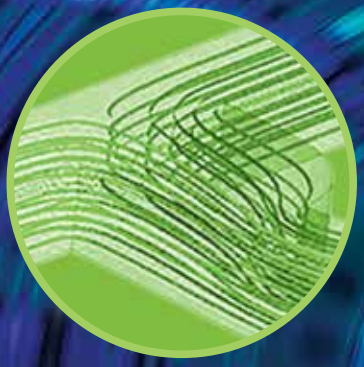
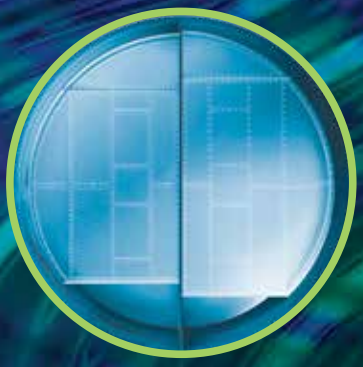
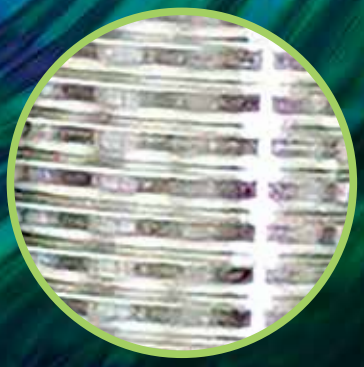
SPECIAL SECTION:

PROCESS INTENSIFICATION







Process Intensification in Practice

A paradigm shift is underway in the process industries. For over 100 years, these industries have maintained that processes were most efficiently treated as a series of standardized unit operations, and that cost-effective scale-up occurred by increasing equipment size to take advantage of economies of scale. These principles still hold in most cases, but process intensification (PI) and modular process technologies are starting to change these perspectives. New thinking and new tools allow engineers to see process development in entirely new ways, and the Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute and its members are helping lead this change in U.S. manufacturing. The news article "RAPID's Quest for Intensification" (pp. 24–28) gives a brief introduction to RAPID and spotlights three of its many projects.

PI is the application of novel process design, technologies, and equipment to substantially increase yield, reduce energy consumption and waste generation, and lower capital and operating costs. Applying PI design principles allows engineers to rethink processes, combine chemical and physical operations, and break the traditional unit operation paradigm.

The article "Introduction to Dividing-Wall Columns" (pp. 30–34) provides an overview of one approach to designing a depentanizer for installation in a refinery. Engineers considered several options, including a series of traditional distillation columns as well as a PI approach using a dividing-wall column. By selecting the dividing-wall column, the manufacturer reduced energy use and lowered both capital and operating costs. Dividing-wall columns are just one example of PI process technology that integrates multiple operations — in this case two distillation columns in one — that manufacturers are adopting at a greater rate.

As engineers become more adept at creating new frameworks for process design, the benefits will become more apparent. Rather than relying solely on traditional unit operations, these modern process synthesis tools simulate fundamental physical and chemical transformations to describe a process system. In modeling a proposed process, these tools often reveal new PI solutions. The next article, "A Building-Block Approach to Process Intensification" (pp. 35–43), describes a modeling approach that uses building blocks to characterize physical and chemical transformations. Blocks are combined to form two-dimensional grids that describe traditional as well as intensified processes. These grids can then be analyzed using numerical optimization techniques. Such modeling approaches may soon become expert systems that predict the next set of PI-enabled operations.

In addition, engineers now have access to sophisticated modeling and simulation tools. Very-low-cost, powerful computing combined with low-cost data storage allow collection of large sets of data from existing processes and simulation of existing and proposed processes in more complex ways — allowing engineers to predict process performance with increasing accuracy and make better process design decisions. Using these modeling tools to assess PI approaches across a range of scales offers the opportunity to modularize process systems to take advantage of distributed resources, such as stranded shale gas and waste biomass, by locating manufacturing where the resources are most plentiful.

"Using Simulation and Digitalization in Modular Process Intensification" (pp. 45–49) explores how simulation and digital twins are impacting engineering and process design, as well as how better integration of computational tools from early-stage conceptual design through final engineering and deployment create more robust models and reduce waste in engineering, procurement, and construction processes. Additionally, more robust simulation tools allow engineers to explore PI and integrate PI solutions that enable modularization.

This special section underscores how PI-enabled technologies and new tools are already impacting manufacturing. The RAPID Manufacturing Institute is working to become the national resource in building and educating a community focused on developing and deploying these innovative PI and modular process technologies. Join us in this worthwhile endeavor.

William Grieco
Chief Executive Officer
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RAPID's Quest for Intensification

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CEP

These and other RAPID-funded ventures could transform industry by making chemical processes cleaner, smaller, safer, and more energy-efficient.

Process intensification (PI) has existed for many years, but it first gained significant attention in the 1970s, when process developers began seeking new ways to improve cost and energy efficiency in industrial plants. The concept is broad — PI encompasses any chemical engineering innovation that creates a smaller, cleaner, safer, or more energy-efficient technology. Over the past decades, there has been renewed interest in PI in Europe, Asia, and the U.S.

But there are several barriers to deploying PI. Companies are often wary of the cost and risk associated with committing to new processes not yet proven on a commercial scale, and intensified systems can sometimes be too complex for easy implementation. In addition, researchers in this field often lack sufficient software or modeling tools to accurately predict the efficiency of novel technologies. Underlying these challenges is a limited understanding of PI across key sectors of the chemical process industries (CPI).

The U.S. Dept. of Energy (DOE) established the Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute in December 2016, with the goal to double U.S. energy productivity by 2030. RAPID focuses on reducing barriers to establish PI, and addresses the development and deployment of PI technologies in domestic industries such as oil and gas, pulp and paper, and other specialty and commodity chemical sectors. RAPID hopes to leverage process intensification to help U.S. manufacturers improve productivity and efficiency, save energy, reduce waste, and cut capital and operating costs.

Modularization is another emerging trend in industry that breaks down chemical processes and facilities into functional building blocks or modules that can simplify design and construction. While PI techniques and modular process technologies can be implemented separately, RAPID also promotes the use of both concepts simultaneously, focusing on modular chemical process intensification (MCPI).

A rapid change in efficiency and design

There are multiple approaches to MCPI, all of which center chiefly on optimizing and consolidating industrial processes. The concept emphasizes advancement in technologies and strategies to combine multiple process steps into smaller process units that can be scaled in number rather than in volume.

This form of intensification has the potential to create more-efficient equipment, and smaller, simpler plants with smaller environmental footprints. Fewer steps and smaller units could reduce recycle streams and improve heat- and mass-transfer efficiencies over stand-alone process steps. Fewer process steps could mean lower capital

▲ **Figure 1**. The six technical focus areas of the Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute.

costs than conventional plants, and reduce risk for companies implementing new technologies for the first time. MCPI techniques could create smaller plants that can be located close to consumers as well as distributers of raw materials, reducing cost and energy needs for feedstock or product transportation.

RAPID organizes its research and development activities into six technical focus areas (Figure 1).

The first three focus areas represent industry sectors that could benefit from MCPI technologies. Chemical and commodity processing deals with research relevant to the CPI and petroleum refining operations, while natural gas upgrading focuses on the processing of natural gas and natural gas liquids (NGLs). The renewable bioproducts focus area looks at the pulp and paper industry, as well as the use of emerging biomass feedstocks that can be converted into fuels, energy, chemicals, and materials.

The three other focus areas address the science and technology that will be required to deploy process intensification. Research into intensified process fundamentals concerns the application of PI, including the scaling of intensified modular manufacturing, while the modeling and simulation area includes research on modeling tools and software for MCPI implementation. And although modularization is relevant to all of the focus areas, the module manufacturing focus area addresses potential supply chains of an established modular manufacturer and other aspects of building modular equipment. These six focus areas are not discrete; projects within every category overlap. However, two common themes are evident — cutting costs and establishing environmental sustainability.

RAPID solicits project proposals from universities, nonprofit research organizations, and companies across the nation. Researchers often propose projects built on collaborations among academic, industrial, nonprofit, and government partners. DOE provides part of the funding for the projects, while the partners share in the cost of performing the work.

Taking another look at fracking

A team of engineers from the Univ. of Pittsburgh received $5.3 million from RAPID in 2018 for work on a project titled "Deploying Intensified, Automated, Mobile, Operable, and Novel Designs (DIAMOND) for Treating Shale Gas Wastewater." The researchers partnered with Texas A&M Univ., the Univ. of Texas at Austin, and Clean Water Technology, a waste solutions company. Their project aims to reduce the amount of freshwater used in hydraulic fracturing and capture high levels of waste heat typical of the process. This project is within the natural gas upgrading focus area.

Hydraulic fracturing, or fracking, is a common practice within the oil and gas industry. To tap into resources such as oil and NGLs trapped under the Earth's surface, companies drill wells into the ground that expose bedrock formations rich with oil and gas.

Pumps inject pressurized water to break up the sediment and release oil and gas, which must then be separated from the injected water and fracking chemicals. This leaves a large volume of contaminated water that must be properly disposed of.

The oil and gas industry is continually looking for better ways to manage this wastewater, and there is an emphasis on recovering clean water from contaminated water for reuse in fracking. The concept of using water separated from the oil and gas collected from one well to frack the next well has already been established. The Pitt engineers want to take this idea one step further.

"We want to go beyond existing solutions," says Radislav Vidic, a project engineer at Pitt. "What if we could treat the contaminated water and recover high-quality freshwater from waste? It's possible to use purified fracking water not only for other wells, but also for agriculture or for other industrial operations. Then wastewater could actually be treated as a resource rather than a waste."

Vidic pictures an oil extraction site with over 20,000 wells — if every well produces water that was both injected and naturally released, at some point, companies will produce more water than they need for reuse in fracking. To treat the excess wastewater, the team is studying a process called membrane distillation.

Membrane distillation uses a hydrophobic membrane to purify fracking water. The researchers pump hot water on one side of the membrane and cold water on the other side (Figure 2). The membrane allows only pure water vapor to pass through it, while contaminated liquid water is rejected. Purified vapor passes from the hot side of the membrane to the cool side, where it is condensed and distilled.

Distillation processes typically operate at temperatures of more than 200°C to sufficiently evaporate components,

driving high energy costs. With membrane distillation, heating the system to even relatively low temperatures creates at least some vapor that can be condensed and distilled. This makes membrane distillation suitable for the utilization of waste heat associated with many industrial processes.

"There's a lot of waste heat produced by plants," says Vidic. "If you can purify wastewater and do it with waste heat you don't have to pay for, that creates an economically attractive alternative for treating wastewater."

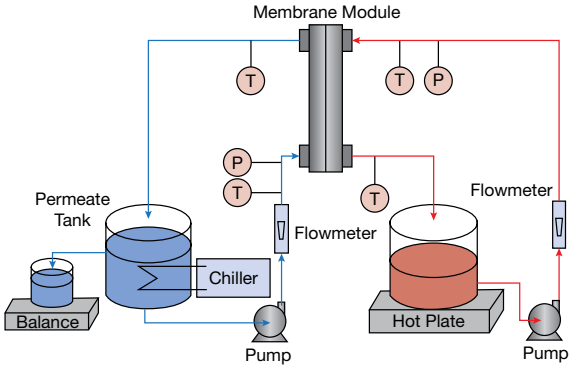
Membrane distillation could improve the overall energy efficiency of the petroleum industry, according to Vidic. By reusing fracking water, the process reduces the amount of pure, unused freshwater needed for injection in the first place. Membrane distillation could also be used to treat wastewater produced through agriculture or other industrial processes.

The process is conducive to modularization, and is relatively easy to scale up. "If we can show how much water we can process per unit area of the membrane, then if you tell me how much water you need to get rid of, I can tell you how many membrane modules you would have to put together to do that," says Vidic.

Vidic's research could have a positive environmental impact. Disposing contaminated wastewater can be risky — pipelines can burst, or trucks carrying fracking water to disposal sites can be breeched, creating an environmental threat. Depending on the pumping rate, disposal wells may also cause minor earthquakes in their vicinity. Reducing the amount of water that needs to be disposed could alleviate these concerns, says Vidic.

The project is still in the early stages, but the Pitt engineers have done some laboratory studies on produced water from well sites in Pennsylvania, with promising results. They plan to study water that differs in composition from various regions, to determine the pretreatment process that optimizes distillation of any wastewater.

They also hope to develop a more-specific membrane; the team is currently using a commercial hydrophobic membrane to separate water. And, they are in the process of developing predictive models that can be used to assess the performance of a system without laboratory experiments. While the project has a long way to go, the researchers are optimistic about its success.



▲ **Figure 2**. Engineers at the Univ. of Pittsburgh partnered with Texas A&M Univ., the Univ. of Texas at Austin, and Clean Water Technology to develop a membrane distillation process that could help purify fracking wastewater. Image courtesy of the Univ. of Pittsburgh.

Saving energy with microwaves

Almost every home in the U.S. has one: a microwave oven, typically used to pop popcorn and heat frozen dinners. But the technology at the heart of this household appliance has the potential to be much more.

