Chemical Product Engineering

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Introduction

We believe that the world of chemical engineering has changed so drastically that our old ways of doing teaching and research are no longer sufficient to ensure continued prosperity, and to entice the most ambitious and talented young students to join our ranks. We have to re-invent ourselves; or to use a more trendy word, we need a new paradigm.

50 years ago, the horizon for chemical engineering was broad. It offered two very different categories of products. On one hand, there were “commodity chemicals,” such as gasoline, aspirin, and sulfuric acid, where the fire of innovation was past, and where many companies made undifferentiated products with similar properties and functions. The goal of engineering here was to manufacture the product at minimum cost, consistent with safety, health, and environmental concerns. The manufacturing came to depend on large volume, continuous processes with dedicated equipment. This manufacturing was capital intensive, rather than labor intensive. It was an efficient operation, adding only a small value in a competitive marketplace.

50 years ago, a second chemical industry also supplied high value-added “specialty chemicals,” such as paints, antibiotics, and missile fuels, where the rate of innovation was fast and where companies competed on product function. The goal of engineering here was to discover ways to combine market pulls with technological pushes to arrive at unique proprietary products. Manufacturing used batch reactions in generic equipment, often with major labor input. The key was not low cost, or even efficient operation, but speed to market.

In the last 50 years, the horizon for chemical engineering narrowed to emphasize the first category, commodity chemicals. Most research focused on perhaps fifty such chemicals, where large, highly competitive markets demanded deep technical insight. While such deep insight was necessarily narrow, it produced a powerful international industry based largely on petroleum feedstocks. Through this industry, we chemical engineers literally changed the clothes on human backs and increased the food on human tables. We can be proud of what we have done.

Now, however, the chemical industry is again changing dramatically, as suggested by the employment data in Figures 1 and 2. In many ways, these changes represent a return to our earlier, broader horizon encompassing commodity chemicals and specialty chemicals. Examples of these specialty chemicals are shown on the cover: buckyballs remain a curiosity, without major applications; adamantane is a potential fuel; and methadone and morphine have different chemical structures, but somewhat similar pharmacological effects. Developing ways to produce molecules like these will alter the way in which chemical engineering is used. We do not think that the skills required will change as much as the ways in which these skills are applied. The change is best summarized by two questions. In the recent past, the key question was: “How will we make our product?” In the future, the key question will be: “What product will we make?” While answering this second question will include the answer to the first, the answer to the second question is too important to be left to management.

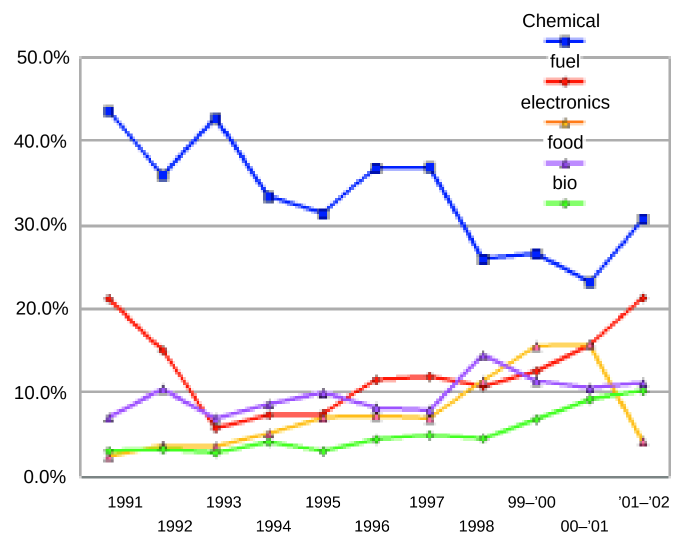

Figure 1. Recent employment of Bachelor’s level chemical engineers.

To explore the consequences of this change, we first consider the steps involved in the creation of new products in industry. We then speculate about how the change from an emphasis on process design to one on product design will alter chemical engineering education and research, including that presented in the *AIChE Journal*.

Product Engineering

Product discoveries can be divided into technology-push and the market-pull cases. One modern example of the technology-push is the Wallace Carothers' invention of the condensation method of making synthetic polymers, which resulted in nylon. An example of market pull is John Hyatt, who sought a substitute for ivory billiard balls, and invented celluloid. As a second example of market pull, the discovery of taxol was motivated by a search for a naturally based cancer cure, a search which analyzed active compounds in 35,000 plant species.

