Perspective

Process Engineering in the Evolving Chemical Industry

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Introduction

The face of chemical manufacturing is changing rapidly, shaped by such powerful forces as:

- Intensified global competition (especially in the production of commodity intermediates and polymers);
- Increased stringency of safety and environmental regulations;
- Increased importance of the expanding fine chemicals, pharmaceuticals, biological chemicals, biomaterials and general biotechnology sectors;
- Increased investor scrutiny of short-term earnings and stock value; and
- Increased customer demand for consistent attainment of high product quality.

The result is an unparalleled transformation of the chemical industry that has created many challenges and opportunities for *chemical process engineering* (CPE), the component of the broader chemical engineering discipline concerned with the development and commercialization of processes for manufacturing chemicals and materials. For example, beginning in 1970, capital productivity—the ratio of revenues generated to the cost of the assets employed in generating the revenues—has steadily declined for the U.S. chemical industry (Figure 1). Many factors are responsible for this decline, including global competition, and new environmental regulations requiring costly process modifications that seldom produce a proportional increase in revenue. The successful evolution of the chemical industry to meet the demands of today and tomorrow, *while remaining profitable*, clearly depends upon how well CPE responds to the forces driving the change.

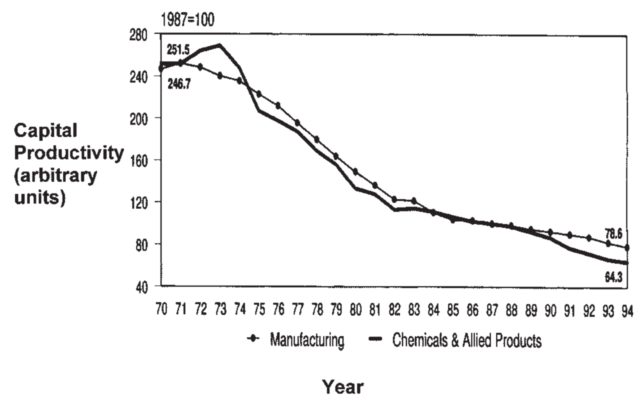

Figure 1. Data from the U.S. Chemical Manufacturers Association indicates a gradual decline in capital productivity, defined as the ratio of the revenues to the cost of the assets (U.S. Chemical Industry Statistical Handbook, 1996).

This communication discusses the changing role of CPE in the ongoing efforts to maintain profitability in the maturing traditional sectors of the chemical process industries, and in shaping the future of emerging sectors. We highlight some of the progress made by CPE and identify some areas that require increased attention as the industry continues to evolve.

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The chemical process and the role of CPE

The chemical process—a single processing unit or combinations thereof, used to convert raw materials and energy into finished product—operates successfully when it meets *two basic requirements*:

(i) ***Comprehensive Safety:*** Process and operator *safety* must be assured; the *health* of workers on the manufacturing site must not be compromised; the overall health and viability of the environment must not be damaged.

(ii) ***Productivity:*** Target *production volume* of saleable product—product satisfying the customer's quality demands—must be met. Observe that the *productivity* requirement as specified here is a combination of the traditionally separated requirements of production volume and product quality.

The "ideal" chemical process (capable of meeting the evolving demands of today and tomorrow) is one that is perfectly safe and perfectly productive, designed, constructed, and operated most efficiently at the absolute minimum possible cost. The role of CPE can be expressed in terms of the following concrete goals, which, if achieved, will produce chemical processes as close to "ideal" as allowable by fundamental thermodynamic and other limitations:

(i) **Design and Operation of Inherently Safe Processes** to reduce or eliminate, by design, hazards of all kinds, including incidents with potential for injury and environmental releases, and chronic emissions.

(ii) **Design and Operation of Inherently Robust Processes** to meet productivity requirements consistently, in the face of unavoidable and persistent variations in external (ambient) conditions, and process and raw material characteristics.

(iii) **Design and Operation of Flexible Processes** to extend the concept of inherent robustness to *multi-product plants* (where quality objectives must be met for two or more products made in a single plant); and to *distributed manufacturing plants* (where the quality objective must be achieved in modular or portable processes).

(iv) **Design for Reduced Capital and Cost Intensity** to reduce, by design, capital investment and operating costs.

The challenges associated with achieving these goals are many; however, here are some of the key issues and how CPE is currently addressing them (see also Keller and Bryan, 2000).

