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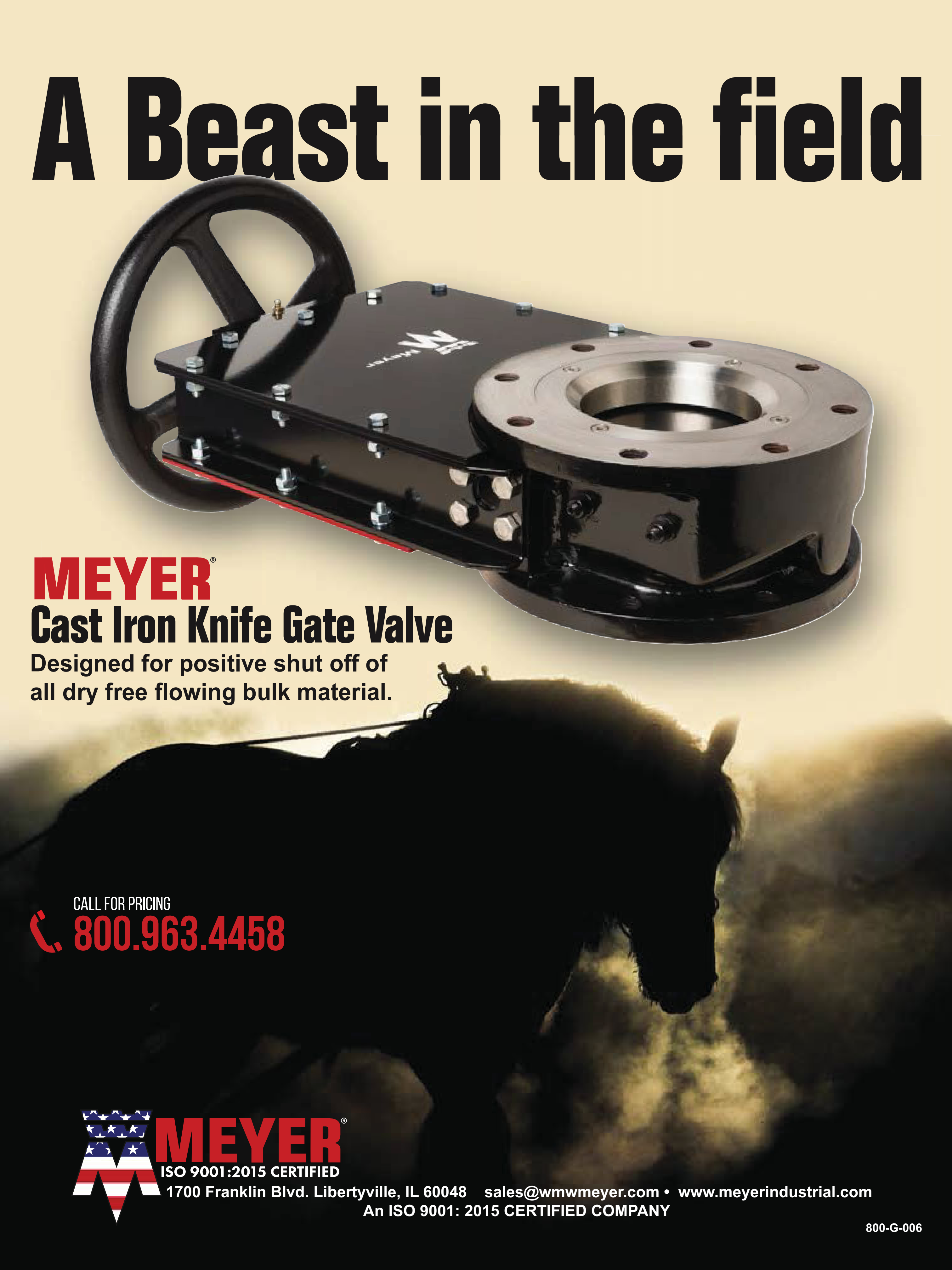
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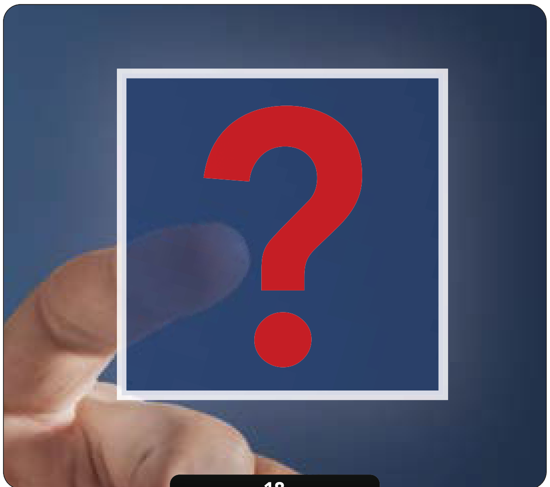

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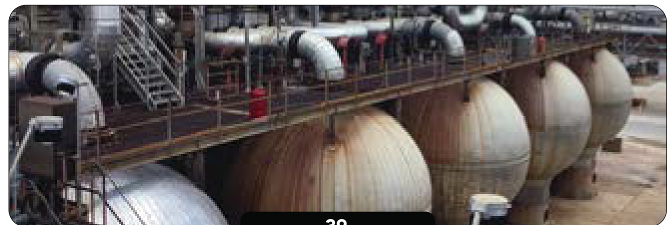

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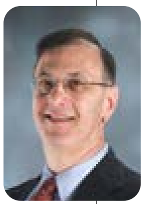
SOCMA Celebrates Centennial

Its diverse efforts aim to bolster the specialty chemicals industry



The group's renaming reflected its evolution to a broader membership.

THIS MONTH marks the 100th anniversary of the Society of Chemical Manufacturers & Affiliates (SOCMA). Founded on October 28, 1921, the group originally was named the Synthetic Organic Chemical Manufacturers Association. At the time, European companies dominated the U.S. market for dyestuffs and other specialty chemicals. However, SOCMA's 36 founding members, most of which were dyestuff producers, felt American companies could successfully compete. Indeed, the group's key objective was "... to take such collective action as may be proper for the establishment and perpetuation of the organic chemical independence of the United States of America."

SOCMA renamed itself in 2009 to better reflect the full breadth of the batch manufacturing value chain, says the group. Because its acronym was so well known, the group came up with a new name that allowed retaining the acronym while still reflecting the evolution to a broader membership. (ISA followed a similar path, going from the Instrument Society of America to today's International Society of Automation.)

SOCMA, since its inception, has focused on three areas: manufacturing and operations; advocacy; and commercial growth.

In manufacturing and operations, key areas of emphasis include facilitating continuous improvement in environmental, health, safety and security (EHS&S); and delivering and fostering best practices in operational excellence.

For example, two decades ago SOCMA worked with member companies to create a training curriculum for plant operators at batch manufacturing facilities. A modernized version of its Chemical Operations Training Tool, which debuted in 2019, has benefited 700–1,000 staff at more than 20 companies.

Today, the tool includes a digital learning module that companies can use to build or supplement their existing programs for new operators or for refresher training of long-term employees. The latest version, released this year, features a system for recording and tracking training progress; integrated 3D animations of process equipment; and additional material on areas such as lockout/tagout and confined space entry.

Another notable effort is ChemStewards, the group's flagship environmental health and safety program that was launched in 2005 to promote safety and environmental compliance at facilities.

SOCMA also bestows "performance improvement awards" in five core aspects of ChemStewards: stakeholder communications; product stewardship; EHS&S in planning and operations; employee training and engagement; and resource management and waste minimization.

Advocacy includes giving industry perspectives to legislators and regulators.

Commercial growth encompasses a variety of efforts aimed at fostering the sharing of business intelligence. SOCMA ran the InformEx trade show until 2005 and in 2020 purchased the Specialty & Custom Chemicals Show, which next will take place in Ft. Worth, Texas, starting on February 28, 2022.

This column only can highlight a few things, so for further details, go to www.socma.org.

SOCMA clearly has played an important and positive role in bolstering the prospects and performance of the U.S. specialty chemicals industry.

The official centennial celebration will take place in New Orleans during SOCMA's annual conference.

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Gain Insights on Topics and Trends

Our monthly polls and economic overviews cover important issues

Our polls and snapshots are meant to point you in the right direction.

IN A world where people overshare many aspects of their lives — from dinner choices to politics — it's nice to focus on straightforward questions. Our anonymous polls offer readers a chance to help us benchmark the industry one quick question at a time.

We've been polling our audience monthly for years and we have a rich database of past results (chemicalprocessing.com/poll-questions). From ethics to workforce issues, we query readers about real issues they face at their facilities. The questions are designed not just to satisfy our curiosity but also to give us insights about trends and prospective topics to cover, which in turn helps us better serve engineers designing and operating plants in the chemical industry. The answers to these questions also help respondents understand where they stand in terms of critical topics faced by their peers.

With a workforce that's experiencing an exit of seasoned engineers, we asked readers how often they rely on specialists at vendors for technical expertise lacking at their sites. Only 3.2% said never; nearly one-quarter (22.3%) said often and 47.3% said sometimes.

In terms of environmental issues, we wanted to know how the attention sites give to water resources has changed over the past three years. Only 0.6% said it decreased significantly; 28.7% said it increased significantly.

As for asset management, a current poll posed this question: How much progress has your site made on the path to predictive maintenance? More than half (53.6%) said some or a lot — it was an even split of 26.8% for both answers. Just 6.3% reported no progress at all.

Looking toward the future of the chemical industry, we asked readers how aware they are of efforts related to open process automation. More than one-third (36.4%) are not at all or only slightly aware; 31.4% are somewhat aware and 28.1% are very aware. (After that poll came out, we published "Open Process Automation Moves Ahead," https://bit.ly/3yu8gwu.)

This information gives us plenty to ponder in terms of future stories as well as areas to focus on regarding webinars, podcasts, news coverage and whitepapers. It also alerts readers to what they might need to work on in their own facilities. In addition, vendors value this information because it tells them where the holes are in their campaigns to serve customers.

Poll questions aren't the only way we help readers feel the pulse of the industry. We also feature a monthly Economic Snapshot. Our database goes back to 2013 and provides a quick overview of how the U.S. chemical industry and the overall U.S. economy are doing. Each month it tracks two chemical-industry-specific indicators: shipments and capacity utilization. It also includes data on the Chemical Activity Barometer. This metric, a leading economic indicator for the overall U.S. economy, developed by the American Chemistry Council, takes into account that chemical industry activity occurs early in the supply chain.

The most current metrics as of press time (numbers are from July 2021) indicate that shipments rose, capacity utilization slipped and the Chemical Activity Barometer remained steady (see page 11 for the Economic Snapshot chart).

Management guru Peter Drucker said, "You can't manage what you don't measure." Whether that's workforce issues or capacity utilization, you must understand where the bars are and if you meet them or need to work on things. Our polls and snapshots are meant to point you in the right direction to search for answers within your own facilities.

ON-DEMAND WEBINARS

There are still a few new webinars on the horizon (Properly Weigh and Batch Powders and Other Bulk Solids (Oct. 27) and Combustible Dust Round Table — Second in the 2021 Series (Nov. 4). And there are several on-demand webinars ready for viewing right now. Be sure to visit https://info.chemicalprocessing.com/cp-upcoming-webinars and take advantage of the presentations from experts in the industry. Their advice and guidance will help you implement new programs and technologies at your facility.

TRACI PURDUM, Executive Digital Editor
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Consider the Effects of Global Warming

We won't recognize chemical processing by 2100

SUPPLY CHAIN disruptions from hurricanes lead to multiple economic impacts as a 2017 fact sheet (https://bit.ly/3ljknbk) from the American Petroleum Institute explains: "When a hurricane disrupts refinery or pipeline operations, the combination of an immediate loss of gasoline and diesel production and a lack of demand for crude can result in a two-tier market — the price of fuel can rise and the price of crude can fall." Of course, other ramifications result, including the need to clean up the devastation.

Skeptics largely have given up arguing against the reality of global warming after Hurricanes Katrina, Harvey and Sandy. The Union of Concerned Scientists says the situation only will get worse: https://bit.ly/3k0HYhf. "It's a forecast nightmare," cautions Kerry Emanual, a professor of atmospheric science at the Massachusetts Institute of Technology. "If a tropical storm or Category 1 hurricane develops into a Category 4 hurricane overnight, there is no time to evacuate people." (See: "What We Know About Climate Change and Hurricanes," *New York Times*, August 29, 2021, https://nyti.ms/3ljllV0.) Logically, this applies to other natural disasters such as tornadoes, wild fires, etc. Warnings may provide only a few hours to prepare instead of two to three days.

Besides causing catastrophic events, global warming certainly will economically impact chemical production. Let's first consider the effect of rising humidity on cooling.

I was concerned with the cooling towers at the plant I work at in Ohio. Using an online program available from SPX Cooling Technologies, www.spxcooling.com/water-calculator, I was able to show the effect of rising humidity. Our current design specification is supply — 83°F; return — 93°F with a wet bulb temperature of 78°F. I assumed a water flow of 10,000 gal/min. Unfortunately, the program is limited to a wet bulb temperature of 90°F but the calculations were revealing. The minimum available supply temperature jumped to 94°F and the return temperature rose to 114°F. The water losses increased by 4%; evaporation increased to 114 gal/min from 110, and blowdown to 57 gal/min from 55. Of course, the loss from drift remained the same; however, atmospheric research on global warming doesn't devote much attention to wind changes.

Projecting SPX's data, I estimate that at a wet bulb temperature of 100°F the minimum product temperature would be at 133°F!

These changes seem modest except for two facts: 1) much of U.S. oil refining takes place along the Gulf Coast (83.5% of the largest refineries are located there); and 2) 133°F is very warm for more delicate chemical products. (I assumed a 10°F minimum approach for heat exchangers.)

As we saw with Hurricane Harvey in 2017, weather can disrupt the U.S. economy for months. Economic forecasters reckon the 3rd-quarter gross domestic product (GDP) dropped by 0.2–0.8% then, a stark contrast to the 3.7% growth predicted before Harvey. If forecasters are right, this economic damage will accelerate with rising temperatures. One conservative estimate is a 1.8% impact on U.S. GDP by 2100; others are higher.

Warmer ambient temperatures directly affect some process operations. As I recall from my experience with fermentation at Anheuser-Busch, sterilized raw materials were stored at temperatures only a little shy of the minimum product temperatures. So, fermentation and most similar processes would have to go to much more expensive refrigeration.

The impact will go far beyond just products; most conventional refrigeration will become useless. Global warming also will affect key equipment. For example, water-cooled air compressors are designed for a maximum temperature of about 120°F — some even lower, 95°F.

Other effects of global warming bear consideration. Storm water controls in our industry generally mandate separating polluted runoff from ordinary runoff such as that from parking lots. Current designs, which date to the 1970s when regulations about separation were created, were developed based on a 24-hr rainfall event from a once-every-25-yr storm. Now, 100-yr floods are happening every five years. Intensities are unpredictable and may reach a wastewater manager's worst nightmares. Few regulators are willing to risk the political backlash from providing specific standards. They won't tell you what you should use for your design standards but will hold your plant accountable if it floods a river with toxic chemicals! It falls to industry to create safe wastewater-handling processes to avoid situations like being banned from sending streams to a municipal wastewater facility.

DIRK WILLARD, Contributing Editor
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Global warming certainly will economically impact chemical production.

