Drive Innovation, Sustainability & Margin in Specialty Chemicals Manufacturing

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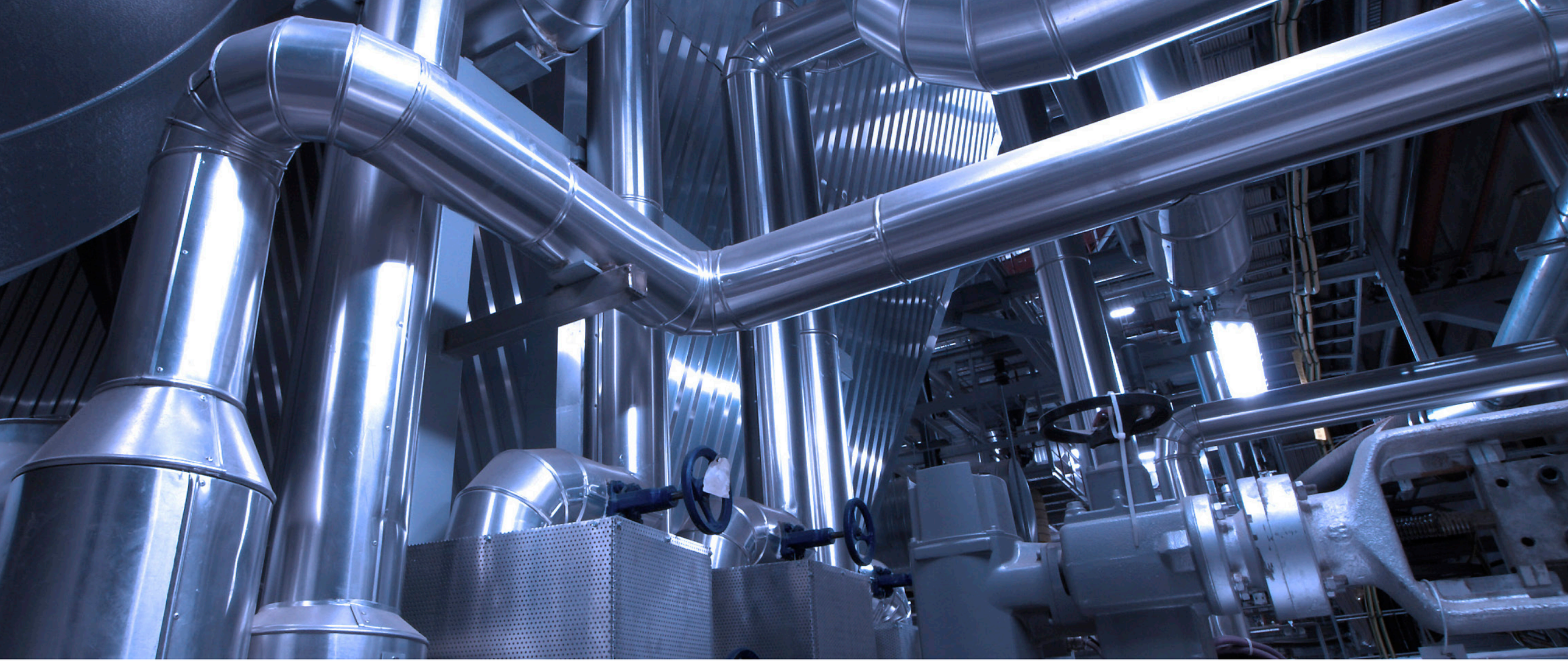

Chemical Industry Outlook

Although the global economy was expected to fully recover from the pandemic by the first half of 2023, the economic downturn continued into 2024. Due to sluggish consumer demand, high interest rates and inflation, chemical companies either reduced rates or downsized less competitive operations. With the pressing necessity of raw materials and energy security, chemical companies are looking to hedge risks either through localization of value chains or creating trusted partnerships.[1] New incentive plans in the US and elsewhere and tougher regulations in Europe are also shaping the chemical manufacturing priorities and landscape.

