WWW.CHEMICALPROCESSING.COM

CHEMICAL PROCESSING

LEADERSHIP | EXPERTISE | INNOVATION

Make Sound Moves With Tolling

Choosing the correct contract manufacturer and developing an effective partnership are key

FEBRUARY 2021

TAKE BETTER CARE OF YOUR LOW-PRESSURE BOILER

PLANTS LOOK OFFSITE FOR INSITES

BUILD SAFER AND MORE RELIABLE SEAL SUPPORT SYSTEMS

PutmanMedia®

WHAT IF...

YOU COULD CLEAN BETTER, FASTER AND MORE SAFELY USING LESS WATER?

SLASH CLEANING TIME, NOT CLEANLINESS

Processors using our TankJet® equipment report dramatic reductions – up to 80% – in the time required to clean tanks, totes, drums, mixers and more. By optimizing impact based on tank residue, TankJet tank cleaners provide faster and more thorough, consistent cleaning than other methods.

REDUCE WATER USE UP TO 60%

Faster cleaning and reduced water use go hand-in-hand. TankJet users report saving millions of gallons of water per year. Using less water also reduces wastewater, chemical consumption and energy use – especially when using heated water.

IMPROVE WORKER SAFETY

Automated cleaning eliminates the need for workers to enter tanks or climb on equipment. It also reduces worker exposure to harsh cleaning chemicals. With TankJet tank cleaners, workers can be deployed to other tasks.

MAKE EVERY DROP COUNT!

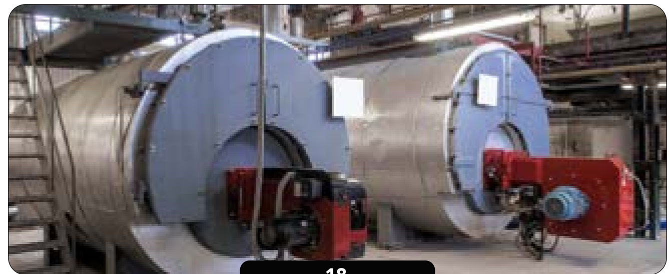
We help companies around the world reduce water, energy and material use, decrease waste, minimize environmental impact and improve worker safety. Let our spray technology advance your sustainability initiatives.

Spraying Systems Co.®

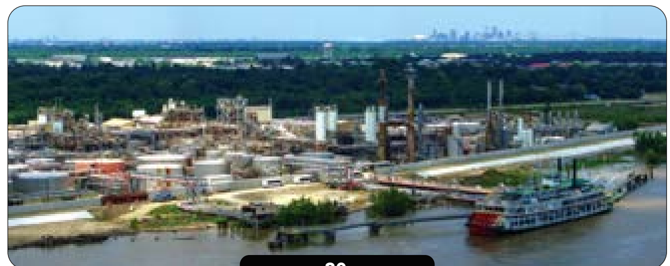
To learn more, visit spray.com/cleanbetter

CHEMICAL PROCESSING FEBRUARY 2021 | VOLUME 83, ISSUE 2

14



18

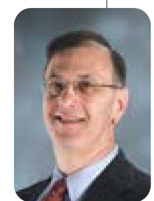


30

Chemical Processing (ISSN 0009-2630) is published monthly by Putman Media Inc.,1501 E. Woodfield Road, Suite 400N, Schaumburg, IL 60173. Phone (630) 467-1300. Fax (630) 467-1120. Periodicals postage paid at Schaumburg, IL, and additional mailing offices. Postmaster: Please send change of address to Putman Media, PO Box 1888, Cedar Rapids IA 52406-1888; 1-800-553-8878 ext. 5020. SUBSCRIPTIONS: Qualified reader subscriptions are accepted from operating management in the chemical processing industries at no charge. To apply for a free subscription, email putman@stamats.com. To nonqualified subscribers in the United States, subscriptions are $68 per year. Single copies are $15. Canadian and other international annual subscriptions are accepted at $200 Airmail. Single copies are $16. Canada Post International Publications Mail Product Sales Agreement No. 40028661. Canadian Mail Distributor information: Frontier/BWI, PO Box 1051, Fort Erie, Ontario, Canada, L2A 5N8. REPRINTS: Reprints are available on a custom basis. For price quotation, contact Foster Reprints, (866) 879-9144, www.fostereprints.com. Putman Media Inc. also publishes Control, Control Design, Food Processing, The Journal, Pharma Manufacturing™, Plant Services and Smart Industry. Chemical Processing assumes no responsibility for validity of claims in items reported.

It's Not Your Father's Industry

Significant shifts are reshaping U.S. chemical manufacturing



VERTICAL INTEGRATION — i.e., making key raw materials and producing a finished product at a single site — can yield important efficiencies. Its application on a large scale dates back more than a century. For instance, Ford Motor Company started production at its River Rouge complex in Dearborn, Mich., in 1918. That massive site included its own steel mill, glass works and power plant. In our industry, the integrated refinery/petrochemical complex probably best typifies vertical integration.

However, in recent decades, the allure of vertical integration certainly has waned in many manufacturing sectors both for economic and strategic reasons.

For instance, large automakers now tend to favor regional factories — e.g., the ones that Japanese, German and Korean car companies operate in the United States — rather than serving all markets from a single, massive plant. This can offer significant benefits in cutting transportation costs and avoiding tariff and other trade issues in key markets. In addition, such factories allow the companies to more easily tailor products to the individual regions and to respond more quickly to local trends.

Foreign chemical manufacturers have flocked to America, too. Indeed, the United States has garnered a massive amount of investment from such companies. This reflects not only their interest in being better placed to benefit from the strong rebound expected for the American economy, as covered in last month's cover story "Brightening Outlook Buoys U.S. Chemical Industry," https://bit.ly/38xTJ97, but also feedstock advantages that American production offers.

A strategic shift also is occurring. Many companies in the chemical industry and other manufacturing sectors have decided to concentrate on their "core competencies," aiming to excel in the most important areas rather than be pretty good at a lot of things.

This shows up in many ways.

For instance, not that long ago, major chemical manufacturers strove to handle much of their engineering internally. They prided themselves on their extensive corporate engineering staffs filled with industry-leading specialists on a broad range of technologies.

Today, many operating companies believe that devoting considerable resources to engineering just doesn't make sense because they are manufacturers first and foremost. So, they have pared their central engineering staffs substantially or dispersed specialists to individual plant sites.

Likewise, the idea that a chemical company must make everything it sells doesn't seem as compelling to many corporate executives nowadays. Sure, some chemical firms long have relied on tollers for specific products. However, I sense that outsourcing of manufacturing is gaining increasing interest. Various factors likely contribute to this, most prominently, the quest to minimize capital expenditure, the lack of suitable in-house equipment and specialists, and the desire for faster product commercialization or response to market changes than possible internally. This issue's cover story "Make Sound Moves with Tolling," p. 14, provides some valuable tips for properly outsourcing production, including how to select the right contract manufacturer and how to forge an effective working relationship.

The famous philosopher Yogi Berra clearly was right: "The future ain't what it used to be." ●

Chemical makers want to concentrate on their "core competencies."

MARK ROSENZWEIG, Editor in Chief
mrosenzweig@putman.net

2021 Webinars Promote Best Practices

Lineup covers myriad topics including safety, conveying, powders and solids, and more.

The new year brings new learning opportunities.

THE NEW year brings new learning opportunities via *Chemical Processing*'s free webinars. We've put together a great lineup of experts to help you achieve success. Here's what is on deck for this year. You can learn more and register for one or more of these at https://info.chemicalprocessing.com/cp-upcoming-webinars. If you can't make the live session, once registered you can view the webinar later on demand.

Feb. 23 at 2 p.m. ET | Exploring Advancements in Pneumatic Conveying Round Table

This discussion will focus on developments and improvements in pneumatic conveying. Our panel of experts, led by panel moderator Todd Smith, P.E., business and strategy manager at the Kansas State University – Bulk Solids Innovation Center, will point out the areas that need the most improvement going forward and answer all your questions.

April 21 at 2 p.m. ET | Powder and Solids Series: Choose the Correct Pneumatic Conveying System

This webinar will review pneumatic conveying systems (dilute and dense phase, and vacuum and pressure systems) and go over the advantages and disadvantages of each type. Experts from the Kansas State University – Bulk Solids Innovation Center will also answer questions from the audience.

May 12 at 2 p.m. ET | Combustible Dust Round Table Series, First Installment

Combustible dusts can pose significant hazards to personnel, plant equipment, and even the surrounding community. In this latest of our ongoing series of exclusive webinars, Laura Moreno, senior engineer and standards lead in the Industrial and Chemical Engineering Division of the National Fire Protection Association will moderate a panel discussion with a number of industry experts on dealing with these hazards. The panel will offer insights on key challenges and provide practical guidance on how to identify, evaluate and effectively address hazards. *The second installment of this series is Nov. 4 at 2 p.m. ET.*

June 16 at 2 p.m. ET | Process Safety Series: Learn Lessons about Operating Plants during a Pandemic

Dr. Stewart W. Behie, P.E., Interim Director, Mary Kay O'Connor Process Safety Center, will discuss lessons learned from three major chemical companies operating during the pandemic. A phased approach in which the level of efforts is adjustable, coupled with multiple layers of protection, makes sense but can pose challenges such as handling contract workers who move from site to site and in allowing employees to work from home.

June 29 at 2 p.m. ET | State of Chemical Industry Mid-Year Update

The chemical industry, like society in general, has faced unparalleled upheaval because of the pandemic. Our annual cover story in January on the state of the industry "Brightening Outlook Buoys U.S. Chemical Industry," http://bit.ly/3qBdYJv, written by experts at the American Chemistry Council (ACC), indicated that a recovery is underway. However, in these uncertain times, the situation quickly can change. This webinar will provide an update from ACC on the current prospects for the industry. Dr. Thomas Kevin Swift, CBE, chief economist and managing director at the ACC, and co-author of the January article, will provide the update.

Sept. 15 at 2 p.m. ET | Process Safety Series: Rethink Process Safety Training for Operators

A recent survey of chemical and refining companies pointed up the need for a structured program for operators that enables them to get process-safety training while continuing to work. This webinar will review that survey and look at what's necessary to achieve faster and more-efficient process-safety training for both current and new operators and to properly assess their knowledge and competency. Dr. Stewart W. Behie, P.E., Interim Director, Mary Kay O'Connor Process Safety Center, will be the speaker.

Oct. 27 at 2 p.m. ET | Powder and Solids Series: Properly Weigh and Batch Powders and Other Bulk Solids

This webinar will provide an overview of how to measure and control the amount of dry ingredients being dispensed. Experts from the Kansas State University — Bulk Solids Innovation Center will cover weighing do's and don'ts, discuss various types of volumetric and gravimetric feeding devices, and go over advantages and disadvantages of each type.

I serve as the moderator for all of these events. If you are in the audience, please make sure you say hello via the chat feature on the webinar platform. I'm planning on asking a few trivia questions before the events begin, so log on a few minutes early to play along. Hope to "see" you soon. ●

TRACI PURDUM, Senior Digital Editor
tpurdum@putman.net.

Don't Put Peddle to the Metal

The benefits of stainless steel sometimes blind users to its limitations

Stainless steel isn't a panacea.

CORROSION CONCERNS often prompt thoughts of using stainless steel. However, even when economics permit, its application requires care. Stainless steel isn't a panacea.

For instance, a chlorine release from a brick-lined carbon-steel vessel spurred discussion on how to avoid a recurrence. The incident investigation showed that acid had worm-holed into the brick and attacked the wall. Some less-experienced engineers suggested switching to a tank made of some exotic grade of stainless steel or even cladding. A better option was to improve inspection of bricks, mortar and the bricking process.

An abrasive mix of paraformaldehyde, tetramethylpentane and who knows what else carved grooves into Type-304 stainless steel in less than a dozen years. Carbon steel, while about 10% stronger than stainless, wasn't an option because it would discolor the product. So, I recommended going with thicker pipe (Schedule 40 instead of Schedule 10), thereby doubling the life of the pipe.

In another case, a Type-304 boiler feedwater line coming out of a deaeration tank gradually thinned out and finally failed. Makeup to the tank is river water — heavily dosed with chlorine that's often poorly controlled. An anti-oxidant protects the pipe. I don't yet know whether the issue stems from overdosing the anti-oxidant, the chlorine reacting with the anti-oxidant to produce HCl or something else. I do know a protective layer of chromium is why a stainless steel pipe doesn't erode away, especially in de-ionized water. If erosion occurs in stainless steel, it's because the chromium can't re-oxidize; levels below 12% chromium provide no protection.

In another example, Type-304 vessels manufactured in Italy showed spider cracks and weld pits. Chlorine exposure in combination with high temperatures, widely varying pH and high salt concentrations contributed to shortened life. Because no records were translated for the tank fabrication process, it was suspected, without proof, that annealing and pickling treatments might have helped.

A common problem with stainless steel is people not respecting the difference between carbon steel and stainless either by welding one to the other or by using carbon steel bolts (generally a good idea) without isolating the contact with the stainless steel. I have seen this go so far as to prompt either the carbon steel fasteners (nuts, bolts, studs) to rust away, fail and cause the connection to leak, or create local corrosion at a flange that weakened the connection enough to leak. It's important to remember that corrosion is like compound interest: a little every day eventually can add up to a lot.

(Using stainless steel fasteners on carbon steel pressure vessels can raise issues, too. See: "Solve the Real Problem," http://bit.ly/2JQ1qhw.)

Then, there's anaerobic attack by bacteria. This corrosion has something in common with the boiler feedwater problem: removal of the protective chromium oxide layer by depriving the exposed surface of renewing oxygen, thus allowing attack of the iron. Raising the pH out of the basic range or increasing the temperature are the best approaches for reducing bacterial attack.

Probably the most common corrosion in stainless steel is pitting at welds. When I worked at Anheuser-Busch, this stemmed from chlorine attack at temperatures above 105°F. Usually, sterilization requirements meant that we couldn't avoid the high temperature, so we specified low-carbon stainless steel — as if this helped! Pitting is especially annoying in the food and pharmaceutical industries because it can result in rough surfaces that hide bacteria.

In tanks and static duty, pitting is easy to spot if monitored: the chromium disappears and the pit turns rusty or black. In pipelines or where erosion sweeps away the rust, detection is more difficult. Ultrasonic instruments can spot thinning — but only once the pitting is difficult to repair; the head of a hand-held ultrasonic gage is about 0.4 in., so I doubt if detection is possible. One precaution, which often is ignored, is to ensure welds in pipes and equipment are accessible to inspectors. Even more important is to perform inspections as often as required per ASME code — and more frequently, if required.

So, what can be done? Make sure the stainless steel is oxygenated to replenish the chromium layer. Watch the pH and temperature; thereby preserving an environment where the steel can survive. Most of all, be aware of process conditions. ●

DIRK WILLARD, Contributing Editor
dwillard@putman.net

Green Hydrogen Looms

Method to convert ammonia to hydrogen targets use in fuel cells

A HIGHLY effective electrochemical process for ammonia-to-hydrogen conversion is a significant step towards widespread, environmentally friendly hydrogen fuel cell production, believe researchers from Northwestern University, Evanston, Ill., and SAFCell, Inc., Pasadena, Calif. The ammonia would serve as a carrier for hydrogen delivery, they note.

"The bane for hydrogen fuel cells has been the lack of delivery infrastructure," says Sossina Haile, professor of material science and engineering at Northwestern's McCormick School of Engineering. "It's difficult and expensive to transport hydrogen, but an extensive ammonia delivery system already exists... If you give us ammonia, the electrochemical systems we developed can convert that ammonia to fuel-cell-ready, clean hydrogen on-site at any scale."

Their process requires a lower temperature than that needed in traditional thermal ammonia-to-hydrogen routes, 250°C versus 500–600°C, and could use renewable electricity, the researchers add.