Product engineering is converting a product discovery into a useful product. After its discovery, any product has a long route to travel before it reaches the market. It took ten years from a polymer pulled out of a beaker at DuPont to the nylon stockings sold in the marketplace. During this time, the engineers involved had to change the chemistry for better product properties. The first polymer, an ester of a sixteen carbon diacid with a three carbon dialcohol, melted below 100°C and swelled excessively in water. Polyamides have much higher melting points than polyesters, and are more suitable for stockings. Moreover, a successful product requires a suitable raw material in sufficiently large supply, with a high purity and at a low cost. For nylon 66, these turn out to be supplied by benzene, which gives polymers which have a melting point of 260°C and which are highly hydrophobic. The engineers involved also developed a multistep manufacturing process to go from benzene to nylon. This process included fiber spinning, knitting, dyeing, and finishing.

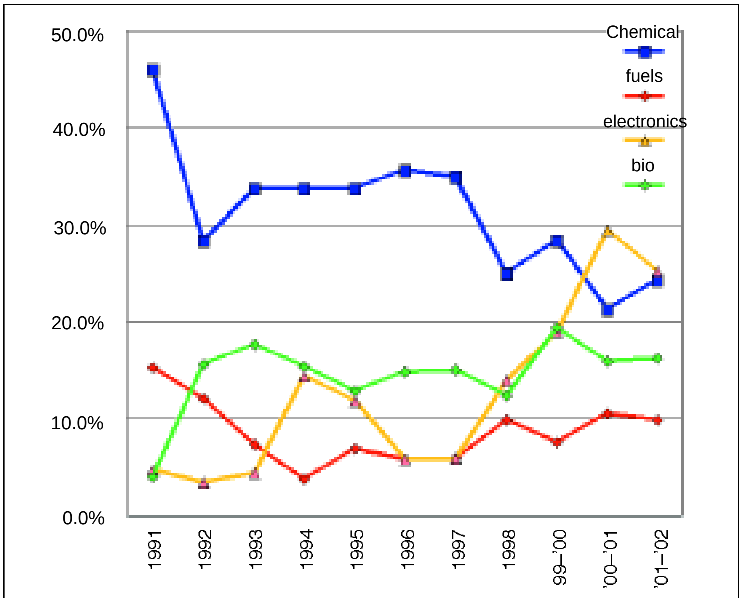

Figure 2. Recent employment of doctoral level chemical engineers.

A second instructive example of product development is taxol. This development took 30 years, from the realization that extracts from the bark of the Pacific yew have anti-tumor activities, through the Food and Drug Administration approval, to commercial availability of taxol. The supply of the century old Pacific yew trees is low, the concentration of taxol in the bark is merely 40 ppm, and harvesting the product means killing the trees, which was fiercely resisted by environmentalists. Thus, commercialization depended on finding a different natural source which could be reacted to produce the product. In addition, taxol has a very low solubility in water, so a vehicle of ethanol and polyethoxylated castor oil was developed to solubilize it.

As these examples suggest, chemical engineers are involved in all phases of product engineering: in discovery, design, manufacturing, and marketing. Our roles are the strongest in design and manufacturing. Product design is different from process design, partly because we are choosing what we will make. In this choice, we use a different design hierarchy than that we normally use for commodity chemicals. Now, our processes will be batch, not continuous, because we will be making small amounts of product in equipment often used for several different products. Now, our process flow diagrams can either involve production of pure species or of pastes, potions, and potpourris. Instead of detailed chemical kinetics, we may care only if our batch process can be finished in one normal working day. We will be much less concerned about distillation and gas absorption than about adsorption and crystallization. After all, many fine chemicals, including drugs, degrade if they are heated past their melting points.

We believe that product design can be idealized as four steps. The first step is to identify what our customers need. The second is to invent ideas—normally many ideas—which can potentially fill this need. The third step in our process design template is to select the best ideas for further development. Once this process is complete, we proceed to the fourth step, the manufacture of our product. Note that this fourth step includes all of the steps of chemical process design.

Needs. Several features of this product design template merit discussion. First, identifying a customer need implies identifying the desired customers. Frequently, these customers will already be using a related product, one which we may hope to replace. These customers will often include some "lead users" who are already improving the product for their own uses. Identifying these lead users and cooperating with them is often a key to product development.

Another part of identifying a product need is the choice of target specifications. These specifications are a part of product design where engineering, rather than marketing, is paramount. We must decide how large a product improvement can be perceived, and how large an improvement is feasible. This task suggests how large a gain can be realized, and, hence, sets limits for any product improvement.

