybrid modeling approach.



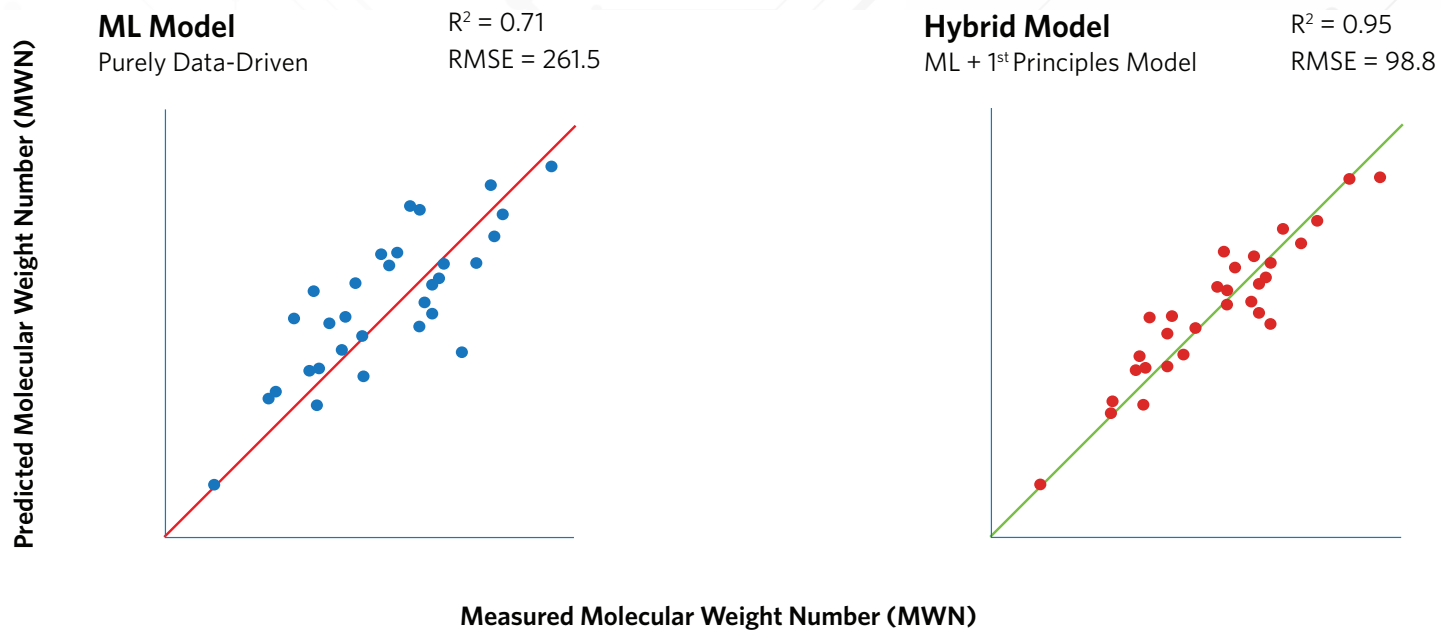


Figure 1. Machine learning model compared to a hybrid model of a polymer reaction process

AI

Three Types of Hybrid Modeling AspenTech Is Developing



AspenTech has developed several key technology components which combine to create hybrid models. These include tools for process and plant engineers to rapidly turn plant and simulation data into AI-based machine learning models without requiring any data science understanding; tools to combine first principles physio-chemical knowledge with these AI-based empirical models and intuitive, automated workflows to deploy these as operational applications.

These will then be provided to industry as three types of hybrid models, which are all industry firsts, namely:

Type 1: AI-driven Hybrid Models

This approach uses machine learning to create an empirical model based on plant or experimental data, augmented with first principles (e.g. thermodynamic properties etc.), constraints (e.g. mass balance) and domain knowledge. A less-experienced user can rapidly generate a completely new predictive, more accurate model, fully democratizing AI's application. Users can now model processes and assets that cannot easily be modeled with first principles alone. Examples include complex reaction unit operations, new material processes and new technology processes.