CONVERSION PROCESS

Figure 1. Zero ammonia crossover and no side reactions result in pure hydrogen product. *Source: Reprinted from Lim et al., Joule 4 1-10 (2020).*

An electrochemical cell with a proton-conducting membrane and integrated ammonia-splitting catalyst drives the conversion (Figure 1).

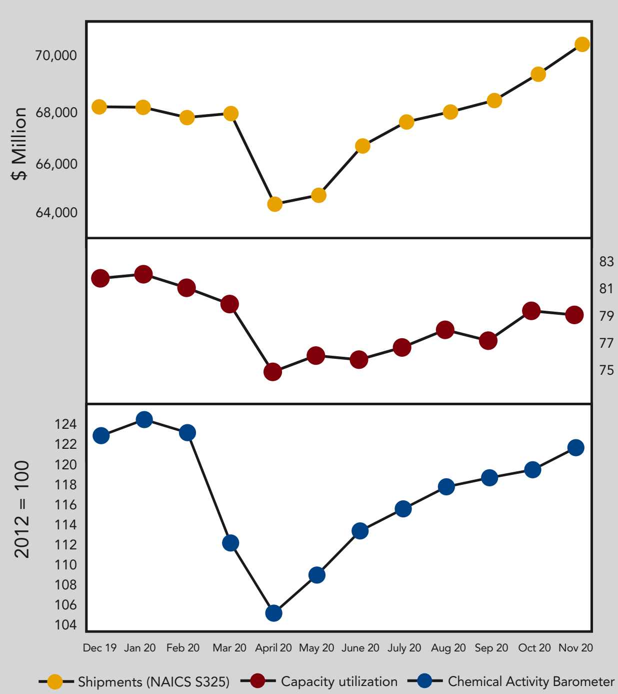
"The ammonia first encounters the catalyst that splits it into nitrogen and hydrogen," explains Haile. "That hydrogen gets immediately converted into protons, which are then electrically driven across the proton-conducting membrane in our electrochemical cell. By continually pulling off the hydrogen, we drive the reaction to go further than it would otherwise."

The pure hydrogen generated doesn't need separation from any unreacted ammonia or other products, and can be directly pressurized for high-density storage by ramping up the electrical power, the researchers note, adding that the device's electrical current directly produces hydrogen, with no loss to parasitic reactions. The journal *Joule* contains more details.

In addition, the cells' metal and polymer components and solid-state electrolyte make them very mechanically, thermally and chemically robust. "Because cells/stacks run at 250°C, they are very tolerant to typical impurities found in 'fuel streams.' These include sulfur components, carbon monoxide and carbon dioxide, most hydrocarbons, and obviously ammonia," says Calum Chisholm, CEO and president of SAFCell. "We have been running our cells and stacks on industrial grade ammonia and have seen no adverse effects up to 5,000 h of operation," he adds.

The team, which has previously focused on electricity production from hydrogen fuel, will next

ECONOMIC SNAPSHOT



Shipments and the CAB rose while capacity utilization slipped. *Source: American Chemistry Council.*

explore methods to produce ammonia in an environmentally friendly way.

"The solid acid technology has potential to produce ammonia from 'green' hydrogen (i.e., hydrogen from renewable sources) and nitrogen from the air in a very simple and economical way. Sossina is currently beginning to explore this option and SAFCell would be more than happy to scale up her successful research," notes Chisholm.

To implement the technology demonstrated by the team for hydrogen production, the stack must be scaled up at least 100× from its present size (1–2 kg H_2/day) to meet the quantity of hydrogen needed at refueling stations (400–2,000 kg H_2/day).

"It is possible that five, 400-kg-H_2/day stacks could be used in parallel for initial 2,000 kg H_2/day systems, but CAPEX [capital] and OPEX [operational] costs will be decreased by using one bigger stack," notes Chisholm. "Whenever you scale up this much, there are always manufacturing and operational 'details' that need to be sorted out. We do not see any major roadblocks, but without a doubt it will take a lot of work," he adds.

The team performed a detailed efficiency analysis based on data taken at SAFCell on scaled-up cells and stacks. "A large system that would be applicable for FCEV [fuel cell electric vehicle] refueling stations, would be around 88% efficient," he says.

Some leading firms are looking into use of ammonia as a liquid hydrogen carrier, with desire to use our scaled-up systems, concludes Chisholm. ●

Electric Reactor Promises Lower Emissions

SIGNIFICANT REDUCTIONS in carbon dioxide emissions could come from using electricity instead of fossil fuels to heat reactors in chemical processes that require high temperatures, for example natural gas reforming, say scientists at research, technology, and innovation organization VTT, Espoo, Finland. The electrification of that process alone would markedly decrease global industrial CO_2 emissions, they note.

VTT is carrying out work on such reactor heating as part of its iBEX program that looks for novel ways to carry out applied research and develop radical technologies to commercialize them.

Research on the project, dubbed the E-Reactor, began in 2020 with an initial survey on potential power sources, for example resistive and induction heating.

"The main challenges have been related to resistive material development," explains VTT researcher Tomi Lindroos.

While the principle is the same as with electrical resistance heating, applying it to very high temperatures and in conditions where chemical reactions are catalyzed is a new application. At the same time, for commercial viability, the E-Reactor also must suit scaling to industrial capacities, which means electricity use in the range of dozens of megawatts.

The lab-scale E-Reactor currently is working at a 2–4-L/min gas flow rate; Lindroos expects this could be scaled-up ten-fold by the end of 2021.

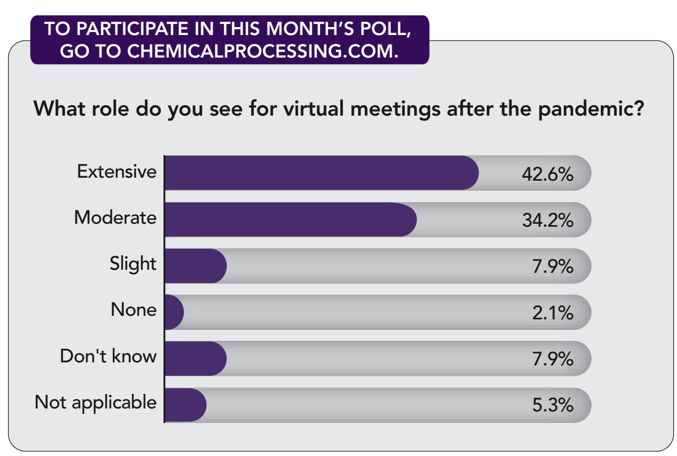
The first target is the reverse water gas shift reaction; the Finnish researchers also plan to investigate other potential applications as the project progresses.

The materials and catalysts used still are under development, with several patent applications lodged already, so process information remains guarded, explains Lindroos.

Besides scaling-up the E-Reactor, the scientists are eager to perform a long-term trial. "This is due to start late this year at the bench scale to test material stability," says Lindroos. "The overall efficiency of the process is of great interest here, too," he notes.

If this work goes well, VTT will decide about scaling-up to demonstration capacity in 2022. "The main challenges here are most likely related to materials and efficiency," emphasizes Lindroos.

The E-Reactor already has attracted strong industrial interest, he reveals, adding that decisions on any follow-up plans such as investment will be made after the long-term testing phase. ●



Most respondents foresee a significant ongoing role for virtual meetings.

Make the Case for PFD Reviews

Identifying improvement opportunities should start with this structured brainstorming activity

By the end of the meeting the operations supervisor was a man with a mission.

WE TALK a lot in these columns about ways to improve energy efficiency in existing chemical processes. However, we haven't spoken much about how to identify energy-saving opportunities for specific plants. Each process is to some degree unique, so it is not always possible simply to replicate ideas. Instead, you must evaluate and understand each plant's needs in order to identify inefficiencies and develop improvement options.

One of the most effective methods for identifying improvement opportunities is a process flow diagram (PFD) review. This is essentially a "structured brainstorming" activity. The procedure resembles that customarily used for HAZOP studies. It starts with a marked-up PFD for the process unit (e.g., hydrotreater, crude unit, etc.), showing the major equipment items and their interconnections, together with the heat and material balance. The inlets and outlets of each major piece of equipment should include temperatures, flow rates and pressures, together with energy flows, such as the thermal duty for each fired heater, heat exchanger or cooler, as well as the power requirements for pumps and compressors. In addition, the PFD should indicate any place where steam is used for heating or stripping, or where steam is generated, with flow rates labeled.

With the marked-up PFD, operations and technical support personnel from the operating site, with assistance from visiting energy efficiency specialists, review each of the main streams, equipment items and systems, to identify inefficiencies and areas of opportunity. The plant operations and technical staff bring their knowledge of day-to-day plant issues to the table. The visiting specialists bring their experience of similar processes at different locations, and the types of energy efficiency opportunities that have worked elsewhere. Together, they brainstorm ideas for the process unit under consideration.

Typically, a PFD review will generate a large number of ideas. These can range from adjusting set points and operating targets, through new control schemes, minor piping changes and equipment modifications, to completely new processes and novel technologies. During the PFD review, document these opportunities, and then later evaluate them more thoroughly to quantify the potential savings, estimate the implementation costs, and identify technical risks. I'll discuss this evaluation process in a future column.

PFD reviews can serve as a stand-alone technique for identifying and organizing opportunities for improving energy efficiency on virtually any type of process plant. However, most often they form part of a larger energy efficiency initiative, such as an overall site energy assessment. They also often are used in conjunction with a pinch analysis to explore a wide range of energy efficiency options for a process or production site.

PFD reviews also provide an opportunity for site personnel to showcase their ideas. An example from a chemical plant illustrates this. The plant's control engineer explained a new control algorithm he had written to optimize the operation of a large compressor. The new application had been ready for several months, but it had not been turned on because the operations department had concerns about how it might impact the stability of the plant.

The operations supervisor was in the meeting, and, initially, he expressed very strong objections to any changes to the existing control scheme. However, the control engineer demonstrated that the energy savings with the new operating mode were far greater than the operations supervisor had realized. Further, the visiting energy management specialist endorsed the new control scheme based on experience at other facilities. An animated discussion followed on strategies for testing the new algorithm and steps needed to safeguard plant operations. By the end of the meeting the operations supervisor was a man with a mission. He was committed not only to testing the new control scheme, but also to making it work.

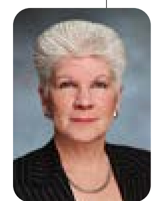
This incident is by no means an isolated case, and highlights a key fact: Successful energy management is not only about good technological solutions. It is also about human behavior, engaging people in the pursuit of energy efficiency, and motivating them to succeed at it.

For further details and examples, see: Alan P. Rossiter & Beth P. Jones, *Energy Management and Efficiency for the Process Industries*, Wiley-AIChE, 2015, pp. 313–325.

ALAN ROSSITER, Energy Columnist
arossiter@putman.net

EPA Proposes Revisions to TSCA Fees Rule

The suggested additions and exemptions will improve fee collection



Stakeholders should consider a tonnage band model.

ON JANUARY 11, 2021, the U.S. Environmental Protection Agency (EPA) proposed to amend the 2018 Toxic Substances Control Act (TSCA) fees rule. This column discusses the proposal and its improvements to the rule.

Under TSCA, the EPA collects fees from chemical manufacturers and processors to help fund TSCA implementation. TSCA requires the EPA review its fee structure every three years and, after public comment, adjust the fees if necessary. The proposed rule suggests modifications to the fees and fee categories through fiscal years 2022–2024, and explains the methodology by which these TSCA fees were calculated.

The proposed rule would establish, update and revise fees collected from manufacturers (including importers) and, in some cases, processors, to defray costs related to activities under TSCA Sections 4, 5 and 6. The suggested updates and changes to the fees rule include:

- adding three new fee categories;
- exemptions for manufacturers subject to fees for EPA-initiated risk evaluations under TSCA Section 6(b);
- exemptions for manufacturers if the chemical substance is imported in an article, produced as a byproduct, or produced or imported as an impurity;
- an exemption for research and development (R&D) activities;
- an exemption for manufacturers of chemical substances produced as a non-isolated intermediate; and
- an exemption for entities manufacturing less than 2,500 lb of a chemical.

Other amendments also are proposed. In addition, the agency notes it won't change the "small business concerns" definition.

Sustained funding is needed to designate chemical substances as high and low priorities for future risk evaluation; conduct risk evaluations to determine whether a chemical substance presents an unreasonable risk of injury to health or the environment; require testing of chemical substances and mixtures; and evaluate and review new chemical submissions, as required under TSCA Sections 4, 5, and 6. Funding also aids collecting, processing, reviewing, and providing access to and protection from disclosure as appropriate under TSCA Section 14.

We commend the EPA for timely issuing this proposed rule and for including provisions that address practical issues that have arisen in implementing TSCA to date, including anomalous and unanticipated challenges in which companies were paying unexpected fees. The three additional fee categories and associated fees — i.e., for bona fide notices ($500/$90 for small businesses); notices of commencement ($500/$90 for small businesses), and an additional fee related to amended test order submissions ($9,800) — are reasonable in light of the costs incurred to handle disclosure information as appropriate under TSCA Section 14.

The addition of new exemptions for manufacturers and importers subject to fees for EPA-initiated risk evaluations especially is welcome and largely motivated by industry stakeholder input. With regard to entities that manufacture chemicals as a byproduct, we wouldn't be surprised to see the EPA refine the exemption so it's consistent with the rule for byproduct producers under TSCA Section 5 Premanufacture Notification and TSCA Section 8 Chemical Data Reporting regulations. Under those regulations, entities that manufacture substances as byproducts for certain separate commercial purposes *must* report; in this light, coverage of these byproduct manufacturers under the fees rule seems both reasonable and practicable.

The EPA's proposed new production/import volume-based methodology for calculating fees for EPA-initiated risk evaluations generally is laudable, but may present additional implementation complexities. It could also result in anomalous situations where small manufacturers are required to bear a disproportionate share of the fees. In addition, circumstances could exist in which the proportion of fees might divulge a particular company's production volume (or average production volume). Stakeholders should consider a tonnage band model as an alternative. That way, a fee proportion can't be used to back-calculate another's production volume.

Given all the surprises potential fee payers faced in 2020 when the EPA published the preliminary lists of fee payers for the "next 20" substances undergoing risk evaluation, stakeholders may wish to consider carefully the implications of the various fee scenarios.

LYNN L. BERGESON, Regulatory Editor
lbergeson@putman.net

Make Sound Moves With Tolling

Choosing the correct contract manufacturer and developing an effective partnership are key

By David Morse, DRM Chemical Process Services

MULTIPLE CONDITIONS may arise when considering toll manufacturing is logical and prudent. For instance, a chemical company may lack the specific equipment, spare capacity or even expertise to make a product or may want to get a product to market faster than it could on its own. In such cases, having another firm handle production or other necessary tasks can make good sense.

Tolling differs considerably from simply buying another company's offering. When you purchase a product branded and sold by another manufacturer, that company sets the product specifications and price — and these can change at any time if the amount you buy isn't large enough to give you sufficient clout. In contrast, in a tolling contract, you set the specifications and process requirements, agree ahead of time to a pricing structure, and get the product exclusively. You also decide how much authority the toller has to make adjustments (think of this as allowing the toller to offer its expertise to improve your product). Yes, a toll deal involves more work upfront but you get what you need in the way you want it and only you have access to that product!

WHEN TO CONSIDER TOLLING

The case for using tolling services is the most obvious for a young company that doesn't have any chemical processing equipment to speak of and likely lacks the experience and expertise to run an efficient and safe chemical operation. The toller's knowhow can smooth out the bumpy beginnings to many chemical products.