Polymers Promise Better Sustainability

Materials offer impressive properties but catalytically depolymerize for monomer recovery

A GROUP of researchers at the University of Akron (UA), Akron, Ohio, believe they have found a promising solution to address the challenges in plastics sustainability. The team has developed recyclable polymers with excellent thermal stability and the high-performance mechanical properties of traditional polymers. Yet, addition of a depolymerization catalyst allows recovery of monomers.

"We are particularly interested in chemically recyclable polymers that can be broken down into the constituents (monomers) from which they are made," says Junpeng Wang, assistant professor in UA's School of Polymer Science and Polymer Engineering. "The recycled monomers can be reused to produce the polymers, allowing for a circular use of materials, which not only helps to preserve the finite natural resources used in plastics production, but also addresses the issue of unwanted end-of-life accumulation of plastic objects."

The team identified the right monomer needed for designing chemically recyclable polymers through quantum chemical calculations, "which demonstrates a promise of exploiting data to discover and develop new materials," notes Wang.

They then synthesized the monomer and polymers using abundantly available starting materials. An article in *Nature Chemistry* explains the research.

SUSTAINABLE POLYMERS

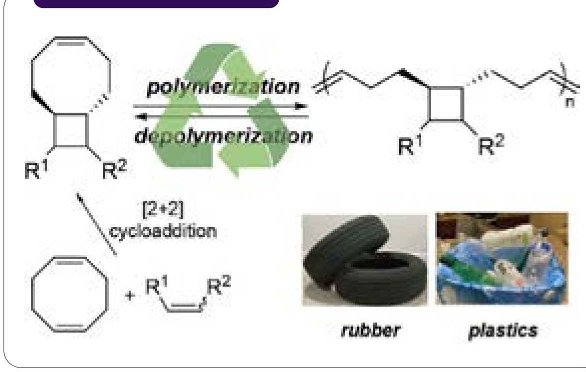


Figure 1. Chemically recyclable polymers with excellent thermal stability and tunable mechanical properties show promise as next-generation sustainable materials. *Source: Junpeng Wang, University of Akron.*

"The chemically recyclable polymers we developed show excellent thermal stability [decomposition temperature >370°C] and robust mechanical properties and can be used to prepare both rubber and plastics," states Wang. "We expect this material to be an attractive candidate to replace current polymers. … Compared to other recyclable polymers that have been demonstrated, the new polymers show much better stability and more versatile mechanical properties. When a catalyst is added, the polymer can be degraded into the constituent monomer for recycling."

Challenges remaining to address include scaling up the synthesis, use of environmentally benign media for depolymerization, and recycling of the depolymerization catalyst. However, the team's current focus is on expanding the scope of the chemically recyclable polymers and to develop carbon-fiber-reinforced polymer (CFRP) composites.

"CFRPs are high-value materials used in the aerospace and automobile industries. Currently, most CFRPs are not recyclable. Since our recyclable polymers have excellent thermal stability and mechanical strength, they are good candidates to replace the polymer matrix used in CFRPs," explains Wang.

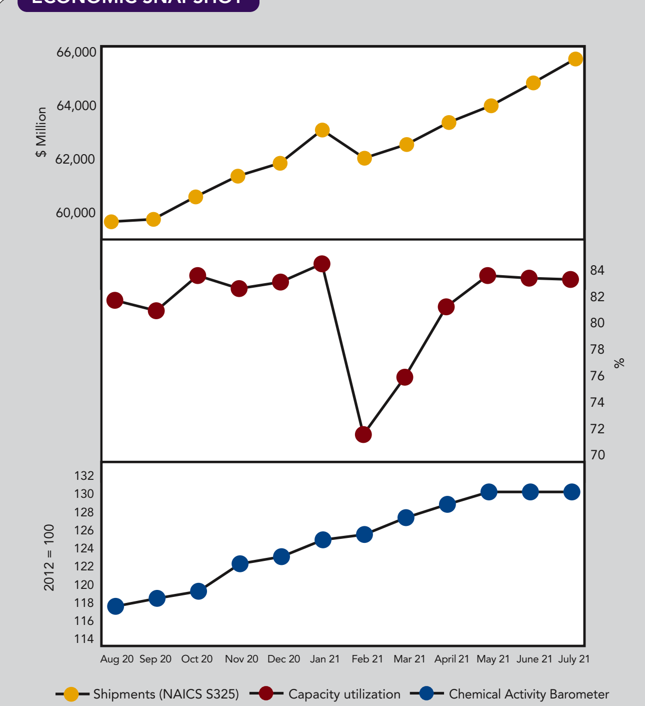
The process also enables preparation of chemically recyclable polymers using bio-based olefins — work on that now is taking place, Wang notes.

The team plans to analyze the economic performance of the process and perform life-cycle analysis for commercialization of the polymers.

"The purpose of life-cycle analysis is to analyze the environmental impact of the chemically recyclable polymers if they are used for certain applications. It is a crucial premise before the commercialization of the polymers," emphasizes Wang.

The researchers are in contact with industrial firms to collaborate on future development.

ECONOMIC SNAPSHOT



Shipments rose but capacity utilization slipped and the CAB remained flat. *Source: American Chemistry Council.*

CO_2 Underpins Microbial Route to Feedstocks

A COMBINATION of heterogenous chemical catalysis, electrochemistry and metabolic engineering pioneered by German researchers has created potentially unlimited uses for carbon dioxide (CO_2) as a raw material in chemical manufacturing.

The researchers, based at the Fraunhofer Institute for Interfacial Engineering and Biotechnology IGB, Stuttgart, use a catalytic step to convert CO_2 to methanol and an electrochemical step to transform CO_2 to formic acid.

What's new here is the methanol and formic acid then serve as nutrients for engineered microorganisms which can produce organic acids used in polymer manufacture and amino acids employed in food supplements and animal feed (Figure 2).

"In principle, the product spectrum is unlimited. Due to the use of synthetic biology and metabolic engineering within the cell, a vast amount of chemical products can be derived from the intracellular metabolites of such engineered microbes," says Jonathan Fabarius, senior scientist biocatalysts at Fraunhofer IGB.

The team chose methanol and formic acid because they are comparably straightforward to produce via chemical and electrochemical processes. Some bacteria such as methylotrophic strains can metabolize these liquid substrates naturally, notes Fabarius. However, metabolic engineering still is required to improve their production capacities, he stresses.

ENGINEERED MICROORGANISMS

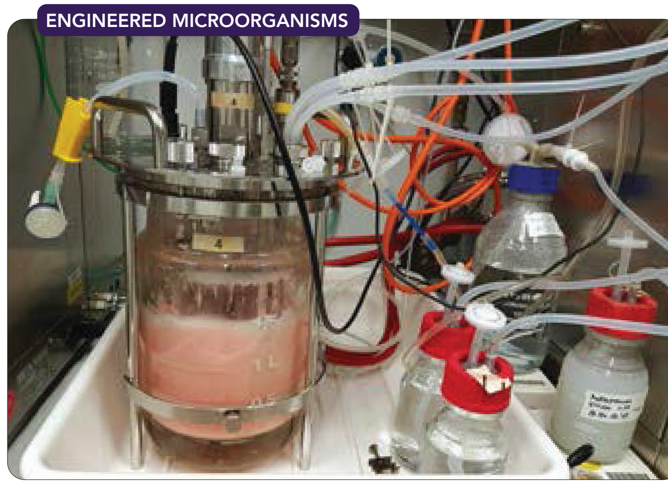


Figure 2. Conversion of carbon dioxide creates nutrients for microbes that can produce a wide variety of products. *Source: Fraunhofer IGB.*

Proper Grab Sampling Can Make A Big Difference

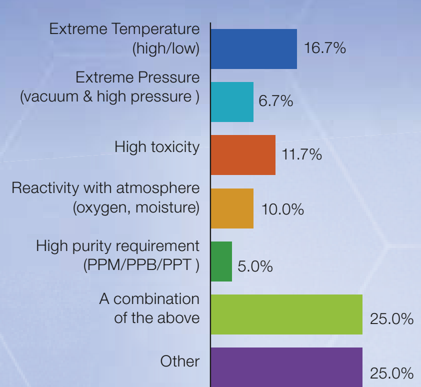
When collecting samples of hazardous chemicals, safety and quality are paramount. It is important to prevent exposure to toxic fumes or spills. A high-quality sample needs to be representative and cross-contamination should be avoided entirely. Having the right tool for the job is essential.

Read the full market insight report at: https://hubs.li/H0V5vgt0

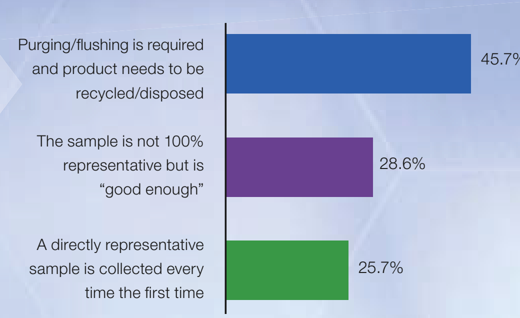
Top 3 areas where improvement is needed in grab sampling:

1. Safety
2. Complexity
3. Reliability

What challenges do operators face when conducting grab sampling?



Are representative samples easy to come by?



"Moreover, liquid substrates provide advantages regarding high solubility in aqueous solution, which circumvent mass-transfer limitations faced in gas fermentation, for example with syngas fermentation or direct CO_2 conversion by algae," he adds.

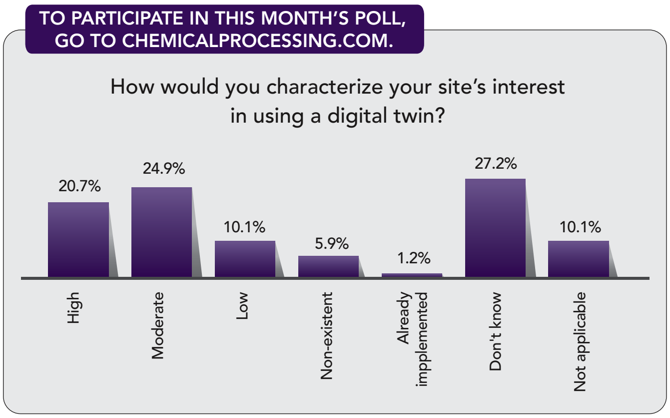
On the catalysis side, the researchers currently are working on two fronts: first, to increase catalyst stability and resilience under flexible-load operating conditions and against possible contaminants of CO_2 from "real" sources such as industrial exhaust gases; and second, to enhance process selectivity and, thus, yields and efficiency through development and engineering of catalyst materials and process conditions.

They have achieved 10-L-scale production of a natural terpenoid dye from a methylotrophic bacterium and are working to get organic acids and amino acids to the same scale.

"We are highly interested to further develop these processes to pilot scale and beyond, both for and in collaboration with interested industrial partners. At Fraunhofer IGB, we have the expertise and infrastructure for the scale-up of biotechnological processes up to 10-m^3 reactor volume," states Fabarius.

However, achieving this requires overcoming two big challenges: the toxicity of CO_2-derived formic acid to bacterial cells, and the flammability of methanol.

"These challenges must be solved with advanced engineering efforts regarding fermentation, for example feeding strategy, and explosion protection — or with enhanced metabolic engineering studies to improve biocatalyst stability against toxic substrate," he concludes.



Nearly three times more respondents report at least moderate interest versus low or non-existent interest.

Change How Your Plant Runs

Focus on operational and engineered advances, proper maintenance, and new technologies

When problems recur frequently, it is wise to explore root causes.

IN RECENT columns, I discussed various ways to identify energy efficiency improvements and implement energy management. These include process flow diagram reviews, online optimization, energy performance indicators (EnPIs), and energy management systems of various kinds. Last month focused on human factors that can influence energy performance (see: "Behold the Impact of Human Behavior," https://bit.ly/2XVHEYH). All are important topics — but to achieve plant energy savings you must translate your ideas into a change in how your plant runs. This happens in four main ways (what I call elsewhere "the four pillars of industrial energy efficiency") — operational improvements, effective maintenance, engineered improvements, and new technologies.

Pillar 1. Operational improvements. Many such improvements involve little or no cost. This makes them particularly attractive where energy prices are low and it's difficult to justify investment in energy-efficiency projects. Also, before committing to projects that require capital expenditure, confirm the existing equipment is being used to its full advantage.

When we identify suboptimal operating practices, the first response generally is to modify operating parameters (e.g., change control valve setpoints). However, this is only a short-term fix. Taking additional energy management steps will ensure the improvement becomes permanent. These might include:

- carrying out additional operator training;
- modifying operating procedures and updating documentation;
- adding control valves and/or automation; and
- implementing real-time optimization systems.

Pillar 2. Effective maintenance. To get the most out of existing facilities, the plant must be properly maintained, especially the equipment and systems that have the largest impact on energy use. These include heat exchangers (especially those in preheat services, and some condensers), furnaces and boilers, steam piping, steam traps, insulation, compressors, pumps and turbines. Common maintenance programs and activities include boiler and furnace tune-ups; convection bank cleaning; steam system management programs, including steam leak and steam trap surveys and repairs; and heat exchanger fouling surveys, analysis and cleaning.

When problems recur frequently, it is wise to explore root causes. For example, with recurrent steam leaks the underlying issue often is poor piping design or inadequate drainage. Correcting the root cause (e.g., re-routing steam lines, adding drop legs or replacing failed steam traps) can eliminate — or at least minimize — the occurrence of future steam leaks, and the cost and inconvenience of further repairs.

Pillar 3. Engineered improvements. Additions and upgrades to existing plant facilities, and modifications to new plant designs can lead to significant improvements in energy efficiency. Examples include:

- resequencing equipment (e.g., heat exchangers in a pre-heat train);
- replacing or upgrading electric driver systems;
- adding or modifying heat exchangers, steam turbines, distillation columns, etc.;
- adopting new control schemes; and
- upgrading catalysts.

Engineered improvements can be expensive, and often difficult to justify based on energy savings alone. However, many such projects bring additional benefits (e.g., improved product quality, reliability or capacity), which enhance the economics. Factoring in "cost of carbon" (e.g., carbon tax) also improves project return.

Pillar 4. New (or breakthrough) technologies. Engineered improvements apply proven solutions to identified problems. In contrast, solutions that incorporate new (or breakthrough) technologies require validation through research and development. They need more time to implement, and their degree of technical and financial risk is higher.

Some of the largest energy efficiency improvements have come through technological breakthroughs. A well-known example is the development of the low-pressure polyethylene process in the 1950s. This was a major advance over the older high-pressure process, and the new process used much less energy per unit of production. More-recent examples include the Dow/BASF hydrogen peroxide to propylene oxide process, which reduced energy usage by 35% compared to earlier technologies; and Shell's OMEGA ethylene oxide/ethylene glycol process, with 20% less steam demand and 30% less wastewater than a traditional thermal-conversion monoethylene glycol plant.

Incorporating new types of equipment — e.g., novel heat exchanger designs and distillation columns packings — in existing processes also can lead to significant energy savings. ●

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EPA Goes Back to the Drawing Board

Agency proposes revising the rules for five PBT chemicals

It's unlikely the EPA will extend the deadline again.