Ideas. To find one successful idea for a new product, we must first discover a large number of ideas. Studies of innovation suggest that different numbers are needed for different industries. For commodities, DuPont suggests 300 ideas are required for one success; for specialties, 3M asserts fewer than 20 are needed. The consensus, expressed by Pfizer and others, is that 100 new ideas produce one new product.

Generating these ideas is most effectively achieved by a design team, including engineers, who have set the specifications and who will follow the new product through development. In their search for ideas, this design team may draw on many resources, including customers, consultants, and the archival literature. The team will probably harvest many of its ideas from widely ranging discussions, sometimes described as “brainstorming.” Many market research firms can facilitate these discussions, which should insure that the core team has a significant investment in the success or failure of the product. Indeed, many business studies suggest that the design team becomes too enamored of its own inventions, and that more new products should be dropped at this point than is currently the norm.

Selection. The next step, to select the two or three best ideas, is the most difficult. In many cases, about half of the ideas for products will turn out to be redundant or obvious folly. Another quarter will turn out to be closely interrelated: for example, some may be special cases of others. However, the results of this editing is still around 20 sound ideas, which is normally too many for a detailed experimental study. Even back-of-the-envelope calculations may be tedious.

In this case, we are forced to use some quick methods by which to screen ideas. These screening methods are often no more than simple matrix estimates, and so will be most valid for marginal product improvements. While we certainly do not expect their infallibility, we do feel that they have considerable value in clarifying the design team’s thinking.

Manufacture. This fourth product design step simply contains the same steps of the process design sequence. Although the steps are the same, the conclusions tend to be different. The process is now normally batch, not continuous. The flow sheet is now more often based on a single pot to which a sequence of chemicals is added. Many of these additions will be reagents; but often some additions will be used to switch from one solvent to another. The batch reactions rarely involve many recycles, but they often require careful temperature control to insure selectivity. Separations tend to be extraction, adsorption, and crystallization, rather than distillation, the workhorse of commodity chemical manufacture.

All these process steps tend to take place in generic equipment, built not for the efficient production of a single product, but for the flexible production of many products. For example, in the drug industry, it is not uncommon for a reactor to be used for 15 different products in one year. As a result, optimization now tends to center on efficient scheduling, not efficient operation.

Design Examples

Let us consider two examples of product engineering and design: guided missile fuels and controlled drug delivery.

When the U.S. Navy or Air Force wants to fire a guided missile to a target, they differ in their needs. The Navy is working on an unstable platform in a warm ocean, where a fuel spill on deck can cause a fire and explosion, so any missile fuel should have a low volatility and flash point. The Air Force works in the frigid upper atmosphere, and does not want the fuel to freeze in flight, so it wants a high volatility and low melting point. Both the Navy and the Air Force agree that the fuel should have the largest heat of combustion possible, so that the missile will have the maximum range, and can be launched at a safe distance from hostile fire. In the past, this led the services to specify the highest heat of combustion per mass. This favors paraffins over aromatics, because paraffins have a higher hydrogen to carbon ratio. However, if the Navy and Air Force wish to use an existing Tomahawk missile with a fuel tank of 150 gallons, their specification implies the highest heat of combustion per volume. Since aromatic molecules are heavier than paraffinic molecules, the desired product is suddenly turned upside down, and aromatics are better than parafins. Multiring aromatics are even better. One idea is adamantane, a multiple ring that is low in hydrogen, but has a density much higher than water, and, consequently, one of the highest BTU/gallon. However, adamantane has a very high melting point, so must be modified to make a suitable fuel. One idea for modification is the addition of multiple methyl groups to spoil adamantane’s diamond-like symmetry.

A second example of product design occurs in controlled drug delivery. Typically, injecting a drug into the bloodstream delivers the drug at a high concentration all over the body, where it may not be needed. This initial drug concentration immediately after injection can be too high and can cause damage, but the drug concentration often declines rapidly to levels too low for therapeutic purposes. Multiple injections may be painful and impractical. What is needed may be a local delivery system that reaches only the desired site, like a tumor but not the bone marrow and the hair. What is needed may be a sustained delivery system that maintains a drug concentration that is just right over weeks, if not years. Any implanted drug depot should not cause immune reactions or be rejected by body tissues, and should completely disintegrate after serving its function, and should be absorbed by the body.