The right toller has the equipment, experience, infrastructure and resources in the area you need. In addition, the toller will free you from responsibilities such as:

- handling chemicals safely;
- training staff;
- providing a chemical laboratory;
- producing pilot-scale batches;
- dealing with waste management; and
- adhering to chemical regulations.

Moreover, opting for a toller avoids the need to invest company capital in a product before its commercial acceptance is established, and can speed the product to market. Remember, in the future, you can buy your own equipment and have gained some experience of your chemical processes in a production environment.

Tolling also can offer advantages to an established chemical company. It provides a way to avoid capital investment or to respond to spikes in demand. In addition, I've heard that some firms like the idea of tolling because it looks more like a raw material in the accounting ledgers while operations sees it as an income source.

For a new product's pilot or launch, sometimes a chemicals maker's own equipment isn't suitable because it's designed to produce large volumes of product. So, using a toller with smaller equipment makes more sense during these early phases.

A contract manufacturer also can play a role in a business continuity plan by providing a second facility to make your critical product.

Table 1 summarizes the pros and cons of using a toll manufacturer.

FINDING POTENTIAL TOLLERS

Locating contract manufacturers with the technical expertise you need can be difficult; this is where an experienced chemical engineer or sourcing person is invaluable. Speedy success depends upon knowing how to search the Internet with key words for your product. A preliminary search should lead you to some tollers' websites. Then, talking to them on the phone — without revealing any details of your product — might give you insight into other key words to refine your Internet search. Now you can implement a project structure such as: Discover, Define, Develop, Deliver, Evaluate, Adjust (Table 2).

Once you have a candidate company or two, make contact with someone at the toll facility and do an initial evaluation for fit. It's often desirable early on to understand the business model of the toller (tolling versus manufacturing for its own sales, distribution, equipment sales, etc.), general business philosophy, quality management program, safety program, project management method, ownership, etc. Keep in mind the toller will be doing the same for your company!

Information sharing. You will need to give the candidate toller some information about what you want done. So, ahead of any of these discussions, carefully consider what information you're willing to divulge before a non-disclosure agreement is in place.

CONSIDERATIONS IN TOLLING

ADVANTAGES	RISKS
Experience of the toller	Loss of intellectual property
Reduced time to market	Scheduling of your product compared to other work
Technical expertise	Higher costs because toller must make a profit
No capital investment	Slow changes in the manufacturing process remain hidden
Flexibility	Incompatible partner chosen

Table 1. Using a contract manufacturer comes with both pros and cons.

A PROJECT SYSTEM FOR TOLLING

Discover	Who might be able to do this as well or better than we can? Have available nonproprietary specifications for the final product, production volumes, the laboratory process you have developed as well as safety risks.
Define	This is the research phase. Put a non-disclosure agreement in place. Share detailed versions of the Discover phase and hear what the toller can do for you.
Develop	This is an encompassing phase. It encompasses the first test batch of your product, and the formation of the back-office logistics. Pay attention to how the relationship is developing.
Deliver	The work agreement is signed and the first production order made and delivered.
Evaluate	You will evaluate the technical specifications but don't forget to assess the back office functions and the overall attitude. This continues forever....
Adjust	As with any process, you want to modify to achieve improvements. You get the toller's input and your company's expertise!

Table 2. Success demands paying appropriate attention as the project progresses.

Plan on sharing the following information (without any proprietary details):

- a description of your company's business, markets, and why you're considering tolling;
- an overview of the product to be made and expected yearly volume for three years;
- any safety risks of which you are aware;
- raw materials that require special storage conditions or handling;
- unit operations needed based on your product development work — the toller eventually may suggest a different path; and
- packaging requirements when leaving the toller's facility.

Photographs are worth a lot. Just ensure you don't show too much information at this point in the process.

Relationship structure. This might be a good time to consider how you will work with the tolling company. I prefer to view tolling agreements as partnerships as compared to dictatorships; in my experience, a partnership mindset provides better results. You want a match that allows the toller to make a reasonable profit while you get your product at a cost you can afford. A partnership should go both ways; so, get a sense if the toller shares that mindset. This does not mean the toller will "invest" in your company by taking a loss early on to reap benefits later. In fact, that's not a constructive approach for a steady relationship.

For a young company, your product quality probably will be higher from the get-go; you can work together on improvements to the product, desirable derivatives or even completely new chemical products for the market.

Disclosure of proprietary information. As discussions progress, sharing your proprietary needs will become necessary; so, you will want a non-disclosure agreement (NDA). Tollers are very familiar with these documents. Therefore, if you sense surprise at your request for a NDA, take that as a warning sign. You likely will end up with a mutual NDA because the toller will want to protect its proprietary information, too. A toller seeking a mutual NDA is being appropriately cautious; this also could signal that it expects to share sensitive information with you.

After the NDA is in place, you'll need to share in some detail what you want to do. That very well may include the chemistry, the process you've developed in the lab and, eventually, the quality specifications and test methods. In return, the toller will share some of its expertise and advise whether its equipment is suitable. Drawings and more detailed photographs can really speed up the information transfer. Don't consider it a failure if you sign a NDA and find out the toller can't accomplish the task. You may have gained some valuable information anyway; so, treat the episode not as a failure but as part of your research! The NDA protects your product information.

Digging deeper. If the initial technical discussions indicate a potentially good match, it's time to get more details about the toller. Don't simply send a generic manufacturing checklist or topics list. Instead, go through the topics and questions to determine what's important to your company. You'll drive yourself crazy trying to get data about all possible topics, so prioritize! The toller will appreciate getting one page covering really important stuff the first time you ask for information rather than having to answer four pages of questions about all sorts of things. You'll ask more questions as you finish each phase; knowing it has moved into the next phase will add to the toller's motivation to answer your next set of questions with care and detail. Take advantage of any opportunities to visit the toller's facility during these discussions. Face-to-face conversations usually add a great deal of value.

For any potential toller, make sure to investigate a number of topics:

- Does it perform the operations your product requires?
- What expertise and success does it have with similar chemistry or unit operations?
- What are its quality control and quality management programs?
- How much flexibility does it have for new projects? How is the toller's management treating your company's proposal?
- What method of new product management does it have to bring your product into its facility?
- What is its corporate culture like?
- How thorough is its regulatory understanding and how good is its compliance?
- What access will you have to its facilities and process data about your products? (You should get the data you want because it's your product!)
- Do you get along with and trust the people — e.g., the project manager, technical people, manufacturing floor operators and supervisors?
- How good is the technology it uses? (After all, equipment and expertise are reasons you are tolling.)
- What vertical services, such as buying raw materials, quality assurance of raw materials, drop shipping, etc., does it offer?
- How financially stable is the firm?

ESSENTIAL FOLLOW-UP

There's no cut-and-dried method for evaluating technical capability and back-office logistics. The possible partnership easily could fall part in this development phase. Here again, it helps to have a plan with priorities. Your company might be most comfortable with the toller showing laboratory proficiency; you may need pilot batches made for your customers (which gives you an opportunity to evaluate interactions with the toller), or maybe you're ready for the first production batch. You will need to pay a fee for service at this point; it could substantially exceed the cost set in the eventual production agreement. You are in product development and

development usually costs more per unit than production for reasons of size and increased risk. Consider any purchase orders at this phase as development expenses. Use this phase to confirm your comfort with the toller's technical ability, willingness to work with you, back-office logistics, shipping, etc. Again, pay attention to how it responds to things that don't go well, as this likely will track over to production.

I encourage you to visit the toller's facility no later than this development phase. Having your technical people on site for some portion of these initial batches is a good idea. Your people can bring insight to the toller's folks, explain quality testing, share anecdotal product/process observations and build a rapport. If you have a supplier audit team, members might attend to evaluate all the other aspects of doing business with this company.

The financial stability of your tolling partner is a serious matter. You are giving up direct control of the manufacturing of a promising product for your business — and, thus, exposing your company to risk if the toller stops making the product. So, you need to check public records on the financial health of the organization. Ask some reasonable questions about cash flow, accounts payable timeline, distribution of its income among different business segments or different customers. While at the facility, look for equipment that appears in disrepair, inventory not neat and orderly, and view posted safety and management notices to employees. You want to feel comfortable that the toller is not near bankruptcy and pays its bills on time. It, too, probably wants to know something about your company's stability. These are all reasonable requests when you want a functioning partnership.

PROCEEDING TO PRODUCTION

To move from development to manufacturing requires a detailed agreement of work. This will legally define responsibilities, e.g., how the manufacturing process and quality information is transferred, and the details of how communications will go between the two companies. The agreement must cover technical aspects and the back-office procedures. This is a supplier agreement with the added complexity of manufacturing to specifications. I suggest starting with your chemical supplier agreement and then blending it with aspects of your company's contract for services. If this arrangement is new to your company, consider asking the toller for a generic agreement that it uses and then build yours from that template.

By work agreement time, you should be very familiar with the toller's project and product management approaches. The work agreement should spell out critical-to-you components from the programs, including:

- communication methods;
- what the toller may adjust on its own;
- when your company can come into the facility;
- contact people at both companies specific to topics;
- practical methods of protecting your information;
- process-control-data tracking and availability; and
- whether the toller may subcontract any portion of your product.

Then, set up scheduled pre-production and post-production information transfer. Have your chemist or chemical engineer at the toller's facility for first production — it's a good investment. Test the back-office flow.

Plan on making adjustments to process and procedures with the toller; this is expected. Pay attention to how the toller responds to your requests and needs. Never lose track of the importance of the toller remaining a willing and able partner.

RELATED CONTENT ON CHEMICALPROCESSING.COM
"Try Before You Buy," http://bit.ly/35hgQCY
"Tap into Tollers," http://bit.ly/3s42Lme

Your initial test of the relationship could be the first time a batch is close to out of specification, misses the spec, or something happens that delays a shipment. Stay calm, listen to what the toller (partner) is saying and then try to work out the best solution to limit damage to both companies. Always remember that your own manufacturing isn't perfect. Expect some difficulties to occur and be prepared to work through them. At least with a tolling company you have additional resources and talent to assist in finding a satisfactory solution.

USE A TOLLER WITHOUT A TOLL

Opting for contract manufacturing often makes business sense. A toller's skilled, experienced production team can speed your time to market while reducing your risk of failure as a company new to chemical manufacturing. Moreover, the tolling option might offer lower manufacturing costs via efficient labor usage, experienced maintenance of equipment, economies of scale, and spreading of capital investment. You also get input from the toller — another set of eyes viewing your process and offering possible improvements in manufacturing and quality testing.

However, you must take steps to ensure you get what you need and leave nothing to chance. Don't assume the other party has all the bases covered; ask questions and get answers you understand. Build a strong, mutually beneficial work agreement that allows for changes as the relationship develops and stay in communication. Once you've selected your partner, give that firm the chance to show you what it can do. Provide the toller with the inputs and feedback it needs to excel. Mutual respect will lead to success of a well-crafted partnership with a qualified toll manufacturer. ●

DAVID MORSE is principal of DRM Chemical Process Services, Keene, N.H. Email him at drmchemicalprocess@gmail.com.

Take Better Care of Your Low-Pressure Boiler

A proper water treatment program is essential

By Brad Buecker and Chad Frierson, ChemTreat

MANY PLANTS use low-pressure boilers to produce process steam for various applications, including heat for chemical reactors, evaporators, building spaces, etc. Often, sites pay less attention to the chemistry programs for these steam generators than to those for high-pressure units. Yet, contaminated condensate return, malfunctions of makeup water treatment systems, and other factors can cause many problems.

Plant staff largely understand that high-pressure boilers require high-purity makeup to minimize corrosion and scale formation in the harsh environment of the boiler and superheaters. In a way, this makes chemistry control more straightforward because the makeup water, boiler feedwater and steam all should meet stringent guidelines. The most-common makeup water scheme for modern high-pressure units uses membrane technologies (micro- or ultra-filtration for suspended solids removal and reverse osmosis for primary demineralization), followed by ion exchange or continuous electrodeionization polishing to produce high-purity water. (For pointers on proper treatment of high-pressure boilers, see "Don't Get Steamed," http://bit.ly/2QzslvC.)

For lower-pressure steam boilers — here, we'll focus on units up to about 600 psi that don't drive turbines — makeup water treatment often is less rigorous. Usually, the leading concern is the potential for calcium carbonate ($CaCO_3$) scaling (Figure 1), as illustrated by the following reaction of calcium ions (Ca^{2+}) and bicarbonate alkalinity (HCO_3-) that can occur in hot water systems and boilers:

$$Ca^{2+} + 2HCO_3^- + \text{heat} \rightarrow CaCO_3\downarrow + CO_2\uparrow + H_2O \quad (1)$$

So, for decades, a typical primary treatment method for industrial boiler makeup was sodium zeolite softening. In this process, the water passes through beds of ion exchange resin that swap the hardness ions calcium and magnesium for sodium. The softened stream, with the remaining impurities, including alkalinity, chloride ions (Cl^-), sulfate ions (SO_4^{2-}), silica (SiO_2) and others, then feeds the boiler. Basic softening offers both advantages and drawbacks. The less-rigorous process, as compared to those techniques needed for high-pressure steam generators, saves the plant money in equipment and operating costs. However, many ions that aren't removed by sodium softening can become problematic upon reaching the steam generator. Alkalinity may convert to carbon dioxide (CO_2) in the boiler, which then carries over with steam. The CO_2 can lower the pH in the condensate return, which leads to potential corrosion issues in these systems. With just sodium softening, the introduction of the remaining dissolved solids to the steam generator increases the general corrosion potential of the water

CALCIUM CARBONATE SCALE

Figure 1. Precipitation from water can cause buildup on internal surface of heat exchanger tube.

due to higher conductivity, especially because the solids "cycle up" in drum boilers as steam is produced. Excess dissolved solids may induce foaming, which can boost impurity carryover to steam. Keeping the solids concentration at reasonable levels may require heavy blowdown. Chloride and, to a lesser extent, sulfate can be nasty impurities, especially in combination with oxygen in the boiler. The compounds also may concentrate under porous boiler-tube deposits, usually iron oxide corrosion products transported from elsewhere, e.g., condensate return systems, to induce acidic under-deposit corrosion (UDC). UDC continues to be a significant problem in industrial steam generators. (Low operating rates caused by the pandemic can spur UDC in other process equipment, see: "Keep Under-Deposit Corrosion Under Control," https://bit.ly/2ZtVq2V.)

Several methods can improve makeup water purity beyond basic sodium softening. Some of the older, established technologies are:

- *Split-stream dealkalization.* Such a setup places a sodium softener and strong acid cation exchanger in parallel, followed by a downstream forced-draft or vacuum decarbonator. Both sets of ion exchange resins remove hardness but the acid generated by the cation exchanger converts alkalinity to CO_2, which is removed in the decarbonator. The process doesn't remove chloride, sulfate or silica.
- *Hot lime softening.* This will remove most of the hardness, alkalinity, silica and iron. It doesn't remove chloride.
- *Ion exchange demineralization.* Demineralizers come in various forms but, in general, if they have both cation and anion exchange capacity, they will remove most dissolved ions, including chloride and sulfate.

The first two methods use somewhat outdated technology. The development and maturation of membrane technologies, particularly for reverse osmosis (RO), have altered the landscape. Single-pass or especially two-pass RO can produce makeup water with very low dissolved solids, including the hardness ions and silica. Keys to successful operation of RO units are pretreatment to remove suspended solids ahead of the RO membranes and optimized chemical treatment to minimize scale formation on the membranes. Careful analysis of RO feedwater is critical for proper pretreatment equipment and chemical selection. Also, RO generates a near-steady wastewater stream that requires handling. For a plant with a cooling tower, the tower basin may serve as a good repository. Otherwise, a site may need alternative disposal methods.

A critical point to note, especially at an existing facility, is that making a change to higher-purity makeup for any application necessitates re-evaluation of chemical treatment programs. The change in water purity, even (seemingly) for the better, may lead to unforeseen consequences if not addressed properly.