RAPID recently accepted a proposal by the Univ. of Delaware (UD) for a project titled "Intensified Microwave Reactor Technology." In partnership with the United Technologies Research Center, this project explores the potential applications of microwave heat for multiple industrial processes. The project is part of the intensified process fundamentals focus area.

The microwave oven has been a commonplace appliance for decades, but the technology underpinning the device is applied very infrequently for industrial processes. According to UD chemical engineers, it has great potential for high-energy/high-temperature reactions, such as methane or hydrogen production.

Conventional fired heaters burn gas to produce flames, which transfer heat via radiation to reactor tubes that contain catalyst. The tubes typically do not sit directly in the flame — rather, they are placed next to the flame and are heated by radiation.

A microwave device heats material by exposing it to electromagnetic radiation, stimulating the polar molecules within to generate thermal energy. Thus, while burners heat matter from the outside in, microwaves heat materials from the inside out.

According to the researchers, direct microwave heating more than doubles the energy efficiency of reactions, from 40% with conventional heating to 90% with microwave heating.

"When you radiate in conventional processes, you don't direct heat in any particular direction," says Dionisios Vlachos, a chemical engineering professor at UD. "The microwave can actually focus its energy on the material, not on the air around it, so you don't lose any energy. All the energy goes where you need it, rather than dissipating, much like a barbecue, where heat goes everywhere."

Vlachos and his team are exploring the use of microwave heat for multiple industrial processes, particularly those with high-energy or high-temperature reactions, such

as petrochemical production from shale gas. There has been increasing demand for products such as ethylene and polypropylene, which are often sourced from hydrocarbons in shale rock. Vlachos hopes to use their microwave reactor (Figure 3) to make petrochemical conversion processes more cost-effective and energy-efficient.

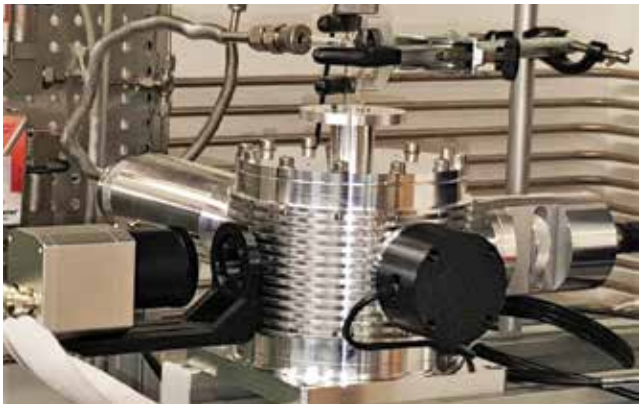
The UD team is also looking to utilize the large quantities of biomass present in the Midwest, namely corn, wood, and manure. Biomass is a potential source of energy that is often overlooked. Converting biomass into energy and using that energy to produce chemicals takes a great deal of power and water, and transporting biomass from the Midwest to refineries on the east coast can be expensive. The UD chemical engineers want to process biomass right on the farms, using small, modular microwave reactors that are more easily integrated on-site.

They are also working with a company that is looking to make airplane brakes of carbon fiber and ceramics that can withstand the immense kinetic energy of an aircraft and are highly resistant to heat shock. Currently, the process to produce these brakes takes about two months. With microwave heat, Vlachos estimates that it could be done in two days.

Another major motivation behind the UD researchers' work is creating carbon-emission-free processes. They plan to use renewable sources of energy such as wind and solar to power their microwave reactors.

"This could be the future," Vlachos says. "Using renewable energy to drive chemical production is a beautiful way of storing power. The cost of solar and wind energy is expected to decrease, and it is likely that renewable energy will become cost-competitive with natural gas and oil."

Powering chemical reactions with a more sustainable source of energy could be a huge step toward sustainability in the CPI. For example, says Vlachos, "hydrogen production produces high levels of CO_2, and ammonia production on its own produces about 1% of total global emissions." He envisions running these reactions with microwave reactors, powered by renewable energy — making the processes emission-free and extremely energy-efficient.



▲ **Figure 3**. A microwave reactor created by researchers at the Univ. of Delaware (UD) and the United Technologies Research Center could help utilize microwave heat for multiple industrial processes, including hydrogen production and shale gas prcoesses. Image courtesy of UD.

The team has made significant progress since they received the RAPID grant in 2018. They are concerned most with increasing their knowledge of microwave reactors, by organizing information and creating design tools. Learning about microwave scaling and modularization is an important precursor to building functional reactors.

"We're looking at developing designs for scale-up and for putting modules together," Vlachos says. "The typical microwave is small, and even laboratory microwaves can't heat up a whole room. The right scale, the economics, that is still unknown. You also want to be able to choose the power/frequency of the microwave, depending on how much energy you need and how much product you want to make. A chemical engineer should be able to tell you what you need in what situation, but at the moment those designs and models don't exist. We want to develop these methodologies."

The rising star of hydrogen production

Many have called hydrogen fuel-cell cars the future of driving. These vehicles use hydrogen gas to power their engines, creating only water and heat as byproducts and completely eliminating tailpipe pollution.

Unlike electric cars, hydrogen vehicles could be refueled quickly at filling stations similar to traditional gasoline stations. They also release less carbon emissions than standard vehicles.

Like most fossil-alternative fuel options, hydrogen is expensive. Electric cars lag commercially because of the high cost of their batteries; likewise, hydrogen fuel-cell cars struggle because hydrogen is expensive to produce, and even more costly to transport. Ultimately, price is the limiting factor. To incentivize consumers to buy emission-free cars, alternative fuels must be cost-competitive with fossil fuels.

Ten years ago, a Pacific Northwest National Laboratory (PNNL) researcher named Robert Wegeng was given an assignment on a project with NASA. At a lunch with rocket scientists and astronauts, his colleagues told him about their attempts to develop solar power technology to create materials on Mars, and asked Wegeng a fascinating question: Why can't we do this on Earth?

Wegeng immediately began work on what has been deemed STARS technology — an innovation in chemical engineering that converts solar energy into chemical energy. He has developed prototypes of the system for nine years, and in 2016, he established the STARS Technology Corp., intending to commercialize STARS technology and use solar

energy to generate mass-produced, inexpensive hydrogen.

While the concept of using solar energy to produce hydrogen is well-developed, Wegeng wants to achieve this via modular manufacturing methods. RAPID awarded the company a grant to pursue its proposed project, "Manufacturing Supply Chain Development for the STARS Technology Modular Solar-Thermochemical Conversion Platform," in 2018.

In partnership with PNNL and Oregon State Univ., Wegeng hopes to see hydrogen filling stations across the country in just a few years.

Most hydrogen is produced via steam reforming of methane, typically by heating the gas in the presence of steam and a catalyst. Extremely high temperatures (in excess of 1,000°C) are required to initiate the reaction. The STARS system uses a dish-shaped solar concentrator that collects energy from the sun to power the reaction, rather than burning fossil fuels (Figure 4).

The STARS process first preheats methane and water, which generates steam that mixes with the methane at temperatures over 1,200°C. This mixture is channeled into a disc-shaped reactor that faces the solar concentrator.

More than 10 kW of solar energy drive the reaction, which produces hydrogen at an energy efficiency that is roughly the same as conventional methods of production. The system is circuitous, using heat created by the reaction to power the initial preheating step. The solar energy is used solely to drive the reaction. This combination of efficiency and inexpensive energy makes the method cost-effective.

Currently, transporting and producing hydrogen is expensive. The cheapest way to make hydrogen is at large facilities, but then it must be transported to filling stations across the country, further driving up costs. The result is expensive hydrogen that most people cannot afford, impeding the integration of fuel-cell vehicles in the U.S. and around the world. Wegeng wants to change that.

▲ **Figure 4.** The STARS Technology Corp. uses a unique system to convert solar energy into hydrogen in an energy-efficient manner. CEO Bob Wegeng is working with researchers to streamline the process for commercialization of STARS Tech. Image courtesy of Pacific Northwest National Laboratory.

"We're trying to produce compact, modular, and process-intensive hydrogen production units that can make hydrogen from natural gas and water right at the filling stations," he says. "Hydrogen can be sold at prices that are cost--competitive to gasoline, and that could allow hydrogen fuel-cell vehicles to compete in the marketplace. We want to be able to provide units for low-cost hydrogen production, but we need to have the manufacturing methods to build these units rapidly, and assemble them cheaply, and that's what RAPID is helping us do."

To compete with fossil fuels, hydrogen prices must drop from $15/kg to $5/kg. The elimination of transportation costs, combined with the cost-effective design and the low cost of hardware, could accomplish this, according to Wegeng.

STARS Tech Corp. places a high value on low-cost hydrogen, but it is also concerned with the environmental component of its system. One of the company's long-term goals is to modify the STARS system so that it produces other hydrocarbons alongside the hydrogen, avoiding any CO_2 emissions.

"With climate change being an important issue now, we need to start creating technology that can operate with a reduced carbon footprint," Wegeng says. "We need to move toward non-fossil energy sources, and doing that in a way that is economically competitive with fossil-fuel sources is very important." Wegeng is confident that consumers will make the ecofriendly choice to drive hydrogen fuel-cell cars if hydrogen costs were lower.

STARS Tech Corp. might become the next company to transform the auto industry. "In less than two years, we're putting our first unit at a filling station," he says. "In five years, we'll be mass-producing units. By 2030, California has pledged to put one million fuel-cell vehicles on the road, with a thousand filling stations. They're going to find it much easier to do so if hydrogen is cost-competitive with gasoline. People are going to want to build these stations to make money, and that means automobile manufacturers will be willing to produce more fuel-cell cars. Consumers could regularly be driving these vehicles, in California and elsewhere."

By supporting projects like STARS Tech, the RAPID Institute hopes to create PI and modularization techniques that can be adapted by companies and manufacturers across the nation. Ultimately, the organization's goal is a cleaner and more efficient chemical process industry. CEP

Introduction to Dividing-Wall Columns

A dividing wall can be added within a distillation column to improve separation efficiency of three or more products.

Manish Bhargava
Anju Patil Sharma
DWC Innovations

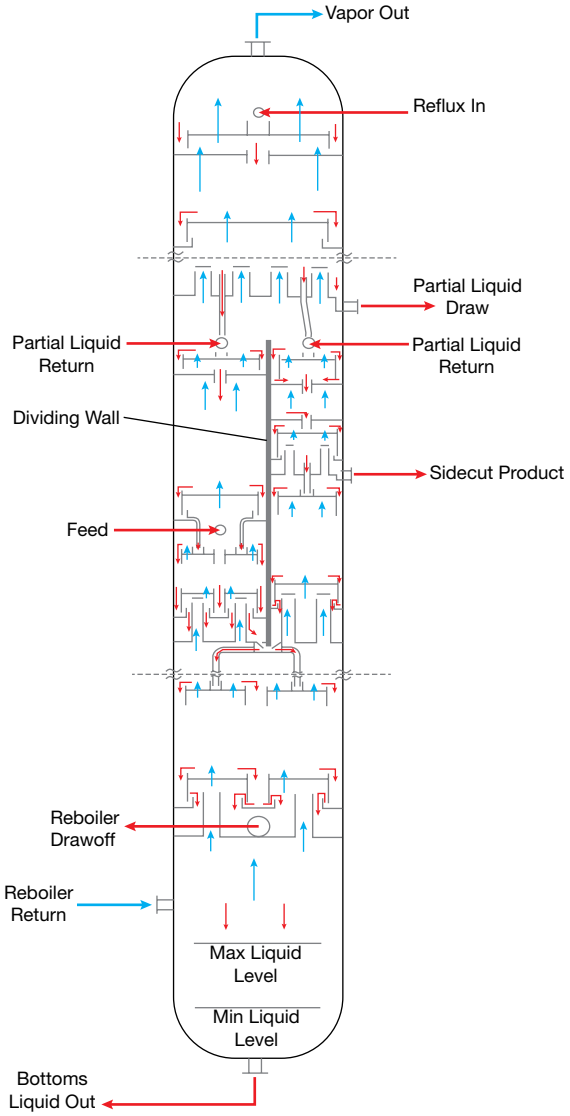
Dividing-wall columns (DWCs) are a type of distillation column that can separate mixtures of several components into three or more high-purity streams (Figure 1). A DWC requires much less energy, capital investment, and plant space than conventional columns in series or parallel configurations. In fact, DWCs can have 20–30% lower capital cost requirements than conventional tower designs *(1–5)*.

Conventional distillation columns are an integral part of the refining and chemical industries. Retrofitting existing columns with a dividing wall to improve separation efficiency is part of a larger push to intensify processes in these industries. Process intensification (PI) targets dramatic improvements in cost and energy efficiencies by rethinking traditional operation schemes. A DWC is one example of an intensified technology.

The concept of DWCs is well established, with much literature focusing on the simulation and control of these columns *(1, 6, 7)*. Several publications have discussed the industrial applications of DWCs in different grassroots and retrofit applications *(8, 9)*.

The technology is quite versatile, and no two DWC applications are exactly the same. Thus, it is difficult to develop a standard protocol for designing these columns. DWCs have been implemented in a variety of applications, such as gas plants, naphtha splitters, and reformate splitters, among others.

