

SPECIAL SECTION:

PROCESS INTENSIFICATION



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Process Intensification in Theory and Practice

In the January 2000 issue of *CEP*, Andrzej Stankiewicz and Jacob Moulijn introduced readers to the concepts of process intensification (PI) and how PI could transform chemical engineering and process development. They covered topics ranging from novel reactor designs and separations equipment to new methods of integrating operations. And they presciently noted that education would play a key role in democratizing PI concepts, suggesting that chemical engineers would need to be “taught an integrated, task-oriented approach to plant design, [instead of] today’s sequential, operation-oriented one” and would need to “gain a much deeper knowledge and understanding of process chemistry.”

Twenty years later, many of their predictions ring true. While chemical engineers still rely heavily on traditional unit operations, many of the technologies that Stankiewicz and Moulijn identified are now more widely used. Intensified operations and multifunctional systems — such as membrane distillation, reactive distillation, and membrane reactors — are becoming more common in manufacturing settings. Investment in process research and development is increasing. New curricula are being deployed to teach PI concepts. And AIChE’s RAPID Manufacturing Institute and its members are working to promote commercialization of new intensified and modular technologies and education in PI design principles.

The articles in this special section offer more insight into the fundamentals that underpin PI and provide examples of the exciting work being done in this field. The authors of the first two articles, Andrzej Stankiewicz and Christophe Gourdon, address the theme “Twenty Years After.” Stankiewicz reflects on the evolution of PI over the past 20 years, from the equipment-centric practice orientation of the field to the fundamental principles and domains derived by the practitioners of PI. Gourdon then examines the application of those fundamentals to the practice of PI, specifically the selection of equipment for PI applications.

In “The Principles and Domains of Process Intensification” (pp. 23–28), Stankiewicz defines the four guiding principles of PI — maximizing the effectiveness of molecular events, ensuring that all molecules undergo the same processing experience, optimizing driving forces and resistances over the greatest specific surface area, and maximizing synergistic

effects. He explains that by observing these principles and designing equipment and processes with unique attributes in one or more of PI’s four domains — spatial, thermodynamic, functional, and temporal — a chemical engineer can capitalize on PI to dramatically improve process efficiency.

Gourdon continues the story in “Selecting Process-Intensified Equipment” (pp. 29–34). He discusses the application of the principles across the domains and offers insight into how engineers can use characteristic time scales for reaction and heat, mass, and momentum transfer to identify process bottlenecks and to assess process and equipment performance. He then describes a methodology for screening and selecting PI equipment.

The third article, “Process Modeling of Intensified Chemical Processes” (pp. 35–42), by Chau-Chyun Chen *et al.*, describes how process modeling is advancing the understanding and development of PI-enabled processes. Through case studies, they identify areas of opportunity — including lack of available chemical kinetic data for complex reaction sets, difficulties in predicting multicomponent adsorption behavior under nonsteady-state conditions, and highly nonideal fluid behavior in membrane transport — where new models are critical to predicting process performance.

In the fourth article, “Sustainable, Modular Chemical Production in Africa” (pp. 43–47), Paul Yelvington and Siphon Ndlela envision modular manufacturing changing the chemical manufacturing landscape in Africa. They cite as examples a gas-to-liquids plant in Nigeria and a chlor-alkali plant in Tanzania, and point out that modular construction can offer significant safety, supply chain, and economic development benefits in the developing world.

Twenty years after *CEP* introduced readers to process intensification, the PI community continues to grow and develop new tools to help chemical engineers design better processes. There is much opportunity for innovation in the process industries, and the RAPID Manufacturing Institute and its members are working hard to build and educate a community focused on developing and deploying PI and modular process technologies in U.S. manufacturing.

*William Grieco, Chief Executive Officer
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The Principles and Domains of Process Intensification

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Apply the fundamental principles of process intensification to the four domains of PI — spatial, thermodynamic, functional, and temporal — to identify possible PI opportunities.

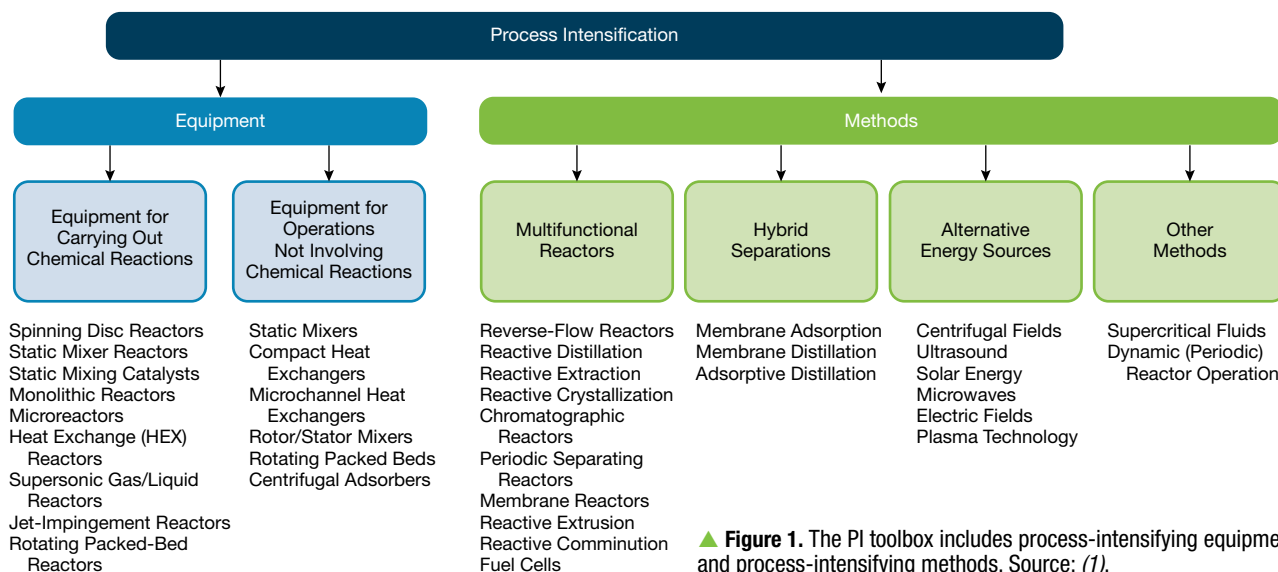
Twenty years have passed since the publication of the seminal paper “Process Intensification: Transforming Chemical Engineering” (1) in the January 2000 issue of *Chemical Engineering Progress*. During those 20 years, many important developments in the field of process intensification (PI) have taken place worldwide. This article and the next one in this special section discuss those developments, focusing on the fundamental theoretical basis of PI and on the practical aspects of selecting intensified equipment.

Born in the industrial laboratories of Imperial Chemical Industries’ (ICI’s) New Science Group (2), process intensifi-

cation, from its very beginnings, has been a practice-driven branch of chemical engineering. Until the early 1990s, PI research concentrated mainly on developing novel processing equipment and methods in four areas: high-gravity operations, compact heat transfer, intensive mixing, and hybrid techniques. Gradually, the practice of PI expanded to new fields, such as microreactors and alternative energy sources.

The toolbox view of PI presented in the January 2000 article (1) was also very much practice-oriented, as it divided PI into two sub-domains (Figure 1):

- *process-intensifying equipment*, such as novel reactors



▲ **Figure 1.** The PI toolbox includes process-intensifying equipment and process-intensifying methods. Source: (1).

and mixing, heat-transfer, and mass-transfer devices

- *process-intensifying methods*, such as hybrid separations; integrated reaction and separation, heat exchange, and/or phase transition (in so-called multifunctional reactors); techniques using alternative energy sources (e.g., light, ultrasound, etc.); and new process control methods (e.g., intentional unsteady-state operation).

This toolbox view was the first attempt at a systematic approach to PI. It has been widely accepted by the community and has been cited often in the PI-related literature.

From practice to principles

To effectively teach PI, a more fundamental approach to this new branch of chemical engineering was needed. Van Gerven and Stankiewicz (3) presented a systematic, fundamental description of PI in 2009. They posited that the ultimate goal of PI is an ideal intensified processing system in which:

- reactions proceed at a maximum achievable efficiency
- all molecules undergo the same processing history
- the hydrodynamic, heat-, and mass-transfer limitations are removed
- the synergies resulting from interrelations between various operations and steps are fully utilized.

This definition is the basis for the following four guiding principles of PI:

1. *Maximize the effectiveness of intermolecular and intramolecular events.* This principle addresses all elementary processes in which intermolecular and intramolecular events play an important role, particularly in chemical reactions. Factors responsible for the effectiveness of a reaction include the number and frequency of molecular collisions, geometry of approach, mutual orientation of molecules at the moment of collision, and the molecules' energy. In this sense, the art of carrying out chemical reactions resembles a game of snooker (or pool), in which experienced players remain in full control of the balls they want to collide by providing them with the right amount of energy, the right geometry of approach, and the right mutual orientation at the moment of collision. Unfortunately, conventional chemical reactors offer a limited degree of control of molecular-level events.

Imagine creating a perfect reaction environment, in which the geometry of molecular collisions is controlled while energy is transferred selectively from the source to the required molecules in the required form, in the required amount, at the required moment, and at the required position. This is the intention of the first guiding principle of PI.

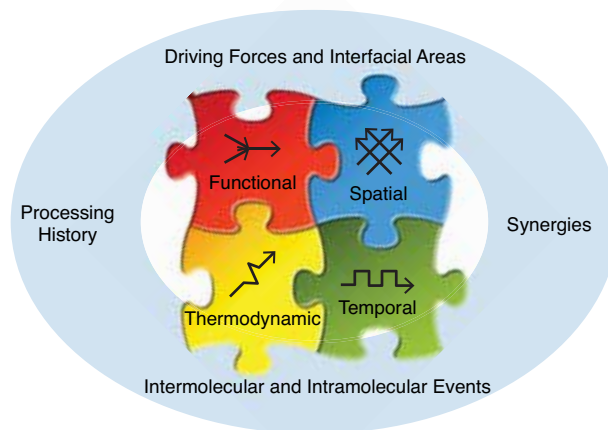
2. *Give each molecule the same processing experience.* Providing each molecule with the same processing experience represents the holy grail of chemical engineering. A process in which all molecules have the same history (i.e.,

undergo the same steps under the same conditions) will deliver uniform products with minimum waste. To achieve such a process, residence time distribution must be narrow, and dead zones (or bypassing), temperature gradients, and local hot spots should be avoided. Mesomixing and micro-mixing also play an important role in providing molecules the same processing history.

A plug-flow reactor is much closer to the realization of this principle than a stirred-tank reactor, in which the distribution of residence times is broad. However, even a plug-flow device does not guarantee real uniformity at the molecular level. Plug flow describes certain flow characteristics at the level of fluid elements, measured by the macroscopic concentration distribution. Gas molecules in a plug-flow system are not in plug flow themselves, as they move freely at high velocities in all directions.

3. *Optimize the driving forces and/or resistances at every scale and maximize the specific surface areas to which these forces or resistances apply.* This principle relates to the transport rates across interfaces. We use the word optimize here because it will not always be necessary to maximize the driving force (e.g., concentration or temperature difference) or minimize the resistance (e.g., in mass-transfer film). The overall effect needs to be maximized, and this is done by maximizing the specific surface area to which that driving force or resistance applies.

Generally speaking, enhanced specific surface areas (or surface-to-volume ratios) can be realized via the structuring of the processing equipment or by application of various forms of energy. For example, the specific surface area for mass or heat transfer in channel-based systems (e.g., hollow-fiber membranes, microreactors) can be increased by reducing the characteristic dimension of the channel. A microchannel with a diameter of 100 μm provides a very high specific area of about 40,000 m^2/m^3 . Nature, however,



▲ **Figure 2.** The four principles of PI (outer circle) are realized in the four domains of PI: spatial, thermodynamic, functional, and temporal.



does better than that — the capillaries in our bodies are about 10 μm in diameter and have specific areas of around 400,000 m^2/m^3 , and (most of them) do not clog!

4. Maximize the synergistic effects of partial processes.

It is evident that in a chemical process, synergistic effects should be sought and utilized whenever possible and at all possible scales. Multifunctionality is the key here. Combining one or more functions within one component (e.g., a process step or a device) often yields significantly better performance than the separate functions executed sequentially.

These principles, in one form or another, are not entirely new to chemical engineering. In PI, however, they are derived from the explicit definition of the goal of an intensified process. And, the PI interpretation of these principles often goes beyond the boundaries of classical chemical engineering. This can be seen, for instance, in the first principle, under which PI looks at molecular-scale methods for improving the intrinsic kinetics of chemical reactions, such as molecular alignment, orientation, and selective bond excitation.

Elementary domains of PI

Process intensification achieves success in realizing these generic principles by operating in four elementary domains: spatial, thermodynamic, functional, and temporal (Figure 2). The following sections discuss these domains and provide real-world examples of intensification in each domain.