BOILER-WATER TREATMENT

Back in the 1930s, as power generating units increased in number and size, trisodium phosphate (Na_3PO_4 or TSP) became a popular boiler-water conditioning chemical for drum boilers. In the utility industry, phosphate treatment programs have undergone much evolution, with a return to just TSP, albeit in low dosages, common for modern units. For industrial boilers, phosphate treatment methods remain a strong choice.

A primary function of phosphate is to generate moderately alkaline conditions in the boiler to minimize general corrosion of carbon steel boiler tubes, drums, and headers:

$$Na_3PO_4 + H_2O \Leftrightarrow Na_2HPO_4 + NaOH \qquad (2)$$

Although TSP is the only recommended phosphate species for utility boilers (to minimize acid phosphate corrosion potential), in industrial units TSP may at times get blended with lesser amounts of disodium phosphate (Na_2HPO_4) and perhaps, although usually not recommended, even a bit of monosodium phosphate (NaH_2PO_4) to control excess formation of sodium hydroxide (NaOH), also known as caustic. Caustic can concentrate underneath porous boiler tube deposits and induce direct corrosion of the boiler metal, in this case due to excess basicity as compared to acidic chloride attack.

A second function of phosphate, which is particularly important for units in which hardness ions periodically may ingress, is to control scale formation. Phosphate, and the alkalinity produced by its reaction with water, can react with hardness ions to form soft sludges as opposed to hard scale. Often recommended with phosphate treatment are sludge conditioners consisting of water-soluble polymers that help keep solids in suspension by a combination of dispersion, crystal modification and sequestration. Such sludge conditioners can enable effective blowdown of otherwise troublesome iron particles from condensate return system corrosion. These polymers sometimes can serve as a stand-alone treatment, particularly if hardness ingress isn't an issue. Another technique successfully employed at times in industrial drum units, but not utilized much today, is chelant chemistry, in which the chemicals directly bind with metals to keep them suspended. Ethylenediaminetetraacetic acid (EDTA) is

RELATED CONTENT ON CHEMICALPROCESSING.COM

"Don't Get Steamed," http://bit.ly/2QzslvC
"Plant Combats Corrosion in Idled Boilers," http://bit.ly/2GS5Bm4
"Don't Foul Up Your Water Treatment Program," https://bit.ly/32rralb
"Improve Your Cooling Tower Treatment," http://bit.ly/2Z3k0Et
"Plants Benefit from Better Cooling Tower Treatment," https://bit.ly/3frCw2p
"Conquer Cooling Water System Challenges," http://bit.ly/2Pq7oDt

the most widely known chelant, and has served for many applications often outside the steam generation industry. However, improper use or control of chelants can cause localized corrosion of boiler components.

The upshot is that several possibilities exist for boiler water treatment. The proper choice depends upon a variety of factors that include boiler design and pressure, makeup-water treatment sophistication and reliability, and the potential for impurity ingress from condensate return. These factors require careful evaluation for each case. A "one size fits all" approach to treatment selection can lead to problems.

Film-forming products (FFPs) for steam generator treatment are under development. These compounds provide a protective hydrophobic layer to metal surfaces to inhibit corrosion. Reports of successful applications of some FFPs continue to emerge but use requires diligent planning and monitoring.

FEEDWATER AND CONDENSATE-RETURN TREATMENT

A large influence on boiler water chemistry can come from ingress of corrosion products or impurities from the feedwater system and condensate return. A top priority is maintaining moderately alkaline conditions in these systems to prevent general corrosion of carbon steel, the typical material for feedwater and condensate return piping. In the power industry, the common pH-conditioner is ammonia, which raises the feedwater pH via the following reaction:

$$NH_3 + H_2O \Leftrightarrow NH_4^+ + OH^- \quad (3)$$

Because this is a reversible reaction, the alkalinity increase is limited, which usually minimizes excessive corrosion to steel in the event of a chemical feed upset. (Copper alloy corrosion is a completely different story.) For industrial boilers, neutralizing amines (Figure 2) are a common choice for condensate/feedwater pH conditioning. These are small-chain organic molecules with an ammonia group attached to or embedded within the compound.

The amines all have a higher molecular weight than ammonia and, thus, won't flash off nearly as extensively as ammonia does to steam — although each has its own distribution ratio, i.e., the amount that remains in the water versus that which departs with steam, whose properties are a function of temperature and pressure. The products also have different basicities, which provides flexibility in selecting a treatment program. Careful evaluation of boiler operating and design conditions is necessary to select the most appropriate amine or amine blend. Some compounds aren't allowed if the steam can directly contact food and other consumable products.

Neutralizing amines often are very important for minimizing corrosion in condensate return systems, particularly if the boiler water contains significant alkalinity. Carryover of CO_2 to steam can depress the pH in the recovered condensate; substantial iron corrosion may result unless the pH is adjusted with a neutralizing chemical.

The potential exists at many plants for impurity ingress from process heat exchangers or other sources. Some form of condensate polishing can prove beneficial but determining the constituents to remove requires careful analysis. If iron particulates from condensate return system corrosion are the major issue, then fabric filter techniques might suffice. Ion exchange can remove dissolved ions such as sodium, hardness, chloride, silica, etc. If organic compounds are the problem, activated carbon filtration or specialty exchange resins may be the answer. Factors that influence condensate polisher selection, such as flow rate, temperature and potential for media fouling, again are specific to each plant.

COMMON NEUTRALIZING AMINES

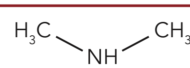
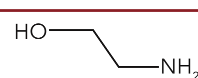
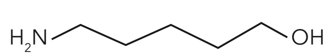
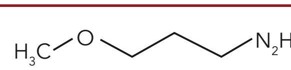
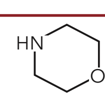
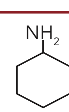
Amine	Chemical Formula	Molecular Weight (g/mol)	Structure
Dimethylamine	C_2H_7N	45.08	
Ethanolamine	C_2H_7NO	61.08	
5-Aminopentanol	$C_5H_{13}NO$	103.16	
3-Methoxypropylamine	$C_4H_{11}NO$	89.14	
Morpholine	C_4H_9NO	87.1	
Cyclohexylamine	$C_6H_{11}NH_2$	99.2	

Figure 2. Boasting higher molecular weights than ammonia, these compounds won't flash off as much.

DON'T FORGET DISSOLVED OXYGEN

The issue of control of dissolved oxygen (DO) can be a bit thorny. For many years, the accepted wisdom in the power industry was to remove all DO from feedwater. Facilities relied on mechanical (deaerators) and chemical (oxygen scavengers/reducing agents) methods to accomplish the goal of zero oxygen at the inlet to the boiler economizer. However, in the 1980s (and continuing to this day), issues regarding flow-accelerated corrosion (FAC) began to appear;

TRAY-TYPE DEAERATOR

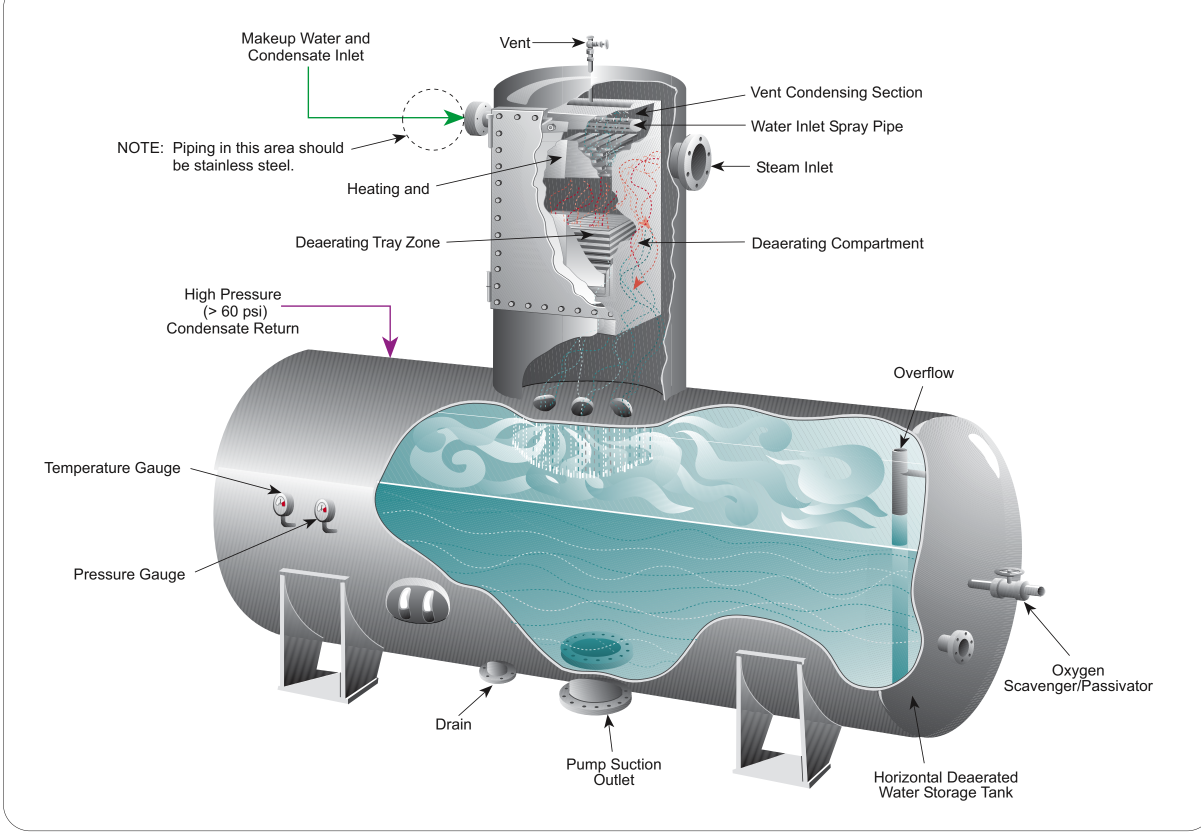


Figure 3. Steam scrubbing of makeup water and condensate return injected at the top of the tray section removes dissolved oxygen.

in some cases FAC-induced failures caused fatalities. This corrosion results from gradual dissolution of the protective oxide layer (magnetite, Fe_3O_4) that forms on carbon steel at startup but leaches away at flow disturbances, e.g., elbows, in the reducing conditions established by an oxygen scavenger. (Temperature and pH also are important factors.) In the meantime, researchers discovered that for units with high-purity makeup (less than 0.15 or 0.2 µS/cm cation conductivity depending upon the particular program employed), some dissolved oxygen in the condensate actually proves beneficial, causing carbon steel to form a tight, reddish-colored, protective oxide layer, different than the gray-black magnetite normally observed. Thus, these mildly oxidizing chemistry treatments now are recommended for almost all high-pressure utility steam generators unless the condensate/feedwater system contains copper alloys.

However, industrial boilers usually receive less than high-purity makeup water, so DO control is quite important to minimize oxygen attack of steam generator components. Most systems come with a mechanical deaerator (Figure 3), which, when operating properly, should reduce the DO concentration to 7 ppb.

In addition, normal practice is to use a chemical oxygen scavenger, often either un-catalyzed or catalyzed sodium sulfite (Na_2SO_3):

$$2Na_2SO_3 + O_2 \rightarrow 2Na_2SO_4 \qquad (4)$$

A common injection point is the deaerator storage tank. The combination of mechanical and chemical methods usually can protect the steam generator against significant oxygen corrosion.

Space limitations prevent a comprehensive discussion of chemistry monitoring here. However, one critical item is iron monitoring, which the power industry has adopted as a standard parameter and which other plants should use as well. On-line and grab sample methods are available to track corrosion products and determine the effectiveness of pH-conditioning and oxygen-control methods. Steam generator protection during outages also is important; “Plant Combats Corrosion in Idled Boilers,” http://bit.ly/2GS5Bm4, provides some insights on this. ●

BRAD BUECKER is a senior technical publicist for ChemTreat, Glen Allen, Va. **CHAD FRIERSON** is a technical consultant with ChemTreat, Glen Allen, Va. Email them at bradley.buecker@chemtreat.com and cfrierson@chemtreat.com.

Plants Look Off Site for Insights

Pandemic fosters use of remote access and virtual attendance

By Seán Ottewell, Editor at Large

THE OUTBREAK of COVID-19 has forced chemical companies and their vendors to find new ways to carry out activities. The experiences of INEOS Styrolution, Endress+Hauser and Emerson exemplify innovative efforts to share valuable information.

"Similar to most companies, at the start of and continuing through the pandemic, INEOS Styrolution significantly reduced and, in some cases, completely eliminated travel. As a result, we recognized early on that we would need to find new ways to complete activities that we normally accomplish in person," says Melissa Cohen, vice president supply chain and procurement, INEOS Styrolution, Americas, Aurora, Ill.

RELATED CONTENT ON CHEMICALPROCESSING.COM
"Wearables Win Wider Role," http://bit.ly/35Efv9x
"Drones Fly Higher," http://bit.ly/3bAb0R1
"*CP* COVID-19 Coverage," https://bit.ly/2A0RX20

With most non-operations personnel working from home, the company clearly needed to find technology to allow staff to view activities and equipment virtually.

After assessing several commercially available options, INEOS opted for HMT-1 and HMT-1Z1 devices from RealWare, Huntsville, Ala. The units, regular and intrinsically safe, respectively, include a camera and snap on to hardhats.

"The intrinsically safe model was very important as this is a requirement for some of our manufacturing areas. Their cameras have great clarity, a very important requisite for remote monitoring, and they have a great deal of software capability including integration with Microsoft Teams. We are still working through a couple of issues to get the technology to work completely. For instance, in our very large sites, Wi-Fi is not always available everywhere," notes Cohen.

At the beginning, the plan was to use the RealWare technology primarily to complete safety and environmental audits. However, the company has continually found new applications for using remote monitoring tools, she reveals.

Here, she cites their value for factory acceptance testing of equipment for a new plant currently under construction at the firm's Bayport, Texas, facility (Figure 1).

"Normally, the engineering team schedules an in-person visit to certify that the equipment meets specifications before it ships to the site. Since some of our equipment is being manufactured overseas, it is extremely difficult and sometimes impossible to complete this testing in person. With the new technology, the vendor can walk us through the testing of the equipment in real time and we can ask questions or direct them to make changes according to our needs," explains Cohen.

Another use is during routine safety and environmental audits of the company's plants — including as part of its membership of Operation Clean Sweep, an international program designed to prevent and help keep plastic litter materials out of the marine environment.

"Earlier this year, we tried to use iPhone technology to reach a wider group of auditors and, although this worked to some extent, the new technology will allow us to be much more efficient."

"There are many possibilities for utilization of the technology that we have not explored yet. Another of our primary objectives is to conduct customer trials remotely, as it is significantly easier to arrange the time for a remote trial based on the customer's availability versus trying to synchronize multiple travel schedules. Other options for use include interior and exterior vessel inspections, and warehouse cycle counting, to name a few," Cohen states.

INEOS Styrolution currently is rolling out the technology both in the Americas and Europe. If the technology continues to prove successful, the company plans to extend its use to its Asian sites as well.

Because of its benefits, the technology likely will continue to play a role even when travel restrictions lift, believes Cohen.

REMOTE SUPPORT

Instrumentation and automation supplier Endress+Hauser, Reinach, Switzerland, found that many of its customers were struggling to conduct critical service work on instrumentation at their sites during the pandemic. Fortunately, the outbreak coincided with pilot tests of the company's cloud-based Visual Support technology that enables audio-visual support for diagnosis and troubleshooting, commissioning and regular maintenance of field devices (Figure 2). With the help of live video transmission and screen casting, its technical support team can work almost as if they were on-site, helping customers in a reliable and flexible manner with their service tasks via remote access, says the company.