Inherent Safety and Environmental Friendliness. A process may be operated safely by the implementation of extrinsic measures, programs, and procedures. A breakdown of any of these extrinsic measures, however, invariably leads to a breach of process safety. The successful design and operation of chemical processes that are inherently safe (i.e., safe by their very design, not merely as a result of external devices appended to the process) is now an important aspect of CPE (Crowl, 1996; Hendershot, 2000). A notable example is the DuPont process for manufacturing Methylisocyanate (MIC), an important but highly toxic and volatile intermediate (Rao et al., 1985). The incumbent process not only involved MIC storage and transportation, but was also based on phosgenation of methylamine to MIC, thus requiring the use of the equally toxic phosgene in the synthesis. The new, inherently safer process achieves the dual goal of reducing MIC storage and eliminating the need for phosgene by employing a new chemistry route based on a two-step carbonylation (of methylamine) and oxidative dehydrogenation (of monomethylformamide). The second reaction is carried out in a short contact time reactor from which the MIC product is immediately converted to products having considerably lower toxicity and volatility.

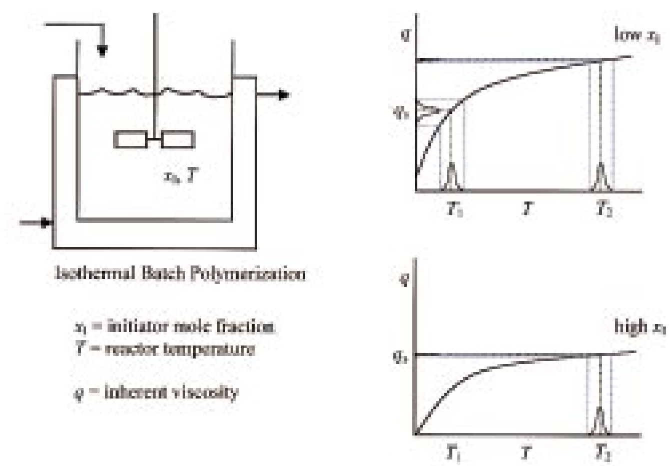

Figure 2. An illustration of inherent robustness by design. By operating at T_2 and high initiator concentration instead of T_1 and low initiator concentration, one obtains a process that is inherently robust to reactor temperature variability.

Similarly, to achieve environmental friendliness by design, the focus is shifting from the more traditional end-of-pipe abatement solutions to "reduction at source" solutions: chemical synthesis routes with little or no byproducts, and/or routes that utilize sustainable/renewable sources (McLaren, 1999). In the production of chemicals from petroleum sources, the focus is on developing more selective catalysts and using more benign solvents such as water and carbon dioxide. The sustainability and molecular functionality of bio-sources provide the primary motivation for moving to such feedstocks as wood, sugars, and grains. Still, developing economically viable processes from these feedstocks remains a major challenge, both in terms of chemistry and process engineering. See Pereira (1999) for a comprehensive survey of environmentally friendly chemical technology, and Biegler and Doherty (1995) for a review of some other examples of process synthesis for waste minimization and plant safety.

Inherent Robustness and "Six Sigma". While the importance of safety is universally accepted in the chemical process industry, the need to achieve high product quality consistently is just beginning to permeate the industry. Process design is still largely carried out with a focus that is often limited to the economics of investment and the utilities of operation. The issue of "dynamic operability" (i.e., how difficult or easy it is to operate a process from day-to-day when process conditions are varying dynamically) is often a post-design, post-construction consideration, if at all. Intrinsic characteristics of the process design such as *controllability*, and *resiliency*, have been proposed for assessing "process operability" (cf. Skogestad and Morari, 1987; Lewin, 1991; Tseng et al., 1999). However, beyond providing quantitative assessments of process operability for any specific design, these concepts cannot be employed for tackling the primary problem of how one actually develops designs that will achieve a specified degree of operability.

In the current competitive climate, it has become essential for the process not merely to be "operable" (even in a well-defined quantifiable sense); it must also now deliver, as economically as possible, products that consistently meet customer quality demands as determined by the metric of "Six Sigma". In the broadest sense, "Six Sigma" refers to a disciplined business management and product improvement/development process for eliminating defects in manufacturing and business systems. In terms of the specific metric it employs, a process is said to operate at the "Six Sigma level" if its products are 99.99966% defect free; i.e., it produces, on average, only 3.4 defects per million basis units (cf. Breyfogle, 1999)! Many chemical companies, including DuPont, Dow, and GE (Plastics) have adopted the "Six Sigma" approach for achieving manufacturing excellence. Concurrently, these companies are beginning to recognize the insurmountable limitations that poor designs impose on the attainment of the stringent demands of the Six Sigma quality metric.

Against this backdrop, we define a manufacturing process as *inherently robust* if (i) its products are virtually defect-free and (ii) its process operational performance is intrinsically insensitive to the variability associated with raw materials and operating conditions. Thus, an inherently robust process exhibits consistency of functional performance by design, regardless of inevitable process variability.