THE IMPLEMENTATION of the Toxic Substances Control Act (TSCA) provisions relating to regulating persistent, bioaccumulative and toxic (PBT) chemicals has been anything but smooth. On September 3, 2021, the Environmental Protection Agency (EPA) announced it intends to initiate new PBT rulemaking and anticipates proposing new rules for five PBT chemicals subject to final risk management rules under TSCA Section 6(h). Additionally, and happily, the agency extended the compliance dates for the prohibitions on processing and distribution and the associated recordkeeping requirements of one of these PBT chemicals, phenol, isopropylated phosphate (3:1) (PIP (3:1)). The action was imperative as EPA's earlier-issued "No Action Assurance" (NAA) lapsed on September 4, 2021. This article provides key points related to this complicated area of TSCA regulation.

NEW RULEMAKING

On January 6, 2021, the EPA issued final rules under TSCA for five PBTs: 2,4,6-tris (tert-butyl) phenol; decabromodiphenyl ether; hexachlorobutadiene; pentachlorothiophenol; and PIP (3:1). The final rules limit or prohibit the manufacture/import, processing, and/or distribution in commerce of these chemicals. On March 8, 2021, the EPA announced it needed additional public input on these rules and opened a 60-day comment period.

In its September announcement, the agency noted it's considering revising all five of the final rules "to reduce exposures, promote environmental justice, and better protect human health and the environment." The EPA will not propose new rulemaking on all five PBT chemicals until the spring of 2023. The current provisions of the January 2021 rules will remain in effect while the EPA works on the new rulemaking effort, with the exception of PIP (3:1), which is described below.

COMPLIANCE DATES

The EPA extended certain compliance dates for PIP (3:1) to March 8, 2022, to address the many "hardships" brought to its attention in the aftermath of the final rule issued on January 6. The EPA did so "to ensure that supply chains are not disrupted for key consumer and commercial goods." As readers may know, following the release of the final PIP (3:1) rule, stakeholders informed the EPA that the prohibition on processing and distribution of PIP (3:1) would significantly and adversely impact articles used in a wide variety of electronics, from cell phones, to robotics for manufacturing semiconductors, to equipment for moving COVID-19 vaccines and keeping them at the appropriate temperature (See, "Better Understand TSCA's Long Reach," https://bit.ly/3gJcZDs).

In response to this, the EPA issued a rare, temporary 180-day NAA indicating it would exercise its enforcement discretion regarding prohibitions on processing and distribution of PIP (3:1). While the six-month reprieve was well received, many stakeholders had advocated for one that would last years, not months.

To ensure supply chains continue uninterrupted, the EPA signed in September a final rule extending compliance dates for PIP (3:1) articles to March 8, 2022. The agency plans to further extend this deadline and the associated recordkeeping requirements to align with comments received and the expected timing for the new rulemaking.

As part of the separate rulemaking on all five PBT chemicals planned for 2023, the EPA will reevaluate the current rules for PIP (3:1) and the other PBTs, and, importantly, describe the information it will require to support any additional extensions to the compliance dates. Without this more-specific information from suppliers, it is unlikely the EPA will extend the deadline again.

DISCUSSION

The EPA's extension of PIP (3:1) compliance is welcome relief. Although some will complain about its seemingly short duration, the agency's approach is fair. After reviewing the many comments received, the EPA's view is that many commenters "did not provide sufficiently specific information about their operations to support their assertions" for more time.

Stakeholders are strongly urged to document efforts taken to-date and immediately to gather more specific facts related to how challenging it will be to survey every supplier of every part. These measures will best prepare stakeholders so when the EPA provides its guidance on commenting, commenters will be prepared to provide feedback during what we expect will be a very short comment period.

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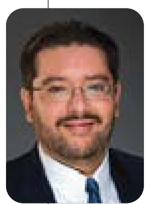
MTP Makes Modular Manufacturing Easier

Time to market is expedited and costs are cut when a common, open standard is applied.



Juan Carlos Bravo
product manager for DeltaV PK Controller and data integration at Emerson

Taking knowledge and finding a way to share it with the next generation without having to spend hundreds of hours teaching them is truly valuable.

A KEY challenge for the chemical industry is the time it takes to bring products to market or change operations to accommodate new products. With many process changes, engineers can spend weeks or longer integrating manufacturing skids and their respective automation systems. Working with industry leaders like Emerson, the User Association of Automation Technology in Process Industries (NAMUR) has been developing Module Type Package (MTP) to create a common, open standard that requires less engineering and makes new equipment integration closer to plug-and-play.

Chemical Processing spoke with Emerson's Juan Carlos Bravo, product manager for DeltaV PK Controller and data integration, to better understand how MTP can standardize and accelerate equipment integration and leverage these benefits to reduce project timelines and costs, improve operations and help the influx of new engineers in the process.

Q: Why does traditional system integration not make sense for today's trend toward more modular manufacturing? And how will MTP solve that problem?

A: In the past when you built a chemical plant, it was a fixed scope. It was one product, it never moved and it operated for 10 to 20 years. Things have changed and facilities need to produce multiple products. In order to change the process, you need to change the equipment.

Everyone has their own process, their own formula and their own twist. The best way to be nimble is to utilize modular production. The industry came up with the module type package standard. MTP creates a common, open standard that dramatically reduces integration engineering effort. It's nearly plug-and-play and you can just remove modules or add new ones and you have a different product.

That's truly the big challenge with traditional systems, they are not equipped for plug-and-play modules. In the past, an engineer would have this big list of signals and have to have conference calls with different OEMs (original equipment manufacturers) and vendors, engineer a plan, and then put it together. If you make changes, that will likely extend the project timeline and increase costs. Instead of spending hours engineering, MTP gives you a file that has a standard configuration and documentation. Load it into a system, and it's configured.

We're also extending MTP into active monitoring equipment. So, if you have rotating equipment like a turbine, you can just bring that complex equipment in and connect to the system. Another big benefit is that you don't need an expert to do this. Someone with very little experience can load a file, go through a wizard and they're done.

At Emerson, we believe a lot in what we call Human-Centered Design. We test numerous different scenarios and we make sure that the person performing tasks is guided safely through the correct steps to accomplish their goals.

Q: How does flexibility in MTP recommendations provide an opportunity for systems providers to better serve manufacturers?

A: Customers can bring products to market faster. For example, we did a large ethylene cracker project. It was 350 modules with 200 signals each. There were multiple protocols for each module and it took thousands of hours. With MTP, we can reduce this by half because not everything will have to be done manually. It makes system vendors more competitive and customers will reap those benefits as well.

Additionally, by not having to do everything manually, you don't have engineers who are just doing the minimum because of the crippling workload. You're bringing more information into a control system that you can reuse for analytics or deep machine learning or for the finance department. In the past you feared performing the engineering to bring in all these elements would overwhelm the system or push the project over budget.

Q: What should organizations consider in order to drive the value gained from MTP beyond project implementation and into everyday operations?

A: One of the bigger benefits of MTP is when you're building a new plant. With modular manufacturing, you'll have to switch equipment, calibrate equipment, validate equipment. So, during everyday operations, MTP is going to help you minimize downtime; it will help you change modules faster to help you produce different lines. We enable customers to have a more flexible production line.

Q: Are there any challenges?

A: MTP is new in the chemical industry. It was born out of NAMUR in Europe. So, a lot more is happening in Europe. In North America, one of the biggest challenges is we still need to see more vendors adopt it. MTP is still evolving.

Another challenge is it's not standardized. MTP right now doesn't have a governing group that validates or certifies MTP vendors or equipment. So, a lot of customers who are adopting it are sticking to a single vendor solution. For example, in Emerson, we support MTP, and we tested our own DCS (distributed control system), our own PLCs (programmable logic controllers) and our own asset monitoring solution (AMS) to ensure that they support all the key elements of MTP and integrate seamlessly.

Q: What about current implementation of MTP?

A: Unfortunately, MTP is so new that there are no full-scale implementations. In Europe a lot of customers are already evaluating and putting equipment in their Greenfield projects. As you know, the pandemic has delayed a lot of these projects. That's why we haven't seen much MTP in the field yet. But I know of some customers who are already putting in their specifications where they're building projects and those vendors who supply MTP were bidding those projects.

Q: Does MTP only benefit integration of PLCs on OEM equipment? Can it be applied to other types of devices typically integrated into the DCS on larger projects?

A: At Emerson, we have also implemented MTP in our asset monitoring equipment. That's an area where we're seeing that you need to bring a lot of data into a system to expose information for analytics, for deep machine learning.

For example, there are a lot of pumps in chemical plants. And some of them are critical. If that pump fails, basically it's going to shut down your production. If MTP connectivity makes it easier to bring pump values into the control system, you can predict that pump is going to fail because it's showing some vibration, because it's showing some cavitation – and if you can predict in advance, it's something that helps the overall productivity.

Q: How can MTP help plants that are struggling to retain a wide base of experienced personnel?

A: There are so few experts now who really know all these protocols. In the traditional project, when you integrate these modules they need to talk different protocols, and some of them are 20-plus-year-old protocols. So, you need to have very experienced people who really know how to map that. There used to be multiple experts on projects to map all these thousands of signals.

MTP-CAPABLE DELTAV OPERATIONS

Emerson's MTP-capable products make it easier to unlock modular manufacturing and bring equipment values into the control system.

Now, with MTP, you can have a more junior engineer do the work because the wizards help map. You can use your experienced people to mentor or work remotely. Or use them in the areas that are critical instead of just doing tedious mapping of modules.

Q: Do you have anything to add?

A: We see signs that MTP is going be widely adopted pretty soon because of the benefits. Right now, the world is in turmoil; customers want and need to be flexible. With supply-chain issues, they're not getting the ingredients they used to get. They need to change their production and change the modules and have a more flexible team.

I think that's what is different from what we have seen in the past, or at least I have seen in my 20-plus-year career. Sometimes standard adoption takes decades. MTP adoption appears to be going faster, maybe because of the current situation, maybe because of the current mentality or maybe because of the loss of experts. We're seeing a lot of people retire who are knowledgeable in a lot of these protocols. So, we're bringing in younger engineers who are used to apps. You ask them to map something and they either don't have the skills to do that mapping or it's going to take them a while to understand.

Vendors like Emerson still have a wide base of people who are knowledgeable and they can transfer and share that knowledge with the next generation by building these wizards. Taking that knowledge and finding a way to share it with the next generation without having to spend hundreds of hours teaching them is truly valuable. So, giving them ways to make the most of what is still in the plants right now while still helping them transition to new technology is really what it's all about.

For more information, visit: Emerson.com/MTP

PSM AUDITS FIND CONFUSION COMMON

Issues with operating/safe limits tables arise all too frequently

By James A. Klein and
James R. Thompson,
ABSG Consulting

PROCESS SAFETY audits [1, 2] serve two main purposes: (1) feedback on process safety program implementation and effectiveness to identify potential opportunities for improved performance, and (2) compliance with process safety regulations such as the 29 CFR 1910:119 Process Safety Management (PSM) regulation of the U.S. Occupational Safety and Health Administration (OSHA) and the 40 CFR 68 Risk Management Program (RMP) rule of the U.S. Environmental Protection Agency (EPA).

A facility with a process covered by these regulations must conduct compliance audits every three years. Facilities in existence when OSHA promulgated its regulation in 1992 now have performed seven to nine compliance audits. A review of recent audit findings for both long-established and newer plants suggests certain shortcomings continue to commonly arise. This article looks specifically at issues related to operating limits, required under the operating procedure (OP) element, and safe limits, required under the process safety information (PSI) element — and provides guidance on how to avoid such findings through appropriate development and implementation of limits tables. Future articles will focus on other common PSM findings (see sidebar).

Operating limits and safe limits tables are important because they define the ranges of safe operation for a process, both as operating limits in the OPs and as the ultimate safe (or design) limits in PSI. Exceeding operating limits can prompt process upsets, quality issues and other problems. Deviating outside safe limits likely will cause significant process incidents and result in possible equipment damage, personnel injuries and environmental harm. Failure to properly document these limits can lead to improper operation as well as major operability and safety issues. So, a plant must spell out the consequences of the deviations from these limits, including the safety and health effects on personnel. The OPs must specify correct operator responses to regain desired control of the process. Many companies choose to combine these sets of limits tables as part of the OPs for ease of reference and use; this, while common, sometimes also becomes a source of confusion if the information is not clearly presented.

Based on our experience, having a complete, accurate and thorough set of operating limits and safe limits tables available to process operators (particularly board operators) as well as engineers, maintenance staff, etc., is invaluable in (1) focusing them on the important process parameters, (2) reminding them of the worst-case consequences associated with going beyond these parameters, and (3) providing a ready reference for actions to take when parameters are exceeded. Limits tables, therefore, are important training tools. Exceeding one flow rate may have minor consequences but exceeding a different flow rate could lead to destruction of the plant. Knowing these differences and how to respond to these deviations are fundamental to safe design, operation and maintenance of the plant.

Many companies refer to "safe operating limits" (SOLs), which also can lead to confusion because the OSHA regulation refers only to safe limits and operating limits. SOL implies that safety, rather than other considerations, determined the operating limits. However, SOLs should not necessarily be equated to safe limits. Auditors should understand company intent and practice relative to the OSHA PSM regulation to determine if requirements are being met.

REQUIREMENTS/BACKGROUND

The OSHA PSM requirements for operating limits and safe limits appear in OSHA 29 CFR 1910:119. OSHA provides additional guidance in its "Petroleum Refinery Process Safety Management National Emphasis Program" [3] and "Process Safety Management Supplement B, Voluntary Protection Program" [4]. EPA mandates basically the same requirements in its RMP rule.

Two basic approaches exist for meeting these requirements:

1. Implementing the PSI and OP requirements separately, with the PSI safe limits tables providing the basic process variables to be addressed in the operating limits tables in the OPs (Figure 1); or
2. Combining the PSI and OP requirements into limits tables in the OPs (Figure 2).

Both approaches are valid for meeting the regulatory requirements — and both have pluses as well as minuses if not implemented and maintained appropriately. For example, combined tables help reduce discrepancies that could develop over time in separate tables as process equipment changes occur.

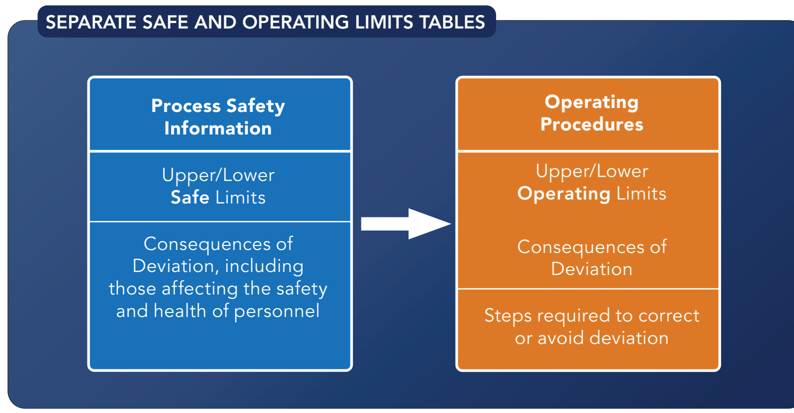


Figure 1. Creating distinct tables can avoid confusion about the type of limit.

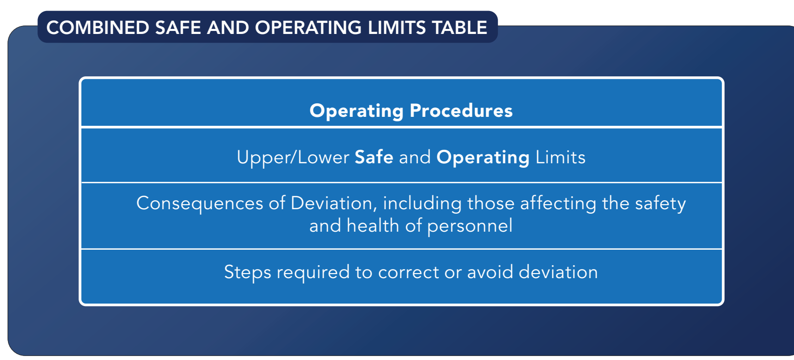


Figure 2. A table containing both kinds of limits can reduce the chance of discrepancies arising over time.