The pilot involved integrating Visual Support into its support services portfolio, giving customers access to in-depth technology and product knowledge, including guaranteed availability and response time from Endress+Hauser's global network of technical experts.

For ten weeks from March to May last year, the company offered the pilot service free of charge to customers. During that time, Endress+Hauser conducted more than 250 Visual Support sessions worldwide.

"Customers gave us a lot of positive feedback," says Franck Perrin, corporate director service excellence.

TEXAS APPLICATION

Figure 1. New camera technology eases handling of a range of activities at the site. *Source: INEOS Styrolution.*

"They are enthusiastic about this new form of support and have experienced how Visual Support can save time and money."

The positive response to the pilot spurred the company to speed up integration of Visual Support into its support service offering.

At the heart of Visual Support is a visual assistance platform developed by Sightcall, San Francisco, targeted specifically at improving the efficiency of field services.

"The application runs on Android or IOS smartphones as well as Windows-based computers. This tool is fully embedded into the Endress+Hauser CRM and service delivery platform. From here, our service engineers have access to all necessary technical information about field devices. Important information from the visual support sessions is captured to give transparency and provide a documented case resolution to our customers," notes Perrin.

"We have seen numerous cases where problem identification took place much quicker and issues were solved faster respectively using the new technology. We learned

Figure 2. Off-site experts use live video streams to help plant personnel deal with instrumentation issues. *Source: Endress+Hauser.*

Figure 3. For the first time, visitors can tour the center virtually as well as in person. *Source: Emerson.*

that we could indeed solve issues remotely that used to require a field service call-out from a specialist," he adds.

For example, he cites the success of the approach in solving a flow measurement problem in the water treatment plant of a food and beverage maker. There, the water flowing through wasn't measured correctly. The local technical staff couldn't detect any visible problems or damage when checking the device; so, they assumed the meter must be damaged because no readings were displayed. The Endress+Hauser technical support team used Visual Support to inspect the installation and check the settings via the device display.

"Our expert identified a problem due to incorrect commissioning of the device. After adjusting the low flow cutoff value, the unit worked properly again — only three hours after the call to Endress+Hauser, with the remote session lasting only one hour from the visual inspection to the adjustment of the unit settings. Most importantly, the customer was able to avoid a field service visit from an expert and the time and cost associated with that," stresses Perrin. Moreover, the rapid solution of the problem meant the customer didn't lose any production.

Now, the company is working on the next extension of its support service offerings. This will enable establishing a remote connection on the Endress+Hauser device configuration tablet, the FieldXpert.

"Remote connection via screensharing to FieldXpert has been piloted extensively and it is clearly seen as an added value. Globally, we launch the new offering together with the FieldXpert bundle in the next coming weeks," he notes.

VIRTUAL ROADSHOW

Meanwhile, Emerson, St. Louis, has introduced a virtual option for its annual roadshow, in which a mobile service center equipped with the latest advances in digital transformation for machine safety, machine automation systems and fluid control, tours multiple countries (Figure 3).

The idea is to give both in-person visitors and virtual attendees access to materials and videos highlighting new products and technologies from the company. How to use Industrial-Internet-of-Things-based technologies as part of a digital transformation strategy, and how to use machine safety in pneumatics to reduce risk without compromising productivity get particular emphasis.

"Due to current travel limitations, we created a digital event that allows us to connect globally with customers in new and exciting ways by virtually touring the mobile service center," said Wolf Gerecke, director of pneumatic product marketing for Emerson's Automation Solutions business, at the launch in November.

The mobile roadshow runs for 11 months across multiple countries. It already has travelled to several customer sites in Germany, with other visits planned for France, the Czech Republic, Poland, Italy and Spain into the spring of 2021. ●

Build Safer and More Reliable Seal Support Systems

Follow some best practices to enhance operations and reduce overall costs

By Sean Hunsicker, Swagelok Co.

CENTRIFUGAL PUMPS at chemical plants and refineries usually rely on mechanical seals to prevent fluid from escaping. Every seal connection is a potential leak point — and any leak can lead to asset damage, unplanned downtime, environmental issues and safety risks. Therefore, taking a holistic view and paying special attention to not only the mechanical seal itself but also the entire seal support system is important.

Mechanical seals became the dominant sealing system for petrochemical processing operations in the 1980s, prompting the American Petroleum Institute (API) to establish a committee to write standards for these components. The committee's work led to the publication of a standard, "API 682 — Shaft Sealing Systems for Centrifugal and Rotary Pumps," in 1994 [1]. Its mission statement read: "This standard is designed to default to the equipment types most commonly supplied that have a high probability of meeting the objective of at least three years of uninterrupted service while complying with emissions regulations."

Now in its fourth edition [2], much of the API 682 standard focuses on mechanical seals. However, it also devotes significant space to seal support systems and their proper operation due to their critical importance in the overall reliability of the entire pump skid. Best practices covered in the standard include proper seal support system design, elimination of potential leak points wherever possible, and selection of components that simplify maintenance. This article will explore these best practices to help plants increase reliability, maximize efficiency and improve safety.

MORE LEAK POINTS, MORE RISK

Most plants historically have handled fluid conveyance with piping, which typically is made from carbon steel and features numerous threaded connection points throughout each run. So, sites often also turned to piping for seal support systems. However, the current edition of API 682 recommends reducing threading and connection points wherever possible. This guideline has fostered a notable shift to bendable tubing systems becoming the preferred

COMPARISON OF CONNECTIONS

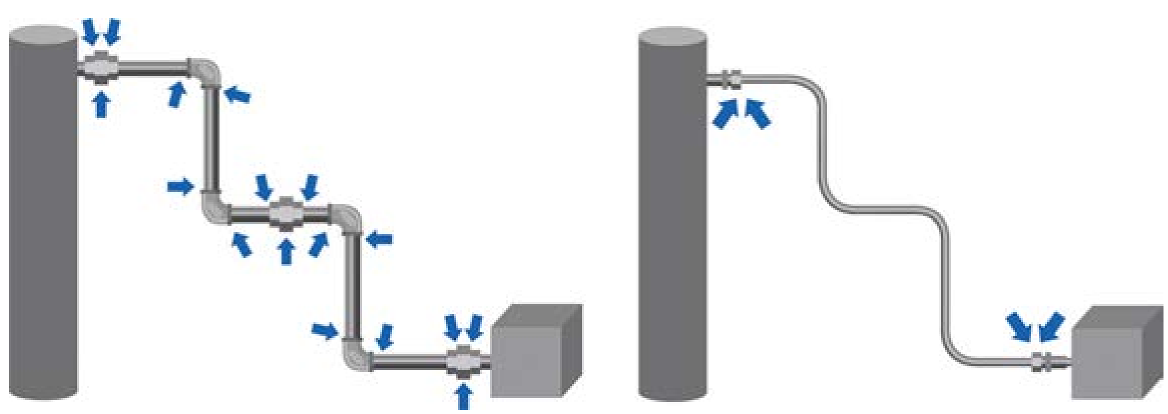
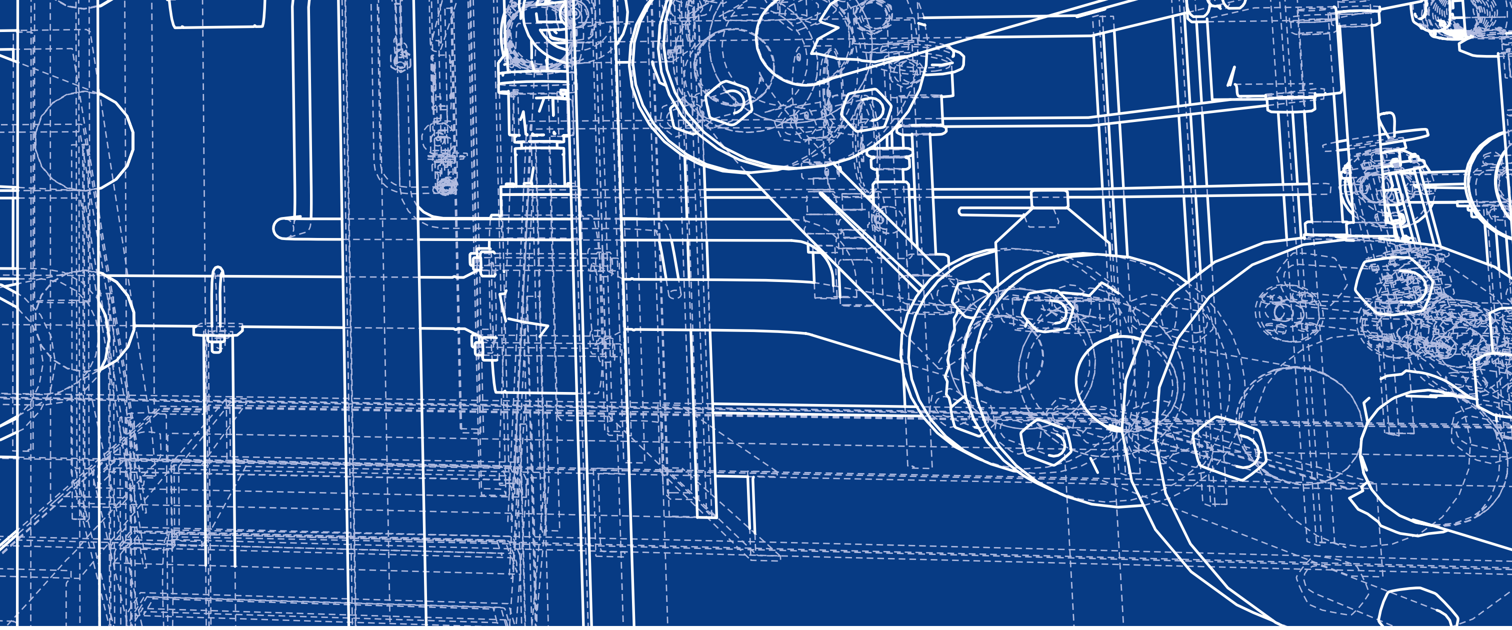


Figure 1. Opting for tubing instead of threaded piping can reduce the number of connection points significantly and, thus, the potential for leaks.



choice among seal manufacturers, end-users, and pump original equipment manufacturers. Plants also have the option to weld carbon steel pipe to minimize threaded connections but the corrosion resistance, flexibility and efficiency benefits of using stainless steel tubing often tip the scales in its favor.

By design, tubing can reduce the number of connections to just those at the mechanical seal and the seal support system (Figure 1). Therefore, the system might only have two to four potential leak points, depending on its configuration. Minimizing the number of connection points and reducing leak potential are possible due to a variety of factors, including:

- Innovative connections, such as flange adapters and extended male connectors; these help decrease the number of connections from threaded ports on seals and seal pots by eliminating the need for multiple fittings.
- Leak-tight tube fittings that can prevent leaks during regular system operation and are easier to service when needed.
- Tubing made from annealed stainless steel, so it can be bent, which lessens the need for fittings and connections. It also resists corrosion, which reduces ongoing maintenance.

The use of tubing provides further financial benefit when examining the maintenance, repair and operation (MRO) costs of the pump, seal and support system. During maintenance operations that require reworking welded piping around pumps, using tubing instead can eliminate the need for costly on-site welding and also speed installation time to reduce downtime.

While bendable tubing offers efficiency benefits to cut installation and MRO labor costs, it is more expensive than carbon steel piping; it can become particularly expensive when using special alloys to combat corrosion. Construction of piping systems in special alloys also is possible but material options are more limited. Therefore, system designers may need to weigh the overall costs of using either tubing or piping — while also factoring in corrosion resistance, aesthetics, MRO activities, supply logistics and more — to make a decision.

Carbon steel piping is perfectly acceptable for many seal support systems such as flush plans. However, it can pose a risk for applications in which moisture is present and internal corrosion is a possibility. For example, the scale that commonly builds up on the inside of carbon steel pipe can break away, flow downstream and then lodge in the gap between seal faces or clog an orifice. Using carbon steel in systems where scaling is a possibility calls for scheduled preventive maintenance (PM) and close monitoring of the system.

Ultimately, the choice between pipe and tubing might come down to the comfort level of the person making the decision. That said, optimizing the system and making it

EFFECTIVE PLAN 32

Figure 2. Installing the plan onto a panel enables proper identification of components and processes and also streamlines system operation.

more reliable necessarily should place priorities on decreasing maintenance, improving performance, and enhancing safety by reducing leak points and threaded connections wherever possible.

SYSTEM OPTIMIZATION

The reduction of leak points is just one aspect of optimizing the system. There also are best practices to follow during the initial design of the mechanical seal and seal support system to help operators ensure proper operation of the seal and pump as well as to improve safety and reliability.

1. Make inspection easier for operators. During turnarounds and other operations such as routine maintenance, pumps and seal support systems often are visually inspected. Simplified designs can facilitate proper commissioning and operation of seal support systems, lowering the risk of operators making common mistakes.

Creating even small obstacles for operators increases the risk of missing trouble signals and, thus, reducing reliability. For example, API 682, 4th ed., shows a Plan 32 design for a flush stream from an external source as multiple instruments and components installed together in a run using either piping or tubing. While functionally correct, this design provides the operator with little information regarding the operation of the system, what information is important, and why it is important. The location of the system can pose further difficulties; if placed next to the seal on a pump, the operator must bend down to read instrument information.

An alternative and more-effective solution is to arrange these components on a panel using the Plan 32 design as a template (Figure 2). Mounting the components to a panel increases awareness that the configuration is a distinct system, which helps operators better identify components and their functions as well as confirm proper operation. A few best practices to follow include:

- Place all instruments at eye level rather than locating components on a less-accessible piping or tubing run.
- Meet API 682, 4th ed., design recommendations (in 9.1.5) that state: "All controls and instruments shall be located and arranged to permit easy visibility by the operators, as well as accessibility for tests, adjustments, and maintenance."
- Clearly display part numbering information, flow path indication and operator instructions to ensure safe and reliable startup and shutdown of pumps and seal support systems.

2. Simplify maintenance. Like the equipment they support, seal support systems typically operate continuously — so, their reliability is crucial. Using high-quality materials (Figure 3) and ensuring the systems are well maintained are important to prevent leaks and costly downtime.