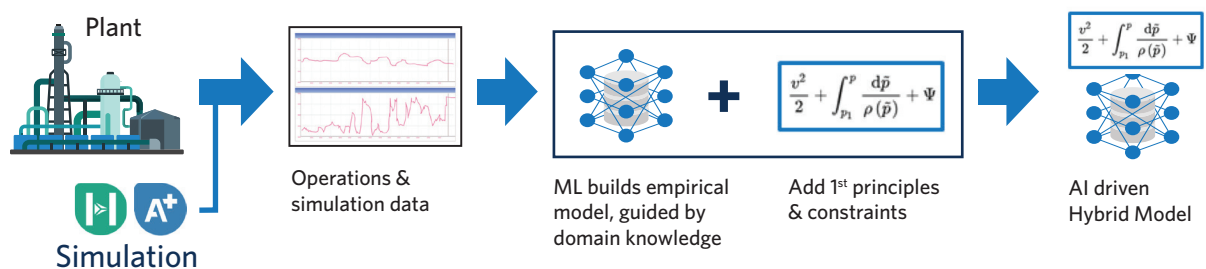


Figure 1: AI-driven hybrid model workflow: process engineers employ data intuitively to rapidly build models of units or processes without having to understand data science.

Type 2: Reduced Order Hybrid Models

In this approach, machine learning is used to create an empirical model based on data from numerous simulation runs, augmented with constraints and domain expertise, to build a fit for purpose, high fidelity, performant model that is accurate within the range for which it has been trained, fully democratizing the application of AI. With reduced order models, users can easily extend the scale of modeling from units to the entire site and synchronize the model across design, operations and maintenance. Examples include building value chain-wide models from crude oil input to finished chemical output, building rapidly deployable and compact models online at the edge, and embedding high accuracy models in the planning linear program.



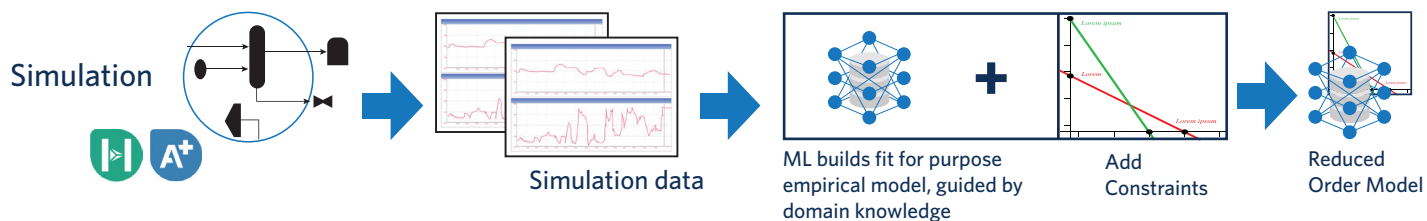


Figure 2: Reduced-order hybrid model workflow. Process engineers employ tuned simulation models to generate machine learning reduced order models that can be deployed consistently in a range of target applications.

Type 3: First Principles-Driven Hybrid Models

This approach augments an existing first principles model with AI, using data from operations to calculate unknown variables and relationships not captured by the original model. Machine learning determines the unknown value and its relationships to continuously calibrate the model as conditions change. This approach is a natural extension to existing first principles models in many brownfield deployments globally; it is quick and easy to adopt and significantly increases accuracy. Examples include embedding AI-created but first principles-governed models for unique batch process units.

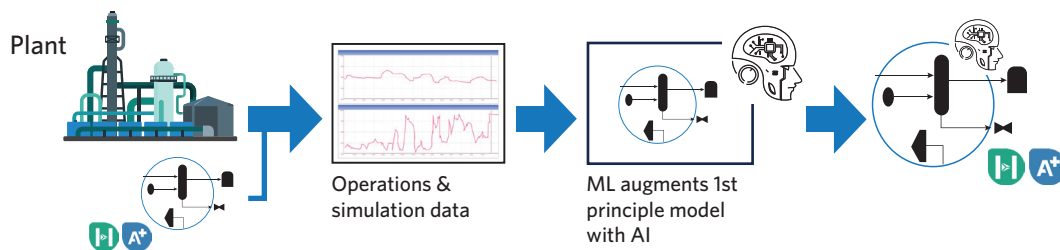


Figure 3: First principles-driven hybrid modeling workflow. Machine learning augments first principles models in characterizing difficult-to-model units, such as many batch processes.