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EXAMPLE OF OPERATING/SAFE LIMITS TABLE

Instrument Tag	Parameter (Process Variable)	Normal Operating Limits	Consequences of Deviation (exceed Normal Limits)	Corrective Action (Troubleshooting)	Interlocks	Safe Limits Do Not Exceed	Consequences of Deviation (exceed Safe Limits)	Corrective Action (exceed Safe Limits)
TC-1700	XX-201 Temperature	Max: 95°C Min: 85°C	Max: Poor yield and increased side reactions; begin to approach runaway reaction. Min: Loss of reaction and lower peroxide concentration in oxidizer; operability/quality issues.	• Reduce air flow to oxidizer. • Increase water flow to circulation cooler.	TC-1700 will activate and: 1. shut off the air to the oxidizer and 2. open water valves to circulation coolers 100% if reading is above 105°C.	Max: 120°C Min: N/A	High temperature leads to runaway reaction. Temperature increases quickly, resulting in a release of gas that may cause a fire/explosion hazard to personnel.	• Shut off air to oxidizer. • Open cooling water valve to circulation coolers to 100%. Divert additional cooling water if needed. • Refer to procedure XX "Response to High Temperature in an Oxidizer" for further steps.
AI-1703A AI-1703B	XX-201 Offgas Oxygen Percentage	Max: 9% Min: 4%	Max: Approach explosive atmosphere in the oxidizer. Min: Poor yield and increased side reactions.	Increase temperature to the oxidizer by 1. reducing water flow to the circulation cooler, 2. increasing steam flow to the pre-heater, or 3. putting steam on the circulation cooler.	AI-1703A/B will activate and shut off the air to the oxidizer if reading above 15%.	Max: 20% Min: N/A	Explosive atmosphere is present in the oxidizer, resulting in a fire/explosion hazard to personnel if an ignition source is present.	• Shut off air to the oxidizer. • Open nitrogen valve to the oxidizer vapor space. • Increase oxidizer temperature before putting air back on the oxidizer.

Table 1. Clearly differentiating between normal operating limits and safe limits is essential

FINDINGS FLAG DIVERSE FAILINGS

Process safety management audits often identify important issues that need addressing. The failings that commonly appear fall into several categories. This article, the first in a series, focuses on operating and safe limits. Future articles will cover shortcomings in operating procedures, training and safe work practices; mechanical integrity issues; and problems in other elements.

ZONES OF OPERATION

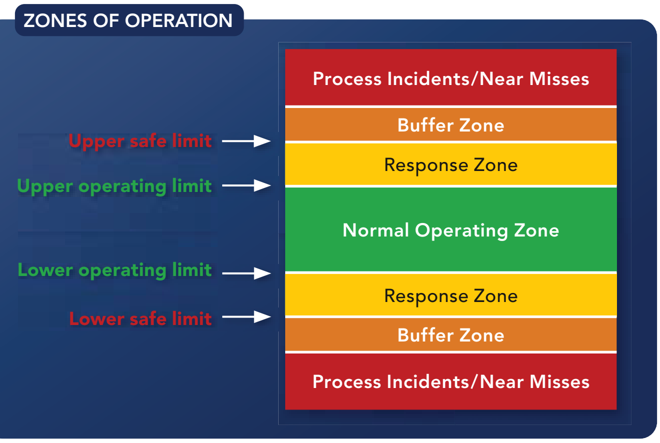

Figure 3. Most processes have a normal operating range with various limits addressing excursions.

Combined tables also undergo periodic scrutiny as part of OP reviews to confirm they are current and accurate; therefore, they frequently are part of refresher training activities. However, improper design and implementation of combined tables can lead to confusion around whether limits are safe limits, operating limits or something else (e.g., control system alarm points). Table 1 shows an example combined limits table.

Figure 3 provides a typical way of thinking of limits. Most processes will have a normal operating zone, such as a temperature range from 100–120°C, based on safety, quality and other operability considerations. This range is used to define the desired upper and lower operating limits. Deviations above or below the operating limits will result in troubleshooting activities by operators and/or automatic response by the control system to return to normal conditions. Usually a response zone is defined before safe limits are exceeded, although the available response time may be very short. In some cases, a buffer zone may exist above the safe limits before worst-case consequences can occur. However, in many cases, the safe limit defines the point where undesirable safety consequences are possible without a buffer. Figure 4 shows these limits and the activation points for possible process safeguards for pressure in a reactor due to a runaway reaction, based on layers of protection as evaluated in a process hazard analysis (PHA).

COMMON AUDIT ISSUES

While the limits table requirements, as shown in Figures 1 and 2, seem relatively straightforward, large processes may need to document literally hundreds of limits. Critical variables may include temperature, pressure, flow rates, levels and many other variables for each piece of process equipment. Developing this information can be a challenge, especially for older processes, due to limited availability of the PSI. With multiple requirements for developing, documenting and maintaining limits, it is not surprising that process safety audits often identify compliance or improvement opportunities related to limits tables. In addition, changing equipment design or regulatory direction may raise issues not found in previous audits.

So, let's now look at five common issues with operating/safe limits observed in PSM compliance audits:

1. Separate operating and safe upper/lower limits are not provided. The OSHA regulation and good industry practice clearly require/expect each covered process to have two separate sets of limits:

- Operating limits, defining the boundaries outside of which a system upset or abnormal operating condition could occur; and
- Safe limits, representing the design safe upper and lower limits of the equipment or process, above or below which operation is considered unsafe.

However, some facilities still:

- Establish only one set of documented "limits" rather than two sets; it often is not clear whether they are operating or safe limits.
- Specify operating limits in tables in the OPs but do not include safe limits in these OP tables or in separate tables as part of the PSI. The reverse of this (i.e., establishing safe limits in tables in the PSI but not operating limits in tables in the OPs) occurs less commonly.
- Reference the alarm/interlock settings in the distributed control system (DCS) and the pressure safety valve (PSV) settings as providing the operating/safe limits.

The first and second instances clearly do not comply with the regulations because they do not provide both sets of required limits. In the third instance, many DCS alarm settings are not established for safety reasons but for quality or operability purposes. Therefore, defaulting to the DCS parameters may indicate the requirements of operating limits are not well understood. In some cases, safe limits also may appear in the tables but be difficult to distinguish from quality, environmental and other limits.

Guidance: Ensure (1) both operating and safe limits are provided in the PSI, OPs or combined tables, and (2) the limits documentation addresses, as applicable, the different zones of operation shown in Figure 3. Also, avoid imprecise terminology when possible.

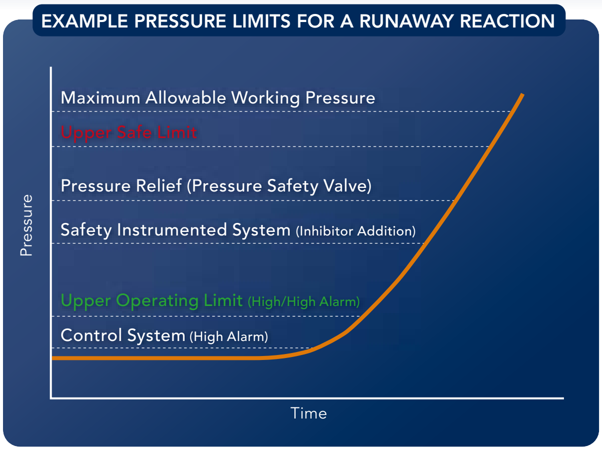

Figure 4. This chart is a modified version of one in "Process Safety: Key Concepts and Practical Approaches" [5].

2. All pertinent operating/safe limits are not addressed. In some cases, inspection of the limits tables may suggest certain critical variables are missing (e.g., temperature in a reactor), leading to additional discussion with site personnel to understand (1) how the limits tables were developed and (2) why, in the case of high temperature in a reactor, the particular limits have not been established. Operating/safe limit tables for all the pertinent process parameters can be effectively evaluated (as time permits) by comparing the limits tables data to the current PHA for the process and other PSI documentation. This can be done by:

- Reviewing the PHA report worksheets for parameter deviations leading to potential hazardous events (e.g., loss of containment) that are not addressed in the operating/safe limits. For example, if high flow or high level in a hazard and operability (HAZOP) table is shown to lead to hazardous events in the PHA, then it would be reasonable that limits for these variables should appear in the limits tables. Note: PHAs typically do not provide the actual limits. Use the PSI to find this information.
- Checking listed safeguards in the PHA (e.g., alarms, interlocks and PSVs) or a separate safeguards table (if available) to determine if the operating/safe limits table includes the associated process parameters. If a high flow alarm or PSV appears as a safeguard, then it would be reasonable for the limits table to contain limits for flow or pressure.
- Scrutinizing PSI documentation (e.g., process and instrumentation diagrams and equipment design files) for specific equipment to see if the limits table correctly lists design limits.

A review of PHAs and other PSI documentation may show the operating/safe limits tables lack a significant number of pertinent process parameters. This situation often develops because the operations and engineering personnel developing/updating the limits tables perform this work independently, without ever looking at the operating/safe limits through the "lens" of the PHA reports or PSI documentation. Audits also provide an opportunity to review the "reasonableness" of the limits. For instance, if the limits table lists a high pressure safe limit of 100 psig while the PSI or PHA shows the related PSV setpoint as 150 psig, a further discussion to understand the difference is warranted.

Guidance: (1) Review PHAs and other PSI documents to ensure the limits table contains appropriate process variables and values appear correct, (2) clearly address both upper and lower limits and note as "not applicable" where no high/low limit exists, and (3) check relevant process change documentation to see if limits tables have been updated as needed.

3. Consequences of deviation are not clearly documented. The impact of exceeding both operating and safe limits must be documented. For operating limits, a simple description such as "process upset" or something similar often appears — but this does not adequately describe the possible consequences. The PSI element also requires the consequences of deviation from safe limits include those "affecting the safety and health of employees," which often is not addressed as part of the consequences. Fundamentally, all these consequences should (1) be consistent, (2) appear in the PHA worksheets, and (3) describe potential safety and health impacts on personnel, as well as effects on processes and equipment. For example, the PHA and safe limits table for high pressure in a reactor might indicate overpressure leading to loss of containment and potential toxic exposure to a specific chemical(s) or fire/explosion hazards.

Audits of consequences of deviation often find:

- Worst-case consequences are not adequately addressed (no column provided or left blank).
- Consequences are worded "leading to a high pressure interlock" or "lifting the PSV" rather than providing the potential worst-case consequence of overpressuring a vessel and loss of containment. Note that activation of a PSV also may result in a hazardous release at the discharge point.
- No mention is made of the safety and health effects on personnel, such as potential toxic exposure resulting from the release of a hazardous chemical.

- Safety consequences are mixed with operability/quality/environmental consequences.

Guidance: (1) Review PHAs to ensure proper documentation of the consequences of deviation outside the safe limits, including possible worst cases and potential safety and health effects on personnel, and (2) clearly distinguish between operating/safe limits and quality, environmental and other limits.

4. Corrective actions are not detailed adequately. OPs must include the steps required to avoid or correct deviation from operating limits. However, this information is not always provided or corrective actions are given for only some operating limits or with varying degrees of clarity. Although the regulation does not specifically require the documentation of corrective actions for deviations from safe upper/lower limits, OSHA's guidance indicates that "emergency shutdown" should be a final corrective action. Obviously, the steps to correct a deviation outside operating limits will help prevent upset situations or going beyond safe limits but the necessary actions likely will differ as a potential deviation approaches or exceeds documented safe limits. For example, operators typically are encouraged to safely shut down a process — even before it reaches an interlock/trip point or safe limit — when in doubt about continued safe operation.

Guidance: Review PHAs, OPs, emergency procedures and other documents as needed to ensure clear guidance is provided on corrective actions for deviations outside both operating and safe limits.

5. Process safeguard setpoints are not included. It is a best practice to detail at what point various process safeguards will activate because this helps operators handle process deviations. What alarms and interlocks are provided and when will they activate? What are the setpoints for pressure relief? This information may be included in the DCS, in the OPs, in training materials or PSI documents. Consider adding this information to the limits tables so an operator immediately can put them in context with the defined limits listed in the table. For example, Figure 4 shows a chart that details several safeguards for high pressure in a reactor to activate as the upper safe limit is approached. Knowledge of these setpoints as operators respond to process deviations is important, both so the operators can anticipate safeguard action and can respond appropriately if the safeguard fails to activate as expected.

Guidance: Consider including process safeguard setpoints, as appropriate, in the limits tables.

AVOID COMMON ISSUES

Well-documented operating and safe limits are an important foundation for safely and reliably operating processes containing highly hazardous chemicals. So, process safety regulations and industry best practices require clear documentation in OPs and PSI of limits, consequences of deviation, and corrective actions. Unfortunately, process safety audits continue to find poor understanding and ineffective implementation of these requirements.

Hopefully, the information provided here will help you better evaluate and improve your operating/safe limits documentation before you receive a regulatory citation or compliance audit finding.