As we closed the first half of 2024, chemical companies are cautiously optimistic for an average 3.4% expansion across all regions led by Asia-Pacific in 2024.[2] Improving markets allow for prioritization of sustainability initiatives and consumer demand for greener and more sustainable products. According to a study published by McKinsey, Total Shareholder Return (TSR) is 2-3 times higher for green leaders vs. green laggards as shown in Figure 1.[3]

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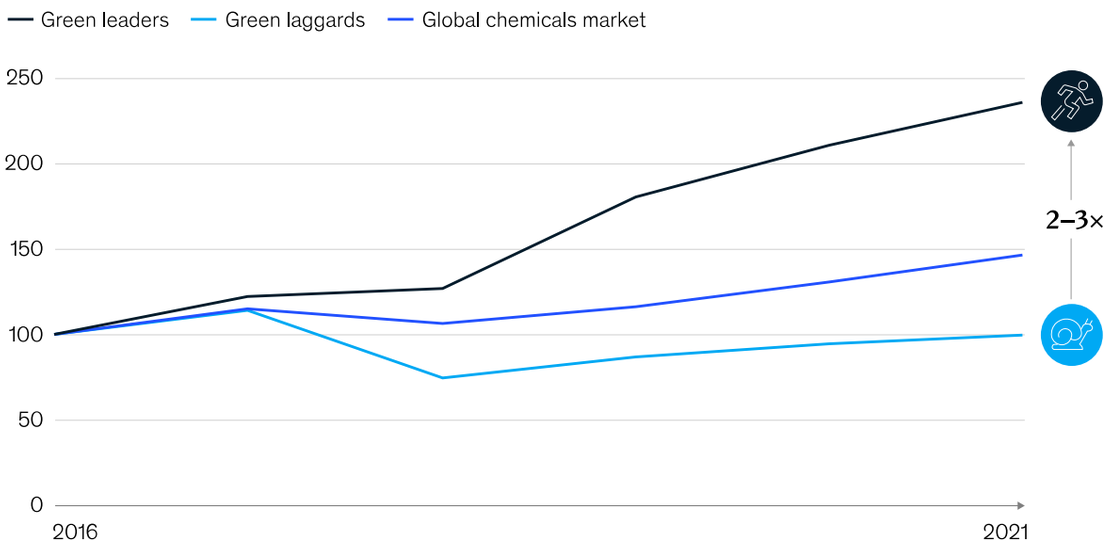
[1]World Economic Forum
[2]American Chemical Society
[3]McKinsey Chemical Markets

There is a widening gap between 2030 – 2050 emission goals and actual industry emissions[4] and a worsening plastic waste pollution.[5] According to the US EPA, the US chemical industry has not been very successful at lowering emissions over the last decade (Figure 2). Therefore, the chemical industry feels to be under pressure to reduce emissions and innovate more circular processes. Sustainability goals cannot be achieved without investments and improvements in efficiency, reliability and process technology. Digital and automation infrastructure upgrades are prerequisites to any meaningful progress in creating a thriving and sustainable chemical industry of the future.

Digital and automation tools are fundamental to technical evaluation, design, optimization and monitoring of operations with a goal of reducing emissions. Digital engineering and control tools enable lowering fuel, steam and electricity use of the plant. Digital supply chain management tools facilitate comprehensive reviews of supply chain operations and identify opportunities to lower carbon intensity of products. Digital engineering tools are also essential to create circular processes such as recycling waste plastic or incorporating renewable feedstocks.

[4]Climate action navigator
[5]Ellen McArthur Foundation



Source: McKinsey analysis

McKinsey & Company

Figure 1 - *The TSR for green leaders is two to three times higher than for green laggards.*