Spatial domain

In the spatial domain, PI focuses on avoiding randomness in chemical equipment and replacing it with structure. Randomly arranged spaces are common in chemical processing. For example, on the meso scale, the distribution of pores in common porous materials (e.g., catalyst particles) exhibits a high degree of randomness due to the manufacturing techniques used to produce the material. On the macro scale, randomness occurs in beds of particulate catalysts in industrial catalytic reactors, such as trickle-bed reactors, where the random character of the packing can cause secondary liquid maldistribution and create local dry zones in the catalyst bed. Such zones in a trickle-bed reactor not only reduce the efficiency of the device in terms of product yield but also present a serious safety problem in the case of exothermic processes.

In general, randomness in the spatial domain at any scale in chemical processing reduces predictability and the ability to control the system behavior. On the other hand, a purposeful introduction of a reproducible structure in the spatial domain should improve both. A defined structure is much easier to understand than a randomly organized space. And, mathematical descriptions (models) of structured systems are simpler and can be created with less time and effort. For

example, modeling the transfer phenomena in a fixed bed of particulate catalysts is complex; the randomness of the bed configuration reduces the accuracy of the model and makes it less reliable for reactor scale-up. Structured catalysts, on the other hand, are reproducible, and therefore the related correlations and models are much more reliable.

Spatial structures can have different forms that depend on the elements of chemical processes they target. Structures targeting molecular events are commonly in the form of cages with characteristic dimensions in the range of Angstroms to nanometers, such as zeolites and metal organic frameworks (MOFs). Structures targeting heat and mass transfer usually have the form of channels (e.g., microchannels, monoliths), corrugated sheets (e.g., column packings, plate heat exchangers), or networks (e.g., solid foams). Structures targeting fluid flow and mixing can also be twisted or folded (e.g., static mixers) or fractal-patterned (e.g., fractal fluid distributors).

Millireactor and static mixer. Ehrfeld Mikrotechnik GmbH designed, manufactured, and supplied a Miprowa production reactor (Figure 3) for Shaoxing Eastlake Biochemical (China). The millireactor has a production capacity of up to 10,000 m.t./yr and a throughput of about 1 m^3/hr . It has a nominal width of 400 mm and a length of 7 m and contains about 150 rectangular reaction channels with exchangeable static mixers.



▲ **Figure 3.** This millichannel reactor is an example of PI in the spatial domain. Image courtesy of Ehrfeld Mikrotechnik GmbH.

Article continues on next page

Shaoxing Eastlake Biochemical successfully launched the production plant in Shaoxing in September 2016. The continuously operated millireactor is used for a fast and highly exothermic alkoxylation reaction and replaces more than 20 batch reactors. The company's decision to select this technology was driven by the achievable product quality, significantly higher yield, inherently safer design, and a quick return on investment. Scale-up from the laboratory scale through a series of channel geometries from the micrometer to millimeter scale was much faster than could be realized for established process technologies.

Thermodynamic domain

The thermodynamic domain of PI focuses on energy. The basic concern is transferring energy from source to recipient in the optimal way, including the best form of energy and energy-transfer mechanism.

Conductive heating is the dominant energy-transfer mechanism in industry, and fossil-fuel-based steam boilers are present in most chemical processing plants. In addition to producing greenhouse gases, steam-boiler-based heating is thermodynamically inefficient and nonselective (*i.e.*, the nonreacting bulk molecules and other reactor components are unnecessarily heated along with the reacting molecules). Thus, the chemical process industries (CPI) need smarter methods of supplying energy that transfer the energy selectively from the source to the required molecules in the required form, in the required amount, at the required moment, and at the required position.

Electrical methods may provide a solution. Electricity can be generated from renewable sources (*e.g.*, solar, wind, geothermal, water, etc.), and is therefore likely to become more widely used in the future.

The thermodynamic domain of PI focuses on the use of

alternative energy forms and transfer mechanisms in order to change the way the molecules are activated or separated, to increase the heat- and mass-transfer rates, or to reduce the mixing time in the system. Many of those energy forms and transfer mechanisms use electricity as the primary energy source. This includes, for example, electric fields, magnetic fields, induction heating, microwaves, plasma, light, and acoustic fields. Other, non-electric energy forms and transfer mechanisms addressed in the thermodynamic domain include the energy of flow, for instance, in hydrodynamic cavitation reactors, ejector-based devices, impinging-stream reactors, and supersonic-shockwave systems, as well as the energy of rotation in high-gravity and high-shear systems (*e.g.*, rotating packed and fluidized beds or spinning discs).

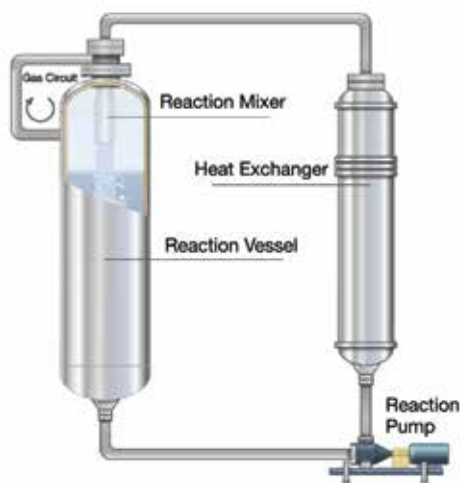
Ejector-based liquid jet reactor. Swiss company Buss ChemTech AG developed and commercialized an ejector-based reactor system called the Advanced Buss Loop Reactor (ABLR). In the reactor (Figure 4), the liquid passes through a venturi-type nozzle, which produces a high-velocity liquid jet. The jet creates a suction and draws the gas into the ejector. Rapid dissipation of liquid kinetic energy takes place in the mixing tube and creates a mixing shock zone, where high turbulence generates a fine dispersion of the gas bubbles and a large specific interfacial area for the mass transfer.

The ABLR delivers very high gas-liquid volumetric mass-transfer coefficients with a relatively low power input, especially compared to stirred-tank systems. For this reason, the device is widely applicable, particularly in fast gas-liquid reactions — such as hydrogenations, oxidations, alkoxylation, or phosgenations — that are mass-transfer-limited in conventional equipment. The very high mass-transfer rates achievable in these reactors significantly shorten reaction times, increase yields and selectivities, and reduce catalyst loads. For example, an oxidation process carried out in the ABLR was almost 15 times faster and had a catalyst load 30% lower than the same process carried out in a conventional stirred-tank reactor.

Functional domain

Process intensification in the functional domain aims to achieve synergy by combining one or more functions (*e.g.*, heat transfer and mixing) in a single device or process step. As stated earlier, maximizing the synergistic effects of partial processes is one of the four principles of process intensification, and multifunctionality is the key here. A combination of functions enhances process efficiency.

Synergies can be sought and realized at the molecular scale, for instance, in multifunctional catalysts. A combination of different energy forms and energy-transfer mechanisms (the thermodynamic domain) can also have synergistic effects. More common, however, is the integration of



▲ **Figure 4.** This loop reactor is an example of PI in the thermodynamic domain. Image courtesy of Buss ChemTech AG.



various functions into multifunctional devices, such as the monolithic stirrer reactor (catalysis plus mixing) and the static mixer reactor (mixing plus heat exchange). Reactive separation systems offer better performance, usually due to the equilibrium shift via *in situ* product removal. Hybrid separations (combinations of two or more separation techniques in one device or process step), on the other hand, facilitate separation in difficult systems, such as close-boiling-point or azeotrope-forming systems.

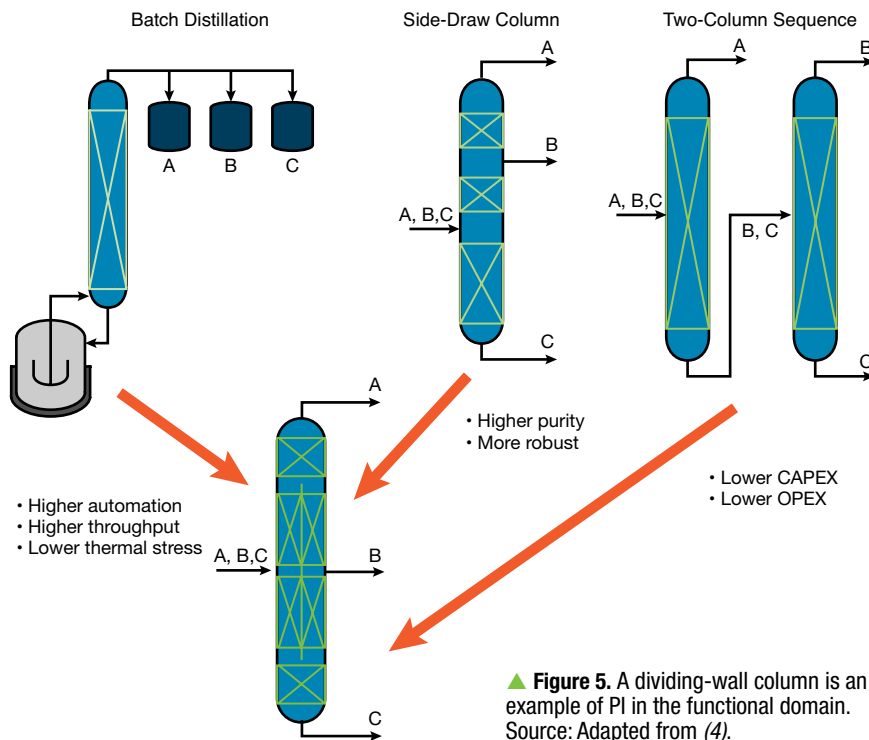
Dividing-wall column. Lonza Goup AG developed a multipurpose dividing-wall column (DWC) that can replace a batch distillation column, a side-draw column, or a conventional two-column sequence (Figure 5). A traditional distillation column can be retrofitted with a dividing wall. Adding a vertical dividing wall across from the feed inlet separates the center of the column into two sections. By adding a side-cut on the opposite side of the wall, a mixture of components can be separated into three or more high-purity streams. To make the DWC flexible for future applications, the positions of the feed and the side-cut stream can be varied over the column height. Moreover, the DWC can be run as a common distillation column by splitting the feed into two equal parts and sending it to both sides of the dividing wall.

Investment costs for one DWC can be 30% lower than for the conventional columns required to achieve the same separation. Replacing a batch distillation column with the DWC increased throughput by 50% and yield by 5%, in addition to increasing product purity from 98% to 99.5% and eliminating component decomposition. According to Lonza, the main advantage of replacing a system consisting of a thin-film evaporator and a distillation column with a DWC is higher product quality in terms of purity and color. Likewise, replacing a side-draw distillation column with a DWC directly connected to the reactor outlet also increased product purity.

Overall, dividing-wall columns have been widely applied for several years, mainly at BASF SE. Currently, there are about 100 columns operating worldwide, and lower capital cost, lower energy use, and smaller plant footprint are commonly reported advantages of the integrated systems.

Temporal domain

In the temporal domain, the underlying parameter for process intensification is time, which can be manipulated in two ways. The first way is to introduce a controlled and



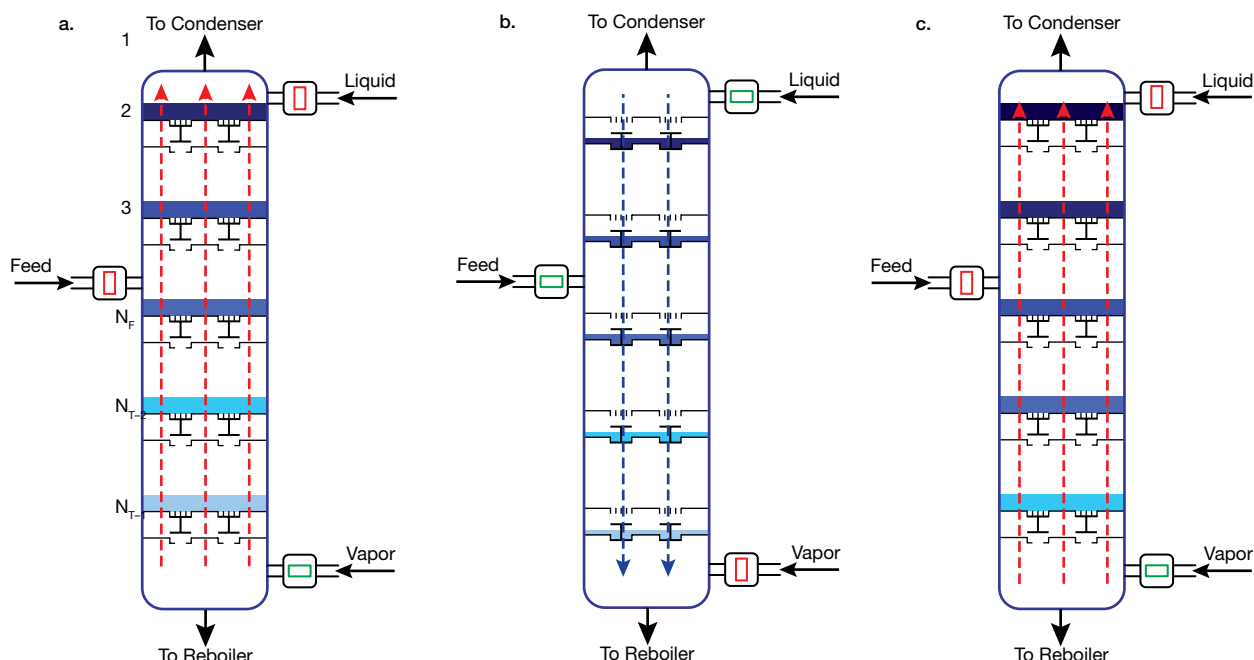
▲ **Figure 5.** A dividing-wall column is an example of PI in the functional domain. Source: Adapted from (4).

optimized unsteady state (e.g., oscillations or cyclic operation) in an inherently steady-state process in order to attain operating conditions that can significantly improve process performance. Examples of PI technologies designed to introduce an unsteady state include oscillatory-flow reactors, reverse-flow reactors, cyclic distillation columns, pressure swing adsorbers, and simulated moving beds.