As already noted, future articles will cover other common findings. ●

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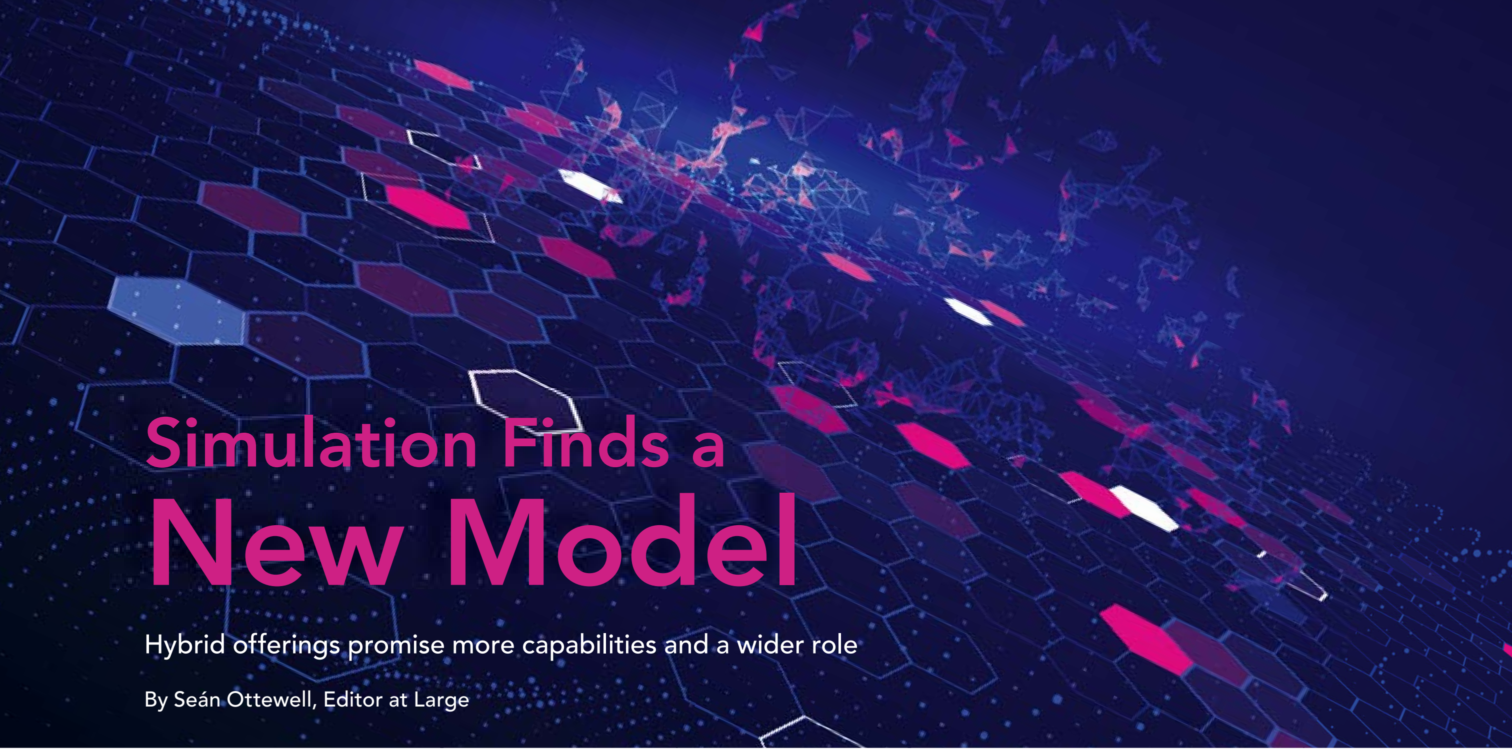

Simulation Finds a New Model

Hybrid offerings promise more capabilities and a wider role

By Seán Ottewell, Editor at Large

POWERFUL DATA analytics such as artificial intelligence (AI) and machine learning (ML) are profoundly affecting the development of process simulation technologies. However, vendors including KBC Advanced Technologies, Walton-on-Thames, U.K., and Aspen Technology, Bedford, Mass., are finding that lots of users don't fully appreciate how simulation is evolving.

A recent KBC user webinar looking at the evolution of process simulation pointed up the disparity. For example, when asked if simulation technology has kept up with advances in software and information technology (IT) technology, nearly 56% of attendees said it hadn't.

"I voted no, too," admits the webinar's host, Andy Howell, KBC's executive vice president, technology.

"I don't think any of the simulation vendors have done enough in the last ten years. It's definitely time to take more notice of third-party solutions such as block-chain, automation and cloud-based technologies, etc. I think that with the advances in data science such as AI and ML rather than just computer science we are on the threshold of a second wave of innovation in process simulation. KBC has been at the forefront of the first wave in thermodynamic computation and intends to be front and center in the second," he notes.

However, Howell is keen to point out that process simulation isn't obsolete — not least because data analytics technologies still have severe limitations with the nonlinear systems that make up many chemical processes.

"The future will be a sensible combination of these things, a hybridization aimed at real world problems [Figure 1]," he adds.

Another poll during the webinar found that half of attendees feel the biggest challenge for process simulation today is integration into other systems. Finding and accessing the data needed for a model came second, with 35% of the vote.

"The integration result was a little bit of a surprise as vendors have made great strides in this area. However, it's a wake-up call to any simulation vendors who think they can do everything. They can't and should never think that they can. Using third-party technologies in cloud-based systems allows users to mix and match simulators and the many add-on analytic tools available today in the way they want," emphasizes Howell.

Figure 1. Simulation increasingly will combine computer science and data analytic technologies to solve real-world problems. *Source: KBC.*

THIRD-PARTY BENEFITS

KBC itself has long associations with many third-party technology providers, the most recent a partnership announced in February giving Petro-SIM users access to the rigorous gas/liquid separation modeling supplied by MySep, Midview City, Singapore.

It's a relationship designed to improve separation expertise at oil companies and engineering/procurement/construction (EPC) contractors, both of which suffer from many disparate and unvalidated design engineering practices for vessels and separation internals.

"Poor separator design causes excessive carryover of liquid from separation vessels resulting in rapid or progressive damage to downstream compressors, contactors, and other pre-treatment facilities. This leads to extended and/or unplanned shutdowns causing operational losses," notes Russell Byfield, KBC global simulation business leader.

KBC also is seeking tie-ups covering a raft of other modeling technologies, including electrolytes, environmental emissions, energy management, bioreactor diesel and synthetic ethanol — so-called e-fuels.

Almost 40% of webinar attendees cited self-tuning as the most important issue for process simulation in the future — well ahead of self-building and closed loop automation. This doesn't surprise Howell at all.

It's one of the reasons KBC parent company Yokogawa, Tokyo, recently signed a partnering deal with enterprise AI developer C3AI, Redwood City, Calif.

"It puts their AI Suite capability into Petro-SIM, giving it the ability to self-tune using whatever quality of data is present in a facility. Ultimately, self-build models will follow on from this," explains Howell.

The company is pursuing two case studies using this technology, one being the tuning of reactor catalysts in refining.

"It's almost folklore how difficult it is to take reactor data, tune it to the reactor model and then be able to predict the operation of the catalyst under current and future conditions with different oils and loads. It's the first time we've really auto-tuned the model... in a reactor/catalyst environment — which is probably one of the most complex situations we get in processing," he notes.

KBC is using the technology in a pilot with several oil companies who have had problems with reactor operations. The challenge for KBC is to find the inherent issues causing these difficulties in an automated way, before they even appear.

"The pilot's been running for about eight months now and it's looking very good. It's due to conclude perhaps in November or December and after that we will be looking to release a commercial product as a bolt-on to our existing simulator," says Howell.

The second case study involves simulations of crude pre-heat trains; one goal is determining which heat exchangers need cleaning first: "So we're doing the hardest units first, with the aim eventually of applying these simulations to a refinery-wide model and ultimately replacing — or supplementing — the LP [refinery linear program] model."

KBC's overall goal is to provide a platform with a petrochemical-wide application, with plug-ins for niche applications from other vendors. Its vision includes cloud-agnostic building blocks, sets of integrated event-based work and data flows, time-series data storage, and use of AI tools to aid model management and updates. It must be self-building, self-sustaining and ultimately in a 3D game style — like Minecraft, declares Howell.

"The digital twin is one step along the way to what I think will be a digital triplet: data analytics and process simulation

THREE MODELS

Model	Approach	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.	• 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.	• Refinery-wide or chemical-plant-wide models • Planning model updating • Fast-solving online models to predict best/worst-case schedules for cleaning • Deployment of process train models online • Advanced-process-control 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.	• Batch unit modeling • Bioprocess modeling • Modeling complex units

Table 1. The target uses of the models differ. *Source: AspenTech.*

connected into a seamless, VR [virtual reality]-type environment. It's that hybridization that will drive the assets of the future," Howell concludes.

NOT FOR DATA SCIENTISTS

AspenTech also is focused on technology hybridization. It recently launched the third of three tools in the Hybrid Models family. These specifically are designed for use by process and plant engineers to rapidly turn plant and simulation data into AI-based ML models without requiring any data science understanding.

They combine first-principles physio-chemical knowledge with AI-based empirical models and intuitive, automated workflows to deploy as operational applications (Table 1).

The company piloted Hybrid Models with 96 companies, including 34 chemical and specialty chemical manufacturers and four with integrated energy and petrochemicals operations.

"The chemicals companies involved were diverse in size and products. We had 15 out of the top 20 largest chemical producers worldwide. We also had representation from global chemical companies, as well as regional players in the U.S., Latin America, Europe, Middle East, Africa, and Asia," says Gerardo Munoz, product marketing manager, engineering. "We received very good feedback," he adds.

"Aspen Hybrid Models are a major advance in the field of chemical engineering. Hybrid models are a major step forward in bringing together AspenTech's process models and machine learning and are a game changer in process engineering and plant improvement," says Karuna Potdar, vice president, technology center of excellence, Reliance Industries, Mumbai, India.

"Using the hybrid model, we were able to create a model that can reproduce real plant data more accurately than the conventional reformer model. We were able to create a highly accurate model in a short period of time," comments Takuto Nakai, who is in the production department of Nissan Chemical, Tokyo.

A third chemical company described the models as a step in the right direction for mission-critical process units, while two others praised the ease and simplicity of the workflows and their excellent diagnostics and analysis capabilities.

More detailed facts and figures about the three Hybrid Models emerged during AspenTech's Optimize 21 virtual user conference in May. Nissan Chemical estimated it decreased steam use by up to 1% in ammonia plants by accurately calibrating reactor kinetics and temperature profiles using models that were created in half the time of a conventional model. Dow reduced the iterations/time for convergence in simulation models by 36% using Hybrid Models as surrogate models to initialize larger simulations. Sabic obtained useful insights on how to improve final product quality after accurately predicting impurity concentration in a distillation process.

Other examples cited by Munoz include:

- a leading European refiner addressed an issue with heat exchanger fouling that was costing $1 million/yr;
- a refining and petrochemical company in the Middle East updated planning models in half the time and estimated gains of 11.3¢/bbl from improved planning model accuracy;
- Lummus Technology reduced time in design and optimization of a gas processing plant by 50%; and
- an engineering consulting company in North America that focuses on oil and gas is using one of the models to optimize an upstream asset, estimating a net present value increase of 8%.

"There is a lot of excitement, and we are looking forward to seeing the benefits as they are being adopted for different use cases. There has been very positive feedback on first-principles-driven Hybrid Models in chemicals, as this modeling technology can be very useful to tune kinetics of reactor models and represent real behavior — for example, real mixing — without having to do a lot of manual tuning. The most positive feedback from users is that this can be done within software with which they are already familiar such as Aspen Plus and Aspen HYSYS, making it very easy for them to use," states Munoz.

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Users have offered inputs on desired enhancements to the hybrids; most feedback focused on usability and how the process could be improved to facilitate the creation of simulation models.

"Some of the feedback and use cases identified by our customers were related to how to use these models to solve key issues in chemicals. The most common cases were modeling key polymer properties, waste reduction and improved product quality, and model creation for special processes such as aromatic upgrading units," adds Munoz.

Like KBC, AspenTech also is forging links with third-party suppliers. The most recent tie-up is with Larsen & Toubro Infotech (LTI), Mumbai. LTI's cloud-managed services will allow access of AspenTech's performance engineering desktop technologies via the cloud.

In addition, AspenTech has bought some companies, for example, industrial analytics and asset optimization specialist Camo Analytics, Oslo, Norway. The company's Unscrambler suite mines big data stores to improve quality and efficiency of output in the pharmaceutical and biotech industries.

Another acquisition was OptiPlant, Walnut Creek, Calif. Its technology focuses on helping EPCs to increase agility and speed of conceptual and front-end engineering design development, dramatically reducing the engineering effort involved. AI-driven 3D conceptual plant layout with parametric asset models and automatic pipe routing enables closer collaboration between owner-operators and EPCs to improve accuracy, reliability and speed of cost estimates from the earliest project stages.

"OptiPlant and Camo can be complementary to Hybrid Models because their focus is different. For example, Aspen Unscrambler from Camo and Aspen ProMV can be used in combination with Aspen Hybrid models. They can be used to analyze the data and identify which are the most relevant variables in a process — then select the data used to create the hybrid model and make the process easier and the model more accurate," concludes Munoz. ●

SUCCEED AT WATER STEWARDSHIP

Using a sensible strategy along with online tools and resources can improve results

By Emilio Tenuta, Ecolab

FOR DECADES, the Dow plant in Tarragona, Spain, withdrew freshwater for its cooling towers from the Ebro, one of the country's most important rivers (Figure 1). However, as economic and population growth raised demand for the Ebro's water, leaders at the Dow plant set an ambitious goal: free up freshwater for other users by operating the facility's cooling towers with as much as 90% reclaimed municipal water.

After ensuring the cooling towers could operate efficiently with treated wastewater, the plant was able to cut its withdrawal by 19%. The drop varies with season but, overall, the plant saves 278 million gal/yr of river water, equivalent to the average daily water use of 25,157 citizens.

The Dow Tarragona plant is not alone in its ambition to reduce freshwater dependence. Increasingly, manufacturers across all sectors, including water-thirsty chemical processors, recognize the urgency to act. They may have seen the latest projection from the World Resources Institute (WRI, www.wri.org), Washington, D.C., of a 56% global shortfall in freshwater supply within the decade or "A Wave of Change — The role of companies in building a water-secure world," the recently released water report from CDP, London, that stresses the need for ambitious action by industry. (For details on the latter, see: "Report Dives into Water Security, https://bit.ly/3Dog46q.) And they may have experienced water scarcity, whether caused by overusing water, a changing climate or increasing pollution. Whatever the reason, a growing number of companies are setting ambitious internal water-conservation goals.

That's good news. Changes in how industry uses water could enormously impact our world's water crisis: on average, industry uses 20% of the freshwater consumed globally and almost 60% in developed countries. However, despite their good intentions and initial efforts, companies worldwide and in the U.S. actually increased their demand for water by 20% between 2015 and 2018. Industry, if it is to do its part to close the projected 2030 supply/demand gap, will need to do much more.

It's not that companies lack the will. In a January 2021 survey of businesses with revenues of $1 billion or more conducted by Ecolab and GreenBiz, 92% — up from 88% in 2019 — said they are likely to take steps to better manage water in the next two years. However, the survey identified a quandary that often stymies water management improvements: corporate leaders typically set water reduction targets but facility managers are made responsible for meeting them. Yet, the plant manager's ability to improve water management often hinges on building a solid business case for corporate investment in individual water projects. Creating the business case is difficult, though, because water typically is underpriced — the plant's water bill does not reflect water's true economic value to operations. Further complicating such situations, facility leaders often lack the methodologies, tools and expertise to make the financial case for water management improvements or to meet water reduction targets.

Would taking a more holistic approach to water management — one that accounts for a range of factors, including the full value of water, opportunities for water saving within the plant, and watershed demand, supply and quality — help companies attain water reduction goals and build resilience to weather unpredictable water challenges ahead?

A growing number of manufacturers — including some chemical processors — are testing such an approach, variously called a "water stewardship" or "water management" strategy. Comprehensive in nature, it marks a major shift from simply managing water to satisfy environmental

SPANISH SUCCESS STORY

Figure 1. Ebro River now provides far less water to Dow plant and others at the Tarragona Petrochemical Complex.

POWERFUL RESOURCE

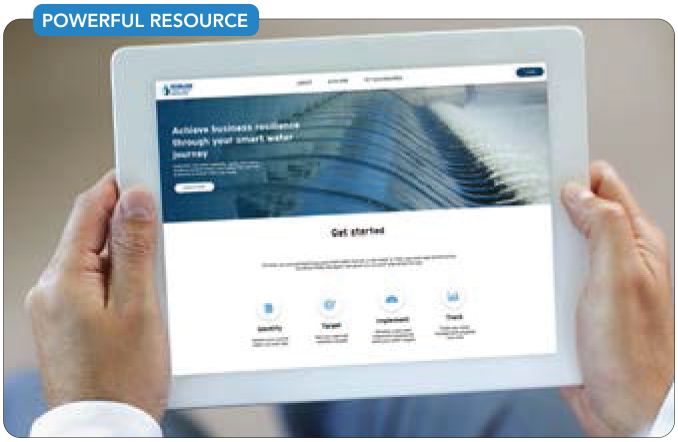

Figure 2. This publicly available online tool focuses on the four key aspects of water stewardship and enables site-specific calculation of risk.

regulations or achieve reduction targets. True water stewardship involves lowering water use internally and collaborating with other water basin stakeholders to ensure water is available to meet all needs and support vital ecosystems. It also involves encouraging effective water management across supply chains, which, when successful, can significantly lower the total corporate water footprint. (For a broader look at chemical makers' sustainability efforts across their supply chains, see: "Sustainability Efforts Link Supply Chain," https://bit.ly/3Bc9AG7.)