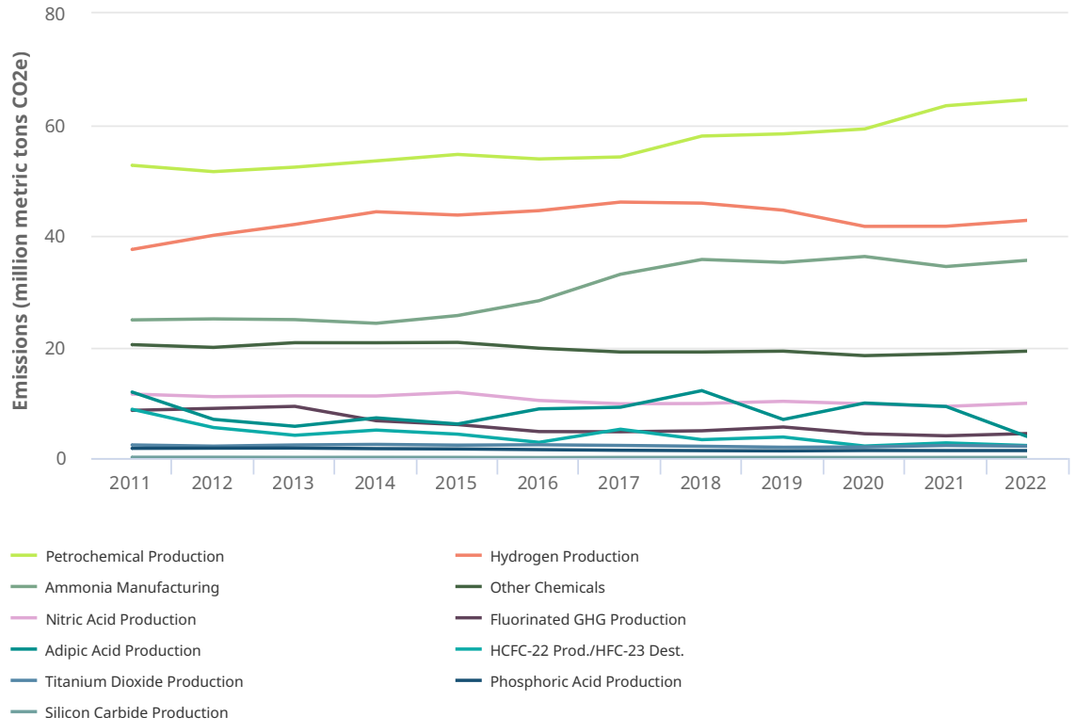


Figure 2 - *Chemical industry subsector emissions data between 2011 and 2022 (https://www.epa.gov).*

Specialty Chemicals Manufacturing

When it comes to specialty chemicals, manufacturers are challenged to bring new and innovative materials to the market faster, more cheaply and more sustainably. The growing demand for higher performance materials requires new areas of research, ultra efficient manufacturing and agility to modify and create value chains. In this article, we will review how digital and automation tools can expedite the innovation process, reduce cost and improve overall operational sustainability.

- **Innovation –** Innovation and speed-to-market are critical for success in the specialty chemicals business. Green pesticides, solar PV cells and new personal care product ingredients are examples of new markets for specialty chemicals producers. Only companies with deep domain knowledge and smart manufacturing capabilities can gain a higher future market share.
- **Operational Efficiency –** With economic headwinds, specialty chemical manufacturers (just like commodity manufacturers) are identifying ways to improve operational efficiency, remove bottlenecks and lower the overall cost of production. Lowering cost can include lowering energy use, finding alternative and perhaps onshoring raw materials, and faster scale up processes. Although specialty chemical manufacturers typically have more flexibility in pricing their products; cost and scarcity of energy and raw materials can impede any operation.
- **Sustainability –** Sustainability is top of executives' mind as chemical companies gear up for a carbon-neutral future. Many large chemical companies have made boardroom commitments and received funding tied to significant, measurable CO_2e reductions. Circularity metrics such as measurable renewable raw materials (e.g., ISCC in Europe) are increasingly becoming dominant. In the next decades, sustainability will drive significant investments in new chemical processes and create new value chains.

Automation Solutions for Specialty Chemicals Manufacturing

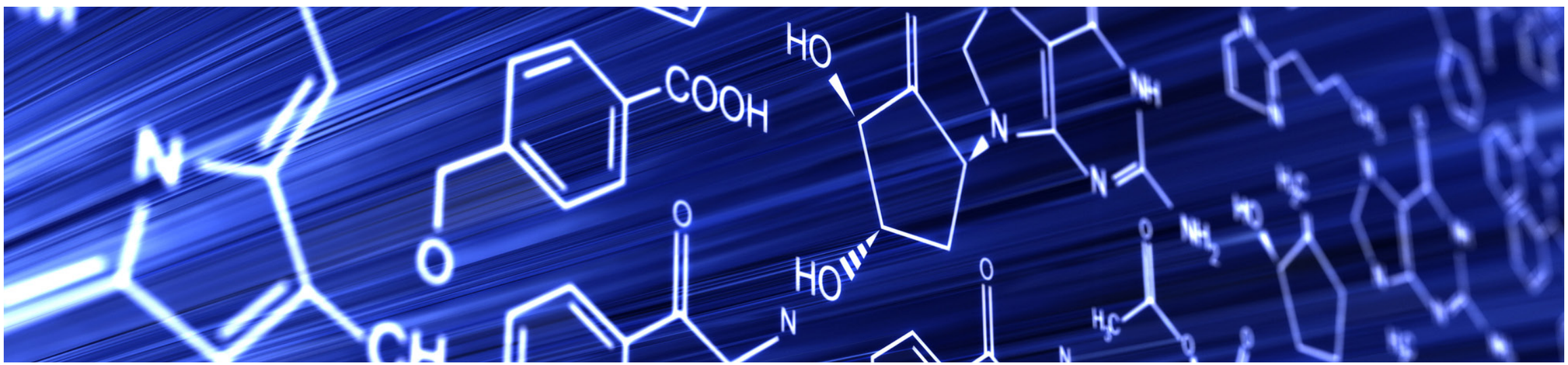
Emerson and AspenTech have joined forces to address production and sustainability challenges for specialty chemicals manufacturers across their wide portfolio of automation and digital solutions. In the following segments we will briefly discuss how some of these solutions can address industry needs and position companies for long-term success.