The second way to manipulate time aims to change (usually extremely shorten) the duration of a process event by dramatically changing process conditions. Milli-

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▲ **Figure 6.** Cyclic distillation is an example of PI in the temporal domain. Source: Adapted from (5).

second reactors, for example, carry out catalytic reactions over extremely short contact times at very high temperatures.

Cyclic distillation. Conventional distillation processes are extremely energy inefficient and require optimization to reduce energy use and capital costs and to improve eco-efficiency. One means of intensification is cyclic distillation, which separates the movement of the vapor and liquid phases (Figure 6). The process is based on the sequential supply of vapor and liquid to the column. During the vapor period, rising vapor prevents liquid downflow by closing a set of valves on each tray (Figure 6a). Vapor runs through the liquid via perforations on the bottom of the tray. The liquid is assumed to be perfectly mixed without a temperature or concentration gradient, and all of the liquid on the tray has the same residence time and a speed of movement equal to zero. During the liquid period, the valves open and liquid moves down the column into a sluice chamber located under each tray (Figure 6b). When the vapor period starts again, the valves close and liquid moves from the sluice chamber to the tray below (Figure 6c).

Maleta Cyclic Distillation LLC reports that its cyclic distillation equipment is smaller than conventional distillation processes, yet it provides higher productivity, higher separation performance, 25% lower energy costs (induced by lower vapor flowrates), and two or more times higher throughput. Cyclic distillation has been applied in atmospheric and vacuum distillation for ethanol dehydration.

Does theory matter?

Practical implications of PI fundamentals

As mentioned earlier, the teaching of PI has necessitated a more fundamental, systematic description and analysis. The principles and domains approach has been used to teach courses in universities and in industry, including those offered by the European Process Intensification Centre (EUROPIC) and, more recently, the AIChE's RAPID Manufacturing Institute in the U.S.

That approach also has a clear practical value — it can help identify possible opportunities for PI improvements in existing plants and processes. Several European organizations, including EUROPIC, have developed systematic procedures, often called PI Scans, that help analyze process intensification opportunities in a given manufacturing process in a structured way. All these procedures consist of several stages, the two most important being: identification of bottlenecks and generation of PI solutions.

The four guiding principles of process intensification can be advantageously used in the bottleneck identification phase, not only to find the bottleneck itself (e.g., low yield or long processing time), but also to determine the underlying causes of that bottleneck (e.g., the presence of thermal gradients [second principle] or insufficient specific interfacial area [third principle]).

Simultaneously, the four elementary domains of process intensification allow structured screening and generation of suitable PI solutions.

CEP



Selecting Process-Intensified Equipment

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Use this approach to
evaluate PI options
and compare technologies.

Process intensification (PI) relies on four guiding principles — maximize the effectiveness of intermolecular and intramolecular events, give each molecule the same processing experience, optimize driving forces and resistances at every scale and maximize the specific surface areas to which those forces and resistances apply, and maximize the synergistic effects of partial processes (see the preceding article by Stankiewicz, pp. 23–28). These principles allow intensified technologies to be classified according to their domain (spatial, thermodynamic, functional, temporal) and their scale of application (micro, meso, macro), and can be used to identify process bottlenecks. Likewise, the domains of process intensification allow structured screening and generation of suitable PI solutions.

This article presents a method for evaluating potential PI options and comparing technologies. This method uses the characteristic scales (time, space) for a process technology to determine process performance and benchmark the associated equipment. An example of the method's application demonstrates how it can be used to select the best available PI technologies at an early stage of the process design workflow.

Characteristic scales

Whatever the process, the chemical or biological transformations are governed by thermodynamics and physicochemical kinetics. The process is driven by the transport phenomena and the intrinsic kinetics of the reaction, which in turn depend on the physical properties of the species and on the operating conditions and equipment. Therefore, the process performance depends on the characteristic scales of time

and space. Table 1 presents some characteristic time scales.

The magnitude of the characteristic scale informs the bottlenecks of the process — *i.e.*, the limiting steps that are worthy of intensification. For example, reactor length L and characteristic reactor dimension R are the characteristic space scales of a plug-flow reactor and a perfectly stirred tank, respectively. Mixing time t_m is the characteristic time scale of the mixing in a reactor or tank. A long time corresponds to a slow (limiting) phenomenon, whereas a short time corresponds to a fast phenomenon.

In Table 1, some of the characteristic time scales are proportional to the space scale to the power of 2, indicating a phenomenon's higher sensitivity to the reactor dimension. This dependence on length-squared also points to processes that are likely to benefit from miniaturization for process intensification. However, design tradeoffs need to be carefully considered, since pressure drop is inversely proportional to the power of 4.

Process performance

A classical way to quantify the efficiency of any chemical engineering process is to estimate the number of transfer units (NTU), which is defined as the ratio of the residence time τ to the characteristic time scale for the phenomenon of interest. For heat transfer:

$$NTU_T = \tau / t_{convheat} \quad (1)$$

where NTU_T is the number of transfer units for heat transfer and $t_{convheat}$ is the heat convection time. For mass transfer:

$$NTU_M = \tau / t_{convmass} \quad (2)$$

Table 1. Characteristic time scales in chemical processing.

Residence time, τ	$\tau = V_r/Q$	V_r = reactor volume Q = volumetric flowrate
Mean residence time (RTD), t'	$t' = \tau = L/u$ if plug flow	L = reactor length u = superficial velocity
	$t'/\tau = 1 + 2/Pe$ if axial dispersion	Pe = Peclet Number = uL/D_{ax} D_{ax} = axial dispersion coefficient
Momentum diffusion time, t_{visco}	$t_{visco} = R^2/\nu$	R = characteristic reactor dimension (e.g., diameter, hydraulic diameter, length) ν = kinematic viscosity = μ/ρ
Mass-transfer diffusion time, t_{diff}	$t_{diff} = R^2/D_m$	D_m = molecular diffusion coefficient
Mass-transfer convection time, $t_{convmass}$	$t_{convmass} = R^2/(ShD_m)$	Sh = Sherwood number = kR/D_m k = mass-transfer coefficient
Heat conduction time, t_{cond}	$t_{cond} = R^2/\alpha$	α = heat diffusivity = $\lambda/\rho Cp$
Heat convection time, $t_{convheat}$	$t_{convheat} = \rho Cp R^2/(\lambda Nu)$	Nu = Nusselt number = hR/λ h = heat-transfer coefficient λ = thermal conductivity
Mixing time, t_m	t_m	
Reaction time, t_R (for a general heterogeneous reaction)	$t_R = C/r$	C = initial concentration of reactant r = transformation (reaction) rate (kinetics law)

where NTU_M is the number of transfer units for mass transfer and $t_{convmass}$ is the mass-transfer convection time.

The characteristic time scales of transport phenomena are derived from the inverse of the kinetics based on the overall transfer coefficients like U for heat and K for mass (and the local coefficients h and k), so that:

$$NTU_T \approx UA\tau \quad (3)$$

$$NTU_M \approx Ka\tau \quad (4)$$

where A and a are the heat-transfer surface area and mass-transfer interfacial area, respectively.

Thus, the performance of any technology can be related to the transport phenomena kinetics and heat and mass transfer — i.e., UA and Ka .

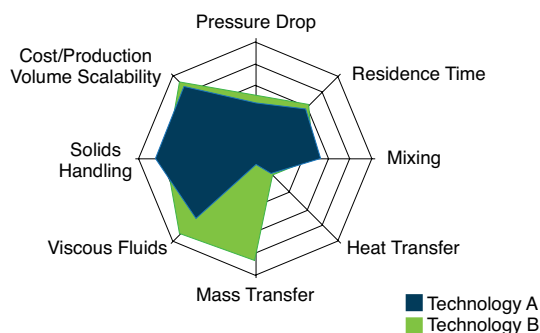


Figure 1. A radar diagram compares the relative attractiveness of technologies along multiple dimensions. Technologies A and B exhibit similar performance for most of the criteria, but Technology B provides much more efficient mass transfer and is somewhat better at handling viscous fluids.

Equipment benchmarking

Once the scales and performance requirements are understood, intensified technologies can be evaluated according to various criteria, such as pressure drop, residence time, mixing, heat- and mass-transfer performance, scalability, etc. Constructing radar diagrams (such as Figure 1) can allow easy comparison of multiple technologies.

The radar diagram in Figure 1 compares the relative attractiveness of Technologies A and B in terms of moderate pressure drop, long residence time, good mixing, good heat and mass transfer, the ability to operate with fluids that are viscous (or complex) or that contain solids, good ratio of equipment cost to production volume, and easy scalability. For instance, the technologies exhibit similar performances for most of the criteria, except for mass transfer and the ability to operate with viscous fluids; Technology B provides much more efficient mass transfer than Technology A and is somewhat better at handling viscous fluids.

Friction factor. Figure 2 plots the friction factor f against the Reynolds number Re for several commercial heat-exchanger (HEX) reactors with various plate designs. The decrease in f with increasing Re is expected. However, some differences among heat exchangers are evident and can be attributed to the specific designs of the HEX reactor plates — the plates with a higher friction factor (and thus pressure drop) provide better mixing.

Mixing time. Figure 3 compares mixing times for several conventional and intensified technologies. The typical stirred tank has mixing times in the range of 1–10 sec, depending on the impeller geometry and the



size of the tank. On the contrary, high-shear-rate and centrifugal intensified equipment can achieve mixing in around 1 msec and sometimes much faster.

Heat-transfer performance.

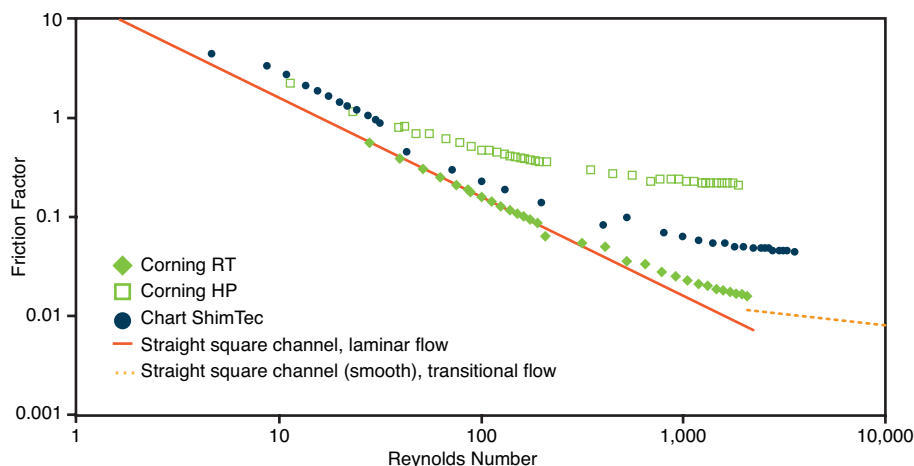
Table 2 (p. 32) compares the performance of several HEX reactors, which combine reaction and heat-transfer functions in a single device. The standard batch reactor is included as a point of reference.

As previously mentioned, the overall heat-transfer coefficient U and the ratio of surface area A to internal volume V of reactor are the key parameters that drive heat transfer and overall process performance. The last row of Table 2 provides an estimate of the overall heat-transfer performance of the HEX reactors — *i.e.*, the product $U(A/V)$, which is referred to as the heat-exchange capacity.