The economics clearly demonstrate why companies should adopt an effective water stewardship strategy. In its "Global Water Report 2020," https://bit.ly/2WuapL9, CDP, www.cdp.net, a nonprofit group to which companies disclose greenhouse gas emissions, water usage and other environmental data, estimated that the manufacturing sector potentially could lose up to $191 billion in business by not addressing water risks, while taking action to avert the risks would cost $2.9 billion. In other words, not acting could be 66 times more costly than acting.

A FRAMEWORK FOR STEWARDSHIP

Both corporate sustainability leaders and facility-level managers have important roles to play in developing and executing a water stewardship strategy.

At the corporate level, successfully implementing a water stewardship strategy requires sustainability leaders to set policy and priority — and provide local support. They must:

- Elevate water on the corporate agenda by ensuring the true risks of water scarcity are appreciated and prioritized, building broad awareness of water-related risks and making saving water part of "the way we do things around here."
- Prioritize water initiatives and investments at facilities across the enterprise. Establishing proper priorities requires understanding the true financial impact of water-related risks to the business: "What would it cost the operation if water were rationed? If prices skyrocketed? If quality drastically deteriorated?" Realistic answers cannot come from relying on the water bill to determine these costs: in most places, water is underpriced and does not reflect water's risk-adjusted value.

Publicly available online tools, such as the Water Risk Monetizer feature found in Ecolab's Smart Water Navigator, www.smartwaternavigator.com (Figure 2), can help calculate the potential financial impact of declining water quantity and quality at specific plant locations. That tool — developed by Ecolab, a global leader in water technologies and services; S&P Global Trucost, a top firm in environmental data and risk analysis; and Microsoft, a major force in cloud computing technology — uses widely respected data sources such as the Aqueduct Risk Atlas of the WRI, https://bit.ly/3mz0dw7, and the Water Risk Filter of the World Wildlife Fund (WWF), https://waterriskfilter.panda.org/. Other data partners and advisors include the CEO Water Mandate of the United Nations (U.N.) Global Compact/Pacific Institute, https://ceowatermandate.org, and the Alliance for Water Stewardship (AWS), https://a4ws.org.

To arrive at the true costs of water risks, the tool uses the latest and most-comprehensive local water basin data sets as well as advanced scientific

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methodologies. The tool's calculations also can help compare water-use efficiency across sites and against industry averages — information helpful in prioritizing initiatives and investments.

- Support facility leaders in developing and executing local water stewardship plans. This includes providing them with a roadmap, tools and motivation to achieve water goals within their facilities — and to connect with other stakeholders in their watersheds.
- Build broad community awareness of, and credibility in, the water stewardship efforts by aligning water reduction efforts with the recommendations of respected global environmental standards organizations, such as the Global Reporting Initiative (GRI), www.globalreporting.org; Sustainability Accounting Standards Board (SASB), www.sasb.org; and CDP, previously known as the Carbon Disclosure Project.

SETTING A LOCAL STRATEGY

At the plant level, leaders can develop and execute a tailored water stewardship strategy aimed at achieving water resilience for both the business and the local community. The following four steps — performable within Ecolab's Smart Water Navigator tool — can serve as a guide for action:

1. Identify how water is being used and calculate its full value to plant operations.

- Start the water stewardship journey by benchmarking how efficiently the facility uses water against industry and organizational standards. A good way to benchmark is by completing the 13-question Water Action Assessment within the Ecolab Smart Water Navigator tool. Responses to the assessment will place the facility in one of four categories on a "water maturity" curve:

  Untapped — Focus is on compliance; smart water management practices are not yet adopted.

  Linear — Water conservation is a primary focus; water reduction pilots are in place.

  Exploratory — Water conservation is mastered; internal piloting of recycling and reuse is underway; outreach to other watershed stakeholders is beginning.

  Water smart — Water is reused and recycled internally; the many needs for water within the watershed are understood.

  Once the plant is placed on the water maturity curve, facility leaders can tap into the Smart Water Navigator's detailed checklists, resources, and business case background, designed expressly for the chemical industry. They also can find guidance on practical, actionable recommendations for advancing the facility to the next level of water maturity.
- Calculate the gap between the true costs of possible water scarcity, poor quality, rationing and other risks and the price the plant currently pays for water. A clear understanding of the potential financial impact of water risks

helps prioritize projects and strengthens the business case for funding water-saving projects.

2. Set sustainable water withdrawal targets. Water quantity and quality vary from place to place, so withdrawal targets should take into account local water conditions and water needs across the watershed. The Water Risk Monetizer contains data sets on local water conditions to establish meaningful sustainable targets.

3. Develop a plan to achieve withdrawal targets — and take actions to attain the next level of water maturity. This involves identifying opportunities to recycle and reuse water within the facility, then applying advanced treatments and technologies to ensure recycled water achieves the level of quality needed for its next use. It also should include regular evaluations of progress toward water reduction goals as well as the return on investment (ROI) of capital expenditures for water projects, basing calculations on the full value of water, not the local water price. ROI data could support the case for further investments in water efficiency initiatives.

4. Monitor and report water stewardship results. Water stewardship is a journey requiring continuous checking, detailing and resetting to next-level targets. So, it is essential to chart water management performance over time to show variations in incoming, outgoing and calculated consumptive water use over multiple years. Presenting the data in easy-to-grasp graphic formats will help quickly convey the interdependencies among production volume, revenue and water use. Finally, reporting water reduction results to the community will build confidence among other water basin stakeholders in the facility's commitment.

COLLABORATE "BEYOND THE FENCE"

Both corporate and site-level managers are responsible for reaching out to other stakeholders in the watershed to drive community-wide engagement — a key aspect of comprehensive water stewardship. Collective action involving business, government, residents and other water basin users is critical to understanding water needs and establishing governance, policy and best practices that will ensure continued water availability. One company alone cannot solve all watershed issues. However, one company can take the lead in building relationships leading to a successful collaborative effort dedicated to "derisking" the watershed.

For example, the Dow Tarragona facility is part of the large Tarragona Petrochemical Complex that includes plants of many chemical manufacturers. Together, these firms are engaged in a project to use reclaimed water for industrial purposes to free up freshwater for local municipal demand and reduce stress on the Ebro River.

A number of organizations provide guidance in organizing community-driven collaborative water stewardship. Among them are:

- AWS, whose International Water Stewardship Standard provides a globally consistent and locally adaptable framework designed to encourage collective approaches to sustainable freshwater use.
- The Water Resilience Coalition, https://bit.ly/3lieGuc, an initiative of the U.N. Global Compact's CEO Water Mandate, which is working to raise corporate awareness of global water stress and preserve freshwater resources through collective action.
- The CEO Water Mandate's free online Water Action Hub, https://wateractionhub.org, which is a global online collaboration and knowledge-sharing platform for water sustainability. It helps companies and other organizations address water risk and advance sustainable water management by raising awareness of water projects around the world and the organizations administering them, and fostering proposals for new projects and partnerships. The hub helps companies connect with relevant water partners and share good water management practices and lessons learned. Many of the site's features complement those available in the Ecolab Smart Water Navigator.

TAKE ACTION NOW

Predicting when, where or how severely water issues will impact operations may be impossible. But given WRI's projection of a global shortfall in freshwater by 2030, we can safely predict that water issues increasingly will challenge chemical and other manufacturers. Implementing a comprehensive water stewardship strategy, one based on water's full value to operations, can help chemical processors build the resilience they are sure to require in the face of water challenges, predicted and unpredicted. ●

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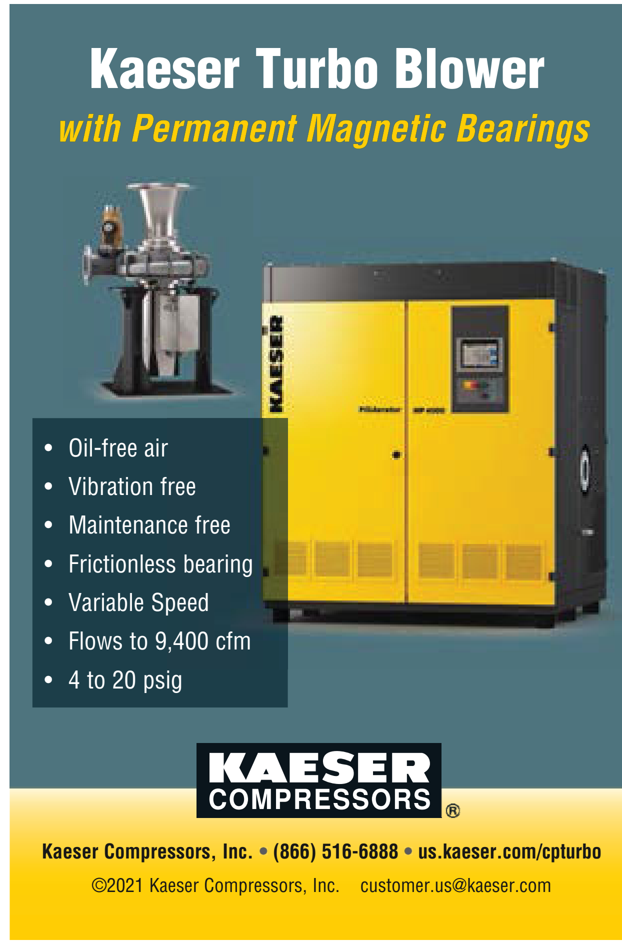

PICK THE PROPER POSITIONER

THE NECESSARY LEVEL OF COMMUNICATION IS AN IMPORTANT FACTOR

By Peter Jessee and Dave Fahlgren, Valin Corp.

POSITIONER SELECTION deserves due diligence — and consideration of several factors before making any firm decision. There's certainly not a typical one-size-fits-all approach for positioners; an uninformed choice can lead to undesirable consequences. On the one hand, selecting a positioner with features that aren't helpful for a particular process likely will lead to spending more than necessary. On the other hand, a purchasing decision made solely on price may result in a positioner that either does a substandard job or needs replacing to perform a required function.

Many vendors categorize the positioners in their line as good, better and best. While that's helpful, it's not enough to pin down the optimum choice. Having a clear understanding of the requirements of a given process and the features of the positioners available will guide the best decision.

When going through the positioner selection process, you typically should focus on two key elements: control and communication. In other words, what precision do you need in controlling the valve, and how much feedback is necessary during the process?

As far as control, the main objective is to facilitate an environment where the valve performs at its very best for the given application. Several options exist depending on the nature of the process. A basic local loop may be well served by a pneumatic positioner, perhaps interfacing to the controller with a current/pressure (IP) transducer, or by an analog electro-pneumatic positioner. When you desire greater capabilities, consider one of the newer microprocessor-based positioners with advanced internal algorithms that can perform more-comprehensive tasks. For example, they can be tuned to maximize performance or adapt the tuning parameters to the loop as time goes on to improve the responsiveness of the valve.

However, although important, control isn't something that many operators need dwell upon. As the communication levels improve, there isn't much fear about inadequate control. In other words, if the communication is robust, the control level will be as well.

COMMUNICATION CONSIDERATIONS

Determining appropriate communication is much more nuanced. Originally, typical positioners relied on one-way communication; they would act on an analog (3–15-psi pneumatic or 4–20-mA electrical) signal from the controller. Smart positioners with digital communication capabilities started to appear in the 1980s and 1990s. Today, many positioners feature two-way communication: the device gets a signal from the control system about required valve position and also sends back digital information, e.g., actual valve position. Such a feedback signal can allow operators to determine whether the positioner is, in fact, following the system commands. Additionally, diagnostics became available with the smart positioner revolution. Now, plant staff can monitor the internal components of the positioner and even the external behavior of the valve to spot when the valve is behaving in an unexpected way. Some manufacturers offer multiple levels of diagnostics from which to choose.

You should strive for the optimum amount of communication needed for the process. With an under-specified communication level, you might not get notifications of potential problems or the valve might not operate as efficiently as possible. On the other hand, over-specifying the amount of desired communication could be a costly mistake. It doesn't make a great deal of sense to pay for technology that is either unnecessary or unutilized.

Basic analog pneumatic and electro-pneumatic positioners still can play a valuable role. The technology is reliable and mature — and performs the job it was designed to do very well. For example, many refineries rely on a large number of basic pneumatic positioners that simply take the 3–15-psi control signal from the controller and modulate the air pressure to the actuator. With no electrical components, the devices fit with the old refinery maxim "no wire, no fire." These and basic electro-pneumatic positioners may adequately handle what's needed under some circumstances; so, upgrading to more-advanced technology wouldn't offer the return on investment required to make such an upgrade feasible. Such positioners lack any kind of digital communication or microprocessor electronics and usually provide a basic level of accuracy and repeatability (0.5–1%).

A bit more capable are advanced electro-pneumatic positioners. These use an analog 4–20-mA input, similar to the basic device, but boast microprocessor-based electronics that allow easy configuration and tuning. However, these analog electro-pneumatic positioners still don't have any kind of diagnostics or digital communications. They do provide a good level of accuracy and repeatability (0.25–0.5%).

The next step up are HART positioners. Such devices come in two basic styles: with zero or just basic diagnostic capabilities; or advanced diagnostics. These positioners usually have a high level of accuracy and repeatability (0.1–0.25%).

HART devices have a digital communications capability thanks to a frequency-shift-key digital signal on top of the 4–20-mA signal going to the positioner. Thus, they are compatible with a 4–20-mA controller. HART positioners are designed to continuously communicate with a control system that has digital communication capability. In addition, someone in the field with a suitable handheld device can communicate with such a positioner to get certain diagnostic information or do an auto-calibration, even if the positioner isn't communicating with the control system digitally.

Smart HART positioners have the widest range of optional capabilities, including international electrical certifications, "fail freeze" functions that lock the valve in its last position on loss of communications or air pressure, explosion-proof or intrinsically safe construction, and others. One of the most common options available is a 4–20-mA position signal. A device with this option has two additional terminals that provide a 4–20-mA position signal connected to an analog input in the control system to give feedback to confirm the valve is moving to the commanded position.

With a digitally integrated control system, you don't need the extra analog input because that information is available in the digital data stream being communicated back and forth between the control system and the positioner.