This concept is illustrated in Figure 2 where the inherent viscosity q of the polymer made in an isothermal batch reactor is shown as a function of the reactor temperature T at two different levels of initiator concentration x_I. The top figure shows how well one is able to meet target inherent viscosity q_s at low initiator concentration by operating at the lower temperature T_1, in the face of reactor temperature variability represented by the indicated distribution around the nominal temperature value. Observe that by moving to a higher operating temperature T_2, the product quality becomes virtually insensitive to the variability in the reactor temperature, but at the expense of higher than desired inherent viscosity. By increasing initiator concentration, one is able to "shift" the q-T curve downwards as shown in the bottom figure and thus obtain a process that meets the desired target and is virtually insensitive to reactor temperature variations.

There are currently no established systematic procedures for designing chemical processes that will intrinsically be capable of operating at the Six Sigma level.

Flexibility in Multi-Product and Distributed Manufacturing. For obvious economic reasons, a single plant is often used to manufacture different products. In such multi-product plants, productivity becomes synonymous with *flexibility:* the ability to meet target production volumes of saleable product—for all the products—by efficiently transitioning from one product type to another. The changes in operating conditions required by the production schedule must be carried out quickly and with minimal out-of-spec products, often while simultaneously increasing throughput for high demand products. A systematic approach is essential in tackling the complex issues of product transition control, asset allocation, and product scheduling, to avoid *ad hoc* solutions that may address short-term customer demands but not improve the overall cost performance (cf. Shobrys and White, 2000).

Rather than manufacture a product in the traditional manner in one location and transport it to the customer, it is no longer uncommon to employ so-called "distributed manufacturing" where production of smaller volumes is carried out at various remote sites typically located closer to the customer base. *Distributed manufacturing* thus

- avoids transportation of toxic, flammable, explosive, carcinogenic materials,
- avoids storage of liquid products with high safety risks, and
- "distributes" environmental impact as a result of the reduced production volume at any one site.

Clearly, such an approach is an attractive option for manufacturing hazardous chemicals. Flexibility is achieved under these circumstances by designing the processes to be modular and/or portable. Kvaerner Inc. (2000) has developed a modular, point-of-use, skid-mounted generator technology in which the toxic intermediate, phosgene, is produced in close proximity of the downstream processing units. This eliminates the need for phosgene storage or transportation. Generators deliver phosgene over a wide range of rates. DuPont has also developed a scaled-down HCN production facility for meeting research and development needs (Koch et al., 1994). The lab-scale system has a capacity of about 1,000 pounds per year with the unique feature of employing inductive energy to provide the endothermic heat of reaction to drive the ammoxidation of methane to HCN. The system has quick start and shutdown capability. Since only the required amount of HCN is produced, this just-in-time facility limits the storage of HCN. The inductive heating process gives a selectivity and yield of HCN similar to that of the Degussa process, and at a residence time comparable to that of the Andrussow process (Kirby et al., 1999). This technology could find significant application in pharmaceutical laboratories and gold mining facilities, both of which require a high yield source of HCN.

Innovative Process Synthesis and Design for Reduced Capital and Cost Intensity. It is commonly accepted that chemical engineering did not fully emerge as a distinct discipline until 1915 when Arthur D. Little developed the principle of "unit operations". *All* chemical processes, independent of size, consist of various combinations of these building blocks. A fundamental knowledge of these units equips the engineer to design *any* plant to manufacture *any* chemical simply by combining relevant operations appropriately, with each unit operation carried out in its own dedicated equipment. Prior to this, chemical engineering was practiced more as an art.

Recently, the drive towards maximizing financial performance has provided ample motivation for developing chemical processes with reduced capital intensity, mostly by (i) reducing the number of chemical transformations (steps), and (ii) by combining unit operations where possible. The first strategy requires carrying out process synthesis concurrently with discovery chemistry, so that process economics can guide the direction and focus of the chemistry scouting efforts. At DuPont, such a concurrent approach is taken in the development of new routes to polymer intermediates (following Lerou and Ng, 1996). Key process issues can thus be quickly identified, paving the way for capital and cost-saving process innovation early in the development. On the other hand, in 1984, engineers at the Eastman Kodak Company established that, by combining several unit operations into a single piece of equipment, it is possible to reduce capital and operating costs significantly (Agreda and Partin, 1984). Integration solutions (such as the use of multifunctional reactors, combined reactive-separation units, etc.) are now regularly sought to simplify processes and reduce investment costs (see also Stankiewicz and Moulijn, 2000).

Process Operations and Control. The issues involved in actual day-to-day operation of chemical processes continue to be a major aspect of CPE. The availability of on-line measurements of process stream characteristics and of conditions within processing units has facilitated the implementation of modern control systems. Robust sensors for pressure, temperature, and single component composition measurements are now commonplace in the industry. More sophisticated on-line or at-line instrumentation has extended to gas chromatography, mass spectrometry, and IR-spectroscopy, among others. Advances in computer technology make it possible to implement advanced process control algorithms (such as model predictive control) in conjunction with real-time optimization systems to achieve unprecedented steady operation of complex chemical processes at optimum operating conditions (Qin and Badgwell, 1997; Edgar, 2000). Intelligent sensors and actuators are becoming more commonplace, providing an added dimension of robustness and reliability and performance to the overall chemical process operation.

