Resource Efficiency in Chemical Manufacturing

Anahita Khanlari, Ph.D., Industry Marketing Director, Chemicals, Aspen Technology, Inc.
Gerardo Munoz, Product Marketing Manager, Aspen Technology, Inc.

aspentech | White Paper

Introduction

With chemical demand increasing globally in the next decade, chemical manufacturers are facing a dual challenge. On one hand, chemical production has to increase to address the growing demands of a growing global population. On the other hand, the industry is facing a climate and an environmental crisis. This dual challenge creates an opportunity for chemical companies to move away from traditional practices and adopt creative solutions like reusing or recycling materials. The United Nations Sustainable Development Goal number 12 highlights the idea of "responsible consumption and production", which many chemical companies have adopted and internalized as a guideline.

Resource efficiency in the chemical industry has different forms. Perhaps the initial example coming to mind is energy efficiency, especially in the face of geopolitical conflicts that have caused waves to ripple through the entire industry. Chemical companies have plenty of opportunities to optimize operations to lower energy use throughout operations—both in the main process and the utility side.

Another form of resource efficiency for chemical manufacturers is reusing materials as feedstock. For example, Kemira Oyj is using by-products from Covestro to make water treatment coagulants.[1] With millions of tons of post-consumer plastics floating in the oceans and buried in landfills, recycling and repurposing plastics has become a focus area for the industry. Global chemical producers are looking to use this waste as part of their feedstock. They are working to come up with technologies to turn it into monomers, polymers, and solvents. For example, Braskem is using waste plastic to create *I'm green*™, a recycled portfolio of products, and LyondellBasell has created *Circulen*, a family of products made from recycled plastic.

Digital solutions are instrumental in the chemical industry's journey to achieve greater resource efficiency. For example, a digital twin can illustrate the economic and environmental impact of every change in an operation. Traditionally, the industry has been relying on isolated models such as optimizing the materials flow and the associated costs, flowsheet simulations, or capital cost estimates to improve efficiency. However, siloed actions can no longer address the profitability, nor the technological or environmental challenges that the industry is facing today.

A comprehensive vision across all segments of the production value chain, from supply chain management to operations and waste management, is needed to improve overall efficiency, profitability and sustainability of the operation. Such a comprehensive approach is rare today. However, there are signs that the industry is moving toward it.

How Can Chemical Companies Improve Resource Efficiency?

To create resource efficiency based on production scale and added value of products, bulk chemical manufacturers might adopt a different set of strategies compared to smaller specialty chemicals manufacturers. For example, reducing Scope 1 emissions is a very pressing topic for an ethylene producer. At the same time, a specialty polymer manufacturer might focus on waste elimination and the circularity of their products. In this paper, we address some of the most critical industry topics.

1. Resource Efficiency via Effective Planning & Scheduling

The chemicals market dynamics have changed frequently over the past several years due to the unprecedented pressure exerted on global supply chains as a result of the pandemic. The subsequent disruptions cascaded through the energy and chemicals industry. While demands for plastics in healthcare skyrocketed, demands for energy plummeted. As the world began to transition back to pre-pandemic dynamics more recently, the conflict in Europe caused even more instability in markets. With market conditions shifting rapidly, integrating upstream and downstream models has helped chemical companies to remain profitable. Production planning and scheduling plays a key role in addressing product demands while conserving resources like feedstock to create the highest production margins.