This article describes the three basic types of DWCs. An example demonstrates how adding a dividing wall can improve the purity of a side-cut stream without requiring the addition of a second column.



▲ **Figure 1.** A standard dividing-wall column (DWC) has a wall that separates the column into two sections. The flow of vapor and liquid is shown with blue arrows and red arrows, respectively.

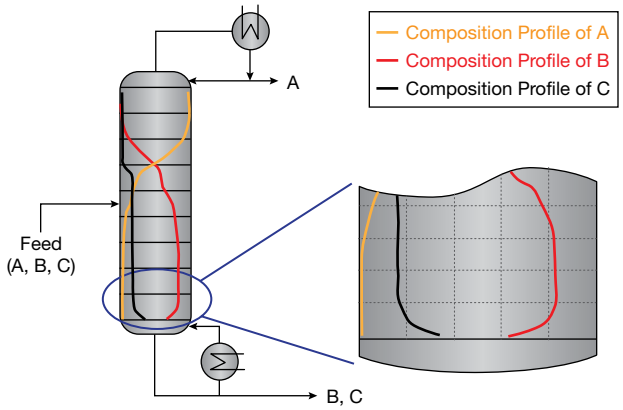
Design and configuration of DWCs

To separate three components, typically a sequence of two distillation columns would be required. Separation in a conventional column sequence suffers from intrinsic remixing (Figure 2). Although the intermediate component develops a concentration peak somewhere in the first column, that component is not withdrawn from the column and instead exits the column in the top or bottom product stream. When the intermediate component travels down to the column bottoms (as in Figure 2), it remixes with the heavier components. The second column in the sequence then has to reseparate the intermediate and heavier components.

DWCs were designed to reduce this intrinsic remixing of components that occurs in conventional columns. By eliminating component remixing with the help of an internal wall, DWCs achieve higher thermodynamic efficiencies than their counterparts, making them more energy efficient than conventional towers.

A DWC is a mechanical and thermal integration of a Petlyuk column *(4, 10)*, which reduces remixing by introducing prefractionation and main fractionation regions in a single shell.

The dividing wall in a DWC separates the tower into two sections and creates different fractionation zones in the column. The area in the column where the feed is introduced separates the heaviest and the lightest components. On the other side of the wall (opposite the feed) is a rectifying zone, where the middle-boiling components are concentrated; the side stream is withdrawn from this area. These distinct separation zones produce three product streams with concentrations higher than can be achieved in a conventional tower with similar heat duties.



▲ **Figure 2.** Precise separation of three components typically requires a sequence of two columns. This figure depicts the composition profile of the three components in the first column of the sequence. Component A (yellow) is most volatile and is concentrated in the top of the column. Component C (black) is the heaviest component and is concentrated in the column bottoms. The intermediate Component B (red) is concentrated in the column center. If it is not removed at the column center, it accumulates in the column bottom, where it remixes with the heaviest component. The downstream column must then undo that remixing to separate B and C. This intrinsic remixing penalizes any conventional sequence of distillation columns.

DWCs are becoming increasingly popular in refinery and petrochemical facilities because they offer several benefits over conventional side-cut columns:

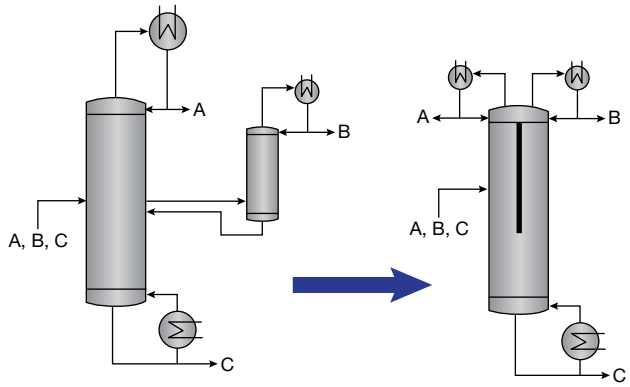
- higher recovery of the desired product
- better product quality for the side-cut and bottom products
- lower reboiler and condenser duties
- fewer necessary equipment modifications, which reduces the capital investment for the project
- robust and flexible design
- smaller footprint than multiple columns in series.

The arrangement of the wall inside the column depends on various parameters. There are three primary ways in which the wall in a DWC can be configured: in the middle, on the top, or on the bottom.

The most widely used DWC has its internal wall in the middle (as in Figure 1). The middle-DWC is an ideal replacement for two columns in sequence. It can also be used to replace a column in which one or more side-cut streams are withdrawn from the middle of the column. Among the DWC configurations, middle-DWCs provide the maximum utility savings. One drawback of the middle-DWC is that the cooling utility is forced to the minimum temperature and the heating utility is forced to the maximum temperature; this may not be desirable in many distillation column configurations.

Top-DWCs are configured to replace a side stripper (Figure 3). There are two separate condensing systems for the two top products. Since the intermediate component condenses at a higher temperature, top-DWCs can be advantageous in some applications, as they provide a means of overhead vapor heat integration. Top-DWCs provide an additional degree of freedom to maintain overhead condensing systems at two different temperatures.

The bottom-DWC is an attractive alternative to combine



▲ **Figure 3.** Top-DWCs can replace a traditional column that is integrated with a side stripper.

columns in an indirect sequence. A sequence of columns is said to be an indirect sequence when the top product from the first column is the feed to the second column (Figure 4). Bottom-DWCs have two separate reboilers and have the advantage of maintaining the bottoms utility at two different temperature levels.

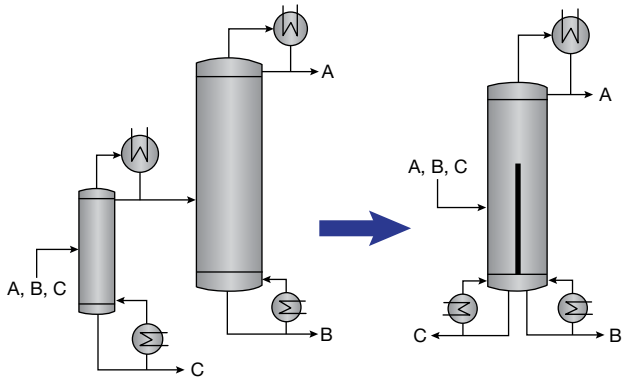
Example: Upgrading a naphtha splitter

A refinery in India wanted to upgrade its naphtha splitter to recover more medium-weight hydrocarbons. Figure 5 shows the original configuration of the naphtha splitter and depentanizer column at the facility.

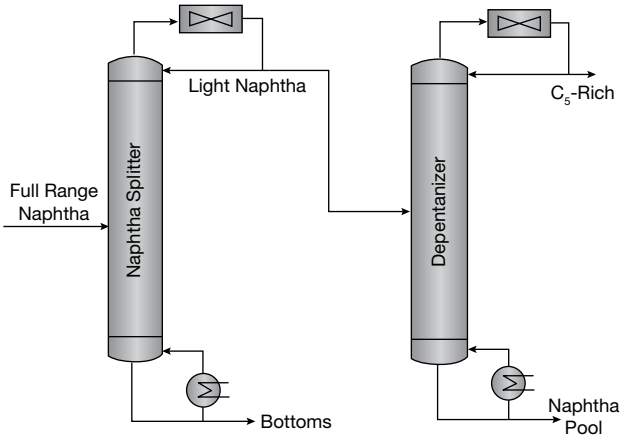
The top product of the naphtha splitter consisted of about 15% nC_5 and 14% iC_5, with larger C_6 and C_7 components making up the remainder. This stream was routed to a depentanizer column, where the C_5 product and heavier naphtha components were separated.

To produce a premium gasoline product with a research octane number (RON) of 90, the refinery wanted to recover a stream of iC_5 with at least 90 wt% purity as a separate product. The refinery considered three possible solutions to achieve this product stream:

- Option 1: Install a third column downstream of the existing depentanizer column
- Option 2: Revamp the depentanizer column by adding a side-cut stream
- Option 3: Revamp the depentanizer column to a DWC.



▲ **Figure 4.** Bottom-DWCs are suitable when the columns to be replaced are in an indirect sequence.



▲ **Figure 5.** A refinery in India wanted to upgrade its naphtha processing system. In the original design, a naphtha splitter was followed by a depentanizer column.

Option 1: Install a new deisopentanizer column

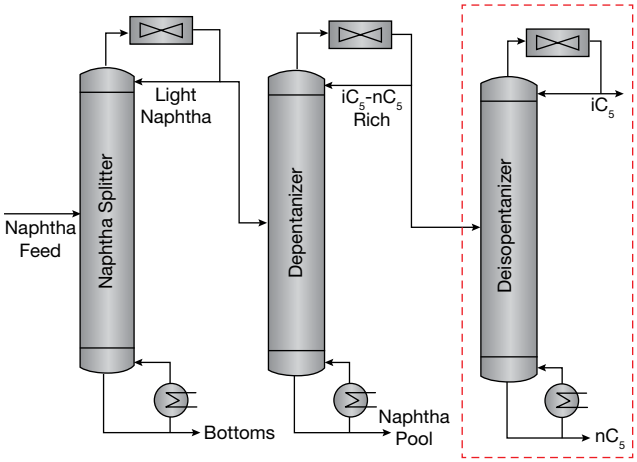
The first option is to build a new deisopentanizer column downstream of the original depentanizer column (Figure 6). The top product stream from the depentanizer, which is rich in iC_5 and nC_5, is routed to this deisopentanizer column, which further separates nC_5 to the column bottom and iC_5 to the top. Although this option meets the necessary product requirements, it requires substantial capital and operational expenditures.

Another drawback to this option is that it has higher energy requirements. The total required reboiling and condensing energy increases as you increase the number of columns in the sequence. As previously demonstrated in Figure 2, this option needs to contend with thermodynamic inefficiency due to remixing.

Option 2: Add a side cut

Another option is to revamp the depentanizer column with new column internals to add a side cut, which would help produce iC_5-rich product at the top by separating a stream of mainly nC_5 from the middle section of the column (Figure 7). Since the side-cut column requires higher duty after the revamp, the column needs to be retrofitted with high-capacity trays. And, tray spacing needs to be reduced to allow the column to accommodate more stages.

Like sequential distillation, remixing of components



▲ **Figure 6.** A new deisopentanizer installed downstream of the existing depentanizer column could be used to recover iC_5 as a separate product from nC_5.

would also be an issue in this conventional side-cut column, which would reduce product quality. However, better product purity could be achieved by increasing the reboiler duty.

A compromise between product quality and duty could be achieved by optimizing the location of the side cut to below the feed nozzle (Figure 8, left). This would allow an iC_5-rich stream to be removed as the top product. However, a large amount of C_6 naphtha components would spill over to the side-cut stream, which would affect the quality of other two products. But, if the location of the side cut were positioned above the feed nozzle (Figure 8, right), then considerable iC_5 would mix and exit with the nC_5 stream.

Option 3: Add a dividing wall

Drawbacks of the two previous options prompted the refinery to consider converting the column into a DWC (Figure 9). In this option, the existing depentanizer is retrofitted with new column internals and converted to a middle-DWC. The new column will produce high-purity iC_5 as the top product without requiring a significant increase in reboiler energy.

A middle-DWC has three separation zones within a single shell. A common rectifying (or enriching) section is followed by a dividing-wall section and, finally, a common stripping section.

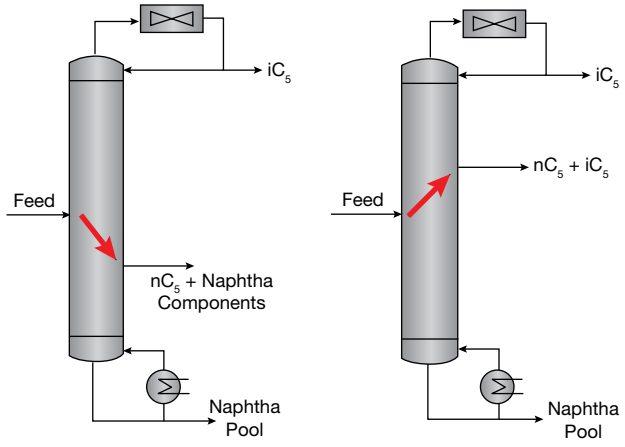
The feed enters on the prefractionation side of the dividing wall. The lightest component in the feed — mainly iC_5 — travels up the column, along with some nC_5. The heaviest components — the remaining nC_5 and the C_6 and C_7 — move down the column. In the common rectifying section, the majority of nC_5 is pushed down toward the dividing-wall main fractionation side. High-purity iC_5 is recovered as the top product.

Similarly, the nC_5 that had traveled down with the heavier components is pushed up in the common stripping section. As a result, a concentration peak of nC_5 is achieved somewhere in the middle of the column on the product side of the dividing wall. A mixed-C_5 stream is obtained as the side-cut product, while naphtha is removed at the bottom.