One idea, for which David Edwards of Harvard received the AIChE 2002 Professional Progress Award, is a new aerosol for drug delivery to the lung. Analysis showed that large aerosol particles are usually intercepted in the tortuous and narrow lung passages and do not reach the alveolae, and the small aerosol particles are quickly consumed by the lung macrocytes. Edwards’ new product uses “whiffle ball” aerosols, of high porosity and large diameter, which escape the lung passages long enough to slowly work in the alveolae.

New products like these require different chemical engineering training and research. We next turn to what directions we expect will be required to fulfill these requirements.

A New Paradigm in Teaching and Research

The switch from chemical processes to chemical products implies a corresponding change in the focus of research and teaching. In some ways, this switch is an echo of the arguments 50 years ago about whether “chemical engineering science” was an oxymoron. From our position today, we can see that chemical engineering science was the consequence of our narrowing horizon, of our focus on commodity chemicals. Now, as we return to the broader goal of both commodity and specialty chemicals, we see that we need a broader scientific basis.

We believe that this new, broader engineering will be evolutionary, not revolutionary. It will center on broader research in chemistry. This reemphasized chemistry will include inorganic and biochemistry. Our interest in organic chemistry will continue to expand beyond simple molecules under 100 daltons to include species with molecular weights of 300–700 daltons. All research areas will include more emphasis on molecular structure-property relations. If we are asked to modify the properties of an existing product, for example, to decrease the volatility or to increase the solubility in water, we must know how the van der Waals forces depend on the skeletal arrangement of the molecules, on the type and number of functional groups, on the rigidity and conformation of the bonds, and on the shape and symmetry of the molecules. The polymer community has been studying structure-property relations for decades, and the rest of the chemical engineers need to catch up.

Fortunately, the information revolution has given us many new tools for the study of structure-property relations. Access to large and varied databases, such as the Chembook of National Institute of Science and Technology, and the encyclopedic Beilstein, is within the reach of undergraduates in doing homework problems and research projects. Quantum mechanical computer software such as Spartan and HyperChem can be used by undergraduates to make molecules, to study their structures, and to calculate a limited number of properties. However, many properties important to product design still cannot yet be calculated *a priori*.

Within this broader chemical basis, we expect that the same key ideas of reaction engineering and separation processes will continue to be central. Reaction engineering will probably focus on near-isothermal batch and fed-batch reactions. Many reactions will be two and three phases. Catalysis will more often be homogeneous; heterogeneous catalysis may involve unexpected twists, like the use of dead cells. Reactions may need low temperatures (-40ºC) and high pressures (*ca.* 1 MPa), but these will be within the skills already developed in the profession. Separations will emphasize crystallization and adsorption. However, the emphasis will be chemical, rather than mathematical: there will be more interest in adsorbent selectivity than in improved models for simulated moving beds or pressure swing adsorption. Interest in extraction will continue to wane, because its unquestioned effectiveness involves too large an environmental intrusion. Distillation will continue the renaissance started by structured packing, but these important gains will interest only specialists on commodities, not the profession as a whole.

Chemical products whose value depends on macroscopic function will continue to gain in importance. For example, customers do not care how a polish shines or an emulsifier enhances shelf life; they only care that the products work well. In many cases, product function depends on the product's nanostructure, rather than directly on its molecular structure. Thus, we can expect an enlarged industrial research effort on nanostructure, but one which will be broader than the current emphasis building nanometer-sized electronic devices. It will include a major effort on sensors, especially biosensors for making real-time measurements in doctors' offices. This research effort will continue to use colloid chemistry, especially for self-assembly of, for example, photonic crystals. It will expand the already productive efforts on particle technology.

We expect that educational changes will, like the changes in research, be evolutionary rather than revolutionary. We need to hang the periodic table on the walls of our classrooms. We need to expand our examples beyond those based on petrochemical feedstocks. We need much more emphasis on batch reactions, as compellingly outlined by Reklaitis. We need to expand our design courses to include both process design and product design. Many of us have begun these changes, and we need collaborations to tell what works and what doesn't.

We find it easy to be startled by these changes, but we recognize that they are the direct result of reclaiming our broadened horizon. Indeed, the goals implied by this altered chemical engineering science are consistent with our renewed emphasis on high value added specialty chemical products, as well as commodity products. In many ways, this "new" science is the natural philosophy which underlies the broad horizon where we started 50 years ago. But, instead of working hard on old problems that we have largely solved, let's work creatively on new problems with higher potential for big advances. Intellectually, we have been away; now, we are coming home.

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