Model	Summary	Examples
AI-driven hybrid model	An empirical model that uses machine learning to build the model based on plant or experimental data, first principles, constraints and domain knowledge to create a more accurate model.	<ul style="list-style-type: none"> Model complex process units and processes Inferential sensors Equipment unit models online
Reduced order hybrid model	An empirical model that uses machine learning to build the model based on data from simulation runs, constraints and domain knowledge to create a fit for purpose model that can run more quickly and efficiently.	<ul style="list-style-type: none"> Refinery-wide or chemical plant-wide models Planning model updating Deploy fast-solving online models to predict best/worst-case schedules for cleaning Deploying process train models online APC nonlinear model deployment
First principles-driven hybrid model	An existing first principles model augmented with data and AI to improve the model's accuracy and predictability.	<ul style="list-style-type: none"> Batch unit modeling Bioprocess modeling Modeling complex units

Table 1: Summary of hybrid modeling styles and example scenarios.

Use Cases Demonstrating Hybrid Modeling's Benefits and Business Value



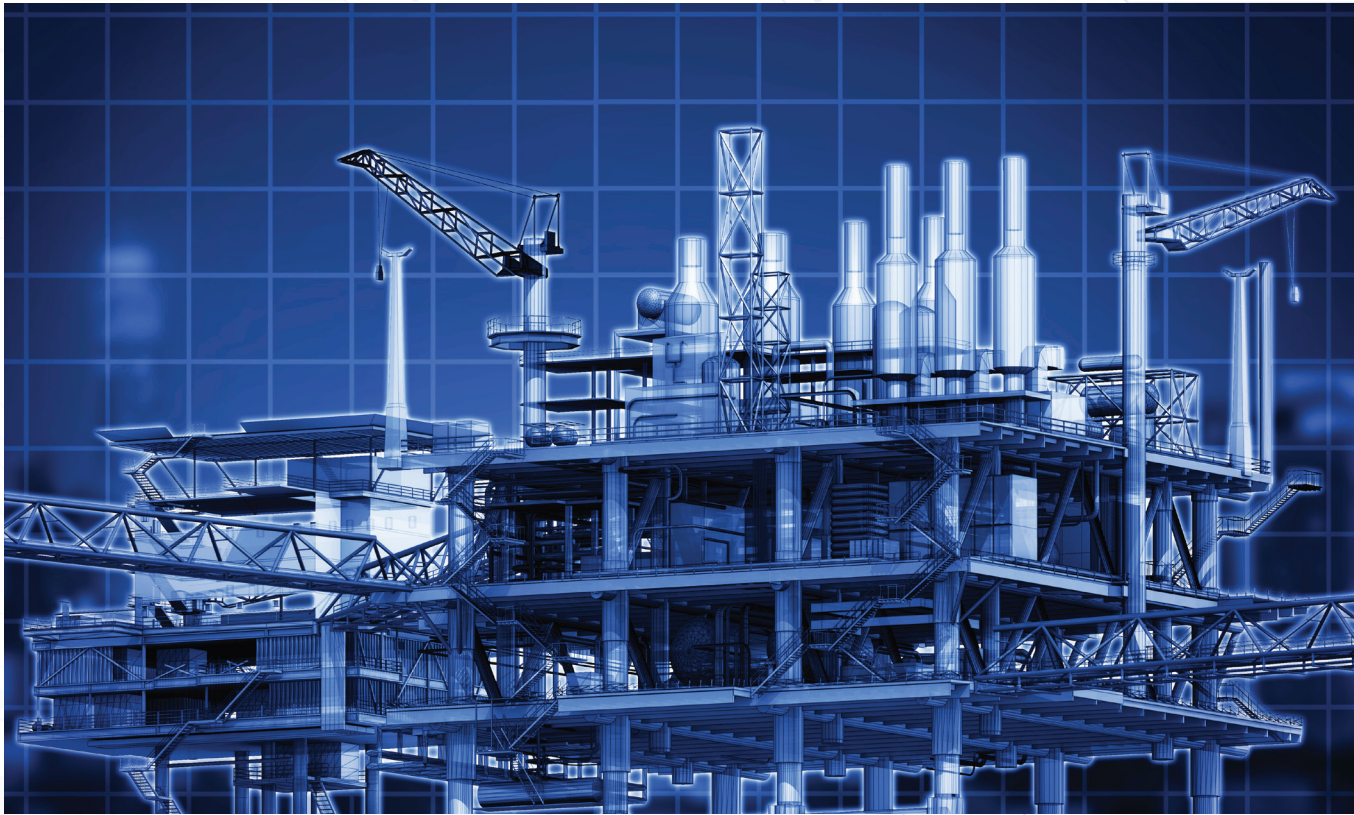
Over 80 companies participated in AspenTech's hybrid modeling tests over the past year; we used over 30 industrial data sets to evaluate the robustness of this approach. Tests identified a variety of high value use cases.