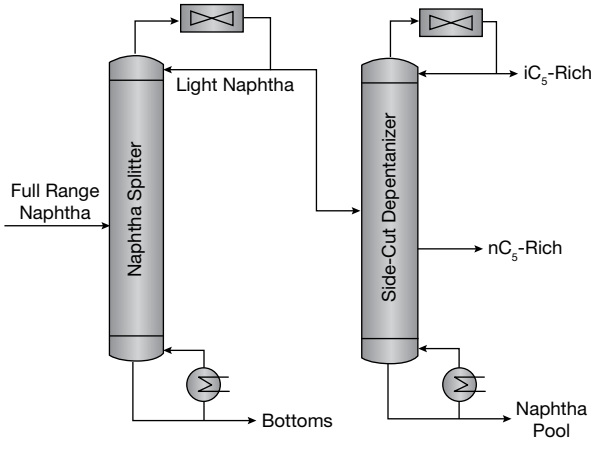
Comparing the options

Table 1 gives the column specifications for various options. In the example, the DWC configuration outperforms the two-column sequence in equipment footprint and energy consumption. Table 2 shows the recoveries and flowrates of the product streams for the column sizes, condenser duties, and reboiler duties given in Table 1.

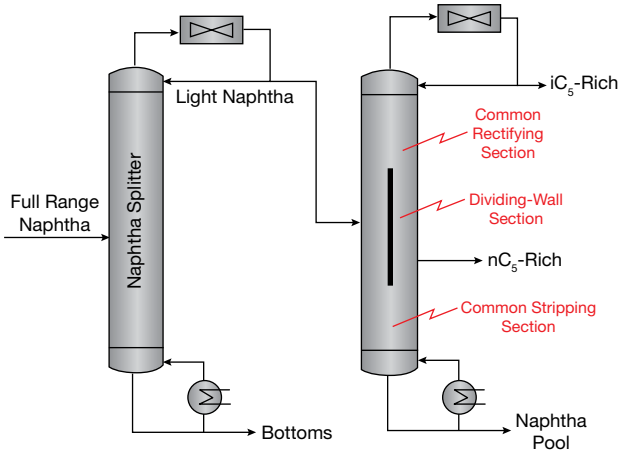
At the same level of condenser/reboiler duty (as shown



▲ **Figure 8.** If the side cut of a conventional side-cut column is positioned below the level of the inlet feed, the top product will have a higher purity, but a considerable amount of naphtha heavy components will mix with the nC_5 side cut. Likewise, if the side cut is positioned above the level of the feed, a large amount of iC_5 will exit in the side-cut stream.



▲ **Figure 7.** The refinery explored revamping the depentanizer by adding a side-cut stream. However, a high reboiler duty would be required to achieve high purity in the iC_5 product stream.



▲ **Figure 9.** Adding a dividing wall to the middle of the depentanizer column creates an iC_5-rich product stream without requiring additional reboiler energy.

in Table 1), DWC product specifications and recoveries are far better than the side-cut column (as shown in Table 2). The DWC can produce an nC_5 stream with the same purity as the two-column sequence, with much lower capital expenditure.

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Table 1. A refinery in India compared three options to recover more medium-weight hydrocarbons. The DWC configuration outperforms the two-column sequence in equipment footprint and energy consumption.

Criteria	Two-Column Sequence		Side-Cut Column	DWC
	Depentanizer (Existing)	Deiso-pentanizer (New)		
No. of Trays	50	75	75	75
Column Dia., m	4.6	3.7	4.6	4.6
Condenser Duty, million kcal/hr	14.6	15.6	18.7	19.1
	30.2			
Reboiler Duty, million kcal/hr	18.4	15.8	23.5	23.5
	34.2			

The refinery engineers evaluated the various options and found the DWC option to be the most profitable. After revamp, the DWC produced three products from the light naphtha feed — an iC_5 top product, a C_5-mix side cut, and a naphtha product.

One of the main objectives of the project was to maximize the utilization of the existing auxiliary equipment by limiting the modifications to the column internals. Since the depentanizer column had to be modified from its original service because the dividing-wall option was chosen, the refinery chose to reuse most of the existing equipment and only use new cost-effective equipment that did not require lengthy lead times.

Though each DWC is unique and tailor-made for its application, the example in this article demonstrates how DWCs can be used to achieve product purities close to those of a two-column sequence. Using DWCs in place of regular distillation columns can help refiners save both capital and utility costs, and create a smaller carbon footprint. CEP

Table 2. In the example, the DWC configuration is able to achieve the same level of product recoveries and purity as the two-column sequence, whereas the side-cut column has lower product recoveries and purity.*

Case Description	Two-Column Sequence	Side-Cut Column	DWC
Feed			
Rate, kg/hr	225,000	225,000	225,000
iC_4/nC_4, wt%	0.45	0.45	0.45
iC_5, wt%	13.97	13.97	13.97
nC_5, wt%	15.59	15.59	15.59
iC_5 Product			
Rate, kg/hr	23,193	20,500	23,193
iC_4/nC_4, wt%	4.36	4.91	4.36
iC_5, wt%	90.00	90.19	90.03
nC_5, wt%	5.45	4.72	5.45
nC_5-Rich Side Draw			
Rate, kg/hr	51,776	84,638	51,776
iC_5, wt%	20.30	15.25	19.98
nC_5, wt%	59.79	36.90	60.10
C_6+, wt%	19.91	47.85	19.92
Naphtha Product			
Rate, kg/hr	150,031	119,862	150,031
iC_5, wt%	0.03	0.02	0.13
nC_5, wt%	1.91	2.40	1.80
C_6+, wt%	98.07	97.58	98.07

*Results were determined using process simulation software Aspen Plus.

A Building Block Approach to Process Intensification

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This new approach represents chemical processes as abstract blocks arranged in a two-dimensional grid. Mathematical-programming-based optimization can identify the best design for intensification at the equipment and flowsheet levels.

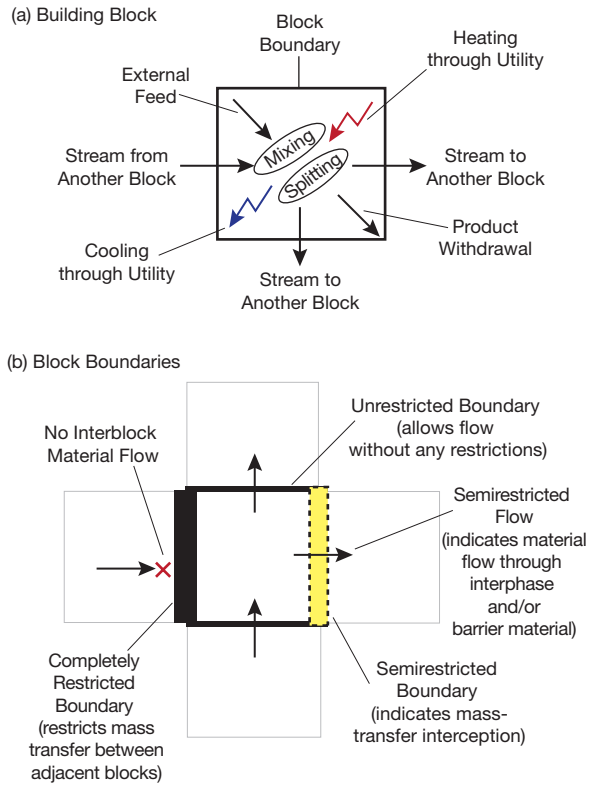
Process intensification (PI) is a design concept with transformative prospects for the chemical process industries (CPI) *(1)*. It is defined as any design activity that substantially improves one (or more) of several process performance metrics, including size, energy efficiency, environmental footprint, and safety *(2)*. Intensification can be achieved by exploiting the synergies, trade-offs, and dynamics between and among multiple competing phenomena that exist within a process. Examples of PI include dividing-wall columns, reactive distillation columns, membrane reactors, reverse-flow reactors, sorption-enhanced processes, static mixers, and more. (Reference 3 provides an extensive review of PI state of the art.)

As CPI companies strive to create processes that are more energy-efficient and sustainable, there is a need to incorporate novel and out-of-the-box solutions when designing an intensified process. Several process synthesis approaches for systematic identification of optimal process configurations have been developed *(4)*. Process integration approaches are also applicable *(5, 6)*.

However, the traditional paradigm of unit-operation-based process synthesis and integration does not always have the mechanisms required for systematic identification of novel designs. At the heart of this challenge remains the question: How should we represent chemical processes in a way that will enable automatic generation and screening of intensification pathways without knowing the equipment and flowsheet alternatives beforehand *(7)*?

Resolving this challenge requires new representation methods to foster creativity at the conceptual design stage. Design methodologies have been proposed in the past that, rather than rely on unit operations, instead employ more fundamental representations, such as generalized modular representation *(8, 9)*, phenomena building blocks (PBB) *(10, 11)*, elementary process functions *(12)*, and the infinite dimensional state-space (IDEAS) approach *(13)*. These methods highlight the usefulness of using fundamental driving forces for transformation *(8, 9)* and/or observing chemical processes as a collection of the fundamental physicochemical phenomena *(10, 11, 14)* that are the basis of all unit operations. These bottom-up approaches enable many more flowsheet variants to be generated than an approach that relies on representations only at the unit-operations level.

Recently, our group has proposed a new representation of chemical processes using abstract building blocks *(15–20)*. These blocks (which are explained in detail in the next section) are different from the traditional blocks that are used to represent unit operations. A systematic arrangement of these building blocks incorporates numerous plausible design and intensification pathways. It also enables a mathematical-programming-based optimization method to simultaneously identify the best design for intensification at the equipment and flowsheet levels. This building block approach shows promise as a systematic design and intensification technique that would not require specification of process alternatives beforehand.



▲ **Figure 1.** Each building block has two elements: (a) the block interior and (b) the block boundary (or border). The interior is characterized by a temperature, pressure, composition, and phase for each material. The boundary between two adjacent blocks defines the interactions between them.

Building block basics

A building block (Figure 1) is an abstract module that hosts or represents a fundamental constituent of a chemical operation. Each building block has two fundamental design elements: the block interior and the block boundary (or border).

The interior of a block (Figure 1a) can be either empty or filled with a functional material such as a catalyst or an adsorbent. Hence, chemical transformations are represented inside the block. The interior of each block is characterized by a temperature, a pressure, and a composition of each chemical species. Based on these physical attributes, a phase is also assigned to each block. There can be multiple incoming and outgoing streams through the block boundaries that are described by their flowrates, temperatures, pressures, and compositions. All outgoing streams from a block share a common temperature and pressure.

The interactions between two adjacent building blocks are defined by the common boundary that separates them from each other. Each boundary (Figure 1b) is classified as either unrestricted, semirestricted, or completely restricted.

An unrestricted boundary indicates that flow through this boundary will not undergo any change in its composition. That is, there is no mass-transfer interception between two neighboring blocks sharing a common unrestricted boundary.

A semirestricted boundary designates that the stream leaving through this boundary has a different composition than the source block; *i.e.,* a mass-transfer interceptor exists. For instance, if one block is in the vapor phase and the other is in the liquid phase, then a semirestricted boundary indicates that a vapor-liquid equilibrium (VLE) dictating the composition differences between the two blocks needs to be established. Permeation-related phenomena such as membrane separations can be represented by assigning a barrier material at the boundary — one block represents the permeate side, the other block represents the retentate side, the semirestricted boundary between them represents the membrane material, and the two blocks and the boundary as a whole would represent a compartment of a membrane module.

A completely restricted boundary imposes a zero-flow condition between two blocks. This may imply a wall that separates two different fluid mixtures, as in the case of a dividing-wall column.