Emerson Capabilities with DeltaV™ Batch & Continuous

The DeltaV™ DCS architecture is based on the ISA88 Batch Standard. Whether it is the physical model, procedural model, or easy-to-use class-based configuration – the DeltaV system is simply "built-for-batch." Like the rest of the system, DeltaV Batch fully supports compliance with the challenging electronic records demands of regulated industries for recipe and campaign management, batch history, automatic version control and change management, and electronic signature support.

As a totally integrated batch solution the system includes process cells, unit modules, phases, equipment modules and control modules. From recipe scheduling to device control, from simple sequencing to multi-stream formulations, the system makes your batch operations easy. Because DeltaV Batch is an integral part of the integrated architecture it uses the same intuitive drag-and-drop engineering interfaces to make configuring your recipes easy.

The system also includes the integrated asset management features to monitor key valves, instruments and pumps to improve availability that would interrupt batch operations and cause costly downtime. The comprehensive nature of Emerson's batch offering has made it the world leading specialty chemical system with 1065 Installations. The extreme ease of use of DeltaV allows end users to easily own and modify control configurations to get the highest return. Integrated Asset Management systems easily connect to smart wired and wireless instruments for cost effective connections to missing measurement and device diagnostics.



Digital Solutions in Specialty Chemicals Manufacturing

Whether to improve your current portfolio or to create new materials, AspenTech's digital portfolio can expedite the creation and commercialization of new chemicals and products.

Engineering Tools for Product Innovation & Process Design

When it comes to new process design, a powerful simulation and optimization tool is critical to ensure future integrity of the operation, maximize efficiency and minimize waste. Digital engineering tools can accurately model the process, generate capital and operating cost estimates and monitor operations in real-time.

Solids Modeling

Solids handling, including tracking particle size distribution, is a complex unit operation. Specialty chemicals and pharmaceutical producers use Aspen Plus® and Aspen Custom Modeler® (ACM) to simulate and optimize crystallization processes. Aspen Plus provides unique capabilities to optimize solid production (sizing and rating of cyclones, fluidized bed reactors, dryers, filters, etc.), reduce energy demand and control particle size distribution (PSD) and moisture content. For example, CJ CheilJedang Bio division (an amino acids producer) used ACM to model physical properties of the amino acid solution to estimate the kinetic parameters of crystallization. After validation with lab data, the ACM model was used as a digital twin (DT) to monitor purity and PSD. This model enabled researchers to improve yield and recovery rate of the operation.

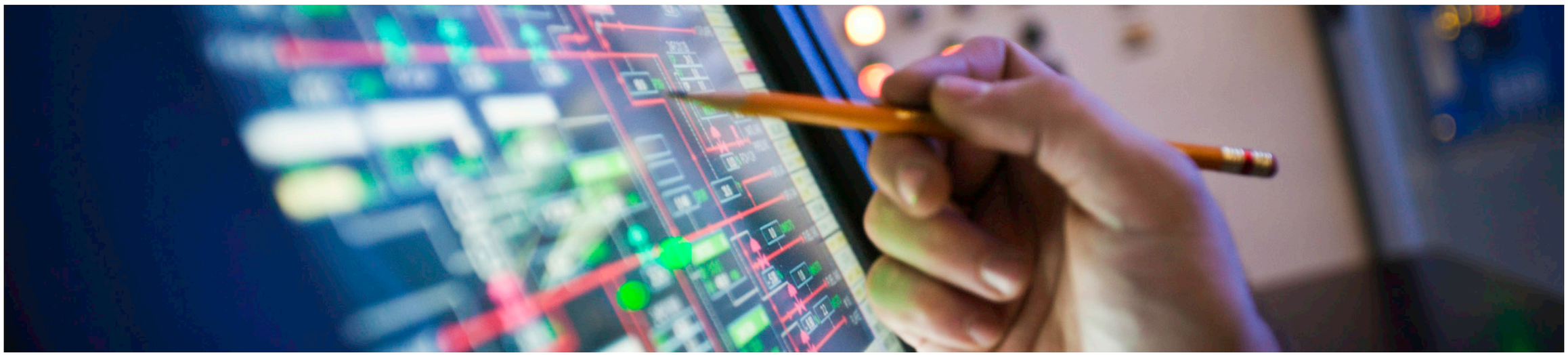
Lilly and Dow Chemical have also used Aspen Plus's solids modeling capabilities to reduce experimentation time, cost, and to calculate residence time of the reactor more accurately.