Seal support systems contain commonly serviced items, such as strainers, flow meters and other instruments. Placing components in inconvenient locations can hinder their getting proper attention and adequate PM, especially if a plant is understaffed. Design should ensure operators can simply

DESIGNING FOR MAINTAINABILITY

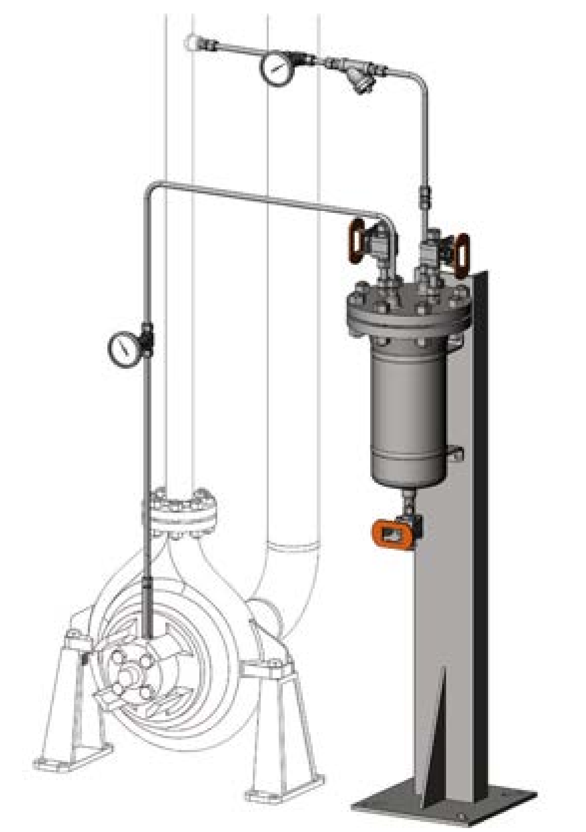
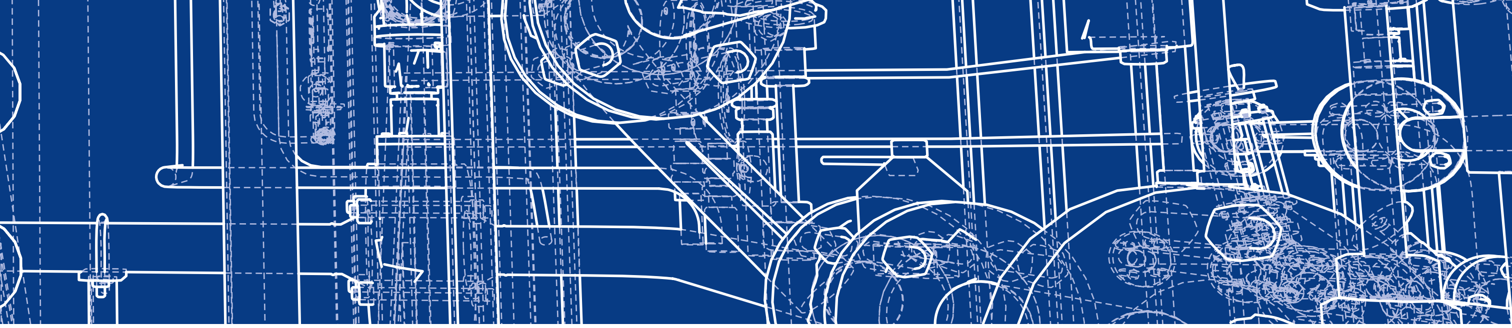


Figure 3. Using high-quality, easy-to-maintain components can maximize uptime of systems such as this API Plan 22 cooled flush system with strainer.

RELATED CONTENT ON CHEMICALPROCESSING.COM

"Rethink Your Seal Support System," http://bit.ly/3rWB3ro
"Consider Air Seals Advantages," http://bit.ly/2XjhADd
"Enhance Centrifugal Pump Reliability," http://bit.ly/2FJhg5t
"Specify the Right Slurry Seal," http://bit.ly/2HGVcyL



and safely perform PM on these systems. A well-designed and dependable system can help a plant reduce maintenance needs and costs.

Consider the process for performing general pump maintenance, which requires blocking in and draining the pump and support system. A well-designed support system can simplify this maintenance requirement by including low-point drains that allow purging of fluids quickly and safely. High-point vents also are important to include for removal of any entrapped air. Providing installers with the proper tubing and components, along with a drawing showing where to place vents and drains, ensures correct system installation and easy performance of future maintenance.

API 682, 4th ed., also recommends using block-and-bleed configurations for all gauges (Figure 4), so technicians can swap out a broken gauge with ease. If systems don't include this feature, as gauges fail, operators likely will lack critical information until the pump and support system can be decommissioned to replace the gauge.

For seal pots, API 682, 4th ed., encourages easy accessibility. It (in 8.1.8) stipulates: "Local operation, venting, filling, and draining shall be accomplished from grade. Unless otherwise specified, systems that require the use of a ladder or step or that require climbing on the baseplate or piping are not acceptable." Many plants have older seal pots with just a pipe plug at the top. Having operators climb a ladder to top off the pot can expose them to process vapors and generally is an unsafe practice; so, avoid this altogether.

Lastly, a wide variety of tubing connections and design options exist that allow easy removal and replacement of every serviceable component in a seal support system while continuing to operate the system. Implement these technologies wherever possible to help simplify and streamline seal support system maintenance and operation.

IMPROVE SAFETY AND RELIABILTY

Mechanical seals are only as good as the systems that support them. Careful design and use of high-quality materials for seal support systems can significantly enhance the operational efficiency, reliability and safety of a plant. Implementing design best practices can help reduce costs and reduce headaches.

To recap the actions plants can take to realize better results with their seal support systems:

- Consider using tubing instead of threaded or welded pipe to decrease installation and maintenance costs.
- Reduce potential leak points and eliminate the use of threaded connections wherever possible.

API-682-RECOMMENDED GAUGE CONFIGURATION

Figure 4. Using a block-and-bleed configuration enables easy gauge replacement without the need to decommission the pump and support systems.

- Make the design intuitive to lessen operator error.
- Mount systems on panels with proper labeling for easy maintenance and to promote system reliability.

Finally, always follow API 682, 4th ed., best practices to avoid seal failures and the associated costs of replacement and downtime, while also creating a safer and more reliable operation. ●

SEAN HUNSICKER is market manager, chemical & refining market for Swagelok Co., Solon, Ohio. Email him at Sean.hunsicker@swagelok.com.

REFERENCES

1. "API Standard 682 — Shaft Sealing Systems for Centrifugal and Rotary Pumps," 1st ed., American Petroleum Inst., Washington, D.C. (1994).
2. "API Standard 682 — Shaft Sealing Systems for Centrifugal and Rotary Pumps," 4th ed., American Petroleum Inst., Washington, D.C. (2014).

Control System Modernization Achieves Multiple Goals

Effort addresses technology obsolescence, enhances lifecycle management and paves way for faster digitalization

By Natarajan Muthaiah, Chevron Oronite; and Marjorie Ochsner, Honeywell Process Solutions

CHEVRON ORONITE, a subsidiary of Chevron Corporation, is a leading developer, manufacturer and marketer of lubricant and fuel additives and chemicals. The company's operations include world-class facilities in the United States, France and Singapore, as well as smaller-scale regional plants.

Chevron Oronite has embarked on a journey to achieve digital transformation — converting data to information, information to insights and insights to decisions. Naturally, the company also kept digital acceleration (i.e., speeding the transformation) in the forefront when starting an ambitious control-system-modernization planning effort as part of its lifecycle management strategy for control system assets. This focuses on upgrading the system for process control, improving workflow efficiencies and operator effectiveness, and digital acceleration initiatives, among other benefits.

Over the years, the company's control platform has included a combination of legacy and new distributed control systems (DCSs) from Honeywell, programmable logic controllers, wireless systems, integration with enterprise resource planning systems, and more. Chevron Oronite's strategic outlook on process automation, based on a roadmap for meeting its modernization requirements at its U.S. site, includes:

- Modernizing in a low-risk direction using a modular approach;
- Furthering the establishment of a multi-year roadmap and buy-in of all stakeholders; and
- Reaping early benefits from new technology such as by adopting some calculated "high-risk, high-return" measures.

The company required new ways to manage the lifecycle of its automation assets while employing new digital technologies combined with data-driven insights to transform operations, boost agility and enhance strategic decision-making. Like other manufacturers, it is managing the retirement of experienced personnel and the training of a new generation of workers not familiar with legacy DCS technology.

STEPPING INTO THE FUTURE

As part of a comprehensive control-system-modernization effort, Chevron Oronite established a multi-year migration plan and undertook one of the first major implementations in North America of Honeywell's Enhanced High-Performance Process Manager (EHPM). It is a process-connected device on Honeywell's Enhanced Universal Control Network (EUCN) that provides regulatory control and sequence operations. EHPM enables unification of control functions and data exchange between devices on the fault-tolerant-ethernet (FTE) based EUCN to help improve operations and control performance. It works in tandem with the updated Experion Local Control Network (ELCN) to preserve existing control applications, graphics and procedures in their entirety while allowing a plant to benefit from the capabilities of a new, advanced control system. This was followed with similar efforts in its Singapore location.

Chevron Oronite's specific migration activities included:

- Retaining its legacy control applications while migrating to a modern control platform;
- Deploying EHPMs as peer-to-peer nodes with existing controllers;
- Using FTE technology to keep existing functionality and embedded applications; and
- Integrating legacy controllers within the new DCS infrastructure.

Planning for the modernization program started in 2013. The first phase — operator graphics conversion, human/machine interface (HMI) and control network implementation, and historian upgrades — began in 2014 and ended in 2017.

The second phase — domain upgrades, virtualization within the process control network, control system integration and implementation of advanced technology — started in 2017 and was completed in 2020.

The third and final phase of the program — migrating to the latest batch control systems, Experion Batch, and deploying modern unit operations controllers, advanced batch visualization, in-batch reporting, etc. — currently is in the implementation stage, covering both its U.S. and Singapore sites. This started in 2020 with two implementations, one each in the United States and Singapore that were completed successfully. In 2021, three more implementations are to occur at these two facilities.

All migration, modernization and upgrade work across these multiple global sites should finish this year, with systems being upgraded to the latest Exp R 520.x release.

Chevron Oronite is translating its modernization strategy to a digital vision by breaking down efforts into step-by-step deployments with clear value propositions:

- Extending the life of its modern control environment;
- Improving configuration and change management;
- Optimizing alarm and operations management;
- Moving laboratory data into the plant historian for a single source of information for process analysis, quick visibility for operators, etc.; and
- Enhancing operator effectiveness and agility through a high-performance HMI, procedural operations functions, advanced reporting, reference/golden batch, advanced batch visualization, etc.

PRESERVING EXISTING INVESTMENTS

The key to the modernization is promoting that different generations of control systems can run in the same environment with a common, seamless interface for plant operators. Saving existing configured applications is a very important aspect of this initiative.

Chevron Oronite is upgrading or replacing current process controllers with modern Honeywell technology to enhance process control performance and address obsolescence. Its objectives are to retain control strategies, operator displays and history/trend information while minimizing disruption to plant operations. Modernization activities have addressed traditional local-control-network and architecture data flow challenges. In addition, they will provide a standalone, class-based, virtualized batch system without the need for a separate batch server.

The project team had the flexibility to choose either physical or virtual options — and opted for virtualization, with an eye toward reducing overall system footprint.

IMPROVED INTERFACE

Figure 1. Control room displays now feature a high-performance human/machine interface that follows Abnormal Situation Management Consortium guidelines.

Virtualization offered a way to preserve and extend investments in decades-old DCS technology. It also increased availability versus a physical platform and helped to simplify the control system architecture. The deployment of controllers and traditional control network nodes in a virtual environment will be the next major undertaking — which is expected to be completed this year following the Experion Batch implementation in its U.S. facility.

For Chevron Oronite, an important part of the modernization program involved upgrading how it detected and averted abnormal situations and implementing effective alarm management aligned with industry standards. This approach helped address alarm configuration problems and decrease alarm floods, established an alarm philosophy for the plant and reduced redundant alarms, and provided operators with a real-time view of the actions needed during an event. Furthermore, a robust boundary-management application now alerts operators to abnormal situations before alarm events occur.

Finally, the company has focused on lifecycle management to enhance its control system infrastructure. The scope of this effort encompasses the DCS, along with control network installations. Migration will help ensure a common DCS front-end platform across all control rooms while keeping the back end on a combination of legacy and new technology.

CHANGING WITH A VISION

When it comes to accelerating digital transformation, Chevron Oronite plans to better manage the lifecycle of its critical control-system assets while providing leadership with enhanced data-driven decision-making capabilities. The company has shown that change must be driven with a vision using a bottom-up and top-down approach, from management and business leaders to plant operators and field technicians.

The ongoing migration, modernization and upgrade work is making sure operations are up to par with current technology; improving operator effectiveness through abnormal situation management, integrated alarm management, automated procedures, etc.; expanding interfaces to the business and third-parties; streamlining data flow from business to DCS and implementing better analytics.

RELATED CONTENT ON CHEMICALPROCESSING.COM

"Control Systems: Cut Cutover Concerns," http://bit.ly/2mHTLpW
"Dodge DCS Migration Startup Surprises," http://bit.ly/2LE9eU8
"A Stragtegic Approach for Upgrading Process Control Systems, Part 1," http://bit.ly/2oiR6DA
"A Stragtegic Approach for Upgrading Process Control Systems, Part 2," http://bit.ly/2p3Qsdr
"A Stragtegic Approach for Upgrading Process Control Systems, Part 3," http://bit.ly/3nBlvGj
"Optimize Control System Migration," http://bit.ly/2ns4jtU
"Migrate Without a Migraine," http://bit.ly/2npau1P

In terms of reaping early benefits, Chevron Oronite's migration strategy provides an effective means of dealing with aging control system technology. This technology, if left unattended, could undermine plant operations and net operating profits because of reduced availability of aged DCS components and knowledgeable resources, as well as increased operational costs related to component failures.

Opting for EHPM allowed modernizing the "heart" of the control system — process controllers — while retaining existing input/output, control strategies, displays and advanced control. At the same time, modernization via EHPM and ELCN enabled the company to take advantage of new functions and technologies such as virtualization platforms, FTE and tighter control system integration.

Chevron Oronite has found that a digital platform for process control can directly increase workflow efficiencies and operator effectiveness. For example, the new technology enables the company to meet change management requirements within its process control environment simply. It can easily determine interactions with the control system; identify when configuration changes were made; and collect and report on system information, configuration history and performance conditions. Honeywell Trace data collection software implemented last year at its U.S. facility also has expanded the visibility of configurations while automating the documentation of actions taken by plant workers.

GAINING IMPORTANT BENEFITS

Chevron Oronite has achieved flexibility and adaptability with its automation technology upgrades. The company's modernization program supports information technology (IT)/operational technology (OT) convergence to eliminate boundaries between IT and OT technologies.

The company has demonstrated that early adoption of new technologies comes with potential risks but can offer significant rewards such as eliminating downtime for system upgrades and preserving valuable configured applications and other legacy assets. Control room operators have gained a future-ready platform that allows them to stay ahead of the technology curve. This paves the way for continuous evolution and the next step in the company's migration journey — more-modern DCS-integrated tools/capabilities and data-driven visualization with new tools providing first-hand information of what is yet to happen in the process.

Most importantly, Chevron Oronite is fostering a culture in which automation, process operations and IT work together as a collaborative team to significantly help improve business results. Now, the company has a clear path to a sustainable future, which allows for technology upgrades while harmonizing new and existing assets, increasing the life expectancy of installed hardware and software, and reducing total cost of ownership with less risk and greater efficiency. ●

NATARAJAN MUTHAIAH is a process control systems project manager for Chevron Oronite, stationed in Belle Chase, La. **MARJORIE OCHSNER** is a senior offering manager — migration solutions for Honeywell Process Solutions, Phoenix. Email them at mutn@chevron.com and Marjorie.Ochsner@honeywell.com.

Revamp a Crystallizer Revamp

Unit needs changes to address difficulties caused by modifications

THIS MONTH'S PUZZLER

We replaced our draft-tube baffle crystallizer for borax (Figure 1 online at https://bit.ly/38GxU7y) six months ago and have suffered a slew of severe problems ever since. Fortunately, the downstream wash-crystallizer can make up some of the production. However, we're under the gun to fix this as soon as possible because we're planning to increase plant capacity.

We're seeing severe corrosion in the propeller; fouling in the draft tube; build-up in the elutriation leg above the steam heat exchanger; fouling in the level measurement float in the settling area; and scaling in the bottoms heater.

Looking at the scant files the corporate engineer left behind makes me concerned. The goal of the project was to increase the output of the crystallizer 50%. This was met in a peculiar way: 1) the volume of the settling area was raised without increasing the agitator power or impeller; 2) the cooling water goes through the same control valve although the coil in the condenser is larger; 3) the volume of the condenser only has been boosted by about 30%; 4) the crystals are larger than desirable, and our product pump is tripping frequently — erosion destroyed the new pump in 8 weeks; 5) now, we're concerned about the feed pump; 6) steam fouling is much worse but we haven't changed the water treatment in the boiler; and 7) the clarifier (the narrow area between the inner and outer wall) has fouled four times in six months.

Corporate has clammed up. However, I am getting help from the company that built the original crystallizer. It says the design of the new unit, which was built overseas, is a mess but can be modified to work.