The design and material of construction of the plates of the silicon carbide (SiC) HEX reactor are responsible for that equipment's outstanding heat-transfer capacity — up to 15,000 times better than that of a typical batch reactor. (For comparison, thermal conductivity, λ , of SiC at ambient temperature is 180 W/m-K, while for stainless steel $\lambda = 16$ W/m-K and for glass $\lambda = 1$ W/m-K (3).)

Mass-transfer performance. Figure 4 (p. 32) plots mass transfer (in terms of mass-transfer coefficient and area, $K_{GL} a_{GL}$) vs. energy dissipation rate for various conventional and intensified gas-liquid reactors. (The subscript GL signifies a gas-liquid process, and the units m_L and m_R are relative to the volume occupied by the liquid and the internal volume of the reactor, respectively.) The nonconventional intensified technologies (*i.e.*, micro packed bed, rotor-stator spinning disc reactor) offer much better mass transfer performances than the conventional non-intensified ones (*i.e.*, packed beds, bubble columns, stirred tank), but at the expense of higher energy dissipation rates (more than 10^3 W/m³).

Technology database. Using all of the equipment benchmarking data available in the published literature, in suppliers' documentation, and developed from laboratory tests with standard model fluids (*e.g.*, water for single-phase systems and air-water in the case of gas-liquid systems), we have compiled a database of technologies related

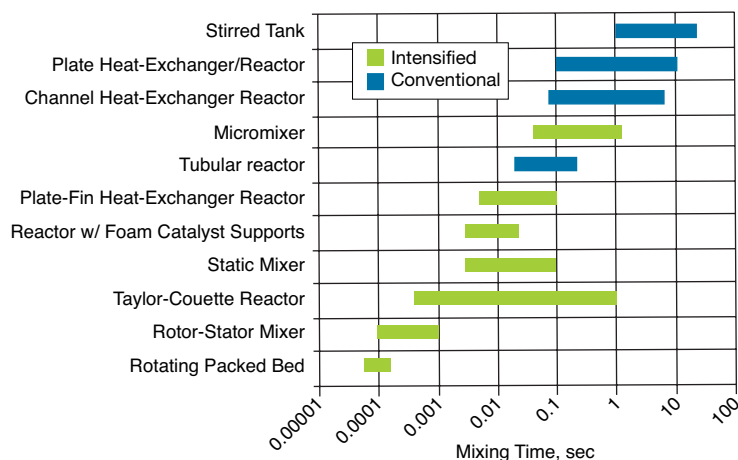


▲ **Figure 2.** Heat-exchanger (HEX) reactors have a higher friction factor and pressure drop — and provide better mixing — than can be achieved in straight channels in laminar flow. Source: Adapted from (1).

to process intensification. That database forms the basis of the equipment selection methodology presented in the following section.

PI equipment selection methodology

A consortium of industrial companies (Elkem Silicones, Solvay, Processium) and French academic laboratories (Laboratoire de Génie Chimique de Toulouse, Laboratoire Réactions et Génie des Procédés de Nancy, Laboratoire de Génie des Procédés Catalytiques de Lyon) developed the equipment selection methodology, focusing initially on reaction engineering. Later, with additional public funding from Agence Nationale de la Recherche, Axelera, and bpiFrance, they extended it to include separation unit operations.



▲ **Figure 3.** Intensified mixing technologies, such as high-shear-rate and centrifugal intensified equipment, can achieve mixing much faster than conventional technologies like a stirred tank. Source: Adapted from (2).

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Table 2. Comparison of heat-transfer performance of different heat-exchanger (HEX) reactors.


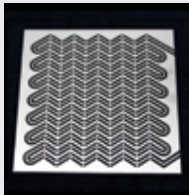


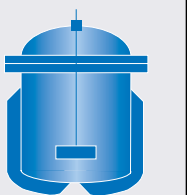
Reactor	Silicon Carbide Plate HEX Reactor	High-Temperature Alloy Microchannel HEX Reactor	Glass Plate HEX Reactor	Stainless Steel Plate HEX Reactor	Standard Batch Reactor
					
Heat-Transfer Coefficient, U , W/m^2-K	7,500	1,500	600	2,500	400
Residence Time	Few minutes	Few minutes	Few minutes	Few minutes	Few hours
Ratio of Surface Area to Volume, m^2/m^3	2,000	2,000	2,750	400	2.5
Heat Exchange Capacity, kW/m^3-K	15,000	3,000	1,650	1,000	1

Figure 5 illustrates the methodology workflow (5).

The first step involves gathering data, as represented by the four blocks at the top of Figure 5:

- Block 1: Identify the objective and specifications of the industrial application, including targeted products and production rate. This block depends on the application and is specified by the end-user.
- Block 2: Compile reaction data, including reaction scheme, reactants, products, byproducts, reaction condi-

tions, kinetics. This block depends on the knowledge and experience of the end-user. Various laboratory tools, such as flow chemistry instrumentation, are available to assist in the acquisition of reaction data. These tools allow high-throughput experiments for screening many diverse conditions, sometimes identifying novel operating windows.

- Block 3: Harness the technology database to benchmark equipment performance. Our database currently includes more than 500 technologies, although the generic methodology can make use of any available information.

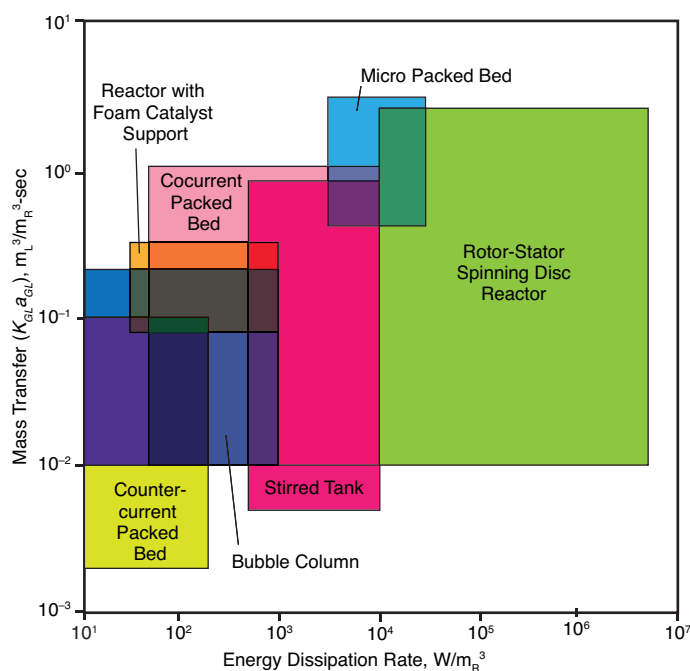
- Block 4: Identify properties of species involved, such as physico-chemical data and phase equilibrium data. We use the commercial database e-thermo, by Processium, but other physico-chemical property data could be used.

After this initial step, three successive stages narrow the options, acting as progressive technology filters:

1. *Feasibility*. This filter checks whether there are any incompatibilities between the equipment and the targeted application. For instance, is the equipment appropriate for the phase of the system (single-phase, multiphase, nature of the phases) and the operating conditions (temperature and pressure ranges, catalyst, etc.)? Is there any suspicion of corrosion or safety issues? If any incompatibility is detected, that technology is rejected. If there is no incompatibility, the technology passes this filter and moves on to the next one.

2. *Technology performance*. The second filter determines whether the performance of the technology meets the requirements of the application. For instance, are the mixing and heat- and mass-transfer performance satisfactory? If not, the technology is rejected.

3. *Pre-sizing*. The third filter evaluates the design



▲ Figure 4. Intensified technologies offer better mass-transfer performance than conventional technologies. Source: (4).



of the process. Does the best available technology fit the desired productivity? What are the different sizes of commercial equipment available? What is the best option: scaling up or scaling out (numbering up)?

This methodology enables the end-user to identify the most suitable technologies that could fit the targeted application.

Filtering based on technology performance

The second stage of the selection procedure filters technologies based on their performance. Figure 6 illustrates this in more detail for heat-transfer performance.

For any application that requires heat transfer, the first step is to determine whether the technology is able to transfer heat. If it is not, that equipment is rejected; otherwise, the screening procedure continues.

The second step of the technology performance screening involves the characteristic scales discussed earlier and shown in Table 1. To compare time scales, another dimensionless number is introduced, the Damköhler number, Da , which is defined as $Da = t_{conv}/t_R$. The variable t_R represents the reaction time and accounts for the reaction kinetics. A Damköhler number close to or less than 1 indicates that the equipment's ability to transfer heat is compatible with the reaction kinetics — *i.e.*, the heat-transfer performance of the reactor is good and heat transfer will not be limiting. If that is the case, the screening procedure continues. If not, the equipment is rejected.

The third step considers the probability of a hot spot developing inside the equipment in the case of an exothermic reaction. This prediction is based on the simulation of the temperature profile inside the equipment (assuming a plug-flow regime and a maximum adiabatic temperature rise determined from the enthalpy of reaction). If a hot spot occurs anywhere along the simulated temperature profile, the ability of the equipment to remove the associated heat must be verified. If it cannot dissipate the heat, the equipment is rejected because of safety issues. If it can, the selection procedure continues to the next step, pre-sizing.

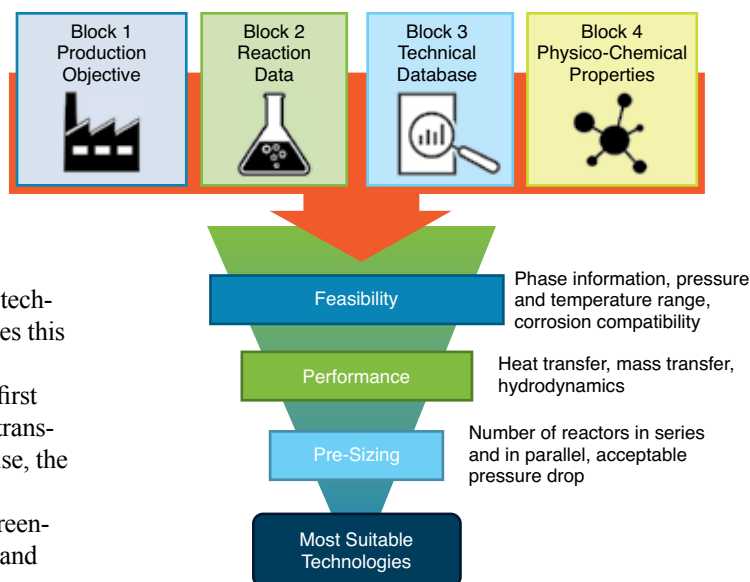
A similar analysis can be conducted for mass-transfer performance.

Applying the methodology

This example illustrates the use of the methodology to choose equipment for an application. Keep in mind that equipment selection typically needs to be done early in the process design workflow and that decisions need to be made even if data about the application are limited (as this example demonstrates).

The end-user provided the following information about the application:

- Block 1: The production yield is approximately

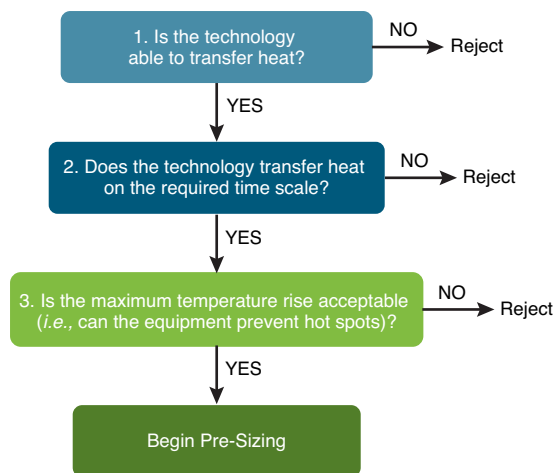


▲ **Figure 5.** The equipment selection methodology follows this workflow.

1,000 ton/yr. The current process is carried out in a conventional 300-L fed-batch reactor.

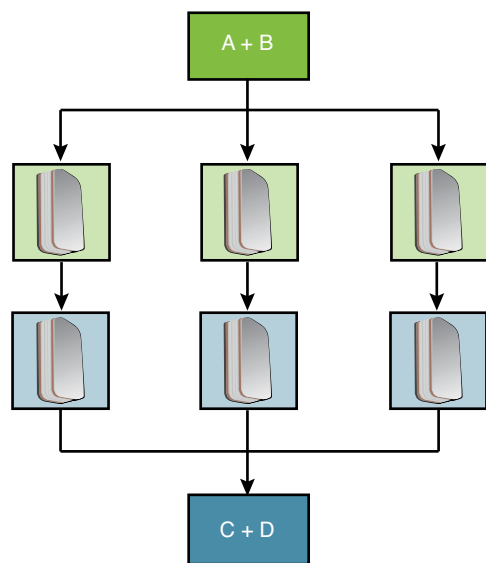
- Block 2: The reaction scheme is $A + B \rightarrow C + D$. It is a liquid-liquid reaction with reactants and products that are well identified. The only information available relative to reaction kinetics is that it takes 1 min to reach 99% conversion. The maximum adiabatic temperature rise is very large, $\Delta T_{adiab} = 300$ K. The user suspects that liquid-liquid mass transfer could be the limiting step.