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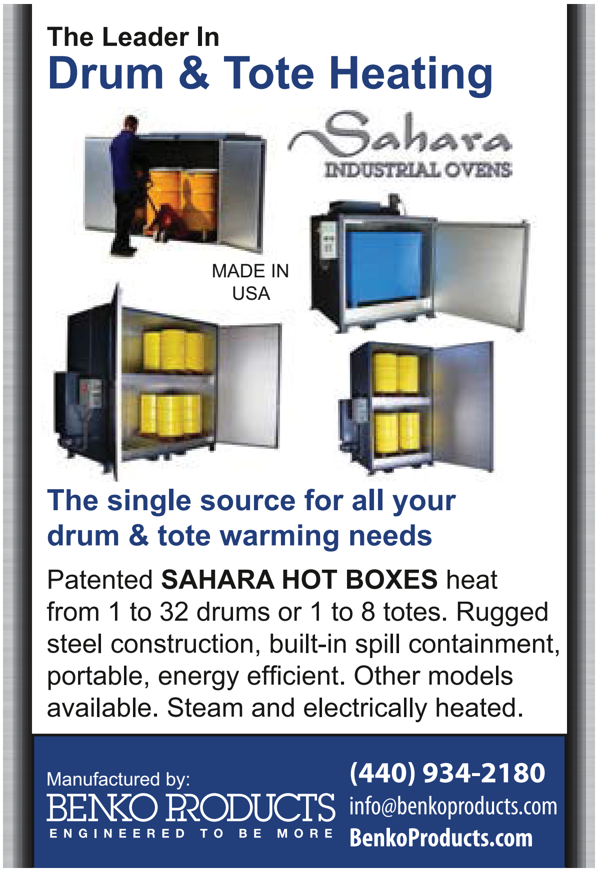
As mentioned earlier, suppliers offer differing levels of diagnostic capabilities in their positioners. Depending on the sensors and internal parts built into the positioner, you may be able to receive information such as the air pressure value, shaft position, housing temperature, etc. Having that digital feedback can foster achieving the best reliability in a control system because operators can determine when certain things of concern are happening. For example, has the air pressure gone away for a particular valve? Is the valve responding correctly? A valve that stops before it gets to the desired position could generate a software alarm that alerts the operator the valve isn't performing the intended way.

Taking this one step further, you can build diagnostic algorithms inside the positioner or control system that look at all the digital data and trigger an alarm if the



valve did not go all the way open. Maybe the valve or actuator has jammed. Maybe air pressure isn't adequate. Maybe some physical damage has occurred. Positioner diagnostics can warn the plant about any of these occurrences.

Keep in mind that optimal communication and diagnostic ability often can significantly impact the bottom line.

INFRASTRUCTURE ISSUES

Unfortunately, limitations due to infrastructure can impact options. For example, a plant may have a variety of different types and generations of input/output (IO) panels that connect to field devices. Sometimes in such cases, an IO panel is an earlier revision that can't talk to these field devices, precluding advanced communications. A variety of other issues also can affect a plant's ability to reach that desired communication level. For example, if the plant has a bunch of programmable logic controllers, as opposed to a distributed control system (DCS), they may lack full communication capabilities — and, thus, may not be able to support an advanced diagnostic system that allows for predictive maintenance.

Fortunately, positioners are available with diagnostic and data historian technology built right in. Thus, even if the control system can't support this capability, those positioners store the diagnostic data internally — which can be retrieved using a handheld device or laptop computer. So, a plant can do predictive maintenance without the expense of a seven-figure DCS system by using a predictive maintenance software application. Or it can upload these data to the control system once full communication capabilities are established, preserving potentially years of diagnostic data.)

The optimum positioner, of course, depends upon the given application. For example, a plant looking into doing more predictive maintenance should select positioners with the level of diagnostics to accurately predict when failures will happen in the equipment. At the same time, perhaps only five loops in the plant may really require the top-tier level of diagnostics. The rest don't need that level of diagnostics and never will use it, so paying for those capabilities makes no sense.

When determining the level of technology necessary, it's critical to understand the needs of the system and options available. Every process is a little different, which is why working with a professional who understands all the options available — after developing a deep understanding of a process' specific needs — is the ideal approach. ●

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Refinery Reduces Octane Giveaway

Teaming an online analyzer with next-generation APC markedly trims reformer output variability

By Mohamed Abokor, Shell Oil

THE SHELL Oil Deer Park refinery is in the middle of its digitalization and end-to-end optimization journey. One recent project focused on our catalytic reformer unit, which converts low-octane feed to a high-octane product called reformate and light hydrocarbons ranging from C_1 to C_{5+}.

In 2019, the site installed an online Raman analyzer on the reformer unit to reduce variability of reformate product octane. At the same time, we commissioned the Platform for Advanced Control and Estimation (PACE) — a next-generation advanced process control (APC) technology jointly developed by Shell and Yokogawa — to optimize the reformer product octane.

Before the installation of the online Raman analyzer and PACE controller, the unit was regulated manually, which required lots of moves from the board operators to keep product on-specification and within the reactors and heater constraints. Monitoring product quality involved sending a sample to the laboratory six hours after a reactor switch (a move necessary to allow catalyst regeneration) and then waiting three to six hours for the laboratory results. This meant the unit didn't reach the target octane until nine to 12 hours after the reactor switch, resulting in a 0.7 octane giveaway for a given target.

The new PACE application, in conjunction with the Raman analyzer, has compressed the decision cycle to two hours from nine, and reduced product variability by 71%, cutting octane giveaway to 0.2 from 0.7.

MODELING AND CONTROL DESIGN

The Deer Park refinery has used APC technology since the 1980s. When the Raman analyzer was installed, we decided to replace the legacy APC with PACE because of its unique

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features and added robustness. The reformer unit process is highly interactive and complex. PACE's modeling flexibility and customizable event logic were a perfect fit for this unit.

The reformer unit's four reactors and their associated heaters were modeled in PACE as one system using a concept called intermediate variables. The idea behind this concept is to create fast and accurate models that represent the process, i.e., a gray box model.

For instance, in modeling a heater and associated reactor, three independent inputs (heater-outlet-temperature controller setpoint, feed rate and feed temperature) were related to an intermediate variable (heater-outlet-temperature controller process variable).

The model accurately captures firing rate and feed impact on the reactor inlet temperature. The reformer reactor inlet temperature determines octane target and final product composition. The next step is to take the outlet temperature and scale it down (one-quarter each to the other three heaters). The last step is to capture and model all four reactors as a single system. This involves calculating another intermediate variable, the average temperature of all four reactors, which then is used to get RON octane.

Increasing the average temperature of the reactors by 1°F will result in a 0.3 octane rise. Board operators can easily understand this when they're analyzing PACE performance and predictions.

Furthermore, if the online Raman analyzer is in maintenance mode, operators now can use the calculated reactors' average temperature as a controlled variable by simply changing it from high and low constraint limits to a single setpoint. Previously, the unit was manually regulated by using average temperature and laboratory samples. The intermediate variable modeling is well suited for this application because fast and accurate models made the controller more robust with minimal deviation from the octane target.

The primary objective of the PACE controller is to keep octane to a given setpoint while balancing the heater and reactor temperature profile.

We set up heater deviation temperature modeling so that operations can adjust the heater and reactor loading profile. Typically, the first reactor runs at high temperature with the other reactors not quite as hot.

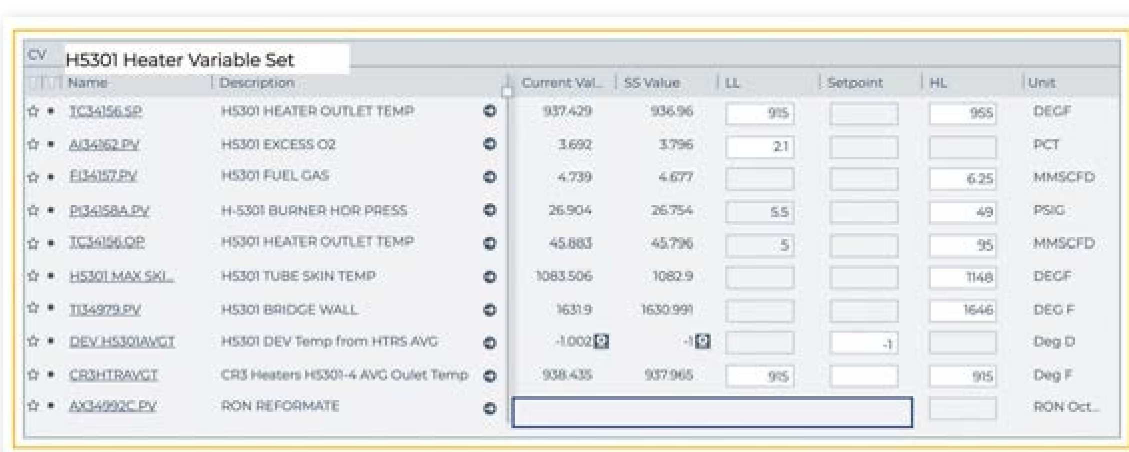
Because PACE enables users to customize the operator human-machine interface (HMI), we created a customized variable set so operators can easily access common and key variables that require frequent adjustments. This allows the operators to display most-used variables without switching back and forth between four reactor HMIs.

The operators decide which heater will be connected to the lead reactor by setting the desired heater deviation setpoint.

Various heater constraints, such as minimum oxygen and maximum burner pressure limitations, determine whether or not the controller can deliver the targeted octane as well as the desired heater and reactor temperature profile. Figure 1 shows typical constraints for one of the four heaters. If a constraint limits a heater, PACE will shift firing load to the heaters that aren't limited. When that happens, PACE no longer can maintain the heater profile temperature setpoint. However, PACE will continue to keep octane at its setpoint if at least one heater isn't constrained.

As already noted, reactor switching is necessary to allow catalyst regeneration. Operations requested automatic shutoff of PACE before a reactor switch is initiated. Fortunately, a very useful feature in PACE called event logic makes setting up event logics based on operator-enabled rules easy. The

EXAMPLE OF HEATER HMI



CV H5301 Heater Variable Set

Name	Description	Current Val...	SS Value	LL	Setpoint	HL	Unit
TC34156.SP	H5301 HEATER OUTLET TEMP	937.429	936.96	915		955	DEGF
AI34162.PV	H5301 EXCESS O2	3.692	3.796	2.1			PCT
FI34157.PV	H5301 FUEL GAS	4.739	4.677			6.25	MMSCFD
PI34158A.PV	H-5301 BURNER HDR PRESS	26.904	26.754	5.5		49	PSIG
TC34156.OP	H5301 HEATER OUTLET TEMP	45.883	45.796	5		95	MMSCFD
H5301 MAX SKI...	H5301 TUBE SKIN TEMP	1083.506	1082.9			1148	DEGF
TI34979.PV	H5301 BRIDGE WALL	1631.9	1630.991			1646	DEG F
DEV H5301AVGT	H5301 DEV Temp from HTRS AVG	-1.002	-1		-1		Deg D
CR3HTRAVGT	CR3 Heaters H5301-4 AVG Oulet Temp	938.435	937.965	915		915	Deg F
AX34992C.PV	RON REFORMATE						RON Oct...

Figure 1. Each of the four heaters typically faces these constraints.

PERFORMANCE SUMMARY

- RON octane is controlled tightly within ±0.2 from a given average target setpoint
- Giveaway was reduced from 0.7 to 0.2
- After reactor switch is completed, RON octane reaches target within 2 hours versus 9 to 12 hours

The spikes on RON octane are related to reactor switch transition PACE is on and RON is on spec - 2 hours

Figure 2. Online analyzer and Platform for Advanced Control and Estimation technology have provided several significant benefits.

controller uses two event logic rules: the primary rule is to shut off when the opening of the reactor bypass valve exceeds 5% — the valve is at 0% normally or 100% before reactor switching takes place; and the secondary rule, which applies when the reactor bypass valve is in maintenance mode, activates shut off when hydrogen injection pressure and flow controllers are switched from manual to automatic mode.

After completion of a reactor switch, the operators put the controller back into active mode when octane lines out and average temperature stabilizes.

IMPRESSIVE PERFORMANCE

Using the online Raman analyzer together with PACE has enabled the site to minimize product octane giveaway by 71%. Figure 2 shows octane variability from a given target remains within ±0.2. Additional benefits include maximizing feed to the unit while keeping heaters at their design point and, after a reactor switch completes, reaching octane target within two hours instead of the previous nine to 12 hours.

We have commissioned the Raman analyzer connection to the reformer unit stabilizer. The purpose of this controller is to separate reformate product and lighter components. We are using PACE to regulate stabilizer bottom reformate C_5s and overhead benzene. The new PACE controller and octane inferential both use the reformer-feedstream Raman analyzer components as feedforwards.

Going forward, the entire site will go through its planned journey with the goal of optimizing the plant.

MOHAMED ABOKOR deploys and maintains PACE applications at the Shell Oil refinery in Deer Park, Texas. Email him at Mohamed.Abokor@Shell.com.

Cooling Tower Capacity Draws Heat

A variety of issues may contribute to current limitations

THIS MONTH'S PUZZLER

We're in the dead of summer — the ambient temperature is already 95°F at 90% relative humidity — and our cooling tower (figure online at https://bit.ly/39bdint) can't cope. We must run at 50% capacity because we can't keep the batch temperature in range; we've offset the process to make product when the ambient temperature is down, such as at night. The condenser on the ammonia refrigeration runs at far above normal temperature, raising the upper system pressure to near the equipment limit of 400 psig. Last week, we blew the relief on the raw materials cooler; on inspection, I saw that the seals on the delivery pump of a cooled product were blown, adding to our troubles. This inspired me to review the entire cooling tower system.

Here's what I discovered: 1) when we pulled the heads off the ammonia condenser, we found it full of assorted muck including tree seedlings and mud; 2) two office chillers replaced early this year never were inspected before they were removed; 3) we pulled the head on one of the distillation column condensers — the smallest one, at the end of the train — and found no fouling; relief valves have popped on the product cooler because of high vapor pressure.

The maintenance engineer strongly believes that one fouled head is no problem. Production wants inspections of the heads of all the exchangers as part of every outage. The project engineer thinks we should add cooling towers but install them to serve the ammonia system exclusively, allowing the reactors and condenser to consume most of the cooling water. Another engineer suggested inspecting more condenser heads and, if needed, installing a filtration system at the discharge of the cooling tower pumps. The instrument engineer recommends automating the cooling tower to increase the cooling and system pressure, thereby improving cooling throughout the system.

Do you think we're in trouble? What's the best bang for our buck?

CHECK MANY FACTORS

Consider the following:

1. First, use a psychrometric chart to determine the theoretical minimum temperature (wet bulb) you can get with the cooling tower at your location. In practice, though, the minimum you can achieve is 4–5°F above the wet bulb temperature. (This is called approach.) Because you have high relative humidity of 90% at ambient of 95°F, psychrometric charts show wet bulb close to 95°F. Compare the temperature of cooling water coming out of the cooling tower with the wet bulb temperature. If this temperature is close, your cooling tower is functioning the best it can. However, if the temperature is much higher (say, approach is 10–15°F), you can improve the operation of the cooling tower.

The key to good performance is effective contact between the water flowing down the cooling tower and air. Factors that can impair this contact are water flow distribution as well as air flow rate and distribution. Check cooling range and compare it with the design value. If the cooling range is much smaller than design, your tower is not working properly. So:

- Inspect the water distributing nozzles at the top of the tower. They can get muddied up if water has high suspended solids. You can rod them out.
- Ensure louvers are not blocking air flow.
- The figure shows mist eliminators. These typically are tightly packed. They could get plugged, resulting in air-flow maldistribution. They are difficult to clean on-line.
- Check the cooling water fans, their rotation, and vibration. They should run smoothly. Measure their amp-draw to get an idea about air flow.

  The above items do not require shutdown of the cooling tower.
- Examine the splash bars, i.e., the slats, which serve to help improve air-water contact. If a large number are missing, you would need to shut down the tower and install new splash bars.
- If the towers contain fill (fill in good working condition can achieve much better air-water contact than slats), look for plugging by suspended solids. On-line cleaning of fill plugging will require lowering the cooling tower pH and increasing blowdown. This is a slow process. Before you do this, carefully review the impact of low pH and increased blowdown on plant equipment and the blowdown treatment facility. If you are using cooling-tower-treatment chemicals from a vendor, seek its help in planning this cleanup.