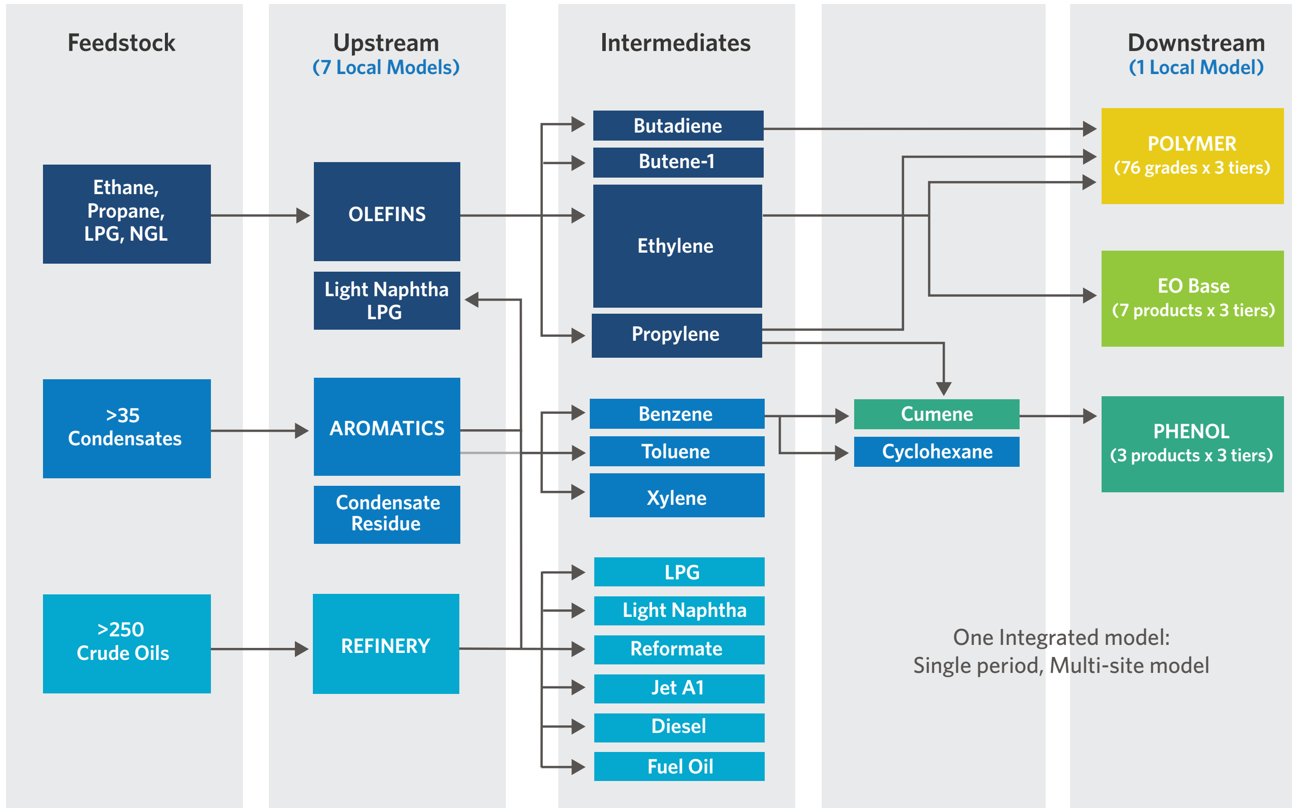
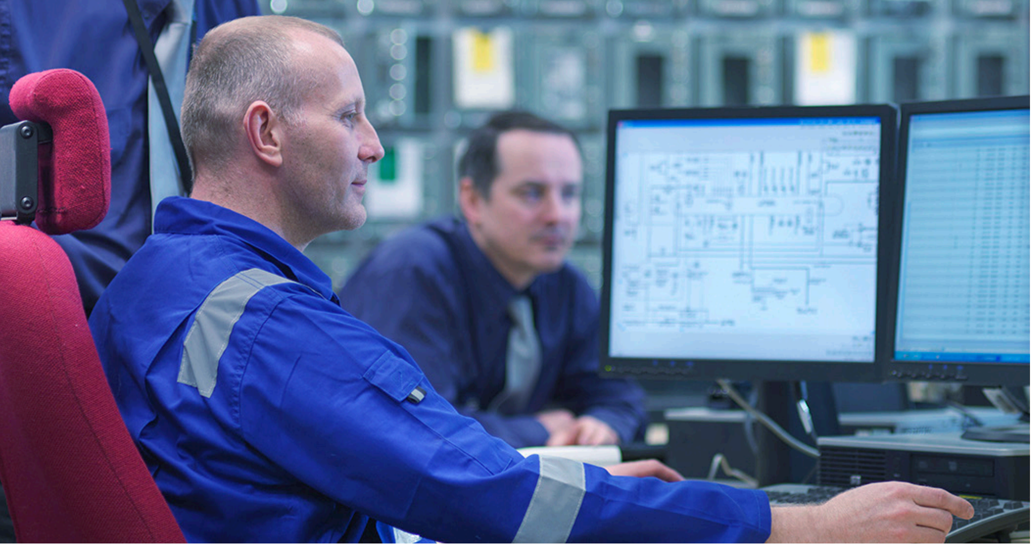