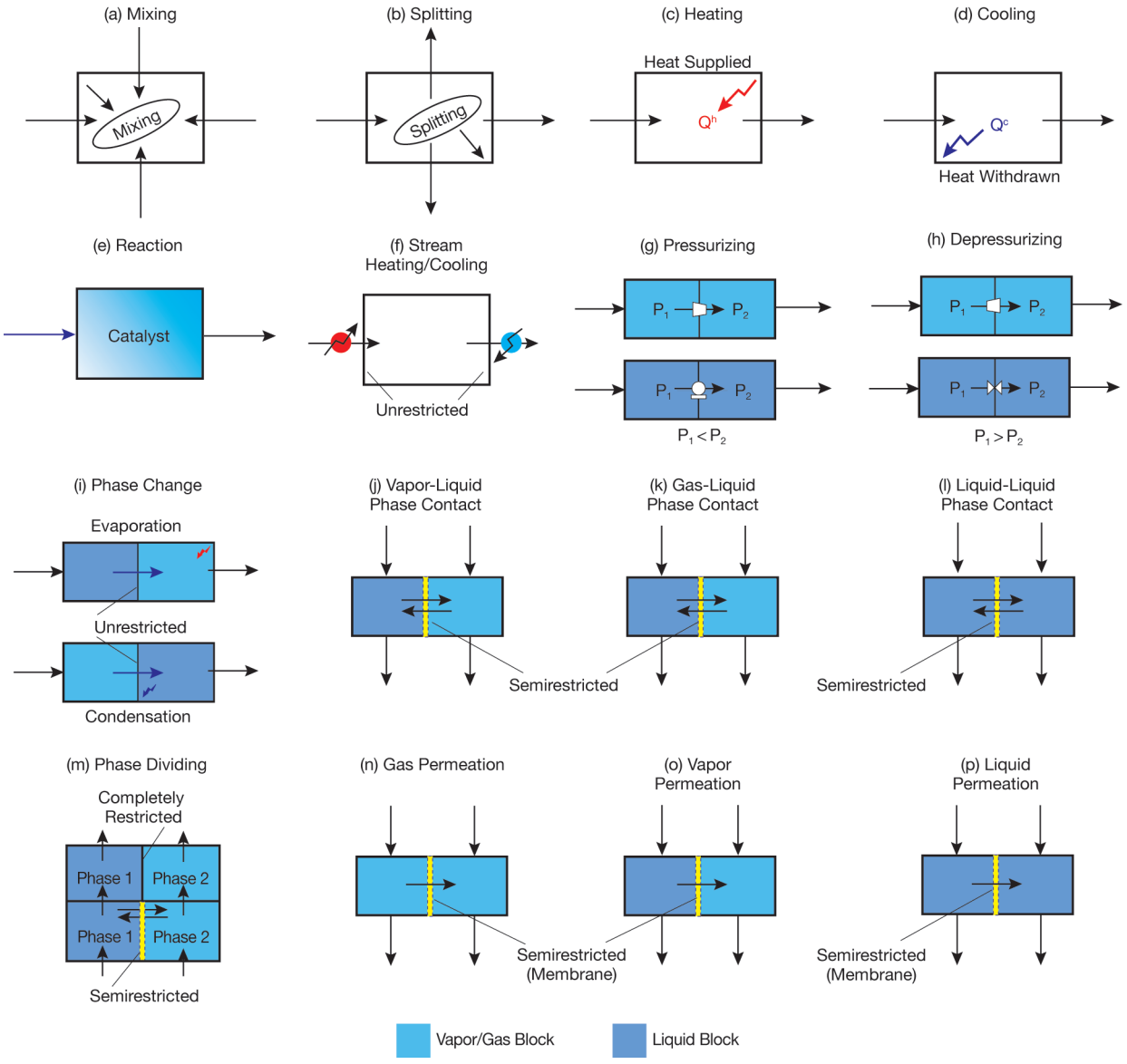
These definitions and notations can be used to represent many key operations and physicochemical phenomena — such as reaction, phase contact, phase transition, mixing, splitting, heating, cooling, etc. — that occur in chemical processes *(10)*. A physicochemical phenomena or task is represented by either a single block or a combination of two blocks (Figure 2).

Simple phenomena such as mixing, cooling, heating, and reaction can be hosted by a single block. Separation phenomena are represented by two blocks sharing a common semirestricted boundary, which can designate either direct contact between two phases (*e.g.,* vapor-liquid contact as in distillation) or a barrier material employed to carry out membrane separations. Splitting and pressure-changing tasks (pressurizing or depressurizing) also require two interacting blocks.

Furthermore, a block is not limited to only a single task or phenomena — a single block can host multiple phenomena. Consider an endothermic gas-phase reaction occurring in an isothermal reactor. The operation of this reactor can be described through a combination of reactant mixing, reaction, and external heating. All of these phenomena can be hosted within a single block (Figure 3).

Building a flowsheet

Many different equipment alternatives can be constructed from these phenomena representations. An array of blocks of the same type represents a classical process unit. For example, an array of catalyst blocks represents a



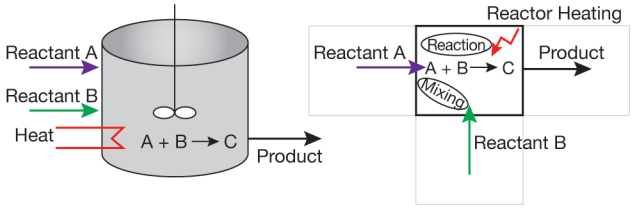
packed-bed reactor and an assembly of blocks packed with adsorbents represents a packed adsorption column.

An array or a closed combination of multiple blocks of different types depicts an intensified unit. For example, a membrane reactor can be represented by two arrays of building blocks, one array containing the catalyst for reaction at a specific temperature and pressure and the other array at a different pressure. A membrane reactor is constructed by placing the two arrays of blocks adjacent to each other with a semirestricted boundary (representing a membrane material) between them (Figure 4).

The building block representation allows a seamless transition from phenomena to task/equipment to flowsheet within a single framework, and makes it easy to incorpo-

▲ **Figure 2.** Building blocks represent a variety of physicochemical phenomena and tasks.

▼ **Figure 3.** A continuous stirred-tank reactor (CSTR) can be described by a combination of reactant mixing, reaction, and external heating — all of which can be hosted within a single building block.



rate various trade-offs and interactions among multiple competing phenomena at the conceptual design stage. Other complex unit operations, such as reactive distillation, reactive absorption, and dividing-wall columns, can be similarly represented.

Finally, an empty block (*i.e.,* with no phenomena assigned) is simply a pipe connecting different units. Thus, an assembly of empty and nonempty blocks would represent a process flowsheet with multiple units connected via pipes (Figure 4).

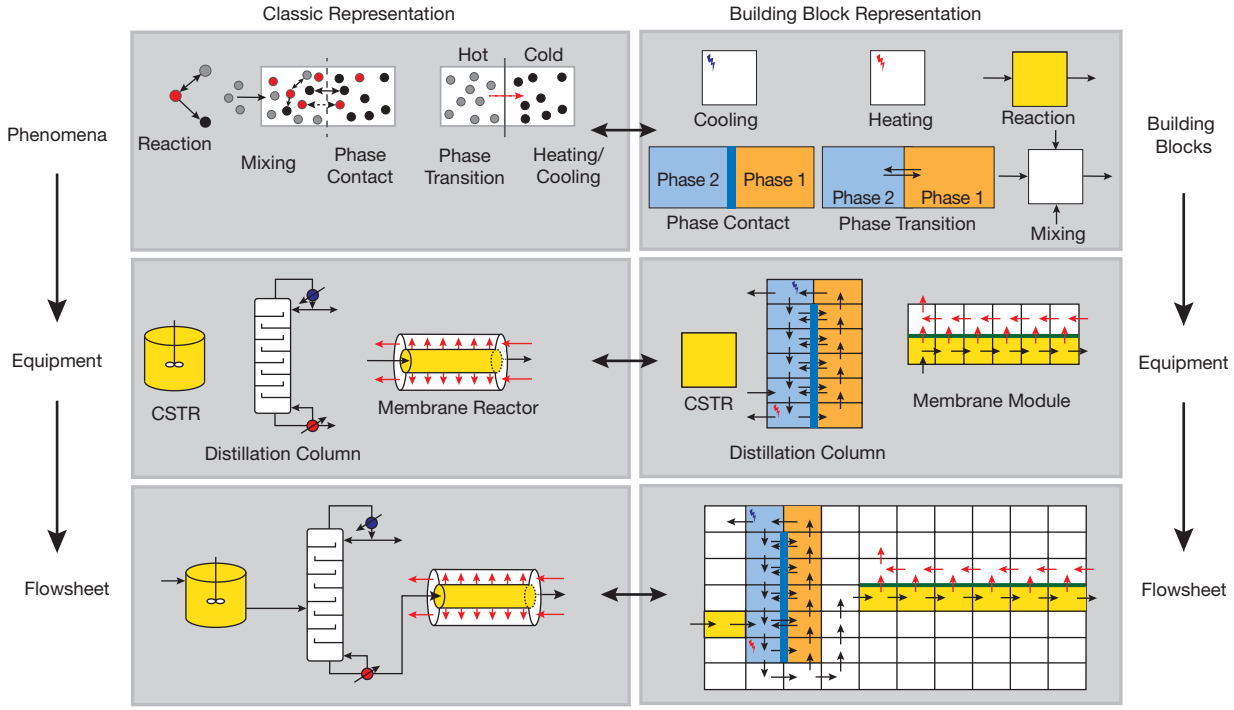
How many building blocks are necessary? The number of building blocks required to represent a particular piece of equipment depends on the type of mathematical models used to describe the system. For instance, with an equilibrium-stage model of a distillation column, each building block pair (*i.e.,* adjacent vapor and liquid blocks separated by a semirestriced boundary) represents an equilibrium stage, and the total number of building blocks required to represent a distillation column is equal to the total number of equilibrium stages required for separation. With a more-rigorous rate-based model of multicomponent mass transfer between vapor and liquid phases (*e.g.,* the Maxwell-Stefan diffusion model), each building block pair represents an actual stage, and the total number of building blocks required to represent a distillation column is equal to the total number of real stages required for separation.

For a plug-flow reactor, if you choose an equilibrium reaction model in which the equilibrium conditions are reached instantaneously, then one building block would be sufficient to describe the operation of the whole reactor. If, on the other hand, kinetic models (*e.g.,* power law kinetics) are used to describe the reactions, then each building block with reaction would represent a single continuous stirred-tank reactor (CSTR) and the operation of the entire plug-flow reactor could be approximated with an array of equal-volume reaction building blocks. This corresponds to a CSTRs-in-series model, and the number of building blocks determines the accuracy of the reactor model.

This discussion of the number of building blocks is valid for the other operations as well. Hence, the number of building blocks required to represent an operation is determined by the type and rigor of the mathematical model used to describe the building blocks.

Generation and automated screening of process intensification alternatives

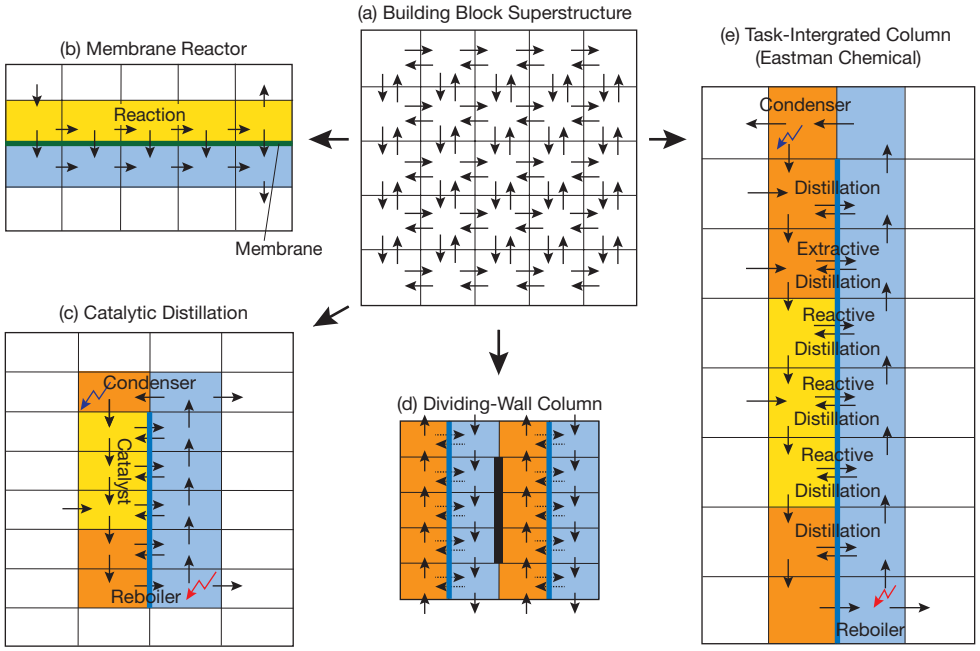
To systematically assign and select different physicochemical phenomena, we can assemble all of these building blocks into a two-dimensional grid, or superstructure, that contains numerous flowsheets in one representation (Figure 5). Blocks are denoted according to their position in the grid (*i.e.,* $B_{i,j}$, where i indicates the row and j indicates the column indices). A block can have multiple entering and exiting streams in both the horizontal and



▲ **Figure 4.** The building block representation allows a seamless transition from phenomena to task/equipment to flowsheet within a single framework.

vertical directions. These are shown as directed arrows in Figure 5a.

The proposed superstructure captures many plausible process intensification alternatives at the equipment and flowsheet levels. For instance, from the block superstructure, it is possible to generate a membrane reactor (Figure 5b) consisting of an array of catalyst blocks surrounded by semirestricted boundaries of membrane material. A catalytic distillation column with liquid-phase reaction (Figure 5c) can be generated by positioning an array of liquid and vapor blocks separated by semirestricted boundaries, where reaction takes place in the liquid-phase blocks with catalyst material assignments. A dividing-wall distillation column (Figure 5d) can be represented as two different distillation regions separated by a completely restricted boundary. Even a task-integrated column *(21),* which can transform an entire process flowsheet by stacking multiple unit operations into a single intensified unit (Figure 5e), can be generated from the same superstructure.



▲ **Figure 5.** From (a) the building block superstructure, we can generate (b) a membrane reactor, (c) a catalytic distillation column with heterogeneous liquid reaction, (d) a dividing-wall distillation column, and (e) a task-integrated column that stacks multiple unit operations in a single intensified unit.

With appropriate choices of blocks, boundary types, flow directions, and functional materials, many intensified equipment and flowsheets can be generated from the same building block representation. Thus, this generic representation serves as the basis for process intensification.