Batch Modeling

Many specialty chemicals processes involve both continuous and batch process units. Modeling both operation modes together ensures maximum yield of the most valuable products. It is possible to simulate batch, semi-batch, and continuous processes (such as batch distillation feeding to continuous fluidized bed) all inside Aspen Plus. This approach makes complex equipment modeling (e.g., reactors, membranes, extruders, etc.) easier and adds to overall process safety. A Japanese pharmaceutical company used Aspen Plus to identify sources of impurities in their crystallization process. Using the Aspen Plus model to convert their operation from batch-to-continuous, they were able to reduce impurities from 100's of PPM to 20 PMM.

Lubrizol and Synthomer have also used Aspen Plus to reduce batch cycle time and increase capacity while minimizing energy use and emissions.

Aspen Plus is the ideal platform to simulate batch and CSTR biobased fermentation processes. The biofeed databank lists more than 500 different feedstocks from agricultural/industrial/municipal waste to micro/macroalgae, grasses, hardwood and softwood sources. The Aspen Plus ferment database includes a wide variety of predefined cell types and common organisms and corresponding properties. As a result, systems with complex kinetics (rigorous pH calculations, multiple substrates and products, anaerobic or aerobic processes) can be rigorously modeled. These models can then be calibrated against experimental data or an AI-enabled Hybrid Model™.



Hybrid Modeling™

Hybrid Modeling™ combines two modeling approaches: Pure First Principles Model and Pure Machine Learning Model. Leveraging Hybrid Modeling, fit for purpose models, can be created to cover the entire asset life-cycle accurately and confidently. First-principles framework provides “guard rails” to keep models consistent with conservation principles and other thermodynamic limits. Here AI guides the first principles fundamentals to match existing process models to actual operation data. Hybrid Modeling use cases include equipment fouling models, predicting brittleness, corrosion, and catalyst deactivation.

DuPont recently used Hybrid Models to address challenges in batch manufacturing. Due to raw materials variation and impurities, operations often required manual adjustments to bring product into specification. Moreover, controlling viscosity of their CSTR reactor was difficult and in-line measurements were not accurate. A rigorous Hybrid Model helped them to identify when the process measurements become unreliable and allowed for advanced process control (APC) adjustments to replace manual changes.

Tools to Improve Batch Manufacturing

Specialty chemicals are often made in batches. Like engineering tools, AspenTech offers a multitude of operation and maintenance tools to batch manufacturers to improve quality and lower operation cost whenever possible.

Data Historian and Batch Manufacturing Record Management

Due to a high number of operational variables, controlling and maintaining batch quality can often be challenging, especially when when common equipment is used to manufacture different products back-to-back. Metrics such as Overall Equipment Effectiveness (OEE) call for reducing unplanned downtime, reducing transition time, maximizing yield and minimizing waste and by-products. Some of these challenges arise from limited data accessibility, lack of visualization and analysis and delayed problem identification. AspenTech MES (Manufacturing Execution Systems) solutions offer greater data visibility, record keeping and visualization to guide and improve production quality.

Many of AspenTech’s specialty chemicals clients have used our data historian and MES over the years. When Chemours (formerly DuPont’s performance chemicals division) had quality issues with Nafion product line, locating data logs and quality reports for multiple customers became overbearing. After implementing Aspen Enterprise InfoPlus.21™ historian and Aspen Production Record Manager® (APRM), the quality team was able to minimize record keeping errors, enable traceability and significantly minimize customer complaints.

Similarly, Owens Corning needed to establish a certification process including all batch records across three different manufacturing sites. When the combination of InfoPlus.21 and APRM were deployed, product tracking accuracy improved to 90% and significantly reduced non-shippable materials quantities.

Evonik also has implemented InfoPlus.21 and Aspen One Process Explorer™ (visualization tool) to engage operators to identify process issues and troubleshoot process sooner to reduce quality excursions and associated cost.

Batch Quality Control Tools

There are several variability sources in each batch process manufacturing. Raw materials inconsistencies, variability in process conditions and operator dependability are to name a few. Optimizing quality, yield and throughput can improve profit margins as well as driving customer satisfaction. Advanced process control (APC) and multivariate analysis are two main solutions to address quality and yield targets.