Here are some of the unique benefits hybrid models provide, based on the test results and feedback on highest potential use cases:

- 1. Expanding Modeling's Scope and Impact:** Complex units often pose yield, performance and quality issues. Hybrid models enable process engineers to model several equipment types that are difficult or impossible to describe using first principles, such as specialty chemical reactor models. Hybrid models expand the scope of modeling from process to total sites, using reduced order hybrid models to make solving these large problems possible.
- 2. Democratizing Modeling:** Organizations have a high proportion of newer engineers today who all need to work off the same information. Hybrid models empower a typical process engineer to develop models for equipment and assets without expert modeling skills, using operational data and the built-in data science to develop reliable and fit for purpose models.
- 3. Creating Accurate, Fit For Purpose Models:** Traditionally, different fit for purpose models have been used in different functional areas, making closing the loop a challenge. Now, reduced order hybrid unit models that represent complex behaviors simply but accurately, in the paradigm appropriate for planning, dynamic optimization and online equipment monitoring, can all easily be derived from the same root refining unit operating data set and simulation model, achieving closed-loop production optimization.
- 4. Better Sustaining Modeling's Benefits:** Since hybrid models have both data-driven and first principles components, they are closely tied to plant data and able to keep in synch with the asset operations closely as the operations evolve and therefore are able to sustain the benefits of modeling more than pure first principles modeling.



5. Accelerating Collaboration Between Disciplines: Reduced order modeling enables model alliance across disciplines. For example, planning models updated by hybrid models from rigorous reactor models in refining improve information sharing and collaboration.





Here are a few use cases successfully tested with industry companies that illustrate how hybrid modeling will:

- expand the scope of business problems that digital twins can solve
- improve profitability and quality
- make technology easily to apply for the new generation of knowledge workers (unseasoned digital natives).

Refining and Olefins Planning Model Updates

Refining and olefin margins are closely related to plant planners and operators' ability to achieve monthly production close to the plan. Gaps can usually be traced to out-of-date or inaccurate planning models, especially for certain key reactor units such as FCCs and hydrocrackers. Existing processes for keeping those models up to date are modeling-specialist intensive.

One of the largest global refiners projects the ability to generate up-to-date revisions of these detailed reactor models as often as needed, using a hybrid modeling workflow, will conservatively deliver value over \$10 million USD annually for a typical 200,000 barrel per day refinery. This is extremely timely as refineries contend with dramatic changes in the products they must produce.

Equipment Monitoring

There are many applications for unit- and equipment-level models, deployed online, to advise operators to improve operational yields, solve performance and safety problems and improve compliance. An example is a preheat heat exchanger train model to provide fouling and cleaning schedule advice, or to even make closed loop decisions. Hybrid models will be easily developed, updated and run. Just the fouling monitoring use case can deliver tens of millions of dollars in value per year for a single heat exchanger train (based on measured case studies).