Figure 1. Aspen PIMS-AO enables short-term tactical planning and optimization for feedstock selection, production level and product mix, furnace line-ups, cracking severity/conversion optimization and energy usage.

PTT Global Chemical, a major producer of olefin and aromatics in Southeast Asia, embarked on a supply chain planning optimization project to improve supply chain visibility. Leveraging AspenTech's multisite integrated planning solution, Aspen PIMS-AO™ , they developed a model for the site operation, that included purchasing orders (e.g. crude, condensates, and NGLs), refined products (e.g. LPG, naphtha, jet, diesel, mogas), intermediates and aromatics (e.g. ethylene, propylene, butadiene, benzene) and polymers (over 240 grades/tiers of polyethylene (PE) & polypropylene (PP)), Figure 1. The model was able to communicate with the site's enterprise resource planning platform (SAP) and could optimize simultaneously for competing businesses like the production of ethylene vs. benzene or polymers. The model also enabled quick decision-making and the creation of consistent "what if" scenarios. By maximizing crude throughput to the refinery, condensate flow to the aromatics unit and production of high value products, the plant's total profits increased by $2M USD/year.

2. Improving Energy Efficiency and Limiting Carbon Footprint

While chemical producers experiment with new business models to take advantage of new feedstocks, new energy sources and new products, many have pledged to reduce their carbon footprint and become carbon neutral by 2050. Similar to the EU's' Emissions Trading System (ETS), other regions of the world are considering implementing carbon taxes in the form of trading markets. Deviations from these targets would impose high operational costs and cut significantly through profit margins. For example, at the time of writing this paper, the permit price of CO_2 in Europe is €67/ton, although it has been fluctuating between €55/ton to €98/ton. Free allowances are expected to be reduced, which will in turn increase permit prices. In such an environment, the energy efficiency of the main process is as important as reducing fuel gas, and steam demand on the utility side. Both measures are no longer simply profitability levers; they have become business longevity mandates, too.



2a. Improve Main Process Energy Efficiency

Considering the competitiveness of the market, feedstock volatilities, and low margins for commodity chemical producers such as ethylene, slight improvements in operations to increase energy efficiency can significantly impact producers' bottom line. Creating a digital twin of the plant can help identify site-wide opportunities to improve energy efficiency without the need for capital investment. For example, LG Chem used Aspen Plus® and Aspen Energy Analyzer™ to create a digital twin of their 900Kton/year ethylene plant in Daesan, Korea. An energy analysis identified about 60 savings opportunities. After reviewing commercial and operational feasibility, 20 of these opportunities were selected for further consideration and implementation. These changes resulted in 3-4 percent overall plant energy reduction, with an estimated $10M USD/year in additional profits for the plant.