The two first blocks of Figure 5 are considered complete and the selection procedure can begin even though we do not have the necessary data to fill Blocks 3 and 4.



▲ **Figure 6.** The second filter of the methodology examines technology performance in more detail. For instance, can it transfer heat, can it do so at the required time scale, and can it avoid the formation of hot spots?

Article continues on next page



▲ **Figure 7.** The methodology identified an intensified option for the example application: a numbering-up of three parallel lines of two heat-exchanger reactors.

The first filter, feasibility, considers the multiphase nature of the reaction (*i.e.*, an organic phase and an aqueous phase that are not miscible) and the heat-transfer requirements associated with a large increase in temperature. Based on these factors, the choices are narrowed from an initial 500 to 38 options that warrant further consideration.

The second filter, technology performance, considers the demanding heat-transfer requirements and the relatively fast kinetics of the reaction. This further narrows the pool of candidate technologies from 38 to seven.

The third filter, pre-sizing, limits the field to only two options. The first is conventional fed-batch reactor. But a second choice — involving an intensified option, a heat-

exchanger reactor configuration — is also identified. As shown in Figure 7, this PI option consists of a numbering-up of three parallel lines of two HEX reactors in series. The numbering-up of the HEX reactors provides the desired capacity (1,000 ton/yr), and operating the reactors in pairs in series provides the required residence time (1 min) necessary to reach 99% conversion.

In closing

Even when the information available at the early stages of process design is scarce, it is possible to propose innovative intensified technologies.

CEP

Nomenclature

A	= heat-transfer surface area
a	= mass-transfer interfacial area
a_{GL}	= gas-liquid mass-transfer interfacial area
C	= initial concentration of reactant
C_p	= heat capacity
Da	= Damköhler number = $t_{convheat}/t_R$
D_{ax}	= axial dispersion coefficient
D_m	= molecular diffusion coefficient
f	= friction factor
h	= local heat-transfer coefficient
K	= overall mass-transfer coefficient
K_{GL}	= overall gas-liquid mass-transfer coefficient
k	= local mass-transfer coefficient
L	= reactor length
Nu	= Nusselt number
NTU_M	= number of transfer units for mass transfer
NTU_T	= number of transfer units for heat transfer
Pe	= Peclet number = uL/D_{ax}
Q	= volumetric flowrate
R	= characteristic reactor dimension
Re	= Reynolds number
r	= transformation (reaction) rate
Sh	= Sherwood number = kR/D_m
t'	= mean residence time (RTD)
t_{cond}	= heat conduction time
$t_{convheat}$	= heat convection time
$t_{convmass}$	= mass-transfer convection time
t_{diff}	= mass-transfer diffusion time
t_m	= mixing time
t_R	= reaction time
t_{visco}	= momentum diffusion time
ΔT_{adiab}	= maximum adiabatic temperature increase
U	= overall heat-transfer coefficient
u	= superficial velocity
V_R	= reactor volume

Greek Letters

α	= heat diffusivity = $\lambda/\rho C_p$
λ	= thermal conductivity
ν	= kinematic viscosity = μ/ρ
μ	= viscosity
ρ	= density
τ	= residence time

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Process Modeling of Intensified Chemical Processes

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Before the benefits of process intensification can be fully realized, a multitude of advances in process modeling will be necessary.

Process intensification (PI) has the potential to speed development of chemical engineering innovations. Among its many benefits, PI can increase the driving forces (physical and/or chemical) for transport phenomena, separations, and/or reactions in chemical processes, and it can inspire novel process configurations with major technical and economic benefits. Examples of PI applications include integrated process units such as heat exchange networks, sorption- or membrane-enhanced reactors, and dividing-wall distillation columns, among others (1).

Given the broad applicability of PI in both traditional and emerging chemical processes and given its focus on increasing energy efficiency in the chemical process industries (CPI), the RAPID Manufacturing Institute has targeted natural gas upgrading, chemical commodity processing, and renewable bioproducts as the initial focus areas for exploration of PI opportunities (1).

To realize the many benefits of PI, engineers will need to combine critical advances in process design principles, process modeling technology, and simulation tools. Process modeling technology captures the knowledge and insights for the experimental measurements, molecular science, and engineering fundamentals that ultimately facilitate reliable prediction of process performance.

There are four key domains required in the development of process modeling technology: data, thermodynamics, phenomena, and unit operations. Each domain forms the scientific foundation for the development of the following one.

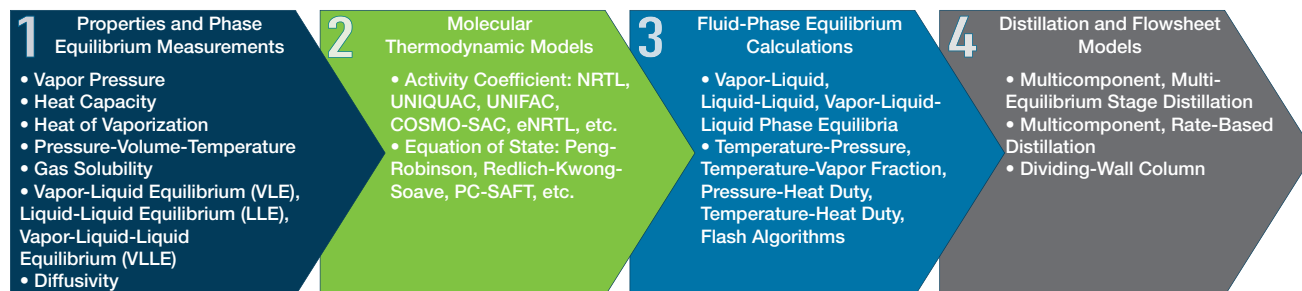
For example, to develop process modeling technology for an intensified distillation process, engineers will need to work toward completing four steps (Figure 1). Each step is associated with one of the four domains:

1. Data: compiling thermophysical properties and fluid-phase equilibrium measurements
2. Thermodynamics: creating molecular thermodynamic models for multicomponent systems
3. Phenomena: modeling fluid-phase equilibria phenomena
4. Unit operations: developing multicomponent, multi-stage distillation unit operation models.

The universal acceptance of existing process simulators for thermal separations has been built on numerous advances in multicomponent mixture measurements and molecular thermodynamic modeling of fluid-phase equilibria, as well as single-stage flash multistage distillation calculation algorithms (2). As we pursue PI opportunities in various chemical processes, traditional or emerging, critical advances in process modeling technology that capture the intensified process fundamentals are essential.

In fact, the RAPID Institute roadmap has clearly outlined many of the key challenges and opportunities in process modeling of intensified chemical processes. Among them are: fundamental data acquisition and/or analysis to generate databases to support process designs involving novel materials for reactions and separations; predictive models that capture intensified process fundamentals; and PI software

Distillation



▲ **Figure 1.** To develop process modeling technology for distillation processes, these four steps will be required. Each step corresponds to a domain of process modeling: data (navy blue), thermodynamics (green), phenomena (blue), and unit operations (gray).

tools that are widely accessible and capable of integrating PI solutions with existing unit operations (1).

This article explores some of the challenges and opportunities in modeling several high-impact, intensified chemical processes: biomass pyrolysis, gas adsorption, membrane separations, and electrochemical systems.

Biomass conversion processes

Modeling of biomass conversion processes can be best described as complicated. Major challenges in modeling these processes include: representation, characterization, and quantification of the individual cellulosic biomass particles and pyrolysis intermediates; thermophysical properties and phase equilibrium modeling for individual components and mixtures of biomass, pyrolysis intermediates, sugar molecules, phenolic oils, and other pyrolysis products; and creation of reaction kinetics models for biomass pyrolysis, secondary gas-phase reactions, and oxidation reactions.

Four key steps will be required to overcome these challenges and develop process modeling technology for biomass conversion processes (Figure 2):

1. Compiling biomass characterization and conversion data
2. Developing thermodynamic and physical property models for biomass, biomass-derived intermediates, and products
3. Developing biomass pyrolysis reaction kinetics and biomass particle models
4. Modeling of reactors and product recovery flowsheets.

Representing biomass particles and intermediates.

Chemical process simulators are designed to track and calculate energy and material streams in terms of specific molecules and components in process flowsheets. Biomass particles and pyrolysis intermediates are not mixtures of a few conventional components with specific molecular structures, as is typically seen in petrochemical process streams. Cellulosic biomass is a complex, mostly solid, heterogeneous substance that is comprised of sugar (holocellulosic) and phenolic (lignin) biopolymers, fats, oils,

waxes, resins, amino acids, and proteins, among other things. A major challenge is representing such complex substances in process simulators to facilitate first-principles-based calculations for heat and mass balances and the various chemical transformations in biomass conversion.

Biomass has been typically characterized in terms of reference components, such as cellulose, hemicellulose, lignin, moisture, and ash (*i.e.*, the holocellulosic components). Under this approach, biopolymer properties are calculated with respect to their monomeric composition. While the monomeric composition of the holocellulosic components is well known and easily represented, the building blocks (and, consequently, the decomposition products) for lignin are much more complex and data on their properties are scant.

Choosing a simplified kinetics model (3) as the basis for modeling pyrolysis, in which similar species are grouped or lumped into model compounds and reactions, Gorenssek *et al.* recently showed that such biomass can be defined in terms of a limited number of conventional model compounds (4). They further showed that the thermophysical properties of these model compounds can be properly estimated to support rigorous heat and mass balance calculations in modeling biomass fast pyrolysis with an entrained flow (5). This approach allows credible estimation of the energy flows and conversion rates in pyrolysis processes.

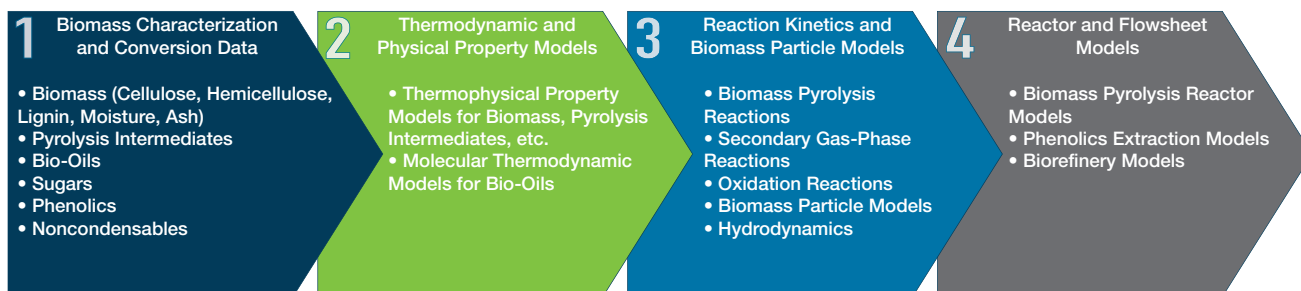
Thermodynamic modeling for bio-oil production.

Another unique challenge is the need for novel thermodynamic models to support development of separation processes to recover valuable bio-derived organic compounds from the raw bio-oil condensate collected following pyrolysis. Bio-oil can be processed for its energy content into liquid fuels, power, and heat. Alternatively, specific biochemical products can be separated from bio-oil and purified, such as levoglucosan and phenolics. In some ways, this is analogous to the recovery of valuable petroleum fractions from crude oil, which is the basis for referring to this type of process as biorefining.

However, unlike crude oil, bio-oil is reactive and can undergo phase separation and other chemical and physi-



Biomass Conversion



▲ **Figure 2.** Four key steps will be required to develop process modeling technology for biomass conversion processes. Major challenges include modeling biomass pyrolysis and secondary gas-phase reactions, as well as creating thermophysical property models for pyrolysis intermediates.

cal changes due to its highly oxygenated nature and water content. The design and optimization of bio-oil separation methods will depend heavily on the availability of experimental measurements and reliable models for fluid-phase equilibria. Classical molecular thermodynamic models, such as nonrandom two-liquid (NRTL) models and UNIQUAC, are incapable of quantitatively correlating the liquid-liquid miscibility data for systems involving phenolics (6).

Incorporating association theory into these classical models to account for the specific chemical interactions between molecules (7) may provide the engineering advance required to accurately describe such complex phase equilibrium behavior.

Reaction kinetics models. In addition to the highly complex biomass pyrolysis reactions, biomass conversion processes involve secondary gas-phase and oxidation reactions. These reactions are collections of complicated sequences of elementary radical reactions and thousands of reaction combinations that are too cumbersome to formulate, inefficient to compute, and have never been implemented in process simulators.