Refining reactor unit models for catalyst degradation and life extension are another example. These models can create economic value of \$5-10 million USD per year per catalyst reactor unit by extending catalyst life and improving yields/performance.



Speciality and High-performance Polymer Process Modeling

Specialty polymer processes are prone to quality problems and waste. However, polymer reactors are inherently complicated, difficult and time-consuming to model accurately. Demand for experts in modelling these processes far exceeds supply. In specialty polymer use cases, hybrid models are able to accurately represent the performance of the key polymerization reactor units.

We have already tested the effectiveness of hybrid models in a difficult polymer production operating application, using actual data and achieving much better results and economic benefit than any other method. We tested the data set with a leading polymer manufacturer who estimates the value of this model is at least \$1 million per line per year, solving a previously unsolvable problem.

Plant-wide Modeling for Optioneering and Optimization

While industry needs site-wide models to solve sustainability- and agility-related business questions, today those models are difficult to build. Reduced-order models can abstract models to enterprise views which inform executive awareness and strategic decision-making. Site-wide models can run faster and more intuitively to drive agile decision-making and optimize assets to achieve safety, sustainability and profit.

Beyond these example use cases, these hybrid, AI-powered models will also fundamentally change how humans work, interacting with intelligent systems in the business. In place of spending many hours building and rebuilding models and handling data streams in largely manual spreadsheets workers will perform higher-level functions, making forward-thinking, data-driven decisions about what to do - thereby increasing overall accuracy, efficiency and performance while reducing system-level risk.

A large, light gray graphic of the letters 'AI' is positioned on the left side of the page. The background of the entire page features a complex network of white and blue lines and dots, resembling a circuit board or data flow diagram. The bottom of the page has a dark blue background with glowing blue circuit patterns.

Conclusion



AI is rapidly proving its ability to provide predictive insights in industrial domains. AspenTech is convinced that for AI to provide effective insights into process industry processes and equipment, domain expertise remains the key. Consequently, we have invented and developed a hybrid modeling approach that brings AI and domain expertise together. AspenTech envisions three types of hybrid modeling, which cover a wide range of high-business-value use cases, that create measurable value for operators and engineers in today's environment. AspenTech involved over 80 of our leading customers, many of whom shared valuable process operating data and models, to test workflows and functionality and to assist in defining intuitive usability.

AspenTech will deploy hybrid modeling capabilities across its existing software suite, through model alliance technology, which synchronizes fit for purpose models in different functional areas to safely, reliably, sustainably and profitably operate an asset.