Effective waste heat recovery from an existing process to generate steam can improve a plant's energy efficiency by lowering the load on utilities and boilers, reducing fuel gas consumption and subsequent greenhouse gas (GHG) emissions. In a recent study to improve energy efficiency in SOCAR acrylonitrile plant, waste heat recovery was improved by 36 percent. In this Sohio process, propylene, oxygen from air, and ammonia go through an exothermic reaction over a catalytic bed to make acrylonitrile. In this propylene ammoxidation reactor there is an opportunity to create steam from the excess heat of the reaction. Leveraging a combination of Aspen Plus®, Aspen HYSYS®, Aspen AI Model Builder™ feature and Aspen Activated Exchanger Design & Rating™, SOCAR developed a model around this fluidized bed reactor and existing steam generation boilers. Aspen AI Model Builder™ was particularly useful for developing a reactor model from operational data and first principles constraints. The model could predict the percentage of acrylonitrile in reactor flue gases and predict the optimal pressure required for the highest conversion. Here, three potential scenarios to maximize steam generation in the reactor were identified and one was implemented. This upgrade helped to reduce the plant's overall emissions by 5 percent.

Compressors are high energy consumers, and improving their efficiency can significantly reduce energy costs. A compressor's efficiency is a function of multiple variables such as feed composition, ambient conditions upstream and downstream operating conditions, and compressor control targets. With constantly changing demand patterns and non-linear relationships, traditional techniques for calculating efficiency seldom reflect real operations. In a recent case, one of AspenTech's global ethylene producer clients focused on improving the efficiency of the plant's cracked gas compressor. Aspen ProMV was used to create a real-time, single model encompassing process inputs, variations, and non-linearities of the compressor operation. When process conditions deviated from normal, or the machine efficiency deviated from the target, Aspen ProMV® Online alerted and guided operations to make quantitative, data-driven decisions to maintain optimum compressor efficiency. The initial result was a five percent reduction in turbine steam consumption. Based on a price of $12.75 USD/ton of steam, this was roughly equivalent to $120K USD/year in savings.

2b. Optimize Utilities (Fuels, Hydrogen and Steam) to Improve Profitability and Lower Carbon Footprint

One way for large chemical manufacturers to improve energy efficiency is through active utilities management. Digital solutions like advanced process control (APC) and digital twins provide visibility and control over utilities operations, emission levels, and opportunities to minimize them. APC has been used in process industries for decades to improve process efficiency. In addition to solving nonlinear problems, leveraging AI and machine learning (ML), new AspenTech APC tools learn from historic performance of the plant and enable users to optimize for desired economic and operational variables in a fraction of the time. Equally, digital twins are strong tools for tracking and managing emissions while providing insights to remove process bottlenecks. Digital twins facilitate monitoring at the equipment level, locating emission sources, and helping to validate and reconcile site-wide data that can be used for reporting and decision-making purposes.[2]

The fuel gas system is a good example of using APC technology in utilities management. Maintaining a balance between the enrichment gases entering the fuel gas network and the overall heating value and volume of gas is a challenge for every utility operator. When the heating value of gas increases, the furnace has to cut back on consumption. This can potentially also cut the enrichment gas flow that had resulted in higher caloric values originally. These cycles, along with the changing volume of the fuel gas, impose non-linearities in the system. A non-linear adaptive process control model brings stability to the network while minimizing flaring, blow-down discharge and ultimately fuel gas use and CO_2 emissions. Figure 2 shows the calorific value of the fuel gas before and after the implementation of AspenTech's APC solution. It is estimated that for a 200,000 bpd refinery, fuel gas optimization can save up to $4.6M USD/year in expenses.[3]