The pyrolysis kinetics model for biomass pyrolysis reactions proposed by Ranzi *et al.* (3) represents an excellent reduced-order kinetics model to be incorporated in process simulators. An earlier version of this reaction scheme (8), in which individual biomass components are assumed to decompose independently, was used by Humbird *et al.* in a one-dimensional (1D) mass, momentum, and energy balance model of an entrained-flow pyrolysis reactor using commercial process modeling software (9).

This approach was modified to make use of Gorenssek *et al.*'s biomass thermophysical properties model (4) and impose a rigorous enthalpy balance, resulting in a pyrolysis process model that more closely aligned with the available experimental data (5). However, conversion to noncondensables was still somewhat over-predicted, while conversion to low-boiling bio-oil components was underpredicted, likely due to secondary gas-phase reactions not being considered. Furthermore, intensified autothermal pyrolysis processes

may take advantage of partial oxidation of the biomass being pyrolyzed to supply the heat required (10). Modeling such a process requires a good grasp of the secondary gas-phase and partial oxidation reactions.

Thus, the challenge remains for the development of reduced-order kinetics models for secondary gas-phase reactions and oxidation reactions. Such reduced-order kinetics models for oxidation reactions, if validated, should be extremely valuable, since many chemical transformation processes, intensified or not, involve oxidation reactions.

Adsorption-based separations

Adsorption is often not well understood and is therefore underutilized for separation. Examples of adsorption processes include mixed-gas adsorption, liquid-phase multi-solute adsorption, chromatographic separations, and ion exchange. Despite the tremendous potential of adsorptive separations as less-energy-intensive alternatives to thermal separations, their broader applications are largely limited to binary separations and greatly hampered by the lack of comprehensive process modeling technology. At present, the design and synthesis of adsorption units requires extensive pilot and on-site testing.

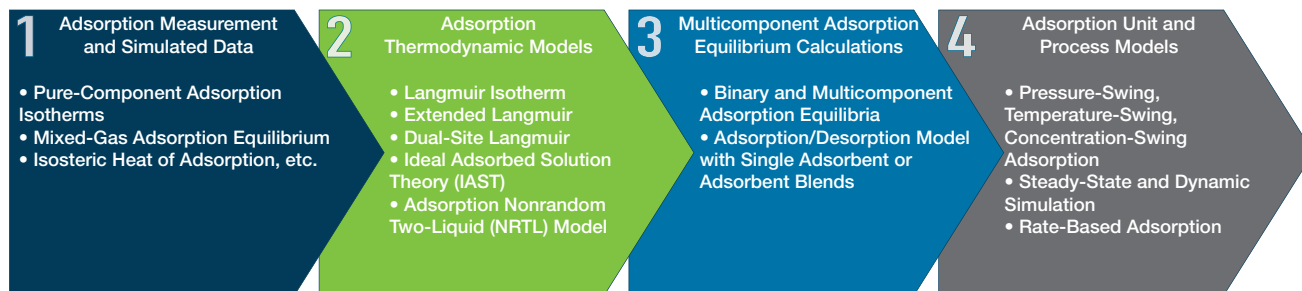
Advances in process modeling technology for adsorption are essential for chemical engineers to reliably simulate, design, and optimize adsorption units. Four key steps will be needed to develop and improve process modeling technology for multicomponent adsorption processes (Figure 3):

1. Recording and gathering pure-component and multi-component adsorption data
2. Improving predictive thermodynamic models
3. Developing adsorption equilibrium calculation algorithms
4. Creating mechanistic adsorption process models.

Among these, Step 2 may be most important for developing accurate adsorption process modeling technology, because thermodynamic models translate experimental measurements into thermodynamically consistent expressions for use in the process simulation models.

Article continues on next page

Mixed-Gas Adsorption



▲ **Figure 3.** Among the four steps required to develop modeling technology for mixed-gas adsorption processes, Step 2 may be most important. Thermodynamic models translate experimental measurements into thermodynamically consistent expressions for use in the process simulation models.

However, current practice remains limited to the use of empirical extensions of the Langmuir isotherm, such as the dual-process Langmuir model (11). These expressions are not thermodynamically consistent because different saturation capacities are assumed for each species on each adsorption site. Their application is limited to binary gas adsorption, and their predictions are questionable.

Therefore, the biggest challenge for adsorption process modeling is the development of predictive thermodynamic models for multicomponent adsorption equilibria. Consistent with the role of molecular thermodynamic models and equations of state for fluid-phase equilibrium for thermal separations, adsorption thermodynamic models need to be capable of accurately correlating pure-component adsorption isotherms and reliably predicting multicomponent adsorption equilibria, including heat of adsorption.

The aNRTL model. The recently developed adsorption nonrandom two-liquid (aNRTL) model may offer the solution to this challenge (12). Derived from the two-fluid theory, the aNRTL model captures the adsorbate-adsorbent interactions in the adsorbed phase with a single binary interaction parameter for each adsorbate-adsorbate pair. A key assumption of the model is that the adsorbate-adsorbate interactions are negligible in comparison to the adsorbate-adsorbent interactions in the adsorbed liquid phase. The model correctly predicts negative deviations from the ideal solution of the ideal adsorbed solution theory (13) and multicomponent gas adsorption equilibria including azeotropic adsorption behavior. The model is currently being extended for liquid adsorption and liquid-phase multisolute adsorption of organic contaminants and heavy metal ions.

The thermodynamic Langmuir isotherm. An interesting extension of the aNRTL model is the activity-based formulation of the Langmuir adsorption isotherm called the thermodynamic Langmuir isotherm. This formulation replaces the species concentration in the classical Langmuir isotherm with the species activity calculated using the aNRTL model (14). Superior in performance to the classical Langmuir isotherm, the thermodynamic Langmuir isotherm

captures the adsorbent surface heterogeneity with a single binary adsorbate-adsorbent interaction parameter. Given that the apparent nonideality of the adsorbed solution in multicomponent adsorption equilibria is determined by the adsorbent surface heterogeneity, the thermodynamic Langmuir isotherm may offer a path to predict binary and multicomponent gas adsorption equilibria from pure-component adsorption isotherms.

Adsorption data. Another challenge related to the adsorption thermodynamic models is the compilation and consistency check of adsorption equilibria and heat of adsorption data for both pure-component and multicomponent adsorption. The National Institute of Standards and Technology (NIST) has established an online database for pure-component gas adsorption isotherms for a wide variety of adsorbates and adsorbents (15). Despite its currently numerous imperfections and transcription errors, the database should become very useful over time as it is periodically updated and refined. It would be highly desirable if the database could be extended to cover binary and multicomponent adsorption data.

Steady state vs. dynamic simulation. Given the availability of predictive adsorption thermodynamic models for multicomponent adsorption equilibria, the simulation and design of adsorption processes should begin with simple steady-state adsorption models. Most modern-day process engineers are well-versed in steady-state process simulation models for thermal separations. Development of steady-state adsorption models should allow this workforce to routinely explore adsorption applications and perform quick and reliable techno-economic analyses.

The development of steady-state adsorption models could benefit from the successful development of the multistage, multicomponent distillation models that are the workhorses of modern-day process simulators for thermal separations. The concepts of theoretical equilibrium stage and stage efficiency are well-established in these distillation models and well-accepted by process engineers. Although these concepts are not applicable for kinetically driven



or rate-based adsorptive separations, it would be very interesting if similar equilibrium stage and adsorption efficiency concepts could be introduced to account for the departure from perfect adsorption equilibria or uniformity in adsorption beds.

Dynamic models for pressure-swing adsorption are currently available in some commercial process simulators. However, existing dynamic models require many inputs that are difficult to determine but have major impacts on process performance. In addition to physical parameters for adsorption equilibria, these inputs include design variables for the desired separation and operational variables for the adsorption unit. These inputs depend strongly on adsorbent properties and are cumbersome to identify by trial and error, but improper inputs may make the model calculations unreliable.

Thus, a key challenge in the development of robust dynamic adsorption models is to improve usability by reducing the user's workload in providing model inputs. For example, it would be very useful to develop a dynamic model that automatically estimates near-optimal flow-rates and step durations for an adsorption cycle based on adsorbent properties. Such a model would require fewer, more-intuitive inputs than conventional models and would eliminate major sources of ambiguity in the calculation of performance metrics.

Rate-based adsorption. Adsorbents that achieve selectivity based on differences in adsorption rates, rather than differences in adsorption affinity, have a better potential to provide an intensified route to several challenging separations. In contrast to conventional thermodynamically driven adsorption processes, in which equilibrium is achieved throughout much of the adsorbent bed by the end of the production and regeneration phases, these kinetically driven processes are deliberately operated far from equilibrium, and this raises unique modeling challenges. For example, the uncoupled linear driving force model used in most adsorption process models becomes considerably less reliable far from equilibrium. However, accurately modeling adsorption rates is critical for these processes. More detailed rate models that consider transport within adsorbent particles can severely complicate the process model.

Thus, accurate rate models of manageable complexity are needed for rate-based adsorption processes, as are improved methods for predicting mixed-gas adsorption rates from pure-component data. The operation of adsorption cycles for kinetically driven separations is also much different and more difficult than for thermodynamically driven separations due to the need to precisely balance cycle timing with adsorption kinetics. Thus, dynamic simulation tools that yield useful results without extensive trial-and-error tuning will require more research into effective operating strategies for kinetic separations, about which little is currently known.

Membrane separation

Selective membranes have become a key enabling technology for intensified processes due to their potential to separate gas, liquid, and electrolyte mixtures with much lower energy consumption, lower capital cost, and smaller footprint than conventional thermal separation systems. Applications of membrane separations with high potential for intensification include water purification, carbon capture, hydrogen separation, olefin/paraffin separation, and benzene derivative concentration (16).

Figure 4 shows the four steps in the development of process modeling technology for membrane separation processes:

1. Compiling membrane properties and performance data
2. Improving thermodynamic modeling for equilibrium partitioning at fluid-membrane interfaces
3. Developing transmembrane flux models
4. Developing membrane module and process models.

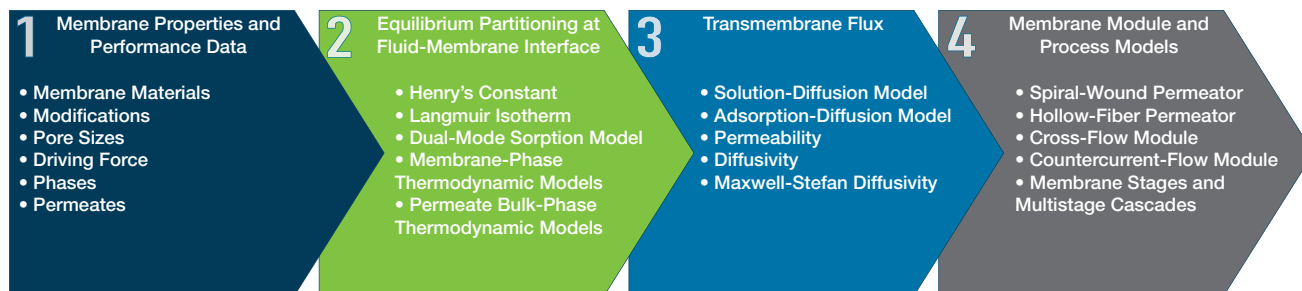
All membrane processes involve a feed stream that contacts a selective membrane, which splits it into permeate and retentate streams. Accordingly, a complete model of a membrane module consists of two sets of mass, energy, and momentum balances — one on the feed/retentate side of the membrane, and the other on the permeate side — coupled by a model of the flux across the membrane.

Transmembrane flux. Estimation of the transmembrane flux is the central challenge facing the development of membrane models with adequate predictive power. Transmembrane flux is governed by a series of steps: transport from the bulk feed to the membrane interface, across this interface into the membrane, through the selective layer of membrane, across the permeate-side membrane-fluid interface, through the porous membrane support layer, and finally from the support layer into the bulk permeate stream.

Under certain idealized conditions, the flux of each permeating species can be represented simply as the product of a linear driving force (depending only on bulk feed and permeate properties) and the permeability (*i.e.*, a lumped, experimentally determined constant of proportionality) (17). However, more detailed analysis shows that this mathematical form is not always justified, and the permeability may depend on conditions that vary considerably throughout a membrane module.

Equilibrium partitioning. The first key element required for a more accurate predictive model of transmembrane flux is a model of the equilibrium partitioning of permeating species at the fluid-membrane interfaces. Viewing the membrane (or the fluid in its pores) as a distinct thermodynamic phase, this equilibrium partitioning can be modeled by requiring the chemical potential of each permeating species to be equal on both sides of the interface. Thus, it suffices to develop accurate models of the species chemical potentials

Membrane Separation



▲ **Figure 4.** The development of process modeling technology for membrane separation processes will require four key steps. Estimation of the transmembrane flux (Step 3) is the central challenge facing the development of membrane models with adequate predictive power.

in both the bulk and membrane phases.