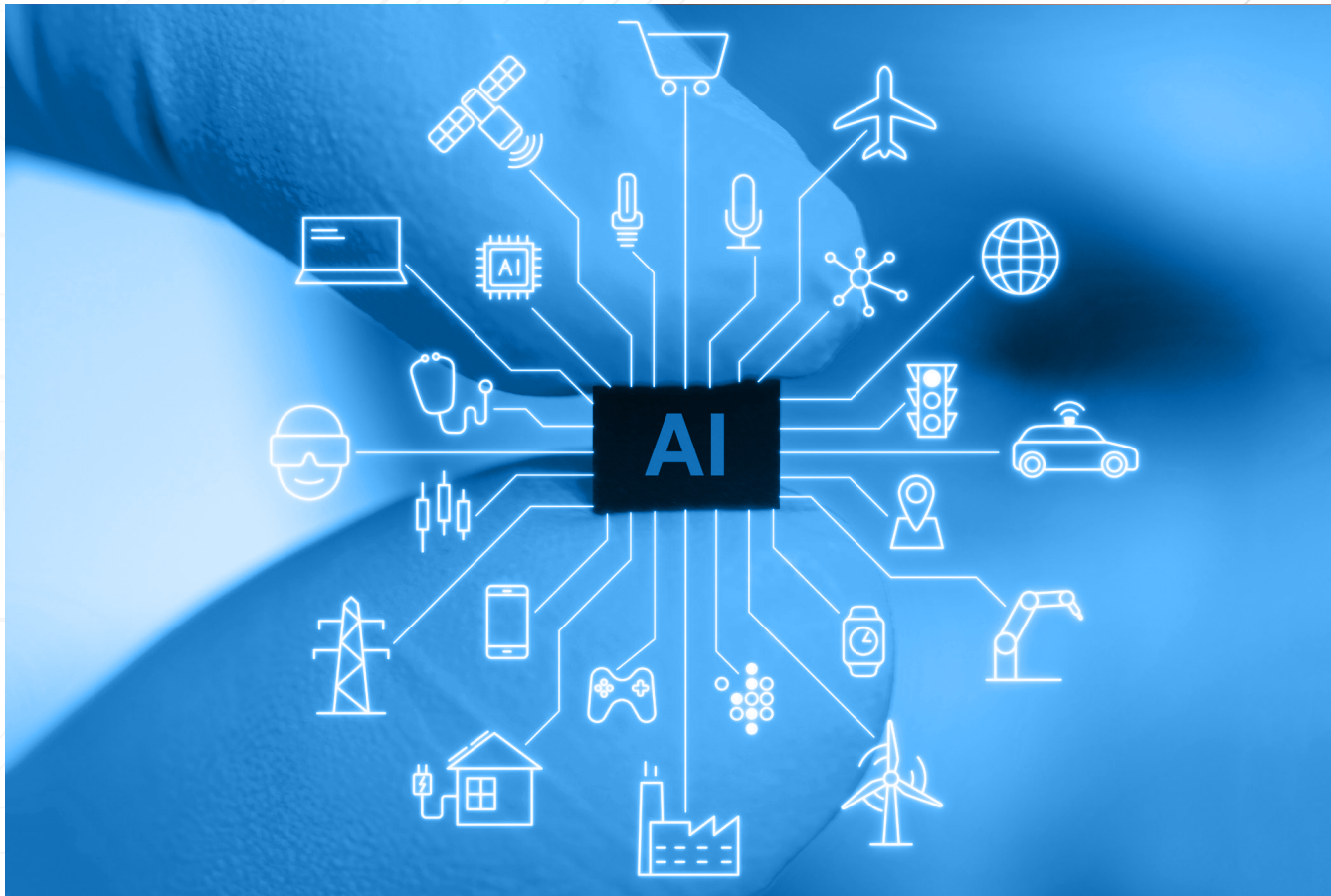
Today, process industry organizations are facing unprecedented challenges. To map a path forward for your business amid demand uncertainty, feedstock and crude price volatility, sustainability pressures and global competition requires agility, insight and enterprise-wide analysis. To execute this in the midst of a wave of retirements, which subtract decades of experience, is even more challenging.

Now is the time to embrace digitalization and AI in a way that provides a smooth path forward, building on the powerful tools you have used for decades, enabling more automation, actionable insights from the models, and remote use of these tools. This will democratize AI in the design and operation of process industry units and plants.

The leading players in energy, chemicals, contracting, and related industries are already working with AspenTech as they see the powerful competitive advantage this technology can quickly provide. These benefits can be translated into dollar value for margin, sustainability and capital savings, as well as a sustainable business advantage.



Contact Aspen Technology today for a briefing on how digitalization and AI can help your business, and for a specific assessment of where it can immediately be applied to improve your business performance.



Contributing Authors:

Ron Beck,
Marketing Strategy Director, Aspen Technology, Inc.

Gerardo Munoz,
Senior Product Marketing Specialist, Aspen Technology, Inc.

About AspenTechnology

Aspen Technology (AspenTech) is a global leader in asset optimization software. Its solutions address 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 artificial intelligence. Its 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 safer, greener, longer and faster.

Visit [AspenTech.com](https://www.aspentech.com) to find out more.

© 2020 Aspen Technology, Inc. AspenTech®, aspenONE®, the Aspen leaf logo, the aspenONE logo and OPTIMIZE are trademarks of Aspen Technology, Inc. All rights reserved. AT-06245