2. Check solids (suspended and dissolved). As a general rule, a dissolved solids level above, say, 5,000 ppm is considered high and can accelerate scaling and fouling. Get an analysis of dissolved and suspended solids. Consider installing a side-stream filter (or,

additionally, softener such as zeolite) depending on the chemicals you find in the analysis. Scaling chemicals such as $CaCO_3$ become problematic above, say, 700 ppm or so.

3. Check cycles of concentration (COC), i.e., the ratio of dissolved solids in the circulating water to those in makeup water. Higher COC is good for minimizing water waste but tends to enhance scaling and fouling. A COC that is too high, say, above 4, will see a substantial increase in scaling and fouling. If you are operating at high COC, consider lowering it by increasing the blowdown.

4. The quality of makeup water also can affect the COC you can live with. Ensure makeup water does not have excessive solids.

5. Now, to deal with heat exchanger fouling, consider in the short term localized additions of dispersants at the water inlet of the heat exchanger. In general, dispersant addition is a part of the overall treatment program. If the tower is heavily fouled, a short shutdown to clean up the entire system is desirable. However, this apparently is not a good option for you; so, instead, consider increasing blowdown and side-stream filters.

The on-line approaches discussed above are slow — improvements will be gradual. As you do these, monitor water quality.

6. You can check if the cooling tower has enough capacity to handle the heat load from your plant: estimate total BTU/h load from all heat exchangers and compare that with the cooling tower capacity. Refer to design data sheets. It is unlikely the tower was undersized initially; however, later additions of coolers may have led to exceeding the cooling capacity.

7. Some long-term options to think about include: side-stream filters; conductivity meters and auto-blowdown; filters and softeners on the incoming makeup water if its quality is not up to par; automatic addition of treatment chemicals including biocides, dispersants, corrosion inhibitors and other chemicals; monitoring the U-values of heat exchangers on-line; and regulating cooling water flows to avoid velocities below 3 ft/s to minimize fouling. Typically, 6–7 ft/s tends to help with heat transfer and minimize fouling.

GC Shah, consultant
Houston

BE SYSTEMATIC

You must start by determining the flow rate required for each cooler using cooling water. First, survey what flow meters you already have in place. If you don't have flow meters everywhere, using portable ultrasonic flow meters may be a good option. These devices have come far in the past 30 years; they will diagnose the flow characteristics — turbulent, laminar, gassy or a slurry. Unfortunately, they do need a good deal of straight pipe, about 10 pipe diameters upstream and 5 diameters downstream — but that depends on other obstructions like valves and bends.

Next, collect all the data sheets for the coolers and material balances, if available. Don't rely on the data sheets to tell you what the flow should be in a particular cooling leg; heat exchangers generally are oversized. Also, don't rely on inputs from design engineers because they may not be experts on the process; get your own data.

Now, you're ready to compare the survey data against the data sheets and material balance. Look hard at any discrepancies between the data sheets and the material balance and the measurements taken for the coolers. The measured flow rates should be *less* than the rates on the data sheets or from the balances; if not, the cooler is too small. Usually, a cooler is designed for perhaps 130% of required flow rate. The first pass probably won't tell you much; you're after a baseline!

Obviously, you'll want to do the first survey when the coolers are free of debris. If not, the data are still useful but will have to be compared to future measurements. The next time you do a survey, use the results to determine if a cooler is fouled.

Some might suggest measuring the pressure drop across the coolers instead. However, this only works if you've got the proper tees set up and ready to go and have a precision gauge you trust. Don't ever leave the gauge in the field; it will become unreliable after a few months. Here's the key thing to know: you must use the same gauge for upstream and downstream measurements across a cooler — the variation in accuracy between two gauges probably will ruin your ΔT calculation. You will find that repeatedly screwing in gauges is more trouble than using an ultrasonic flow meter. Plus, you may not see much difference in pressure drop between a fouled heat exchanger and a clean one.

CHECK OUT PREVIOUS PUZZLERS

To see all the Puzzlers that have been published over the years, go to: www.ChemicalProcessing.com/voices/process-puzzler/.

Filtration is a good idea if you've got the money. You will have to separate continually and blowdown the solids from the filter back into a sump with a screen on top. The screen will foul unless you skim it; fortunately, continuous skimmers are available.

Automating the towers makes absolute sense. I cut our plant electrical bill by 10% by doing just that.

Something else you should be thinking about is global warming. (See: Consider the Effects of Global Warming," p. 9.) Most cooling towers are designed for about 80°F wet bulb. Much of the United States will be well above that during future summers. If you're popping relief valves now, imagine what risk you'll be running at 95°F wet bulb temperature! You may want to opt for better refrigeration for key processes in your plant.

Do the study first! Then, consider the economics. The cost of an ammonia release is perhaps $5,000/each depending on the severity and maybe $200,000/d in downtime. So, any project under $2 million probably is worth consideration.

Dirk Willard, consultant
Wooster, Ohio

DECEMBER'S **PUZZLER**

I'm fresh out of college and have been handed a project for which I need help. I'm installing a centrifuge for concentrating a pharmaceutical product from a reactor's mother liquor. This is an expansion plant, designed by corporate engineering, for handling a new process.

The mother liquor is fairly sticky. I only have two data points: 31 cP at 108°F and 72 cP at 72°F. With the product, in a concentration of 13% by mass, the viscosity is 52 cP, and 101 cP, respectively. I am told the product starts to degrade above 115°F.

The density ratio between the product and the liquor is 1.3:1 for the batch stack centrifuge. I read that upstream factors could affect this ratio.

I still haven't figured out how I'm going to do the cleaning-in-place, given the sensitivity of the product to low pH and high pH. I'm worried about residual materials.

My problem primarily is instrumentation because we are under orders to reduce the labor costs per batch. I'm kind of on my own here. I have some ideas on what controls are critical versus just nice to have. What do you suggest as far as instrumentation?

Send us your comments, suggestions or solutions for this question by November 12, 2021. We'll include as many of them as possible in the December 2021 issue and all on ChemicalProcessing.com. Send visuals — a sketch is fine. E-mail us at ProcessPuzzler@putman.net or mail to Process Puzzler, *Chemical Processing*, 1501 E. Woodfield Rd., Suite 400N, Schaumburg, IL 60173. Fax: (630) 467-1120. Please include your name, title, location and company affiliation in the response.

And, of course, if you have a process problem you'd like to pose to our readers, send it along and we'll be pleased to consider it for publication.

Don't Simply Blame the Piping Designer

Bizarre layouts often stem from poor communications

A TOP-NOTCH piping designer was asked to train a group of process engineers after a revamp hadn't gone well. He bluntly counseled them that complaints "only a fool would do piping like that" probably are misdirected — the engineer often is at fault for not understanding what the piping designer needed to know.

A recent review of a project involving a compressor train, with cooling and liquid knockout between the stages (Figure 1), highlighted this issue. After the cooler, a knockout drum removes liquid condensate. The condensate then is pumped to a different part of the unit for further processing. The piping from the bottom of the knockout drum goes up through an inverted-U loop. The top of the loop is a high point ten feet above the liquid level in the drum. The end side of the inverted U drops straight into the suction nozzle of a horizontal pump. The horizontal pump uses a between-bearings shaft and has both the suction and the discharge nozzles pointed upwards.

At first glance, the piping layout looks horrifying — and at second glance, too. The liquid in the drum is near its bubble point. As long as there's enough static head of liquid in the system, this head provides pressure for flow out the bottom nozzle and along the pipe without vaporization.

As the liquid rises along the upward side of the inverted U, the pressure of the liquid drops until it reaches its bubble point. Then, the liquid starts to vaporize. A vapor pocket forms in the top of the inverted U. Liquid flow stops.

If the pump is running, it can "suck" some vapor out of the feed pipe, reducing the pressure. This may create enough suction lift to get flow over the top of the inverted U. However, the flow to the pump always will be two phase. The lower pressure drawn by the pump suction causes vaporization. This is an extreme case of what happens when a pump has vaporization due to insufficient net positive suction head.

Two situations might make this system "work" — but not well. The first is if the system has enough heat loss in the piping that the liquid entering the piping is subcooled. For this application, that's unlikely because it would require approximately 7°F of subcooling. At the flow rates involved, the surface area of the pipe simply won't lose enough heat to the environment, even on a very cold day. The second is if there's enough vaporization and velocity in the upward line; then, it might be possible for liquid to get to the top of the inverted U and fall down the other side with the vapor being recompressed and condensing. I've never seen this happen in practice. However, a colleague swears he's seen such a system. Unfortunately, that system had to have exactly the right flow rate to work and had significant damage to both the pump and the piping.

Some questioning clarified the reasons for the strange piping layout. The piping designer was using a standard that required a minimum of 15 diameters of straight pipe at the pump suction inlet. By itself, this is good practice. It makes for smoother inlet flow into the pump and more-reliable pump operation. However, the upward-facing suction nozzle meant the 15 inlet diameters were straight up. Combining the entry pipe requirement with the already selected equipment elevations and layout forced the creation of the inverted U. What the piping designer didn't understand was that the line from the drum to the pump suction had to have no pockets. (For more on this, see: "Piping Geometry: Grasp Line Layout," https://bit.ly/2AXkbuX.)

Some questioning clarified the reasons for the strange piping layout.

COMPRESSOR INTER-STAGE COOLING

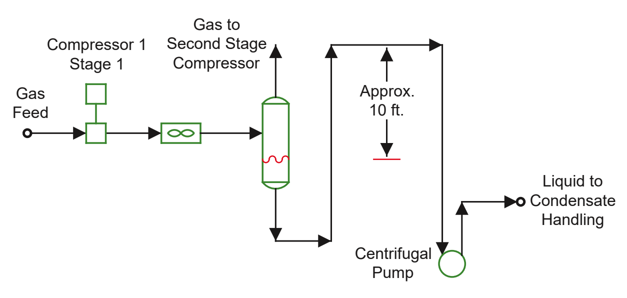


Figure 1. The piping's 10-ft-high inverted U promised to undermine reliability.

Here, reliable plant operation demands a change in piping layout. The most straightforward solution is to switch to a pump with a side suction nozzle. Unfortunately, the pump already had been purchased. Nevertheless, the economic penalty incurred from changing the pump order clearly is the cheapest option over the long term.

This episode points up the importance of team members helping each other understand what's important in locating and piping equipment. Experience accumulates over time. Even the best of us has to start somewhere.

ANDREW SLOLEY, Contributing Editor
ASloley@putman.net

Tablet Provides Accurate Global Positioning

The Cedar CT8X2 rugged tablet offers increased processing power, RAM and storage, running on the Android 10 operating system. Powered by an octa-core Snapdragon CPU from Qualcomm, the tablet is designed to run demanding applications. The increase in RAM allows easy handling of larger files and data-intensive tasks. A bump in onboard storage prevents users from needing to offload data frequently and provides plenty of space for applications. With global navigation satellite system (GNSS) accuracy of around one meter in open skies and five meters in tree canopy, the tablet offers GNSS positioning that exceeds the accuracy of typical consumer devices, the company says.

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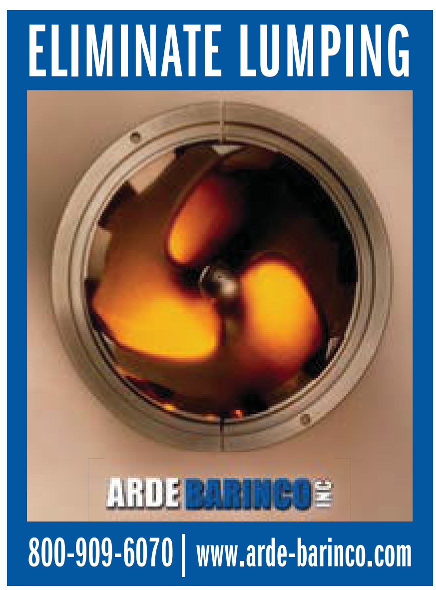

Algorithm Tackles Process Simulations

Method quickly identified novel materials for gas storage

The algorithm works by intelligently selecting which simulations are worth running.

SCIENTISTS AT IBM, Cambridge, Mass., the University of Liverpool, U.K., and the University of Southampton, U.K., have developed an algorithm that could vastly reduce the time and cost of running engineering, materials chemistry and new drug discovery simulations.

The algorithm works by intelligently selecting which simulations are worth running, and then focuses resources on them.

A report in *Science Advances* explains how the researchers used their method to quickly identify novel materials for gas storage. It saved 500,000 central processing unit hours (CPUh) over traditional simulation methods.

On the face of it, combining machine learning and virtual computational screening should produce a powerful means for discovering new functional organic materials.

However, while this is true for calculating thermodynamic stability and the associated functional properties of candidate materials, tackling a broader range of problems remains difficult, caution the authors. A big hurdle, they say, is the prohibitive computational expense of accurately calculating energies and properties for every candidate material to be screened.

Especially difficult is the a priori design of functional molecular organic crystals with desirable materials properties. Unlike framework-based crystals such as zeolites and metal organic frameworks, molecular crystals rarely obey the kind of simple geometric principles that can be exploited for rational design.

"Even very small changes to molecular structure can have marked effects on crystal packing and, hence, the resultant solid-state properties. Molecular crystal packing is often dictated by weak, competing intermolecular interactions. Hence, the a priori design of materials with predetermined, desirable properties requires a more subtle approach than for materials where structure (and hence function) can be 'built-in' through the use of intuitive bonding rules, such as adherence to known framework topologies or other geometric bonding principles," they write.

One tool for virtual screening candidate organic molecules for desirable properties such as natural gas storage capacity is an energy-structure-function (ESF) map. Such maps pair lattice energy and function to show if a particular molecule has the desired properties. This information can help guide an experimental campaign.

However, the authors note that while this is an effective strategy, ESF map generation can be computationally intensive. The methane storage predictions carried out in this project, for example, took around 800,000 CPUh to compute an ESF map for just one molecule under investigation.

Of course, the cost of creating ESF maps grows as the molecules of interest become more computationally expensive and the number of candidate structures increases. Porous materials pose even more challenges because the energy range that includes all observable crystal structures is extended by solvent templating and sometimes by multiple components such as co-crystals.

"To overcome these, we have packed all of our algorithmic advances into a simple service called IBM Bayesian Optimization (IBO), which means that users can easily get the value from using these algorithms without themselves having to become Bayesian optimization experts," the authors explain. In general, IBO answers the question: "With what I know now, what should I do next so that I get the best overall result in the future?"

Two main challenges remain, however.

"Being able to work in complex situations without passing that complexity to the user is a key facet of IBO's application processing interface design. One such example is explainable AI [artificial intelligence] techniques to help the user understand why the algorithm is asking them to do certain actions or experiments," says Kirk E. Jordan, IBM engineer and executive in the company's research division's data centric solutions center.

Another is handling data from multiple sources.

"Being able to take in many different pieces of information is still a challenge. … the authors address one part of this by allowing each property to have its own model. They are now working on a method which allows them to choose between different ways of testing the same hypothesis (which might have different costs or accuracies) in real time and [fusing it] into a single model, which means maximal usage of the available information. Initial results … are promising, so keep your eyes peeled for a publication soon," adds Edward O. Pyzer-Knapp, research lead, AI enriched modelling and simulation and visiting professor of industrially applied AI at the University of Liverpool.

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