- **Batch APC –** AspenTech's batch APC is a closed-loop model predictive control system. The model can predict product quality and use available handles to achieve a desired target. In operations, batch APC relies on decision points. These are intervention points where the outcome can be affected by manipulating key variables. It means, the controller automatically adjusts the batch recipe at these decision points, as needed, to keep product quality within specifications and optimize cycle time. Once this solution is implemented online, it will consistently adjust those key variables, batch after batch. The error between prediction and actual value is considered and used in the next batch.

  Recently one large food ingredients manufacturing company used AspenTech's batch APC to improve 2.7% product yield. Batch APC predicted & controlled product concentrations at multiple decision points along the cycle time. Based on these predictions, optimized ingredient rates (aka manipulated variables) at each decision point were sent as targets to the underlying DMC3™ for controlling pH.

- **Aspen ProMV™ –** Troubleshooting quality issues with muti-variate analysis is another accessible digital solution for specialty manufacturers. Finding sources of variation in production processes is difficult when all the variables are correlated. Aspen ProMV analyzes interrelated process data to identify minimum critical set of variables driving quality and performance. Aspen ProMV exploits tens of thousands of recorded "experiments" in plant historian to develop a robust model of the process. When deployed on-line, it can diagnose subtle shifts from optimal process operation enabling early, informed intervention by operations personnel.

FMC used Aspen ProMV to determine that simple changes in the batch herbicide process could save close to 50 percent of their production. For years plant personnel had thought the problem was in the chemical composition of the raw materials. However, the Aspen ProMV analysis showed that batch size and heating rate were the culprits. The improvement in recovery was worth millions of dollars per year.

Improving Asset Reliability

In a fast-paced manufacturing environment, executing orders on time and ensuring minimum waste and downtime is key to push the economic envelope of the operation. Aspen Mtell™ is an asset management tool to monitor rotating equipment and predict the time to failure. In this way, operations can allow for planned maintenance, preventing unexpected downtime and product loss in addition to the HSE consequences of each failure.

In one example, a specialty chemicals manufacturer had problems with an agitator shaft. Due to product accumulation at the top of the shaft, the shaft would get stuck and eventually break. It would take up to five days of downtime (revenue loss) to change the shaft plus maintenance cost adding up to about $400k per year. After deploying Mtell, operators were able to identify future failure events for up to 30 days in advance. In another example, the separation column primary pump would lose capacity and eventually fail with the deposition of salt. By monitoring column and pump, Aspen Mtell was able to provide a four-day warning to the operators. Operations would then switch to the spare pump and prevent a process shutdown.

Improving Value Chain Agility and Resiliency

After the pandemic, especially with the start of war in Europe, chemical companies became more cognizant of localized reliable value chains. With changing demand patterns and raw materials scarcity, companies need to laser focus on their long-term, medium-term, and short-term planning. This is in addition to successful execution of production plans. Multi-term planning enables companies to optimize value chains at different levels to drive sustainability, agility, resiliency and profitability.

AspenTech SCM solution offers a comprehensive set of tools to accomplish longer term and shorter-term planning and execution. Aspen Collaborative Demand Manager™, Aspen Supply Chain Planner™, Aspen Plant Scheduler™, and Aspen Schedule Explorer™ have been used by specialty chemical companies to meet their planning and scheduling needs.

Dow Chemical used Aspen Schedule Explorer to bring visibility to order execution and identify bottlenecks. Schedule Explorer enabled them to visualize raw material projection shortages with more accurate inventory forecasting and granular minute-to-minute scheduling visibility. Through this process, Dow was able to achieve 20% increase in unit throughput.

Albemarle (global provider of lithium and bromine) used Aspen Supply Chain Planner to incorporate GHG emissions associated with raw materials and utilities across the entire supply chain. They were able to reduce water usage by 11% and carbon intensity by 6% through process intensification.

Data Driven Operations

As business leaders are trying to change organizational culture to data-driven, real-time KPI's and enterprise-level dashboards for analyzing data in real-time are becoming prevalent. Integration and contextualization of process data allows the application of AI and advanced analytics into developing issues – in time for early resolution. Integration of planning & scheduling functions with operations, laboratory, logistics and compliance will streamline business processes. The benefits of this integration include improving agility, customer service, troubleshooting capabilities and overall operational efficiency.

AspenTech Inmation™ is an Enterprise-grade OT/IT system Integration Platform. All operational components and IT systems (such as LIMS, lab data, plant DCS, plant historian, etc.) can be connected across entire geographic and enterprise network infrastructure. Inmation would then contextualize the data and transform it into actionable information, which is presented to every decision-maker on any device, anytime, at any location. BASF, Cabot and Takeda have all used Inmation to create data governance, improve cyber security and create a harmonized and scalable data platform.