For gas separation, equilibrium partitioning is well understood and available models are typically adequate. As an example, with dense glassy polymer membranes, uptake of gas permeants is commonly understood to occur by the parallel mechanisms of dissolution into the condensed polymer phase and adsorption onto polymer packing defects. Since most gas separation processes operate at low membrane loading, it is adequate to model these two sorption mechanisms by Henry's law and a simple Langmuir isotherm, respectively, the combination of which produces the well-established dual-mode sorption (DMS) model (18).

In contrast, equilibrium partitioning of liquid mixtures and some gases at high pressure is considerably more complex and less well understood, and the lack of reliable thermodynamic models is a critical challenge. For example, accurate activity coefficient models are needed for the polymer solution formed by the uptake of liquid mixtures into a dense polymer membrane (e.g., in pervaporation and reverse osmosis). The resulting membrane-phase concentrations are typically much higher than in gas sorption, which often leads to highly nonideal behavior.

Molecular thermodynamic models. Several molecular thermodynamic models have been developed for polymer solutions, including the Flory-Huggins model with various extensions, lattice theories, two-fluid theories, group contribution methods, and equation-of-state approaches such as PC-SAFT (19). However, it remains to be seen which model, if any, achieves the balance of accuracy, predictive power, and simplicity needed for effective process modeling and simulation.

Membrane processes are often used to treat complex aqueous organic and inorganic electrolyte solutions, such as black liquor in the pulp and paper industry and high-salinity produced water from oil and gas production. The challenge in the process modeling of such membrane systems is actually associated with the availability of molecular thermodynamic models for both the complex aqueous solution and

the membrane phase. These models provide not only the thermodynamic basis for the equilibrium partitioning of the permeating species at the fluid-membrane interfaces but also other thermodynamic properties such as boiling point elevation, osmotic pressure, and scaling potentials that are essential operational considerations.

Fortunately, recent research has yielded molecular thermodynamic models for high-salinity produced waters (20) and for mobile ion partitioning between the bulk solution and the polyelectrolyte membrane (21).

Transport within the membrane phase. The second key element of a predictive model of transmembrane flux is a model of transport through the membrane phase. This remains a major challenge for dense and nanoporous membranes, where transport is strongly affected by permeant-membrane interactions. For gas separations at moderate pressure, simple diffusive models consistent with dual-mode sorption are typically sufficient and are easily parameterized by pure-component experiments (18). However, for liquids and some nonideal gas mixtures at high pressure, high permeate concentrations within the membrane can lead to permeate fluxes that are strongly dependent on local composition (22). Specific factors that cause such nonideal behavior include:

- changes in the activity of a permeant due to the presence of other permeants
- coupled motion of two or more permeants due to strong intermolecular forces
- changes in critical membrane properties due to high permeant concentration, such as changes in free volume, polymer chain mobility, or pore size.

Empirical composition-dependent diffusion coefficients have been proposed to address these factors, but these models lack predictive power and require many coupling parameters. The first two factors are more rigorously addressed by methods based on nonequilibrium thermodynamics, of which the most practically useful is the Maxwell-Stefan approach (23).

This approach requires binary Maxwell-Stefan diffusivi-



ties for all permeant-permeant and permeant-membrane pairs, which could be prohibitive for complex mixtures. Moreover, these diffusivities are still commonly observed to be concentration-dependent. However, several empirical and theoretical mixing rules have been proposed to estimate the required diffusivities from measured values for only permeant-membrane pairs at infinite dilution. In short, more research is needed to find the right balance of predictive power, data requirements, and computational complexity for a general-purpose model of nonideal multicomponent transport in membranes.

Modeling the membrane module. Once an appropriate flux model has been determined, the governing differential equations describing the membrane module need to be solved. This model generally takes the form of a boundary value problem (BVP) in nonlinear partial differential algebraic equations. Models in only one spatial dimension are sufficient in some important cases, but two- or even three-dimensional models are often needed to describe the cross-current flow patterns used in spiral-wound and some hollow-fiber modules. Multidimensional models may also be required to explicitly model the transmembrane dimension, *e.g.*, to capture external mass-transfer resistance (24).

General-purpose numerical methods for such problems involve spatial discretization followed by the solution of the resulting algebraic equation system using a Newton-type method. However, the computational complexity and unreliable convergence of such methods are prohibitive for solving membrane models in the context of a larger process flowsheet simulation.

For 1D models, which are most often two-point BVPs, another approach is to use a shooting algorithm. A shooting algorithm reduces a BVP to an initial value problem, in which you “shoot” different trajectories from the initial condition that satisfies one boundary condition until you find one that satisfies the other boundary condition. This is usually achieved by setting up a root-solving algorithm.

The key advantages of shooting are adaptive spatial discretization, superior numerical error control, and potentially higher efficiency provided that the shooting iteration converges quickly. Unfortunately, the convergence of shooting algorithms has also proven to be unreliable, especially for systems with many components or high stage cuts (24).

Several simplified models and custom algorithms have been developed to address these numerical issues. Notable examples include the seminal cross-flow model of Pan (25), which reduces a 2D BVP to a 1D BVP, and the custom discretization method with improved convergence by Coker *et al.* (24). However, such methods apply only to binary separations, and they require the use of simple constant-permeability flux models. This constitutes a critical technology gap because the use of more sophisticated thermodynamic

and transport models is likely to make the efficiency and convergence problems associated with general purpose algorithms much worse. Thus, there is a critical need for new research into simplified membrane models and custom numerical methods that are efficient and converge reliably, even for nonideal multicomponent mixtures with complex thermodynamic and transport models.

Notably, similar challenges arose in the past for highly nonideal thermal separations and were largely overcome by the development of the inside-out algorithm of Boston and Britt (26). The algorithm solves the separation module equations with local thermodynamic and transport models in the inner loop and then further converges on the local model parameters in the outer loop. Similar advances for membrane simulation could prove to be equally transformational.

Electrochemical systems

Process modeling and simulation of electrochemical systems is in its infancy and no general-purpose electrochemical reactor modeling capabilities exist in process simulators today. However, process modeling will be critical for the intensification of electrochemical systems.

Chemical reactions follow drastically different mechanisms in electrochemical systems. The imposition of an external electric field further perturbs the system and contributes to nonideality. From the process modeling perspective, the key challenges include developing:

- an accurate database for the thermodynamic redox potential for each reaction step at the appropriate reference state
- concentration corrections to the redox potential due to solution nonideality
- calculation of overpotentials due to presence of an electric double layer on the electrode surface
- activity-based microkinetic models for specific electrochemical reaction systems (27).

Additional modeling challenges involve calculation of electron density on electrodes as a function of electric poten-

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DISCLAIMER

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tial and the kinetics of electron transfer in solutions (28).

With proper thermodynamic and kinetic models, an electrochemical reactor can be modeled by incorporating macroscopic mass- and heat-transfer equations. The molecular thermodynamic models that already exist in today's process simulators should be very useful for the calculation of ionic and molecular species activities in solution and concentration corrections to the redox potential. However, reliable databases for transport properties and estimation methods are essential but lacking. Ion diffusivity data might not always be available, so estimating ion diffusivity will also require research and development.

Concluding remarks

Successful development of process modeling technology for PI will require vision, group learning, creativity, teamwork, and support from the chemical engineering community. It is expected that, through the development of process modeling technology, new insights into the intensification of chemical processes can be developed and shared with the engineering profession at large. Furthermore, through the subsequent application of novel process simulation tools to intensified processes and phenomena, the pursuit of PI opportunities can be greatly accelerated and expanded.

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Sustainable, Modular Chemical Production in Africa

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Developing countries have an opportunity to leapfrog old technologies and adopt advanced manufacturing techniques such as modular chemical process intensification.

Modular chemical process intensification (MCPI) has a unique role to play in the developing world. It can provide a means for sustainable and inclusive chemical manufacturing that reduces reliance on limited natural resources and promotes better productivity. It offers a way to leverage resources and circumvent cost barriers in the development of more efficient chemical production processes. By implementing MCPI and advanced manufacturing techniques, developing countries have the opportunity to bypass older, traditional technologies and take a different trajectory and approach to chemicals production.

This article focuses on the application of MCPI in Africa. However, these same benefits could be realized in other constrained areas. The article discusses early successes in modular chemical manufacturing in the developing world that demonstrate the benefits of smaller, decentralized, and sustainable systems.

The concept of bypassing old technologies and adopting new, better tools is often referred to as leapfrogging. For example, over the past decade, hundreds of millions of Africans gained the ability to make phone calls and send text messages via mobile phones, often in areas where landlines were never installed. The spread of mobile phones demonstrates the benefits of leapfrogging — rural areas of developing countries bypassed 20th-century landline technology in favor of 21st-century cellular technology. In some cases, the penetration of mobile phones has even outpaced that of electricity; for example, 59% of Kenyans have mobile phones while less than a quarter have access to electricity (1).

Many places on the continent avoided the installation of landline infrastructure and telephone-switching equipment. In the process, access to phone and internet service was democratized, sidestepping state-run, monopolistic phone companies. Leapfrogging the old phone technology rippled into other aspects of life; for example, mobile payment apps gave banking capabilities to many Africans who otherwise would not have had access to a traditional bank account.

Overview of MCPI and its advantages

Analogous to the introduction of mobile phones, small, modular chemical manufacturing may represent a way to leapfrog the conventional, large, centralized chemical processes found in the developed world. These modular chemical processes could be more efficient, less expensive, and more environmentally friendly than their large, centralized counterparts.

Two types of modular manufacturing are possible, which we refer to as unitary modular manufacturing and parallel modular manufacturing.

Unitary modular manufacturing refers to the concept of dividing a plant into a set of smaller modules (e.g., air-separation module, reactor module, utility module, etc.) that are each factory-built and later assembled and installed at the plant site. A plant constructed in accordance with unitary modular manufacturing can have process units that are just as large as those in a traditional chemical plant. The design process of breaking down a flowsheet into modules is called cubing the project and is often driven

by shipping constraints and the complexity of the process module interconnections.

The unitary modular manufacturing concept is well established and has two key advantages: It can make the manufacturing process easier at a construction site that is remote or difficult to access. And it can reduce the time required to bring a new plant online because module fabrication can be done in parallel with site preparation.

Parallel modular manufacturing, a focus of the RAPID Manufacturing Institute, is less well established but may provide additional benefits for chemical production in Africa. This type of modularity refers to the practice of obtaining the desired production output by operating multiple units in parallel — *i.e.*, numbering up rather than scaling up. For example, a required throughput of 50 m.t./day could be achieved with ten 5-m.t./day modules or five 10-m.t./day modules.

Parallel modular manufacturing offers several potential advantages in addition to those realized from unitary modular manufacturing. These modules can be skid-mounted and transported by truck or rail; thus, they can be repositioned as markets or feedstock availability shift, providing additional operational flexibility. This type of modular processing, in which capacity is increased through numbering up instead of building one monolithic unit, enables producers to grow into a market with a smaller initial capital outlay. This strategy reduces upfront financial risk and helps to improve utilization of plant assets.

Furthermore, small, modular plants can be sited close to the point of use of products or near the source of feedstocks, thereby simplifying transportation logistics. This distributed manufacturing strategy can improve safety by reducing the risk associated with transporting toxic products (*e.g.*, ammonia or chlorine). It can also reduce operating expenses by minimizing the transport of low-density feedstocks (*e.g.*, biomass). Another potential advantage: Alternative energy sources (*e.g.*, renewables like solar or wind, which are inherently distributed) can be more easily utilized to provide process energy than traditional, fuel-derived process heat and power. Process intensification (PI), which assists in creating smaller and more efficient processes, can also play a key role in providing the cost savings necessitated by a small, modular approach.

Shifting from a bigger-is-better paradigm to a small, modular paradigm is not without challenges. Principal among them is the loss of economies of scale at lower throughputs, which translates to a higher capital cost per unit of production. However, we are beginning to see that economies of mass production (something that is well known from automotive or electronic device manufacturing) can provide cost savings similar to those realized through economies of scale (2).

The economies of mass production are the cost savings gained from experience when a manufacturer produces many copies of the same product. Chemical plants themselves are not often thought of as products, but they would essentially be products under a factory-built, modular plant paradigm. The automotive industry provides strong evidence that mass production can apply to chemical plants. Automotive engines — essentially chemical plants comprising compressors, pumps, fans, piping, heat exchangers, batch reactors, catalytic monolith reactors, sensors, and controls — are today factory-built and mass-produced.