Furthermore, the building block superstructure can be used to automatically generate intensified flowsheet variants. This can be achieved by allowing any phenomena included in the search space to be positioned in any block within the grid. To enable this, we use an optimization-based approach that assigns the materials and phenomena within the grid, as well as flows through boundaries, with respect to an objective function, such as minimization of total annualized cost, utility consumption, waste generation, etc.

Table 1 summarizes the optimization problem, where x represents the vector of continuous mass and energy flow variables between lower and upper bounds x^L and x^U, respectively, and z represents the vector of binary variables. These binary variables can take a value of only 0 or 1, and they are used to determine the position of active material and phenomena selections. The objective function, represented by $f(x,z)$, can be any intensification target related to the economics, energy, and/or environmental impact of the innovative process solutions.

The term $h_t(x) = 0$ represents linear and nonlinear equality constraints describing mass and energy balances and thermodynamic models that are satisfied at each block within the superstructure. The model has three types of inequality constraints: $g_w(x) \le 0$ denotes process specifications (*e.g.,* minimum product purity, recovery, waste, etc.) that must be satisfied, which are formulated based on continuous variables alone; $g_q(z) \le 0$ denotes constraints used to assign materials, tasks, and phenomena to each block

Table 1. The optimization assigns materials and phenomena within the grid and flows through boundaries with respect to an objective function.

$\min_{x,z}$	$f(x,z)$		(1)
subject to	$h_t(x) = 0$	$\forall t = 1,\ldots,T$	(2)
	$g_w(x) \le 0$	$\forall w = 1,\ldots,W$	(3)
	$g_q(z) \le 0$	$\forall q = 1,\ldots,Q$	(4)
	$g_l(x,z) \le 0$	$\forall l = 1,\ldots,L$	(5)
	$x^L \le x \le x^U,$	$x \in R^M,$	$z \in \{0,1\}^N$

and boundary in the superstructure, which can be formulated using only binary variables; and $g_l(x,z) \leq 0$ denotes logical constraints that enforce the relationships between continuous and binary variables (*i.e.,* 0 or 1).

This optimization model is a mixed-integer nonlinear programming (MINLP)-type model that can be set up in a modeling environment that supports mathematical optimization. (Reference 15 provides detailed descriptions of the equations needed to formulate the MINLP model.) The major benefit of the MINLP model is that it can be used to automatically generate intensified flowsheets. Given the reaction stoichiometry, kinetics, equilibrium data, material properties (*e.g.,* membrane permeance), and bounds on process temperature, pressure, etc., the solution of the MINLP model will determine the optimal position of the phenomena within the given grid size and the interconnections between the phenomena. This building block superstructure result can then be translated into a traditional flowsheet representation. This is a unique approach to automated flowsheet synthesis.

From building blocks to flowsheet

After solving the optimization problem in terms of block variables, the results need to be converted into a flowsheet.

Consider a gaseous stream containing an equimolar mixture of A and B that has a flowrate of 0.5 kmol/sec. Component A is a hazardous chemical that we want to convert to B at the highest conversion possible before the gaseous stream is discharged to the environment. A catalyst material (*Cat*) is available to convert A to B according to the following heterogeneous, reversible, isothermal gas-phase reaction:

$$\mathrm{A} \leftrightarrow \mathrm{B} \qquad -r_A = 0.3P_A\left(1-\frac{P_B}{4P_A}\right) \quad \left(\text{kmol/bar-kgcat}\right)$$

where r_A is the consumption rate of the reactant A, and P_A and P_B are the partial pressures of A and B, respectively.

Alternatively, A and B could be separated by a membrane (M) that is highly selective to B; the membrane has a maximum available area of 1,000 m^2, a permeance of 3.125×10^{-7} mol/m^2-sec-bar for A and a permeance of 4.689×10^{-5} mol/m^2-sec-bar for B.

The objective is to maximize the yield of B from the process. This is the basis for the objective function, Eq. 1 in the MINLP model summarized in Table 1. No purity specifications for the product stream are specified, as the goal is to remove as much of the hazardous material as possible. The equilibrium conversion of A at equimolar inlet conditions is 60%.

To solve this problem through the block superstructure approach, we use a 3×3 block superstructure (*i.e.,* three rows and three columns). Thus, all the process alternatives must be embedded within at most nine building blocks. A smaller superstructure may not contain all plausible process alternatives, whereas a larger superstructure will increase the size of the model.

Any one of the nine blocks, but only one block, is allowed to be assigned with catalyst (*i.e.,* with reaction); the decision as to which block should be assigned with catalyst is determined by the solution to the optimization problem. In addition, at most one of the block boundaries is allowed to be semirestricted. This implies that of the 12 block boundaries within the 3×3 grid, at most one of the boundaries can be assigned with the membrane material. The decisions as to whether the membrane material should be used, and if so where to position it, are also determined by the solution to the optimization problem. These decisions are modeled via the binary (0,1) variables; because this problem has nine blocks, nine binary variables are involved in determining the position of the catalyst material within the 3×3 grid. Similarly, as this problem has 12 boundaries (excluding the exterior boundaries, which are impermeable to material flow), 12 binary variables are involved in determining the position of the membrane material.

Solution of the MINLP problem yields an objective value of 0.451 kmol/sec B. This corresponds to a process with 80.3% A conversion, which is 34% higher than the equilibrium conversion. Figure 6a shows the block structure for this result.

Solving the MINLP model gives the optimal values for the continuous and binary variables included in x and y. The positions of the reaction block and the semirestricted membrane boundary are indicated by the values of the binary variables. For instance, for the reaction, the optimizer gives the binary variable associated with Block $B_{2,1}$ a value of 1, and all the other binary variables associated with reaction for the other blocks are zero. Hence, reaction takes place only in Block $B_{2,1}$ (shown in yellow in Figure 6a).

Similarly, membrane material is assigned to the block boundary that is on the right of Block $B_{2,1}$ (green in Figure 6a). At this boundary, the semirestricted boundary variable has a value of 1, and at all of the other positions, the semirestricted boundary variables are zero.

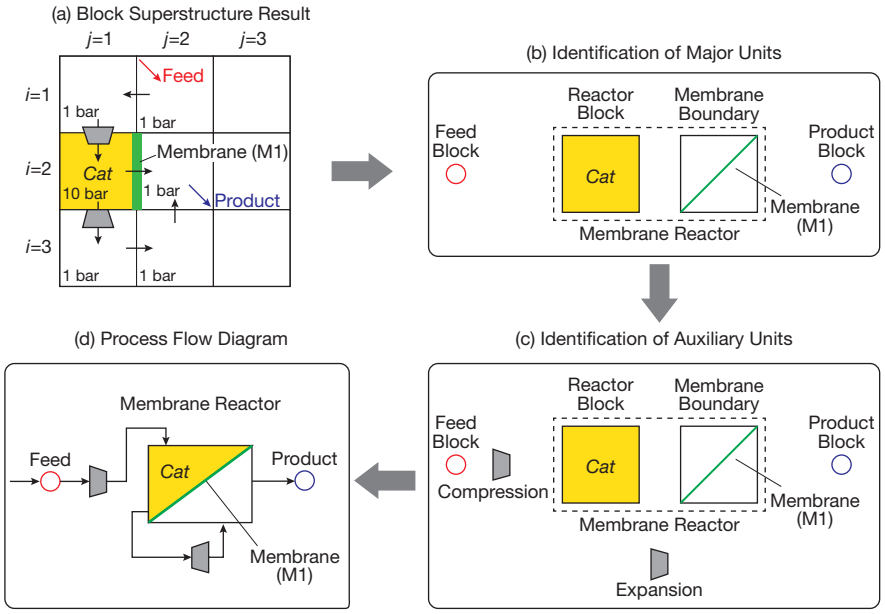
The values of the interblock streams (which are continuous variables) indicate the direction and the amount of the material flow between building blocks. If the amount of flow associated with an interblock stream is zero, then no stream is shown at the corresponding position on the grid. Similar to the interblock streams, external feed and product streams that carry the fresh materials in and take the product streams out from the superstructure are also indicated by the value of the continuous variables. For instance, in

Figure 6a, the feed stream variables for Block $B_{1,2}$ are non-zero, while for all the other blocks, they are zero. This indicates that external feed stream is only fed into Block $B_{1,2}$.

The next step is to convert this building block structure to the corresponding process flow diagram. In general, the transformation (Figure 6a–d) involves the following three-step procedure:

Step 1. Identify the primary phenomena and material assignments and the external feed and product positions (*e.g.,* reactors, separators, feed, product, and waste streams) that will form the basis of the process flowsheet.

The block structure in Figure 6a has one feed stream assigned to Block $B_{1,2}$ and one product stream assigned to Block $B_{2,2}$. These blocks indicate the starting point and the end point of the flowsheet, as shown in Figure 6b. The catalyst material is assigned to Block $B_{2,1}$ and the boundary between Blocks $B_{2,1}$ and $B_{2,2}$ is assigned to the membrane. Block $B_{2,1}$ is the retentate side of the membrane and Block $B_{2,2}$ is the permeate side. As the reaction proceeds toward B in the retentate side, reaction product B is simultaneously separated from the reaction block through the membrane boundary. Reaction and membrane act simultaneously, and we can identify a membrane reactor as combination of Blocks $B_{2,1}$ and $B_{2,2}$ (Figure 6b).



▲ **Figure 6.** Transforming (a) the superstructure into a flowsheet involves identifying (b) major units and (c) auxiliary units, as well as (d) the connectivity between phenomena and materials.

Step 2. Identify auxiliary unit operations (*e.g.,* heaters, coolers, expanders, compressors, mixers, splitters).

The existence of any utility consumption is indicated by the block and stream heat duty variables, which are determined through energy balances. In this example, the operation is isothermal, so no energy balance constraints were considered; accordingly, there are no heaters or coolers. Similarly, energy required or released through pressure change is not considered. However, the pressure increase on the retentate side suggests a compressor on the reactor inlet stream, and the pressure decrease across the unrestricted outlet stream suggests an expander (Figure 6c).

Step 3. Identify the connectivity between phenomena and materials to complete the flowsheet.

To build the explicit connections between the units identified in the first two steps, start at the external feed streams and follow the active streams (*i.e.,* non-zero flow variables) around each block. In Figure 6a, two streams leave Block $B_{2,1}$ — the permeating stream through the membrane boundary, and the stream that enters Block $B_{3,1}$ through the unrestricted boundary. The latter stream is then carried through Block $B_{3,2}$ to Block $B_{2,2}$, where it mixes with the permeating stream and acts as a sweep gas to dilute product B on the permeate side (Figure 6d).

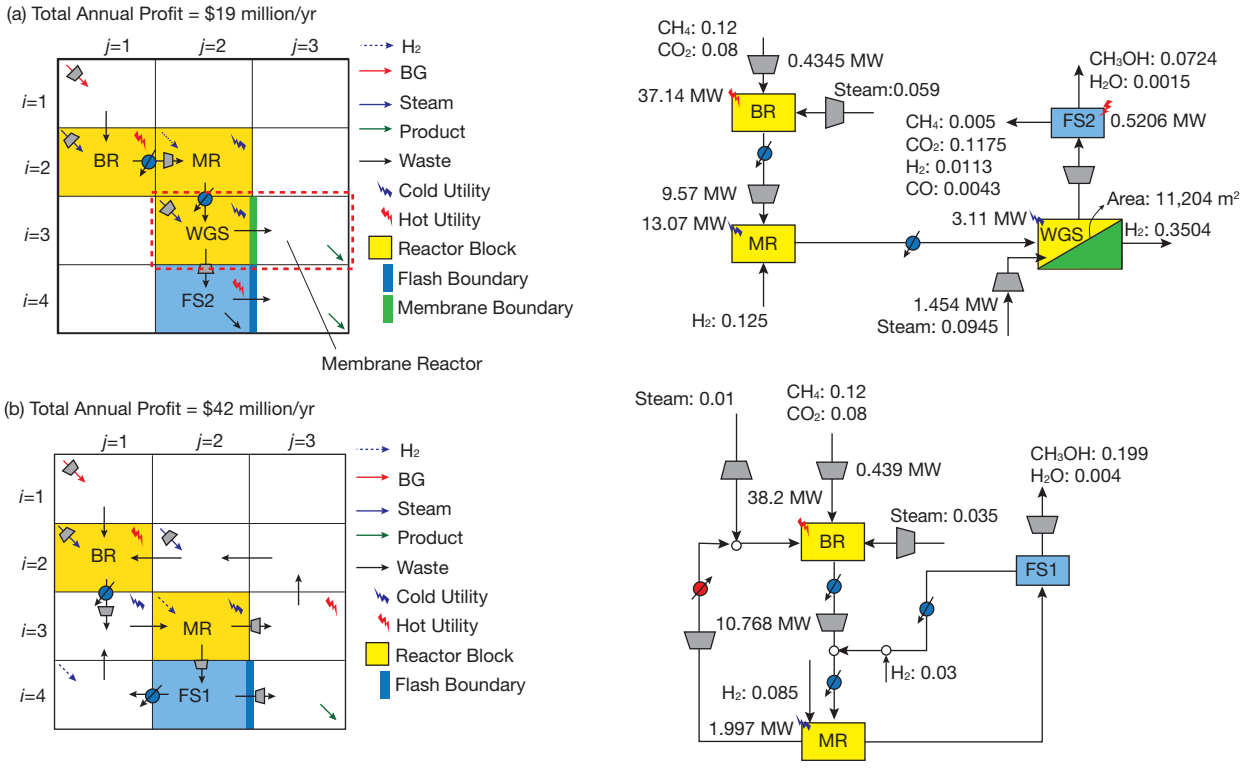
The use of the reactor outlet stream as sweep gas reduces the concentration of B on the permeate side of the membrane, which increases the separation driving force. This allows a higher concentration of reactant A to be obtained in the reactor block and increases the overall conversion to 80.3%.