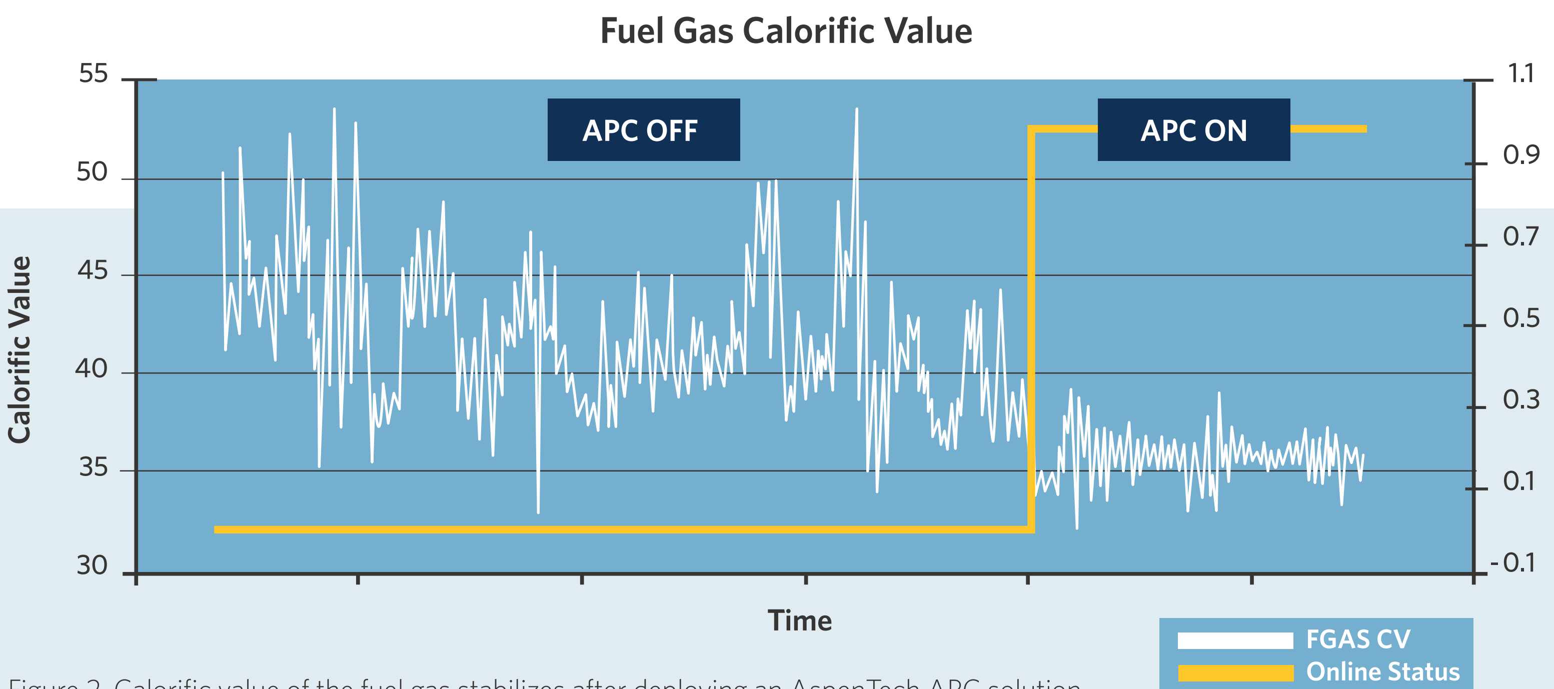


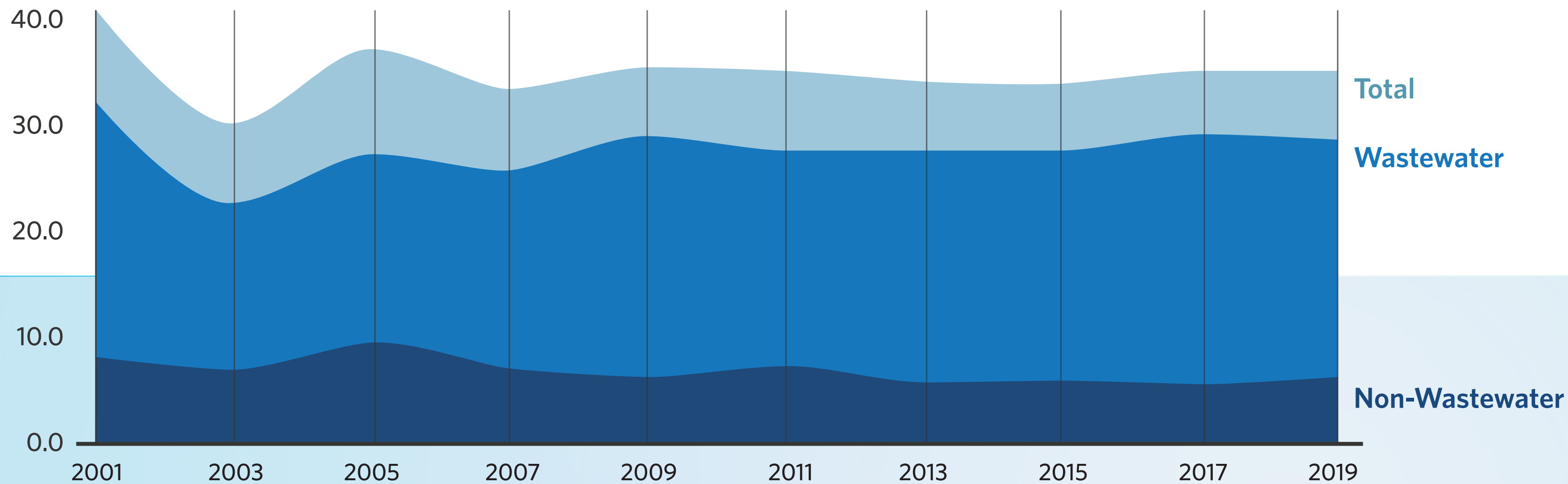
Figure 2. Calorific value of the fuel gas stabilizes after deploying an AspenTech APC solution.

As for the fuel gas network, using APC to optimize the steam network can improve the plant's' overall energy efficiency and save millions of dollars in fuel costs while significantly reducing the carbon footprint of the process. Any amount of lost or degraded (i.e., let-down) steam changes the fuel consumption and rate of CO_2 generation. Here, a non-linear adaptive process control, in addition to an APC optimizer, enables users to stabilize high, medium and low-pressure headers while maximizing boiler efficiency, distributing loads between equipment and continuously minimizing let-downs.

Utility digital twins provide a holistic view of the utility system, which enables managers to identify and implement key actions to improve overall efficiency. In one example, SABIC developed a utility digital twin model in one of their sites in the Middle East using Aspen Utilities Planner™. The model could determine energy losses at the equipment level and perform an overall utility system optimization to maximize energy gains. This model helped to identify site-wide opportunities and answer questions such as boiler selection; steam source; the impact of maintenance activities on steam system optimization; steam supply balance in high, medium, and low-pressure levels, and the selection of proper driving force (i.e., steam vs. electric motor) for the equipment. The findings of the model were used to implement changes which ultimately resulted in 130GJ/hour savings in energy usage. This is equivalent to nearly 60,000 tons of CO_2 reduction per year (assumes natural gas usage).[4]

3. Reducing Waste Generation

Waste generation in the chemical industry accounts for a large portion of total waste produced globally. This waste can be in the form of liquid, solid or gaseous material. According to the Environmental Protection Agency (EPA), 34.9 million tons of hazardous waste were generated by 23,700 active generators in 2019[5]. Since the chemical industry consumes significant amounts of water to cool down processes or as part of the process, wastewater accounts for the largest stream of waste produced. Figure 3 shows the reported wastewater and non-wastewater quantities generated by the chemical industry between 2001 and 2019, per EPA data.



Source: Environmental Protection Agency • Get the data • Created with Datawrapper

Figure 3. Total hazardous waste reported to the EPA between 2001 and 2019 (in million tons).

To minimize waste generation, the chemical industry has leveraged digital solutions in different ways. Figure 4 summarizes how digital solutions influence production, process optimization, maintenance and reliability, waste management, conditioning, and ultimately recycling. Instead of a typical linear view of the chemicals value chain, here we are looking at a circular approach. The right half of the circle outlines proactive strategies to prevent or minimize waste generation in the first place. The left half of the circle defines strategies to manage generated waste. Both halves of the circle heavily benefit from the implementation of digital solutions.