Is the crystallizer company just bad-mouthing the competition or do you think it can fix the unit? Do you suggest any changes to the setup? Should we go to the fabricator of the new unit to try to get it to address the problems under warranty? What else should we consider?

MAKE PROPER MODIFICATIONS

Although the inquirer supplied a considerable amount of information, some assumptions are necessary for this preliminary analysis. As I understand the situation, the plant achieved a 50% active volume increase on the existing draft-tube-baffle (DTB) crystallizer by extending the straight side of the vessel, eliminating the cone but not changing any mechanical details on the draft tube, agitator and baffle area. The updated figure (on p. 34) reflects this.

As a crystallizer consultant, I often have worked on DTB- and Oslo-type crystallizers, including ones for processing of borax. My comments are as follows:

1. It appears that the modifications now make the unit function as both a DTB and modified growth/Oslo unit.
2. The lack of modifications of the draft-tube (DT) location and agitator means the bed of crystals at the bottom is not fully suspended and, thus, is well above the crystal bed. The additional 50% active volume without more circulation increases the temperature rise around the draft tube, which significantly boosts supersaturation — resulting in severe encrustation/scaling throughout the circuit, including the vessel bottom, baffle, fines destruction piping and the heat exchanger.
3. Because the bottom of the vessel is not fully circulated, the unit is acting like a modified Oslo (fluid-bed crystallizer), which can grow large crystals that swirl around, do not reach the boiling surface where the highest level of supersaturation occurs, and exit out of the elutriation leg based on particle-size-distribution/settling velocity. The leg is susceptible to encrustation due to the high level of supersaturation. The larger particle size distribution can cause damage to the product pump. Although not mentioned, the improper location of the feed type perhaps was an attempt to provide some mixing in the bottom settling zone.
4. The result of the increased supersaturation is that the mother liquor and some of the slurry exit into and salt up the baffle area because it originally was designed with a small area between the baffle and inside wall. Another problem is the location of the feed pipe; by not actually going into the draft tube, it potentially is leading to fines short-circuiting around the draft tube, causing entrainment at the surface and high levels of supersaturation.

5. You should measure the wt-% fines in the fines destruction loop. The baffle area was not modified, so, a much higher wt-% solids than in the original design is likely; this can result in baffle plugging plus erosion of the circulating pump and heat exchanger. For many systems, the fines destruction circuit should have less than 1 wt-% solids. Although not mentioned, I assume the flow rate in the fines destruction circuit has been increased.
6. The issue concerning treatment of the condensate at the boiler most likely is due to tube failure in the heat exchanger because of abrasion with a large wt-% solid in the fines destruction unit. In my experience, I have found that borax is an abrasive crystal that can erode pump impellers, DT impellers, plus heat exchanger tubes and tube sheet.
7. Although not mentioned, I assume the heat exchanger was not changed, and perhaps is old and subject to erosion.

If a simple fabricator made the modifications, it usually only provides a mechanical warranty and no process warranty. It often does not have the technical background to properly design a unit.

The unit requires a detailed investigation regarding the current operating parameters as well as some significant modifications to correct the apparent design and operational deficiencies.

Wayne J. Genck, crystallization consultant, Park Forest, Ill.

CRYSTALLIZER ISSUES

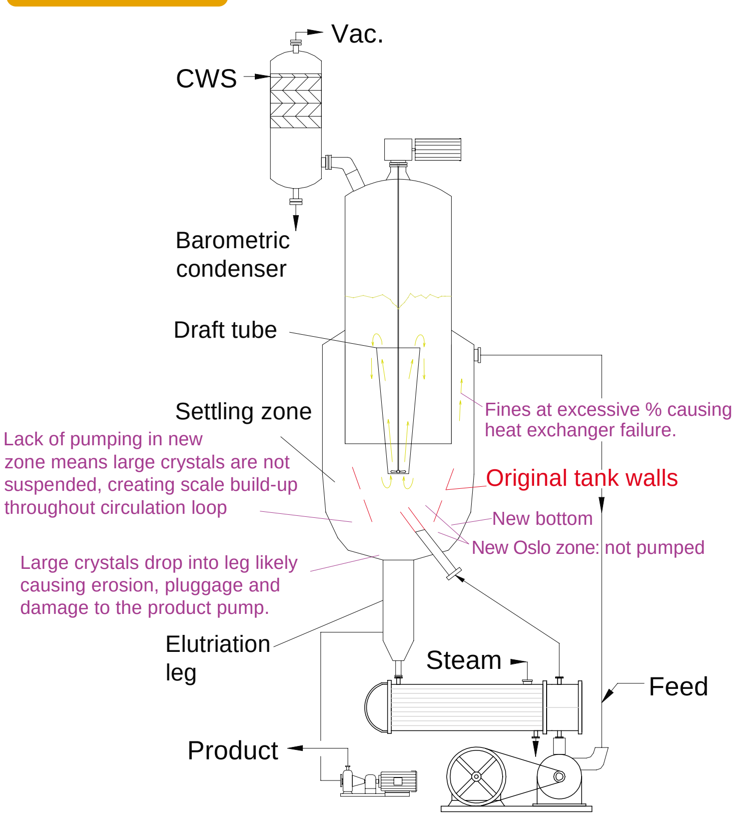


Figure 1. Ill-conceived modifications have led to a variety of serious difficulties.

REVIEW THE SCALE-UP

Key variables that control crystal size and distribution include: slurry density, supersaturation, crystallizer geometry including diameter of impeller/diameter of the crystallizer, impeller tip speed, circulation rate as well as pressure and temperature. In scale-up, you should attempt to maintain as much geometric and operational similarity as practicable.

Consider the following:

- Ensure the levels of supersaturation and slurry density of the scaled-up equipment are close to those for the original set-up. In addition, poor agitation, or shear, would contribute to larger crystals. Evaluate scale-up of the agitator (power per unit volume, impeller diameter, and locations).
- Crystallizer pressure and temperature also affect crystal size. So, keep them the same in the scaled-up equipment as in the pre-scaleup equipment. You will need to do a heat/material balance to get an estimate of cooling load on the overhead condenser and the vacuum system.
- Lower rates of circulation and slow velocity zones (flow discontinuities) could contribute to excessive scaling or fouling. Match circulation rate as much as possible to that of the original equipment.
- Plugging of the level transmitter could be an issue. The problem statement does not state the type of technology used. If the level transmitter is head pressure based, e.g., a differential pressure (DP) cell, realize that a capillary-type transmitter such as a regular DP cell with impulse legs is prone to plugging in slurry service. Similarly, displacers also are susceptible to fouling in slurry service. If capillary application fails to perform, you may need to consider other techniques such as nuclear or guided-wave radar with a stilling baffle. (A stilling well also could work

but excessive fouling could cause maintenance headaches.)
- For frequent tripping of the pumps, check for high motor speed (RPM), and the condition of mechanical seals, bearings, shaft, and operation of the pump too far (high flow rate) on the head capacity curve.
- As you establish operation of the scaled-up equipment closer to the original pre-scale operation, erosion problems conceivably could subside. However, in the meantime, check with the pump vendor for erosion-resistant materials such as stellite or ceramic-coated parts, etc.
- As stated in the problem, poor boiler-feed and return-water treatments could cause corrosion (general corrosion due to CO_2, pitting from poor oxygen scavenging), and scale problems (silica, hardness). Consider local (to the steam heat exchanger) addition of amines, oxygen scavengers and scale inhibitors. Also, possibly discuss localized treatment options with your water treatment provider.
- Poor circulation or stagnant zones could foster excessive fouling (e.g., in the clarifier region). So, upgrade circulation rates proportionate with the scale-up.

GC Shah, consultant
Houston, Texas

APRIL'S PUZZLER

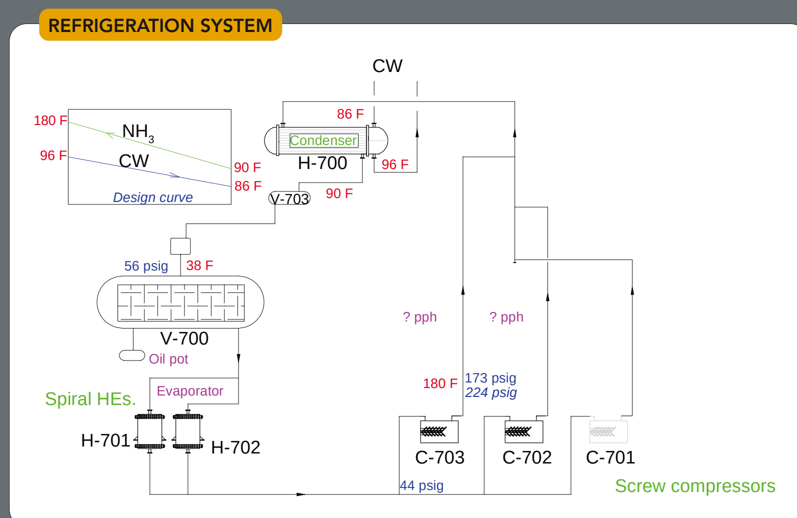


Figure 2. Spiral heat exchangers (H-701 and H-702) always are in service, as are two of three compressors (C-701, 702 and 703).

Simultaneous failures of our ammonia compressors shut down our refrigeration unit. I've been asked to specify a couple of rentals so we can cope until we get spare parts from Germany. However, I face a difficulty because the file only contains the original design; the ammonia refrigeration system was expanded about 30%. (In addition, our load center is maxed-out, so current draw is a problem.)

A corporate engineer compounded the problem by attempting a material and energy balance based on the condenser data sheet. This undated exercise seems to confuse the total ammonia flow through the screw compressors with the individual flow through the condenser. It shows a mass flow rate much higher than compressor horsepower would allow. Also, the flows through the condenser and evaporators don't add up. Fortunately, I found a useful website for a pressure/enthalpy chart: http://bit.ly/35DTSX4.

We need two compressors to operate the plant (with an additional unit on standby) and keep two spiral heat exchangers in service at all times (see Figure 2).

These compressors have run so smoothly that their simultaneous failure caught us by surprise. It took two days of frantic searching to find suitable oil filters.

Operations is wondering if we can continue to run the plant without refrigeration because the daytime high temperature now is about 30°F.

How do I resolve this puzzle? Can we safely operate the plant temporarily without ammonia refrigeration? Should we believe the ammonia flow calculation based on the condenser?

Send us your comments, suggestions or solutions for this question by March 12, 2021. We'll include as many of them as possible in the April 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.

Keep Cool with Heat Transfer Calculations

Always assess the applicability and accuracy of the approach you're applying

Many users erroneously assume that method selection isn't that important.

ENGINEERS ROUTINELY use simulators to evaluate equipment and calculate thermophysical properties. However, you never should take any result as accurate unless it's tested against measured data, as one recent case exemplifies. It involved investigating the performance of a heat-transfer-fluid system.

The system, which uses a fluid with a proprietary blend of propylene glycol, water and corrosion inhibitors, wasn't working as desired. One possible cause was deposition of corrosion products.

To understand the problem, first we must consider the real nature of the fouling factor in heat transfer calculations. Conventionally, it serves to make the calculated heat transfer match the observed result. The factor incorporates all the sources of difference — including not just fouling but also disparities between calculated methods and reality, errors in data, and flaws in estimating physical properties.

Most programs calculate single-phase heat transfer in turbulent flow in tubes based on the Sieder-Tate equation:

$$Nu = 0.023 Re^{0.8} Pr^{0.33} (\mu_b/\mu_w)^{0.14}$$

where the Nusselt number, Nu, incorporates the film coefficient, and both the Reynolds number, Re, and Prandtl number, Pr, contain a number of fluid properties. Properties required include specific heat, density, viscosity and thermal conductivity. Also needed are the viscosity at the bulk temperature, μ_b, and at the wall temperature, μ_w; the effect of the viscosity term to the 0.14 power is small, so we'll ignore it in this discussion.

Simulator packages take two different approaches to these properties. Composition and fundamental relations, often expressed in an equation of state (EOS), can provide some properties. Most models determine specific heat this way. Simulators derive other properties such as density and transport properties, e.g., viscosity and thermal conductivity, from the values for pure compounds adjusted by blending or mixing rules to represent the mixture.

You only should apply an EOS and mixing rules for their intended specific mixtures and ranges. Extrapolation outside the range of applicability can lead to serious errors. To cover a wide variety of conditions, all commercial simulator packages include multiple options for EOS and mixing rules. Unfortunately, many users erroneously assume that method selection isn't that important. Aggravating this, figuring out the data sources and applicability ranges for the different simulators and their options often is very difficult.

Now, let's examine the simulator results for the propylene-glycol/water system compared to using the literature values for the fluid properties. Table 1 shows the variation in calculated heat-transfer coefficient.

The base tube-side heat-transfer coefficient came from using literature values provided by the fluid vendor for the properties of the mixture. These were checked by curve-fitting values from the open literature that bracketed the 50/50 composition range. The property values from the vendor and in the open literature matched well.

In comparison, the closest simulator values for system properties result in heat-transfer coefficients more than 10% away from the base value. In some cases, deviations reached about 30%.

Table 2 gives ranges of heat-transfer coefficients for each of the properties. These numbers don't add up to the ones in Table 1 because some deviations offset each other. Table 2 shows that

Continued on p.38

COMPARISON OF RESULTS

Data source	Tube-side heat-transfer coefficient
Literature values	Base
Simulator 1, EOS and Transport property set 1	0.888 Base
Simulator 1, EOS and Transport property set 2	0.788 Base
Simulator 1, EOS and Transport property set 3	1.272 Base
Simulator 2, EOS and Transport property set 1	0.696 Base
Simulator 2, EOS and Transport property set 2	0.862 Base
Simulator 2, EOS and Transport property set 3	0.882 Base
Simulator 3	0.707 Base

Table 1. The simulator results differed significantly from the one obtained via literature values.

PROPERTY INFLUENCE ON VARIATION

Property	Average deviation in heat-transfer coefficient
Density	1.3 %
Specific heat	10.1 %
Viscosity	18.3 %
Thermal conductivity	21.1 %

Table 2. Three of the properties can cause substantial deviations.

Blender Provides Gentle Agitation

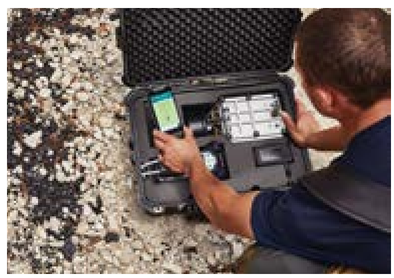
The Model DCB double cone tumble blender is designed for large-scale yet intimate blending of free-flowing solids in a full suite of laboratory, pilot and production sizes. In a highly repeatable process, minor and micro ingredients are thoroughly distributed throughout the batch more gently than in the more common V-shaped geometry without damaging fragile or sensitive components. Rated for vacuum up to 29.5 in. Hg, the jacketed 75-ft^3 double cone blender efficiently heats and dries product as it is being blended. Other features include a gas purging capability, a 16-in. pneumatically-operated discharge valve, 5-passage rotary union, explosion-proof brake motor and PLC controls.

Charles Ross & Son Company
800-243-7677
www.mixers.com

Large Enclosure Suits Hazardous Environments

The Bebco EPS 6100 series purge and pressurization system for use with large enclosures in Zone 1 hazardous areas can purge an enclosure over 450 ft^3 (12.2 m^3). The fully automatic system does not require an operator to initiate purging or pressurization. Additionally, there is automatic pressure compensation for excess leakage from the enclosure. The system consists of a control unit, vent, low pressure sensor, and optional temperature sensors that can be mounted around the enclosure for alarm notification or cooling. The intrinsically safe user-interface can also be mounted in a separate enclosure near an operator for quick access and easy system monitoring.