Note that this flowsheet was obtained by solving the MINLP problem. Although no mention of a membrane reactor or information on flowsheet connectivity were provided beforehand, the solution suggests that this approach can automatically generate an intensified flowsheet with a membrane reactor and complete flowsheet connectivity.

Example: Methanol production from biogas

An example problem involving the production of methanol from biogas demonstrates the capabilities of the building block superstructure approach. Biogas is produced from organic waste and is composed mainly of methane and carbon dioxide. Currently, its principle use is in the production of heat and electricity. It can also be used as a feedstock for the production of value-added products, such as methanol. This example investigates several processing pathways to convert biogas into methanol.

The objective of the problem is to obtain an optimal flowsheet with maximum total annual profit. The annualized profit constitutes the objective function (Eq. 1) in the



▲ **Figure 7.** Building block results and corresponding flowsheets for the example biogas-to-methanol process.

MINLP model. We consider four reactor alternatives: dry reformer (DR), bireformer (BR) (which combines steam and dry reforming reactions), water-gas shift (WGS) reactor, and carbon monoxide hydrogenation methanol reactor (MR). Equilibrium reactor models are used for the DR, BR, and WGS reactor, and the MR is modeled with a fixed conversion. We also consider four separation alternatives: two flash tanks for separating methanol and water from other gases at low and high pressures (FS1 and FS2, respectively), a distillation column (D) for methanol-water separation, and an H_2-selective membrane (M). Both methanol (with minimum 98% purity) and hydrogen are considered viable products.

We use a 4×3 block superstructure and the previously mentioned MINLP model to automatically generate the optimal flowsheet. We allow all the reaction and separation alternatives to be assigned to any block and boundary, respectively, within the superstructure in the search for the optimal configuration with maximum annualized profit. The positions of these reaction and separation alternatives are indicated by the binary variables included in the MINLP model. Solution of this MINLP model yields several flowsheet variations *(16),* including the two shown in Figure 7.

The first flowsheet alternative (Figure 7a) is for a process with both methanol and hydrogen as end products. This process starts with biogas being fed to a bireformer. The effluent from the BR is cooled and compressed then sent to the methanol reactor. Additional hydrogen is also fed into the MR. The outlet stream from the MR is then sent to the WGS reactor, where additional hydrogen is produced and simultaneously removed via the membrane (M). Note that the WGS unit assigned to Block $B_{3,2}$ and the membrane boundary assigned to the right side of that block suggest a membrane reactor. The block superstructure can identify the existence of this intensified unit without its existence having been prespecified and can use it to increase the conversion obtained from the WGS reactor (96% CO conversion is achieved, vs. the equilibrium conversion at the same conditions of only 86%). The hydrogen stream that permeates through the membrane is removed as a co-product. The effluent from the WGS membrane reactor is sent to flash tank FS2 for recovery of methanol and water from other gases. The methanol stream is the product from $B_{4,3}$. This flowsheet provides a total annual profit of $19 million/yr.

The process depicted in the second flowsheet alternative (Figure 7b) makes only methanol as a product. It employs only the bireformer and the methanol reactor (without the WGS membrane reactor) and has two recycle streams: one from the MR outlet to the BR inlet and one from the FS1 outlet to the MR inlet. These two recycle streams enable all of the carbon in the biogas feed to be converted to methanol. Because of this higher yield, the process has an annual profit of $42 million/yr — 120%

higher than the process depicted in Figure 7a.

As these results show, the building block superstructure can automatically generate and screen different flowsheet alternatives with intensified or traditional unit operations.

Final remarks

The systematic process design and intensification method presented here marks a departure from the classical unit-operation-based representation of process units, flowsheets, and superstructures. It generates optimal intensified designs by solving a generic MINLP model without the need to develop different process superstructures for different applications. While this approach brings everything within a single optimization-based framework toward a unified method for design, synthesis, integration, and intensification, the focus is on the method rather than on design of intricate equipment such as microwave heating, magnetic separation, and jet-impingement reactors.

Challenges remain in quickly finding globally optimal solutions. Due to the model's nonlinearity and nonconvexity, good starting points are very useful in finding an optimal solution.

Further work is needed to address the symmetry and degeneracy of the block-based superstructure. In the current block superstructure, the assembly of blocks remains the same after geometric operations like translation, rotation, and mirroring, so many combinations of blocks correspond to the same process flowsheet. Hence, effective symmetry-breaking constraints may help in obtaining results more efficiently.

Finally, the operability, controllability, and safety of the resulting intensified process systems also need to be considered for practical implementation *(6, 9, 22)*.

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Acknowledgments

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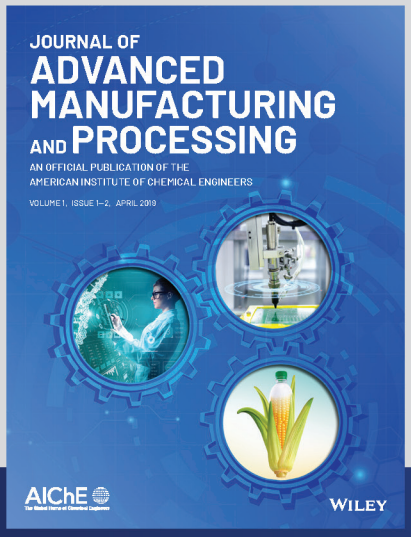

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Using Simulation and Digitalization for Modular Process Intensification

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John Lusty
John Nixon
Siemens

These tools enable engineers to create a digital twin of a process, which can be key to developing new technologies and testing them virtually at a rapid pace.

The chemical process industries (CPI) have been built upon two fundamental tenets: economies of scale and unit operations *(1)*. Traditional chemical processing takes advantage of economies of scale by building large plants, which make better use of capital and resources. And, the processing steps are grouped into unit operations, which are combined like building blocks to design and build plants.

Recently, these tenets have been challenged by smaller plants that combine more than one function in a single piece of equipment — *i.e.,* process intensification (PI) — and by the modularization of processing units. To exploit the capital, resource, safety, environmental, and other benefits of PI and modularization, engineers need to develop and test technologies at a rapid pace. Digitalization and simulation are key tools for virtually developing and testing intensified technologies.

Digitalization provides a new way of creating, sharing, storing, and analyzing data that enables an integrated engineering approach and eliminates the "silos" typical in many organizations. Simulation can play an important role in the creation of data, supplementing traditional data creation and collection via experimental methods.

This article demonstrates how these tools help achieve the broader goals of PI.

Modularization

Globalization has changed the pace and nature of business and innovation around the world. Materials with new and innovative functionalities are driving change in many industries, and product cycles are becoming shorter. Kockmann *et al. (2)* promoted the "50% idea," which aims to reduce the time to market by half. As explained in the white paper published by DECHEMA *(3)*, five key elements will be integral in achieving the 50% idea: microreaction technology, process intensification, resource-efficient continuous chemistry, modularization, and standardization. Many of these elements are related.

An important driver behind modularization is its ability to reduce time to market; a standardized approach and modular units allow faster and easier plant construction. Modularization offers several more benefits *(3),* including:

- improved sustainability attributable to reconfigurable multipurpose production plants
- lower capital costs achieved by the reuse of modules
- an easy way to increase capacity by numbering up
- shorter construction phase and partial elimination of the plant start-up phase realized through the centralized manufacturing of processing modules.

Modularization allows for easier scale-up. Instead of scaling up a process by employing larger pieces of equipment, smaller modules are numbered up to achieve larger production capacities. Traditional scale-up typically entails a long period of experiments at various scales — laboratory, bench, and pilot — to derive correlations and scale-up rules on a case-by-case basis.

Combining processing steps into a single step in smaller devices removes some of the heat- and mass-transport barriers. However, these modular units are fea-

sible only if the traditional unit operations can be replaced by a multifunctional unit operation or if several unit operations can be combined into a single processing step — that is, if the process can be intensified *(4)*.

Digital twins

A digital twin *(5)* is a virtual representation of a piece of equipment or a process. It generally consists of multiple interconnected representations that address the various aspects of the process, *e.g.,* mechanical function, control variables, process conditions, etc.

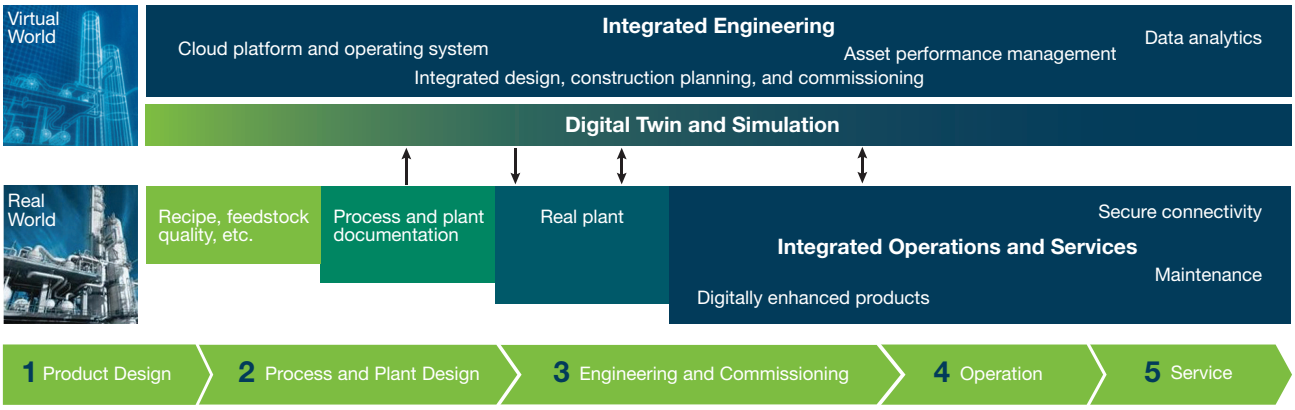
To ensure accurate modeling of the process or equipment, a digital twin uses data from sensors within the unit or plant to determine real-time performance, operating conditions, and changes over time. Using these data, the digital twin evolves and continuously updates to reflect any change to its physical counterpart throughout the lifecycle, creating a closed loop of feedback in a virtual environment that enables companies to continuously optimize their products, production, and performance at minimal cost.

A digital twin helps in understanding and predicting the physical counterpart's performance characteristics. It can simulate, predict, and optimize equipment and production systems before the company invests in physical prototypes and assets. This article describes how a digital twin can be designed and deployed through virtual integrated engineering.

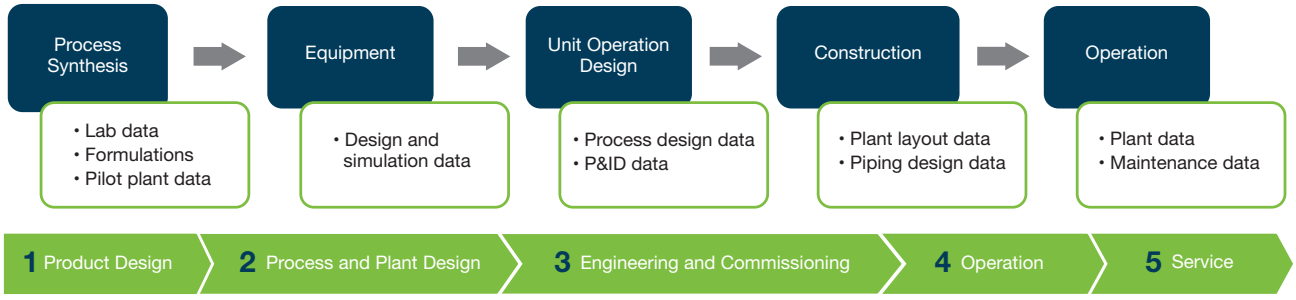
Virtual integrated engineering — the future of modular plant construction

Virtual engineering begins with a conceptual design of the process and equipment during research and development. The integrated virtual engineering workflow (Figure 1) uses various digital solutions, such as simulation, engineering data management, requirements management, virtual commissioning, etc., to create the digital twin during the process and plant design phase and to update the digital twin during the engineering/commissioning and operation phases.

Throughout the life of a process plant, an organization deals with various types of data. In the initial stages, computer-aided design data generated in the laboratory provide the basis for the design of unit operations. During the engineering and commissioning phases, piping and instrumentation diagram (P&ID) data, detailed engineering



▲ **Figure 1.** The integrated engineering approach connects the virtual world with the real world via a digital thread. Software and simulation tools create a digital twin (top) of the real-world plant and engineering workflow (bottom).