Flaring in manufacturing plants is an example of waste generation with environmental impacts on nearby communities. For example, at a **Braskem** production site in Brazil, large quantities of C_4 products were lost to flaring due to over pressurization of the debutanizer column. The over-pressurizing was in fact due to propane escaping from the bottom of the upstream depropanizer column. The facility's management considered the addition of a secondary reboiler to the depropanizer column to ensure effective separation of propane. However, the addition of a reboiler required both capital expenditure (CAPEX) and maintenance investments. As an alternative, Aspen ProMV was used to study over 15,000 data points and 45 different variables that impacted the operation of the depropanizer column. Its analysis identified the best control temperature for a proper separation using the existing reboiler. As a result of this study, over $1M in annual C_4 losses to flare were prevented.

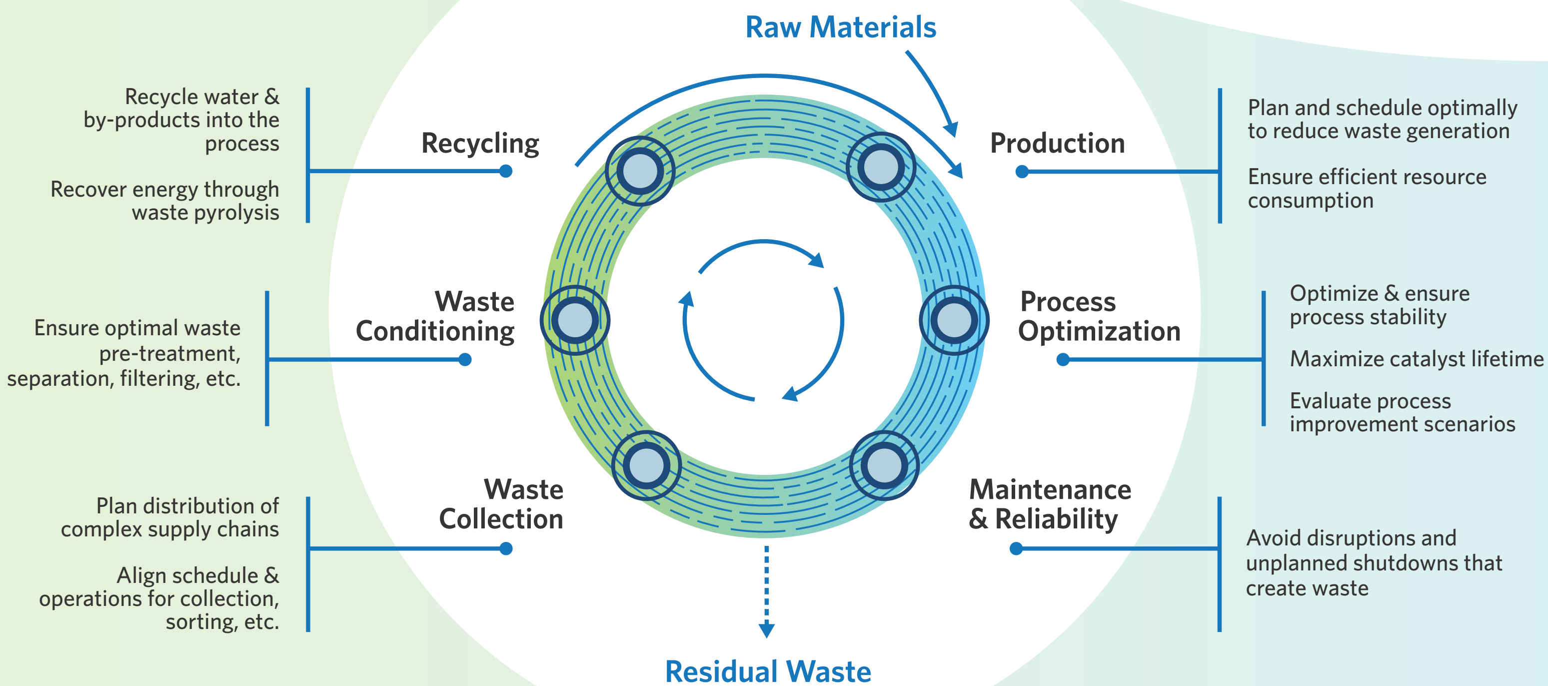


Figure 4. A circular value chain view for the chemical manufacturing industry. In each segment, potential opportunities for leveraging digital solutions to minimize waste are listed.

Reducing the need for further product treatment or minimizing catalyst decay are other examples of waste minimization in the chemical industry. **Petrocuyo** uses peroxide treatment on one of their resin products if the melt flow of the resin does not meet specifications. Generally, they had to use peroxide treatment on 80 percent of the product as it did not meet the required indices. To address the issue, Petrocuyo implemented Aspen ProMV to map production variables against the product's quality and melt flow properties. In this case, 1,800 data points from more than 60 different variables were fed to Aspen ProMV. From this dataset, Aspen ProMV identified 6 key variables of the temperature, pressure, and hydrogen ratios and how they have to be set to result in a qualified product. After implementation, the need for peroxide treatment in this product line reduced by 60 percent. This resulted in monetary savings in addition to requiring less storage and handling of a harmful chemical.