Digital Solutions in Sustainability

Reduce Energy Use and Emissions to Lower Scope 1 and 2 Emissions

The chemical industry is aware of the impact of chemical manufacturing on global emissions. Following the Paris Climate Accord and subsequent amendments, many global chemical companies have pledged to a net zero future. However, unfortunately the economy and geopolitics haven't made it easy for chemical companies to make significant strides on this path. Nonetheless, chemical companies are investing heavily to make meaningful progress to reduce and abate emissions. Digital solutions bring visibility and provide control levers to optimize energy use and reduce emissions.

Optimize Production

Lowering Scope 1 or 2 emissions is an immediate priority for chemicals manufacturers. Based on the existing capabilities, every company is tackling this challenge with a distinct approach. Many focus on immediate Scope 1 emissions through optimizing existing operations. Boilers, furnaces and reactors requiring significant amounts of heat are subject to evaluation and optimization. Utility planning allows plant managers to predict utilities supply and demand more accurately and incorporate cheaper fuel and power whenever possible.

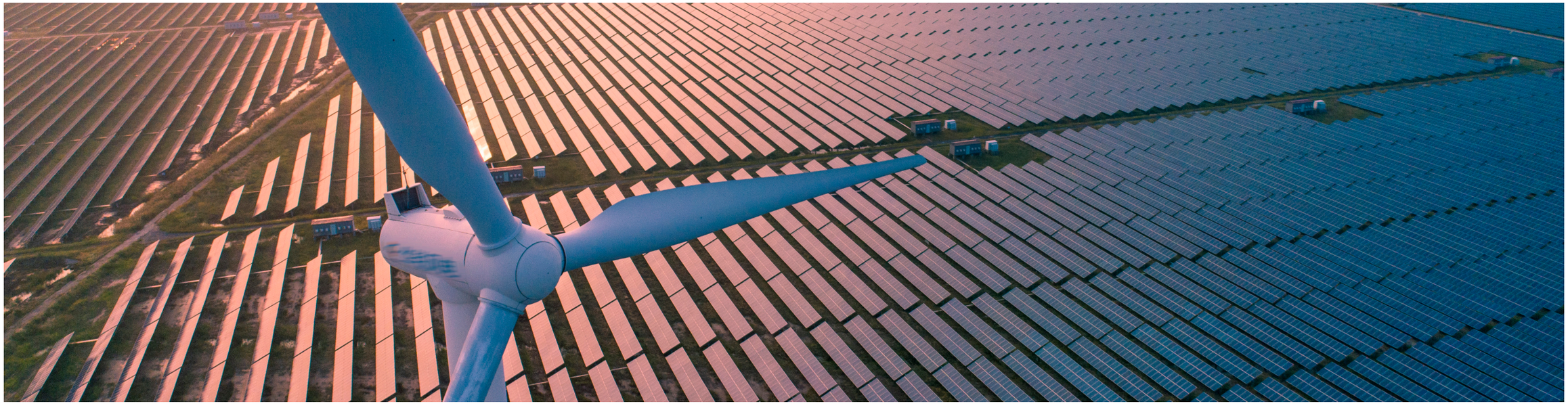
Huntsman has used Aspen Plus and Aspen Utilities Planner™ to identify $50M in annual energy savings opportunities.

Bring-In Renewable Power and Green Hydrogen

Swapping fossil-based fuels with renewable solar, wind, geothermal or hydroelectric power can in theory significantly lower GHG emissions. However, there is not enough harvested wind or solar energy, and availability patterns of renewable sources are somewhat unpredictable. Whether it is generated or purchased power, Aspen Tech's OSI digital grid management tools can help chemical manufacturers manage their microgrids. Improving situational awareness, enhancing grid cybersecurity, and improving safety, reliability and efficiency are some example benefits.

AspenTech Fidelis™ is a capital project modeling tool based on Monte Carlo probability analysis. Fidelis provides visibility and planning tools to de-risk any new project including sustainability and renewable energy projects. Aspen Fidelis can help to identify future bottlenecks and estimate economic variables as well as to complete RAM studies once the unit is operational. Braskem has used Aspen Fidelis to develop a roadmap to cut greenhouse gas emissions.

Envision (a producer of green ammonia) has used Aspen Fidelis to understand uncertainties associated with green power and green hydrogen generation.