Pepperl+Fuchs
330-425-3555
www.pepperl-fuchs.com



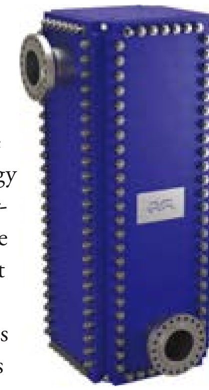
Kit Monitors Both Gas and Radiation

The Dräger X-site Live is an area monitoring kit for both gas and gamma radiation hazard monitoring. It also integrates with FirstNet, a nationwide wireless broadband network that provides priority and preemption for first responders and those who support them, affording reliable public safety communications. It features a smart gateway for Wi-Fi and cellular communication in the cloud. It also includes a removable X-am 8000, for personal gas monitoring detection, that displays up to seven gases at one time. Live readings can be sent back to a central monitoring station. The kit reportedly is easily configured within minutes for operation.

Dräger
800-437-2437
www.draeger.com

Heat Exchanger Handles Higher Pressures

Compabloc+ bloc-type heat exchanger technology is designed to support a greater number of heavy process industry applications. Its new sealing concept reportedly ensures safe operation with no risk of media leaks at pressures up to 60 bar. A fully confined, graphite gasket, dubbed the +Seal, enables the technology to safely handle higher operating pressures than possible when using a traditional flat gasket. Its design also protects the gasket and prevents overtightening of the panels during service, making maintenance easier, safer and faster for operators. The performance capabilities suit its use as a replacement for shell-and-tube heat exchangers.



Alfa Laval
866-253-2528
www.alfalaval.com

Radar Transmitters Detect Weak Signals

The Sitrans LR100 series of 80-GHz radar transmitters now includes the Sitrans LR140 and Sitrans LR150. These high-frequency, compact transmitters are said to deliver reliable measurements in challenging environments. Both offer fast, easy setup. The LR140 features 4–20-mA simplicity and is configured via Bluetooth wireless technology and the Sitrans mobile IQ App. LR150

offers a four-button user interface on an optional HMI for configuration or monitoring. Configuration also is available via Bluetooth and the IQ App or remotely with 4–20-mA/HART using Simatic PDM. The Quick Start Wizard will have the transmitter operational in minutes, says the company. The transmitters' fast response and high sensitivity help to detect weak signals.

Siemens
800-241-4453
www.usa.siemens.com

Flow Meters Withstand Corrosive Liquids

The compact, lightweight QCT_PA12 series of in-line liquid ultrasonic flow meters are intended for use in low-viscosity liquid applications. The meters' construction and nylon-12 material suit many high purity and corrosive liquids. A unique measurement section within the meter where flow is conditioned and temperature differential is measured along the meter's axis reportedly helps achieve high accuracy and repeatability. The meter measures the time difference of an ultrasonic wave traveling with and against the flowing medium; this is directlly proportional to the fluid's flow rate. The meters have non-wetted sensors, no moving parts, and nothing in the flow stream to cause an obstruction to the flow path.

FTI Flow Technology, Inc.
480-240-3400
www.ftimeters.com

Strong Magnet Attracts Contaminants

The Xtreme RE7 rare earth circuit incorporated in the company's tube and grate magnets provides magnetic separation to recover fine iron contamination and reduce product wash off. The RE7's high gauss strength reportedly is ideal for chemical applications, where the level of inspection or ability to attract small metal pieces is most demanding. In addition, its greater holding force and improved separation efficiency surpass

previous models, the company says. The magnetic separators require no electric power, and can last a lifetime with very little loss of magnetic field strength. The magnets suit a range of applications including dry bulk materials, liquids or slurries and even high-temperature applications.

Eriez
814-835-6000
www.eriez.com

Monitoring System Boasts Communication Versatility

The HawkEye365 online inventory asset and monitoring portal is an in-plant and cloud-based measurement and monitoring system. Power over Ethernet (PoE) connectivity provides secure communications as well as remote sensor setup, diagnostics and troubleshooting abilities. The portal monitors PoE transmitters and is sensor agnostic to monitor any type of field device such as level, flow, pressure, temperature and pH. Multiple communication methods include RS485, HART, Modbus, Ethernet TCP/IP, cellular, Bluetooth and PoE. The portal has the ability to monitor multiple tanks and applications worldwide in real-time. It provides accessibility to critical data such as volume, space, material height, historical trending, alarms and alerts, sensor setup and diagnostics.

Hawk Measurement Systems
888-429-5538
www.hawkmeasurement.com

PLANT INSITES

Continued from p.36

density errors aren't that significant but deviations in estimated specific heat are — and that thermal conductivity and viscosity differences are most important.

The film coefficient is only one part of the heat-transfer evaluation. The total deviation will be less than that shown here but errors of up to 30% can lead to significant misses when evaluating fouling.

What's interesting is that the simulators mostly predicted lower heat-transfer rates than those using the literature values for the fluid properties. The simulator physical-property estimates lead to a lower predicted fouling than that derived via the vendor-supplied physical properties.

The key lesson here is that, before making a decision based on simulator results, you must understand the methods involved to generate the physical properties, how they differ among methods, how they compare to data, and what that may mean for your conclusions. (For more simulation tips, see "Stifle Simulation Snafus," http://bit.ly/3pSSOpR.)

ANDREW SLOLEY, Contributing Editor
ASloley@putman.net

AD-LITS

VENTING SYSTEM FOR MANAGING COMBUSTIBLE DUST EXPLOSION RISKS

An NFPA-compliant indoor flameless venting system by the inventors of indoor flameless venting, REMBE, the Q-Rohr-3 eliminates the need for relocating dust col-

lectors and other equipment outside. The recently introduced Q-Rohr-3-6T/6T-AL are now approved for use with dusts, gases, hybrid mixtures and metal dusts. The Q-Rohr-3 products are the perfect solution for applications found in pharmaceutical, coatings, steel, iron and other industries.

REMBE, INC., 704-716-7022

www.rembe.us

PutmanMedia®

PUBLISHING HEADQUARTERS

1501 E. Woodfield Road, Suite 400N
Schaumburg, IL 60173
Phone: 630-467-1300
Fax: 630-467-1109
Web site: www.chemicalprocessing.com

Brian Marz, Publisher
E-mail: bmarz@putman.net,
Phone: 630-467-1300, x411

Carmela Kappel, Assistant to the Publisher
Phone: 630-467-1300, x314
Fax: 630-467-0197

SALES

FAITH ZUCKER, District Manager
Digital Sales Manager
Email: fzucker@putman.net
Phone: 216-316-8203

CLASSIFIEDS/AD-LITS

PEGGY HARRINGTON-MARZ,
Inside Sales Manager
E-mail: pharringtonmarz@putman.net
Phone: 708-334-9348

REPRINTS

Jill Kaletha, Reprint Marketing Manager
574-347-4211
jkaletha@mossbergco.com

ADVERTISER INDEX

Artificial Intelligence Tunes MOFs

Machine learning and AI could help target metal organic frameworks to specific applications

"MOFs discovered here are strongly competitive against some of the best-performing MOFs/zeolites ever reported."

A NOVEL automated discovery platform developed by a team of North American researchers eases the creation of custom reticular frameworks for use in gas storage, separation, catalysis and a host of other important chemical processes.

Such frameworks include metal organic frameworks (MOFs) and covalent organic frameworks (COFs), both of which are effectively tailored sponges that can form into a vast number of different molecular arrangements. MOFs are increasingly gaining traction as absorbing materials for removing carbon dioxide from flue gas and other combustion processes.

The researchers, based at the University of Toronto in Canada and Northwestern University, Evanston, Ill., are using machine learning and artificial intelligence (AI) to craft the best building blocks in the assembly of such frameworks so they target specific applications.

Described in a recent issue of *Nature Machine Intelligence*, the work started in a conventional way by constructing a large number of MOF structures on the computer and simulating their performance using molecular-level modeling.

From this, the researchers generated a "training pool" of MOF candidates that could be used in a specific carbon dioxide separation application. In the past, each member of the pool would be screened computationally until a list of top candidates could be isolated for further study.

However, for this work, they created an automated nanoporous materials discovery platform powered by a supramolecular variational autoencoder (VAE) for the generative design of the reticular materials.

"What's new here is that the automated materials discovery platform developed in this collaborative effort is more efficient than such a 'brute force' screening of every material in a database. Perhaps more importantly, the approach uses machine learning algorithms to learn from the data as it explores the space of materials and actually suggests new materials that were not originally imagined," explains study co-author Randall Snurr, professor and chair of the Department of Chemical & Biological Engineering in the McCormick School of Engineering at Northwestern.

"Designing reticular materials is particularly challenging, as they bring the hard aspects of modeling crystals together with those of modeling molecules in a single problem," says senior co-author Alán Aspuru-Guzik, research chair in theoretical chemistry at Toronto. "This approach to reticular chemistry exemplifies our emerging focus … of accelerating materials development by means of AI. By using an AI model that can 'dream' or suggest novel materials, we can go beyond the traditional library-based screening approach."

The study authors conclude that their model shows high fidelity in capturing MOF structural features and that the autoencoder has a promising optimization capability when jointly trained with multiple top adsorbent candidates identified for superior gas separation.

"MOFs discovered here are strongly competitive against some of the best-performing MOFs/zeolites ever reported," write the authors.

Another branch of the industry pursuing VAEs is cheminformatics. Here, the concept of molecular similarity implies that molecules with similar structures tend to have similar properties. So, for example, knowing that a certain molecule shows a desirable chemical activity, the question then arises how many — if any — candidates in potentially massive online collections might have similar properties.

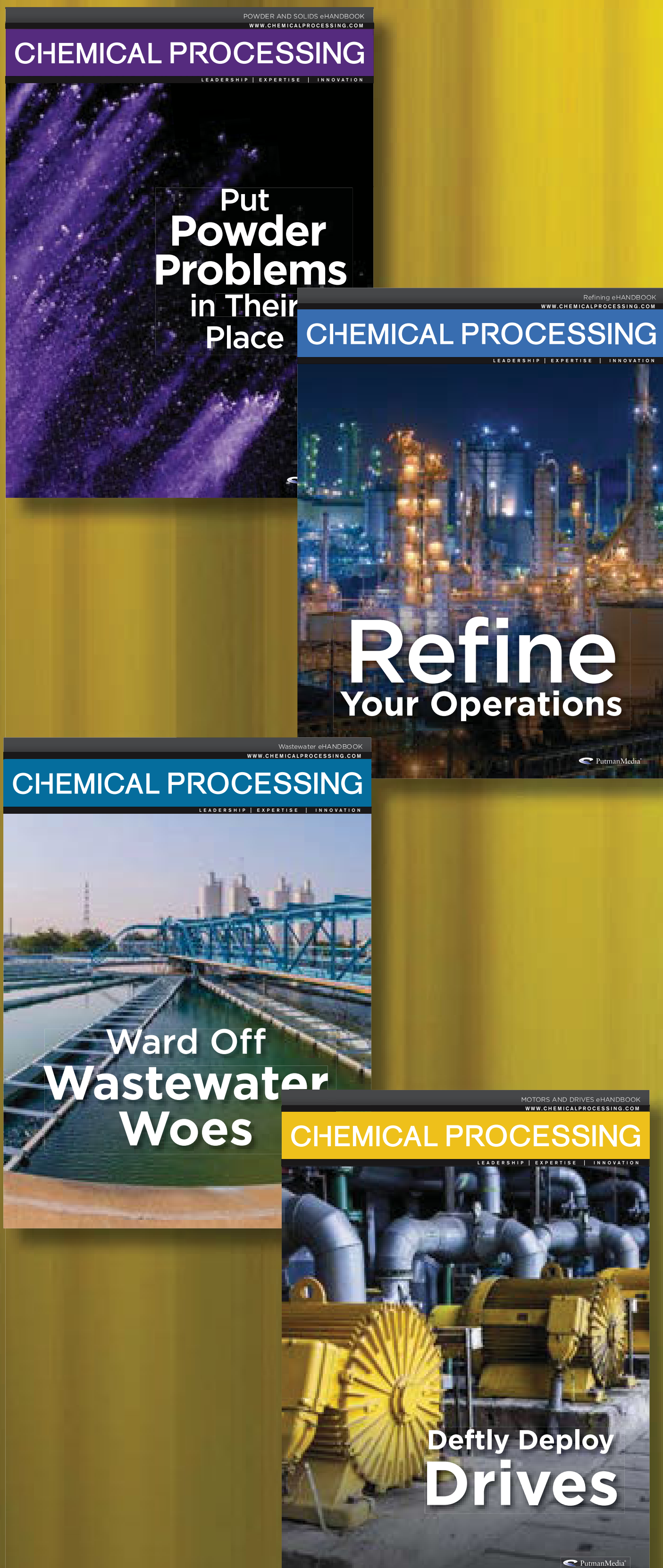
However, defining such similarity is a far from simple procedure and different methods have their own inherent problems. They can be highly variable, and prone to both false negatives and false positives, for example.

To try to overcome this, a team of researchers from the universities of Liverpool and Manchester in the U.K. and Lyngby in Denmark are using a VAE to target over six million drug-like molecules and natural products.

Writing in a recent issue of *Chemical Biology*, the researchers say their approach provides a rapid and novel metric for molecular similarity that is both easily and rapidly calculated.

As well as leveraging a new method of encoding the molecules themselves, the researchers note that methods which involve VAE are generative and allow for the creation of entirely new molecules. "This opens up a considerable area of chemical exploration, even in the absence of any knowledge of bioactivities," they write.

SEÁN OTTEWELL, Editor at Large
sottewell@putman.net


POWDER AND SOLIDS eHANDBOOK
WWW.CHEMICALPROCESSING.COM
CHEMICAL PROCESSING
LEADERSHIP | EXPERTISE | INNOVATION
Put Powder Problems in Their Place
Refining eHANDBOOK
WWW.CHEMICALPROCESSING.COM
CHEMICAL PROCESSING
LEADERSHIP | EXPERTISE | INNOVATION
Refine Your Operations
PutmanMedia
Wastewater eHANDBOOK
WWW.CHEMICALPROCESSING.COM
CHEMICAL PROCESSING
LEADERSHIP | EXPERTISE | INNOVATION
Ward Off Wastewater Woes
MOTORS AND DRIVES eHANDBOOK
WWW.CHEMICALPROCESSING.COM
CHEMICAL PROCESSING
LEADERSHIP | EXPERTISE | INNOVATION
Deftly Deploy Drives
PutmanMedia

CV TECHNOLOGY®
FIRE AND EXPLOSION PROTECTION

EXCITING & NEW ANNOUNCEMENT

PATENTED REVOLUTIONARY NEW DEVICE
We are proud to announce the Interceptor® QV,® the first of it's kind, a passive isolation device based on flameless venting technology.

INTERCEPTOR® - QV®
PASSIVE ISOLATION

At the core of the unit is a stainless steel mesh cartridge, which is located directly in the pathway of clear air return. If a deflagration propages through the clean line return then it will make contact with the mesh cartridge which will immediately and passively remove energy from the flame front of the deflagration as it passes through the torturous path of the mesh, forcing the flame to transfer its energy to the high surface area of the mesh, therby quenching the deflagration and not allowing any flame to pass beyond the Interceptor® -QV®.

WITHOUT THE QV INSTALLED

Fires headed down a line typically result in an explosion or secondary incident. The threat is real, instant, and often times, lethal. The image to the left illustrates an unprotected line.

QV INSTALLED

A passive system, the I-QV is always on the job 24 hours a day, 365 days of the year. There is nothing to arm and no power source required to activate. This device provides pressure drop monitoring, thermal sensing and signaling, and an easy-to-service cartridge.

WATCH THE INTERCEPTOR® - QV® IN ACTION
CVTECHNOLOGY.COM/INNOVATION/QV