In another example, **Air Products** was challenged with a complex network of steam methane reformer (SMR) reactors feeding 600 miles of a gulf coast hydrogen pipeline. When there was an unexpected situation like a power trip, the feed to the reactors would drastically change, damaging the catalyst and imposing an unexpected shut-down to the plant. Here, an Aspen Plus model was created to monitor process conditions and to report deviations. This allowed process engineers to proactively monitor the reactor's performance and adjust operations. Additional conversion and increased capacity following the implementation of this model resulted in additional revenue of between $250K USD/year and $500K USD/year.

Summary

Increasing demand for chemicals globally, greater pressure on businesses to become more sustainable and a complex, volatile global market are all requiring higher levels of operational agility, flexibility and insight from today's chemical manufacturers. Industry leaders are accelerating the adoption of digital technologies to improve resource efficiency and minimize the carbon footprint of their operations. We highlighted a few of the companies who have already successfully implemented digital solutions to improve asset reliability, productivity and efficiency across their plants without making any new CAPEX investments. Digital solutions provide operational insight and create value throughout the chemicals value chain—from supply chain visibility to process design, production optimization and asset reliability and maintenance.

Citations:

[1] https://cefic.org/a-solution-provider-for-sustainability/chemistry can/driving-the-circular-economy/making-chemical-plants-more-resource-efficient/

[2] Digital Twins: Essential to Driving Sustainable Operations for Chemical Producers, Morse P. M., Pherwani G., AspenTech, 2021

[3] Save energy and reduce CO2 emissions with closed-loop optimization of utilities network, S. Lodolo, Aspen Technology, Hydrocarbon Processing, May 2022, p 43-48

[4] SABIC Continuously Optimizes its Utility System to Reduce Emissions and Increase Plant Energy Efficiencies, AspenTech case study, 2021

[5] https://rcrapublic.epa.gov/An Overview of Hazardous Waste Generation

About Aspen Technology

Aspen Technology, Inc. (NASDAQ: AZPN) is a global software leader helping industries at the forefront of the world's dual challenge meet the increasing demand for resources from a rapidly growing population in a profitable and sustainable manner. AspenTech solutions address complex environments where it is critical to optimize the asset design, operation and maintenance lifecycle. Through our unique combination of deep domain expertise and innovation, customers in capital-intensive industries can run their assets safer, greener, longer and faster to improve their operational excellence.

aspentech.com