Circularity and Scope 3 Emissions

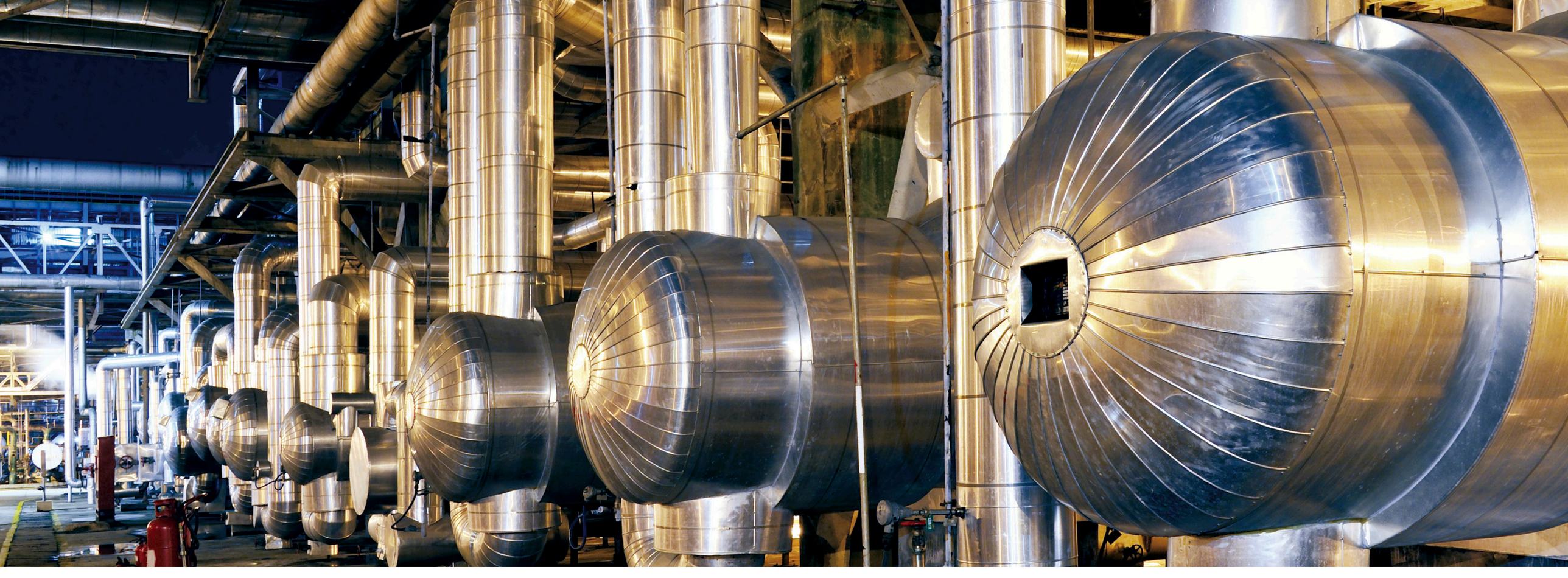
To reduce indirect Scope 3 emissions, chemical companies are evaluating value chains and adopting circular economy principles. This can include sourcing raw materials more sustainably, optimizing logistics to reduce fuel consumption, and incorporating renewable feedstocks. Developing plastic recycling technologies and incorporating bio-based feedstocks would lower fossil fuels dependency and minimize waste and emissions.

Aspen Plus brings tremendous capabilities to create circular processes. Designing biobased processes to use palm or waste cooking oil and lignocellulosic materials are some capability examples. Existing plastic recycling models include dissolution, pyrolysis and glycolysis. These models can be further optimized either by feeding experimental data or using AI-enabled Hybrid Modeling. For example, Equinox used Aspen Plus software to streamline the design of a Polyester Recycling process. These models allowed for a complete techno-economic evaluation while also optimizing feedstock blends to the process.

Tracking biobased portions of products through the entire value chain is a complex undertaking for a global manufacturer. Different countries and regions with different regulatory environments demand different modes of reporting. A digital platform to track and report renewable materials along with their associated emissions can address this complexity. OMV has used Aspen PIMS to track and report bio feedstock content in 35 of their blend grades heading to 5 different European countries.

Conclusion

Upgrading automation, digital, and data infrastructure is a necessity to position chemical companies for long-term growth. Whether improving existing operations or innovating new materials for new applications, chemical manufacturers use digital tools to ensure technical and economic feasibility. AspenTech and Emerson offer a wide portfolio of digital and automation solutions designed to ensure productivity, margins and safety. Through our websites, users have access to a vast library of use cases and success stories in chemical manufacturing.



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