▲ **Figure 2.** Data is a raw material that serves as an input to the digital twin in each phase of the workflow.

data, and process simulation data are generated. After the plant is constructed, operational data are used to monitor and maintain the plant. At each stage of the facility's lifecycle, tremendous amounts of data must be generated and fed as input to the next stage.

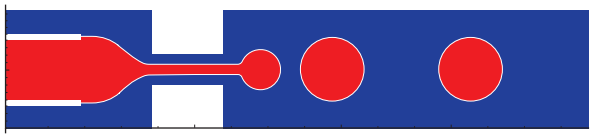
However, not all organizations can connect the data across all of the stages. A common digital thread provides continuity and makes the overall process more efficient. A digital twin that replicates every aspect of the real process in digital form using data structures, physics-based simulations, control models, etc., provides such continuity. Data is a raw material that the digital twin processes in each stage to reach the next step in converting an idea into reality (Figure 2).

Using simulation to overcome hurdles in process intensification

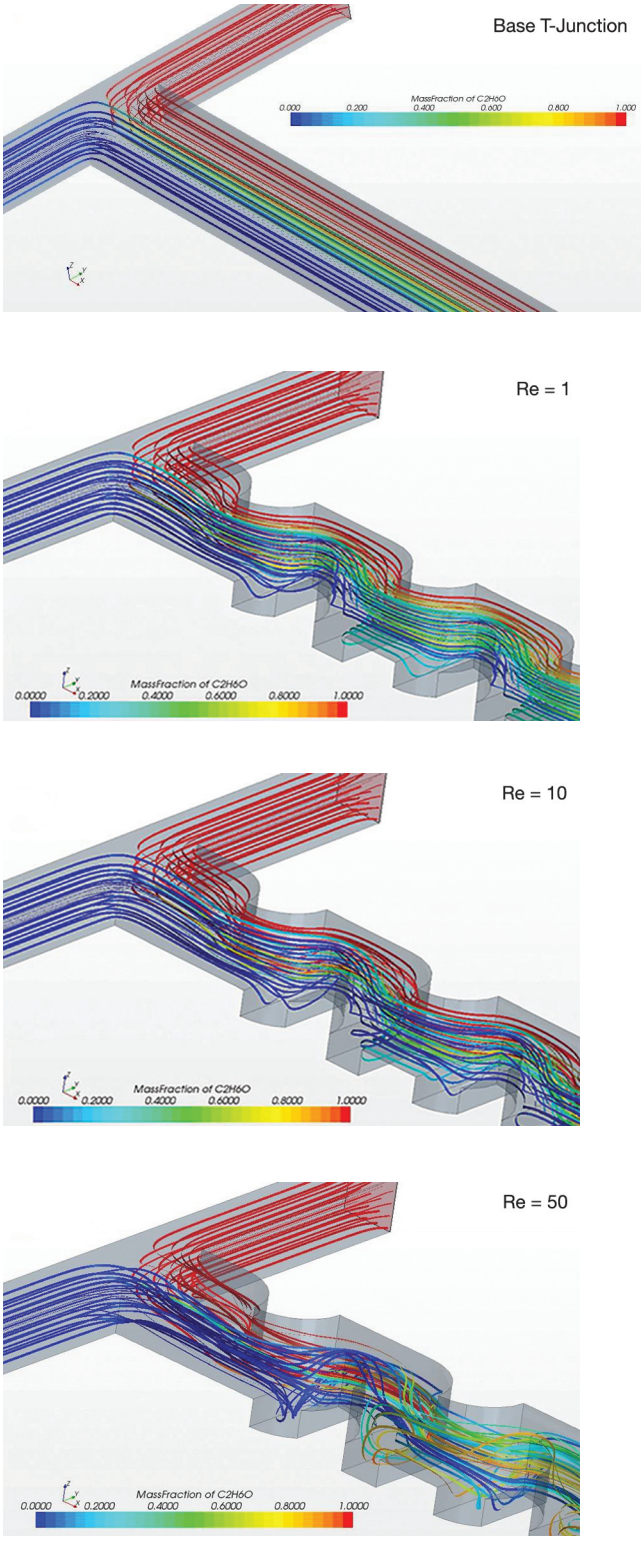
Heat- and mass-transport limitations make it difficult to intensify traditional equipment designs. To ensure performance, reliability, manufacturability, and successful scaleup, as well as to reduce cost, the intensified units must simultaneously overcome these transport limitations. In order to meet the fundamental transport needs of an intensified process, engineers often attempt to employ complex reactor structures and processing approaches to enhance these phenomena. The following examples demonstrate the role of simulation in studying and designing such intensified systems.

Microfluidics deals with the study of fluids that are geometrically constrained to very small channels, with channel sizes of around 100 nm to 500 µm. It typically involves control and manipulation of very small volumes of fluids, on the order of nanoliters. Microfluidic devices find applications in cooling, emulsification, filtration, and reaction processes. A microfluidic device can combine multiple steps, for example mixing and reaction, in a small, intensified operation. Such a device can then be numbered up to create a module.

Investigators at Indian Institute of Technology (IIT) Delhi performed a numerical analysis of a microfluidic device used for mixing fluids at small scale known as a T-junction device (Figure 3) *(6)*. Software and simulation tools helped them elucidate the squeezing, transition, and



▲ **Figure 3.** Researchers used simulation to analyze the squeezing, transition, and dripping regimes of droplet formation in a microreactor. Source: *(6)*.



▲ **Figure 4.** Simulation was used to study the effects of various geometric design parameters and changing Reynolds number on the mixing efficiency of a T-junction microreactor. Source: *(7)*.

dripping regimes of droplet formation as the liquid passed through the device. Numerical modeling is quite flexible in characterizing the physics of the problem, which would be very difficult to do experimentally. It helps engineers understand and rationalize the effects of the geometrical parameters, which otherwise may require the creation of a large number of prototypes.

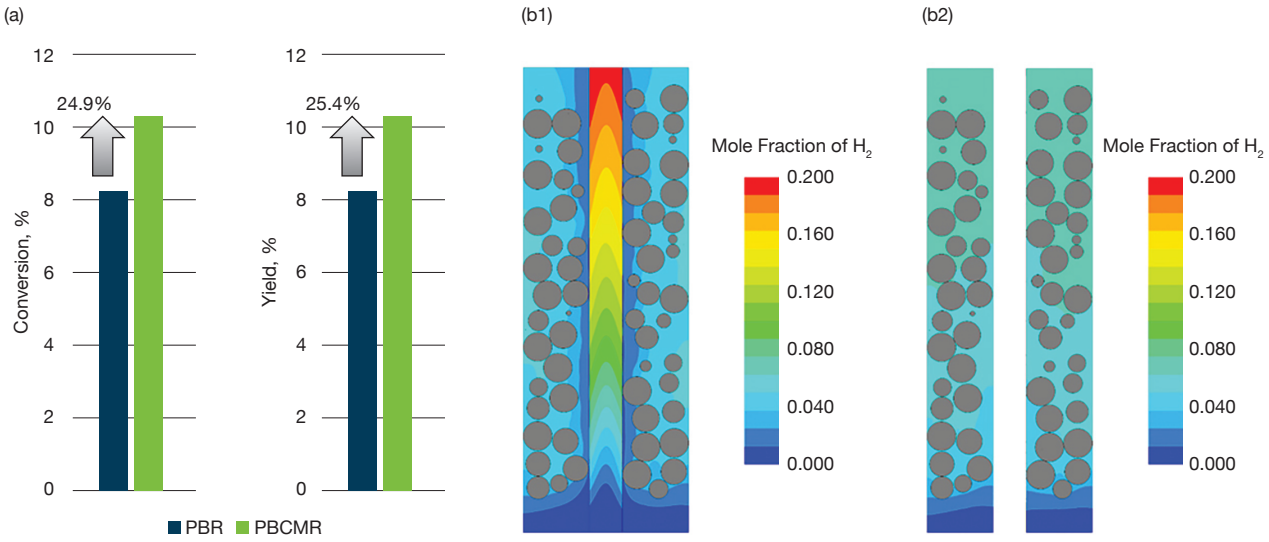
Similarly, researchers at Hertfordshire Univ. used STAR-CCM+ to investigate the effects of various geometry design parameters on the mixing efficiency of a microreactor (Figure 4) *(7)*. The study identified the effects of strategically located and dimensioned grooves (in addition to the typical baffle structures) on flow patterns and mixing levels. With the help of simulation, the researchers were able to easily identify designs that had regions with poor mixing characteristics, eliminating the need to prototype several of those designs.

Half of the world's hydrogen is produced via steam methane reforming (SRM), which is traditionally carried out in packed-bed reactors. Using a membrane to remove the products *in situ* may increase the yield by shifting the chemical equilibrium, thus intensifying the process. Researchers at TU Berlin investigated the convection and diffusion flow effects on the conversion of methane to hydrogen in a packed-bed membrane reactor (Figure 5) in order to evaluate and scale up the process *(8)*. They used computational fluid dynamics (CFD) simulation to evaluate three critical parameters — fluxes, temperature, and heat transfer. The work demonstrated an increase of about 25% in the yield and conversion to hydrogen.

Once a design is verified for performance, the next step is to evaluate its manufacturability and begin the computer-aided design of a module. A simulation-based approach to process intensification employing a digital twin of the design makes the entire engineering workflow more amenable to modularization by, in effect, eliminating the laboratory work involved in traditional scale-up. This approach to scoping and configuring equipment could be considered a necessary starting point for many new technologies being explored for plants of the future *(9)*.

Connecting the dots with virtual integrated engineering

Engineering, procurement, and construction companies (EPCs) realize that fabrication and engineering must be closely integrated when it comes to modularization. As a project evolves, the fabrication department will request modifications. That information needs to be communicated back to the engineering department and the changes need to be well understood by both teams. Such close collaboration is missing in today's typical workflow. This results in wasted materials and unnecessary labor requirements, both causing financial burdens on an organization. In one such case, the engineering department did not properly inform the fabrication department of a change that was made to the design of a particular component in a plant. Unfortunately, the fabrication department had already purchased approximately $20 million worth of valves that could not be used.



▲ **Figure 5.** Researchers used computational fluid dynamics (CFD) simulation to investigate the convection and diffusion flow effects on the conversion of methane to hydrogen. (a) The conversion and yield were about 25% higher in a packed-bed membrane reactor (PBMCR) than in a packed-bed reactor (PBR) system. (b) Comparison of hydrogen concentration (mole fraction) in the PBMCR (b1) and PBR (b2) under similar operating and design conditions. The membrane is in the form of an annulus; there is no flow in the annulus of the PBR because the membrane was deactivated in the simulation to allow one-to-one comparison. Source: *(8)*.

The transition toward virtual integrated engineering is grounded in the ability to look across the entire project lifecycle to understand how each element in the overall schedule is related to, and impacted by, everything else. A more granular and integrated understanding of the project design and execution affords the opportunity to apply and benefit from a modular engineering approach, which then creates further opportunities for process intensification.

Based on many discussions with customers in the CPI, we have defined a holistic digitalization concept stretching over the complete value chain. We are particularly focused on the current lack of integration between engineering and operations during data handover at the conclusion of a major capital project. A benchmark study by the National Institute of Standards and Technology (NIST) in 2004 *(10)* concluded that the cost of inadequate interoperability and information management to U.S. capital facilities (*i.e.,* commercial and institutional buildings and industrial facilities) was $15.8 billion each year across the project lifecycle. Given the explosion in the amount of data and documentation and overall project complexity since that time, the cost is likely much higher today, and thus the need for integrated project execution has never been greater.

With that in mind, we are particularly focused on the transition between the design/engineering phase and the startup/operations phase. How do we move from integrated engineering to integrated operations? By consolidating and integrating the data that were created and received across the project execution lifecycle — the as-designed, as-built, and as-operated systems — within the digital twin.

With stronger integration of all engineering steps, the time from process and plant design to operations can be shortened, and the improved information processes at the data-handover stage positions the owner for more successful start-up and operations. At project data handover, the owner-operator receives an organized digital twin of the new facility and is better prepared to support high rates of plant utilization and regulatory compliance, as well as capitalize on opportunities for optimizing and intensifying plant operations and maintenance.

The product of the integrated engineering approach is the digital twin of the plant. The digital twin provides for a common data model and allows for the creation of an accurate 3D model of the plant for simulation for training purposes. During operation and maintenance, all changes to the as-operated plant condition must be incorporated into the model. In this way, the closed-loop digital twin stays up-to-date over the entire lifecycle of the process or facility.

Leveraging next-generation tools. Vertical integration brings together the different views from the virtual world to the real world during operations in support of an integrated operations approach. By combining all available data from the field and the automation (operations) level with the management (enterprise resource planning, or ERP) level, the cloud can optimize operations and increase productivity and flexibility by leveraging today's artificial intelligence (AI) and internet of things (IoT) capabilities in pursuit of operational excellence.

A critical enabler for this will be secure and reliable communication and connectivity — within all levels of the orgainzation, between them, and to and from the external world. CEP

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