Opportunities and constraints specific to Africa

According to the 2016 Economic Report on Africa (3), a publication of the United Nations Economic Commission for Africa (ECA), Africa has made significant progress in economic development over the past decade. However, the continent's economy continues to rely on the production and export of commodity chemicals and raw materials, making it vulnerable to fluctuating commodity prices. In addition, its focus on exporting products to the global market instead of its own regional markets limits job opportunities for a growing young population and contributes to the high level of poverty throughout Africa.

Sustainable development in the chemicals and materials sector is key to moving from a historically mining and raw material extraction model to a value-added model. The 2016 Economic Report on Africa suggests that the current industrialization trajectory in Africa is not only unsustainable, it also reduces the rate of growth in the long term (3).

The need for sustainable development was first articulated in the Brundtland report (4) in the 1980s and reinforced by the National Academies 2006 report on sustainability in the chemicals sector (5). Expansion of sustainable, chemical production in Africa through modular manufacturing works toward several of the UN Sustainable Development Goals (6), namely reducing poverty, improving health, providing clean water, providing clean energy, supporting decent work, improving industry and infrastructure, and promoting responsible production.

Stemming poverty and stimulating economic growth is not a straightforward endeavor. It will require a novel approach. While this approach will take many routes, this article focuses on the application of small, modular process technology to capitalize on the continent's abundant mineral resources, rich soil for productive agriculture, and young workforce to ignite a sustainable chemicals industry.

Several success stories demonstrate the potential benefits of modular chemical manufacturing in the developing world. The three projects discussed next in the article exemplify the breadth of possibilities.

Chloralkali plant in Tanzania

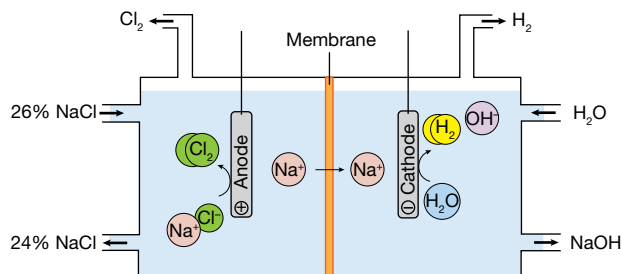
The chloralkali process plays a pertinent role in the chemical process industries (CPI). Its products — chlorine and caustic soda — are used in more than half of all industrial chemical processes. In Africa, chlorine is commonly used as a disinfectant in water treatment. However, the quantity of chlorine used in Africa is low, which makes it uneconomical to build a large-scale plant; thus, most African countries import chlorine. Transportation of liquid chlorine carries a risk of accidental release and is subject to increasing regulatory pressures. Widely available feedstocks, distributed demand, and safety concerns make chlorine a prime candidate for small, modular chemical manufacturing.

Modern chloralkali plants use an electrochemical process, based on membrane electrolysis cells (Figure 1) that are inherently modular and scalable, to convert water and sodium chloride into chlorine and sodium hydroxide (caustic soda) (7).

Within the electrochemical cell, sodium chloride brine travels to the anode chamber, where chloride ions (Cl^-) are oxidized to chlorine gas (Cl_2). At the cathode, electrons from the electrolytic current pull hydrogen ions (H^+) from water and reduce them to hydrogen gas (H_2), releasing hydroxide ions (OH^-) into solution. Sodium ions (Na^+) pass through an ion exchange membrane that separates the cathode and anode chambers and recombine with OH^- to produce sodium hydroxide (NaOH) in the electrolyte.

Chlorine production is an energy-intensive process, consuming roughly 12,000 kJ per kg of product. The process is also somewhat unusual in that most of the energy consumption is in the form of electricity, which presents an opportunity to use distributed, renewable wind or solar power.

Recognizing this opportunity, a joint venture of Junaco (Tanzania) and Serba Dinamik Holdings (Malaysia) contracted the engineering and procurement company ThyssenKrupp in 2018 to build a modular, skid-mounted chloralkali plant in Tanzania — a first of its kind in sub-Saharan Africa (8).



▲ **Figure 1.** Modern chloralkali plants use membrane electrolysis cells to convert water and sodium chloride into chlorine and sodium hydroxide. At the anode (left), Cl^- is oxidized to Cl_2 . Na^+ ions pass through the membrane (center) to the cathode (right), where they react with water to produce NaOH and H_2 gas.

The modular plant can produce 15–45 ton/day (14–41 m.t./day) of chlorine and is composed of modules that fit into 40-ft shipping containers, an example of unitary modular manufacturing (Figure 2). The modules consist of stacks of electrochemical cells to convert water and sodium chloride into chlorine and caustic soda. In theory, several plants could be arranged in parallel to number up to the required demand, providing scalable production near the point of use. The plant is being built in Tanzania, providing local work opportunities for its construction and operation.

Escravos gas-to-liquids (GTL) plant in Nigeria

In contrast to the small, modular chloralkali plant being built in Tanzania, the Escravos GTL plant in Nigeria is the fourth-largest GTL plant in the world, after the Pearl plant in Qatar and a handful of others (9). At peak production, the Escravos plant converts 325 million ft^3 /day of natural gas into 33,000 bbl/day of liquid fuels — primarily synthetic diesel, along with a small amount of liquefied petroleum gas (LPG) — via the Fischer-Tropsch process. The plant sits on a remote site in the Niger delta that was originally a mangrove swamp. Because of the remoteness of the site and the demanding local conditions, much of the plant was prefabricated off-site as modules and shipped in by barge — another example of unitary modular production.

The plant was developed through a partnership between Chevron Nigeria Ltd. and the Nigerian National Petroleum Co. Through another partnership between Sasol (South Africa) and Chevron (U.S.), the plant uses Sasol's proprietary Fischer-Tropsch process along with Chevron's isocracking technology, which upgrades waxy syncrude intermediates into lighter fuel blendstocks. Some of the plant's products are used domestically in the region and others are exported to foreign markets. Engineering, pro-



▲ **Figure 2.** This skid-mounted module is part of a chloralkali plant that can produce 15–45 ton/day of chlorine; a modular plant based on this design is being installed in Tanzania. Image courtesy of ThyssenKrupp Uhde Chlorine Engineers.

curement, and construction of the plant was performed by a consortium consisting of KBR (U.S.), JGC (Japan), and Snamprogetti (Italy).

The plant comprises more than 130 modules, including 12 process modules, the largest of which weighs more than 2,600 tons and measures approximately 22 m × 29 m × 32 m (Figure 3). The other 118 modules are used for pipe racks, air separation, and various other auxiliary or utility functions (10). The plant, which cost US\$10 billion to build, began operation in the summer of 2014. Although the cost of the project did escalate significantly over the course of its construction, the modular approach was key to developing the plant in a demanding location (9).

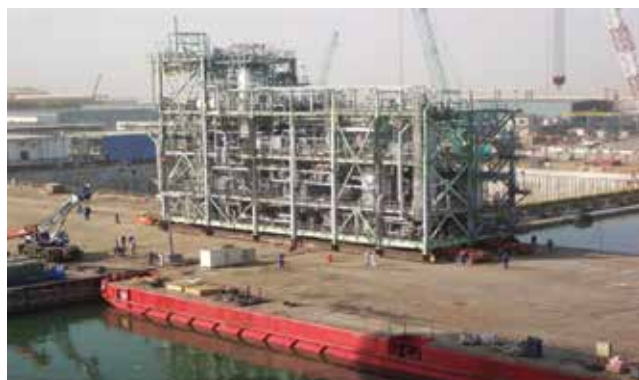
Tupelovox decentralized wastewater treatment

South Africa, like many countries across the continent, is facing a growing water shortage. Contributing factors to this crisis include population growth, water pollution, and deteriorating infrastructure. The discharge of inadequately treated wastewater into rivers and streams harms water quality and is the primary cause of eutrophication and algae growth in waterways in South Africa (11).

Although centralized wastewater treatment facilities are ubiquitous in the developed world, they are not practical in Africa. Traditional centralized wastewater treatment systems are simply too expensive for many smaller municipalities. In addition, these areas lack the technical expertise required to manage and operate wastewater facilities.

Decentralized, modular systems, on the other hand, offer many benefits:

- Developers and home builders do not have to wait for local water management authorities to complete an extension of the sewer system in order to finish a project, which fosters economic development.
- Small municipalities do not have to spend limited financial resources to expand their centralized water treatment facilities in order to cope with local growth.



▲ **Figure 3.** A module for the Escravos gas-to-liquids (GTL) plant is loaded onto a barge headed to Nigeria, where it will be connected to additional modules. Image courtesy of Chevron Nigeria.

• The systems provide affordable long-term solutions to wastewater management challenges.

• Engineers can easily adapt small decentralized wastewater treatment systems to a variety of site conditions.

• Officials can provide their communities with public health protections and preservation of natural resources without excessive expenditure of limited taxpayer funds.

• Treated water can be reused for nonpotable uses, *i.e.*, toilet-flushing, irrigation for landscaping and green areas, machine and floor wash down, cooling towers, fountains, etc.

Tupelovox Pty. Ltd., a South-African company, has successfully built several decentralized wastewater treatment systems in South Africa. They designed and built a system for the telecommunications company Vodacom, which opened one of the largest corporate rainwater harvesting systems in the country (Figure 4). The harvesting system has a storage capacity of one megaliter and overall annual capacity to harvest 12 million L/yr. The rainwater is collected in a storage dam with a total access area of 0.04 km² (almost 10 acres). The scale of the project and the fact that the system harvests surface rainwater and uses the harvested water for a cooling tower makes this a unique project in South Africa. The main components of this state-of-the-art system are a stilling basin to reduce the turbulence of inlet water and an underground reservoir.

Future opportunities

The Tanzanian chloralkali plant and the Escravos GTL plant are examples of modular chemical manufacturing that span two orders of magnitude in plant capacity, from approximately 50 m.t./day to 5,000 m.t./day. Especially at the lower end of the spectrum, smaller modular plants could provide decentralized economic development that benefits both urban and rural populations. The decentralized paradigm could be applied to various fields and scenarios, helping to advance sustainable industrialization in Africa. For example, recent progress in cleaner leather tanning in Uganda, sustainable forestry in Gabon, biofuels production in Malawi, geothermal power production in Kenya, and



▲ **Figure 4.** Tupelovox Pty. Ltd. constructed a rainwater harvesting and treatment system capable of capturing 12 million L/yr of stormwater. These photos show the stormwater sediment trap during and after construction. Photos courtesy of Eugene Sihle Ngcobo.



solar power generation in South Africa could benefit from distributed, modular production (3).

Malawi, a landlocked country, recognized its dependence on road transport and transportation fuels and developed a plan to minimize sensitivity to supply chain disruptions. The government established a national biofuel policy that incentivized the commissioning of two ethanol plants that use molasses, a byproduct of sugar production, as a feedstock. As a result, gasoline in Malawi contains approximately 20% ethanol and higher blend ratios are being explored.

Unfortunately, both plants operate at 50% capacity as a result of inadequate molasses feedstock, which now must be imported from neighboring Mozambique (3). If these ethanol plants had been smaller and modular, it might have been possible to redeploy them to areas that had sufficient feedstock to maintain high utilization rates. In this case, a modular approach could improve not only sustainability, but also resilience of the plant, as redeploying the plant would allow it to recover from feedstock supply chain disruption.

In another example, the government of South Africa is promoting small, decentralized solar installations. As a result, South Africa is now the 10th-largest solar market in the world for installations less than 5 MW. Majozi and Veldhuizen (12) recently reviewed various other chemical industry projects in South Africa.

Small, modular chemical manufacturing certainly is not a one-size-fits-all solution, and it requires careful examination of the regulatory and market forces. A previous CEP article by Baldea *et al.* (13) provides a framework for evaluating small, distributed chemical production versus large, centralized production. This framework, which defines a value density metric, may be a useful tool for quickly screening potential projects in Africa. Potentially attractive projects resulting from the screening can then be subjected to more detailed supply chain analysis, like the one completed by Kis *et al.* (14) for distributed vaccine production in Kenya. For example, distributed, point-of-use ammonia production for fertilizers is one potential project that could establish local jobs and support sustainable agriculture. Distributed ammonia production that uses electricity from renewable sources to produce the required hydrogen feed via water electrolysis would provide an alternative to large-scale fertilizer production, which is the current norm in Africa.

The Nigerian Dangote Group recently announced a US\$2 billion plant to convert Togo's vast phosphate resources to fertilizer. Currently, Togo's phosphate resources are mostly exported in their raw form, so establishing a fertilizer manufacturing plant would provide for value addition. It is too early to say whether this plant might be modular along the lines of the Escravos plant, but clearly there are opportunities for modularity across a variety of scales.

Africa has a unique opportunity to chart a more sustainable, efficient trajectory for chemical production than the course taken by the West. With the annual growth in real GDP in sub-Saharan Africa outpacing that of the U.S., an abundance of renewable energy and natural resources, and a young and increasingly well-trained workforce, Africa is positioned to become a driving force for sustainable chemical production in the future.

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