Emerging opportunities for CPE

With the maturing of the traditional sectors of the processing industries (e.g., chemicals, energy and materials), and the emergence of newer sectors (e.g., electronics, biomedical, biomaterials, etc.), comes new challenges and opportunities for CPE. This "emerging opportunities" landscape is so rich and vast as to make it virtually impossible to provide anything but the briefest high-level sketch of a few very promising elements.

Synthesis and Design of New Products. CPE has traditionally focussed on processes at the macro level. With strong economic forces driving the need for product specialization and differentiation, there is significant incentive for the development of synthesis and optimization tools to aid in the discovery and design of new products. Analogous to process synthesis, what is required is an approach for formulating and solving the *inverse problem:* starting from an *a priori* specification of product attributes for a particular application, identify the molecular species that meet these specifications. The challenges are daunting, but the potential impact is enormous and there is already evidence of progress. For example, Venkatasubramanian et al. (1994) have developed genetic algorithms that use more detailed chemical information and improve the efficiency of discovery of new molecules.

Synthesis and Design of Small-Scale Chemical Systems. The past decade has seen the development of mini-chemical systems at several industrial and academic research institutions. For example, some work at DuPont has focused on the application of micro-fabricated chemical devices for the manufacture of hazardous chemicals for which storage and transportation are to be avoided (Lerou et al., 1996). Microfabrication tools provide intricate geometries for mixing, mass transfer, and heat transfer tailored to meet the specific needs of the reaction system of interest. The challenge here is to *scale out* the single unit into a cascade of parallel, replicated units. There is also considerable potential and interest in mini-chemical devices, such as miniaturized analytical tools (e.g., mini-gas chromatography and mass spectrometry, chemical sensors), portable medical diagnostic tools (e.g., DNA analysis chips (Burns et al., 1998)), and portable energy devices (e.g., mini fuel cells, lithium ion batteries). In spite of their vastly smaller scale, mini-chemical systems are *bona fide* chemical processes. As such, there is potential benefit in bringing to bear on these systems the tools and methodologies of CPE, including modeling, systems integration, optimization and control that are traditionally employed on large-scale processes.

Synthesis and Design of Biochemical Processes. Because bio-based syntheses take place under naturally milder conditions, typically in aqueous media, and usually with the potential for much higher desired product selectivity, they offer a potentially attractive alternative to the traditional approaches. From bio-based polymers, bio-catalysts and nano-structured materials to cosmetics, neutraceuticals and tissue engineering, the application areas of bio-based processing are numerous and the potential for growth is significant. Yet, the successful design and operation of economically viable bio-based processes presents several challenges to CPE, including:

- A molecular focus for process design and synthesis (in light of the considerably more sophisticated chemical functionality of bio-materials);
- Innovative separations techniques for economically extracting desired component from a stream that typically includes several other like-components in a large excess of water;
- Improved bio-catalyst performance, perhaps via genetic engineering complemented by advances in process technologies; for example: novel reactor configurations for carrying out enzyme catalysis in biphasic media; and immobilization methods; and separation strategies which maximize biocatalyst and cofactor recovery.

Cellular Process Engineering. The traditional role of CPE within the general field of biotechnology has been limited to simply "choosing and providing a particular environment for cells within the process" (cf. Bailey, 1995). With the quantitative molecular biology information provided by the genome sequencing projects, and such micro-chemical technologies as the PCR (polymerase chain reaction) technique for producing, very rapidly, working quantities of any known DNA sequence, it is now possible to introduce precise changes in just about any aspect of cell function at the molecular level. (See Shuler (1999) for a discussion of the uses and limitations of single-cell models as a tool for relating genomic information to cellular regulation and dynamics.) The cell quite literally may now be considered as a chemical process, and all the methodologies of CPE can be employed for creating and optimizing cell types and cell functions. The potential implications of this possibility are quite staggering and not yet fully appreciated.

Conclusion

The face of the chemicals and materials industry is changing very rapidly and CPE must also evolve with it to meet the challenges and take advantage of the opportunities. For the maturing sectors, perhaps no more is required than a re-shaping and re-sharpening of the traditional tools. For the emerging sectors, however, major technical innovations will be necessary, requiring even more deliberate integration of science and engineering, and more vigorous interaction across multiple disciplines including biology, materials science, and computer science.

Acknowledgments

The authors gratefully acknowledge input and comments from their DuPont colleagues Carmo Pereira, Ray Zolandz, and Arthur Boxman.

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