CHEMICAL PRODUCT AND PROCESS DESIGN EDUCATION

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Abstract

This paper discusses approaches for providing chemical engineering students a contemporary experience in product and process design. Current trends and issues in chemical engineering education are reviewed, as well as the interaction between business decision-making and product and process design. Then, the Stage-Gate product development process is examined as utilized by product and process engineers and business decision-makers (BDMs). The overlap between the Stage-Gate process and a template introduced to teach the steps in product and process design is examined next. For product design, problems involving molecular structure design, batch process synthesis and simulation, and configured consumer product design are recommended for undergraduate instruction. These involve quantitative synthesis and analysis to generate and select from among alternatives.

Keywords

Product design, Process design, Simulators, Stage-Gate, Equipment design, Configured product design

Introduction

This section is intended to examine several trends and raise questions regarding product and process design education, as a frame of reference for the concepts presented in subsequent sections of this paper.

As chemical engineering graduates become more involved in: (1) nano- or meso-scale analysis and synthesis, (2) molecular modeling (quantum chemistry and molecular simulations), (3) bench-scale genetic manipulations and separations, and (4) 3D configured consumer products, design synthesis continues to be important, but on smaller length and time scales. See, for example, the proceedings of the workshop on *Frontiers in Chemical Engineering Education* (Armstrong, 2003). A key question concerns how to blend the associated engineering science and design strategies into the chemical engineering curriculum. In this regard, it is noted that more involvement in microbiology, molecular modeling, and structured materials is being added gradually to the curriculum, with an increasing number of young faculty having completed doctoral research at the nano- or meso-scale. Yet, processing continues to be the principal emphasis, especially in courses on transport phenomena and chemical reaction engineering.

Given the increasing emphasis on the design of consumer products, design instructors have been challenged to introduce product design strategies. Since product and process design activities are often not easily decoupled, a challenge has been to find a template that introduces the steps in designing most products and processes. Related challenges in product design arise because most of the idea generation and screening steps are qualitative in nature, and the feasibility analysis step often involves experimentation and possible consumer testing. Since some form of quantitative analysis is usually important in product synthesis, educators are challenged to find ways to enable design groups to examine alternative ideas more quantitatively, using experiments when necessary. This seems to be an important requirement because qualitative, rather than quantitative, design studies are often not sufficiently challenging and interesting for students. Other questions concern how to introduce design throughout the curriculum and whether to have one or two courses at the senior level. Given the close relationship between process and product design concepts, the proposal to teach process design first followed by product design (Cussler and Moggridge, 2001) seems less attractive. In addition, the placement and conduct of *capstone* design projects continues to remain a challenging problem. Yet, a related concern is the changing faculty orientation, with the retirement of experienced process design instructors, often replaced by young faculty who have relatively little experience with plant-scale equipment. Finally, with the diversification and growth of software and databases, the opportunities for their use in obtaining more realistic solutions to design problems have grown significantly. It has become more challenging to assist students in the effective use of these extensive systems without becoming overwhelmed by details.

In this paper, our objective is to address the strategies for introducing product design concepts into the senior process design courses. This paper expands upon our introduction in “PSE and Business Decision-Making in the Chemical Engineering Curriculum” (Seider et al., 2003). It adds more definition to the mechanisms of business decision-making, especially as regards the Stage-Gate product development process (Cooper, 2001, 2002). Furthermore, it shows the relationship between the steps in product and process design and the steps in the Stage-Gate process. Finally, it examines case studies that involve quantitative analyses in product design with foci on molecular structure design, batch process scheduling, and configured product design.

Product and Process Design

The design of chemical products begins with the identification and creation of potential opportunities to satisfy societal needs and to generate profit. Thousands of chemical products are manufactured, with companies like Minnesota Mining and Manufacturing (3M) having developed over 50,000 chemical products since being founded in 1904. The scope of chemical products is extremely broad. They can be roughly classified as: (1) basic chemical products, (2) industrial products, and (3) consumer products. As shown in Figure 1a, basic chemical products are manufactured from natural resources.

1. Basic chemical products include commodity and specialty chemicals (e.g., commodity chemicals – ethylene, acetone, vinyl chloride; specialty chemicals - difluoroethylene, ethylene-glycol mono-methyl ether, diethyl ketone), bio-materials (e.g., pharmaceuticals, tissue implants), and polymeric materials (e.g., ethylene copolymers, polyvinylchloride, polystyrene).

2. The manufacture of industrial products begins with the basic chemical products, as shown in Figure 1b. Industrial products include films, fibers (woven and non-woven), and paper.

3. Finally, as shown in Figure 1c, consumer products are manufactured from basic chemical and industrial products. These include integrated circuits, dialysis devices, solar desalination devices, drug delivery patches, fuel cells, hand-warmers, Post-it notes, ink-jet cartridges, detachable wall hangers, cosmetics, laundry detergents, pharmaceuticals, transparencies for overhead projectors, and many others.

Many chemical products are manufactured in small quantities and the design of a product focuses on identifying the chemicals or mixture of chemicals that have the desired properties, such as stickiness, porosity, and permeability, to satisfy specific industrial or consumer needs. For these, the challenge is to create a product that has sufficiently high market demand to command an attractive selling price. After the chemical formulation is identified, it is often necessary to design a manufacturing process.

Other chemical products, often referred to as commodity chemicals, are required in large quantities. These are often intermediates in the manufacture of specialty chemicals and industrial and consumer products. These include ethylene, propylene, butadiene, methanol, ethanol, ethylene oxide, ethylene glycol, ammonia, nylon, and caprolactam (for carpets); together with solvents like benzene, toluene, phenol, methyl chloride, trichloroethylene, and tetrahydrofuran; and fuels like gasoline, kerosene, and diesel fuel. These are manufactured in large-scale processes that produce billions of pounds annually in continuous operation. Since they usually involve small, well-defined molecules, the focus of the design is on the process to produce these chemicals from various raw materials.

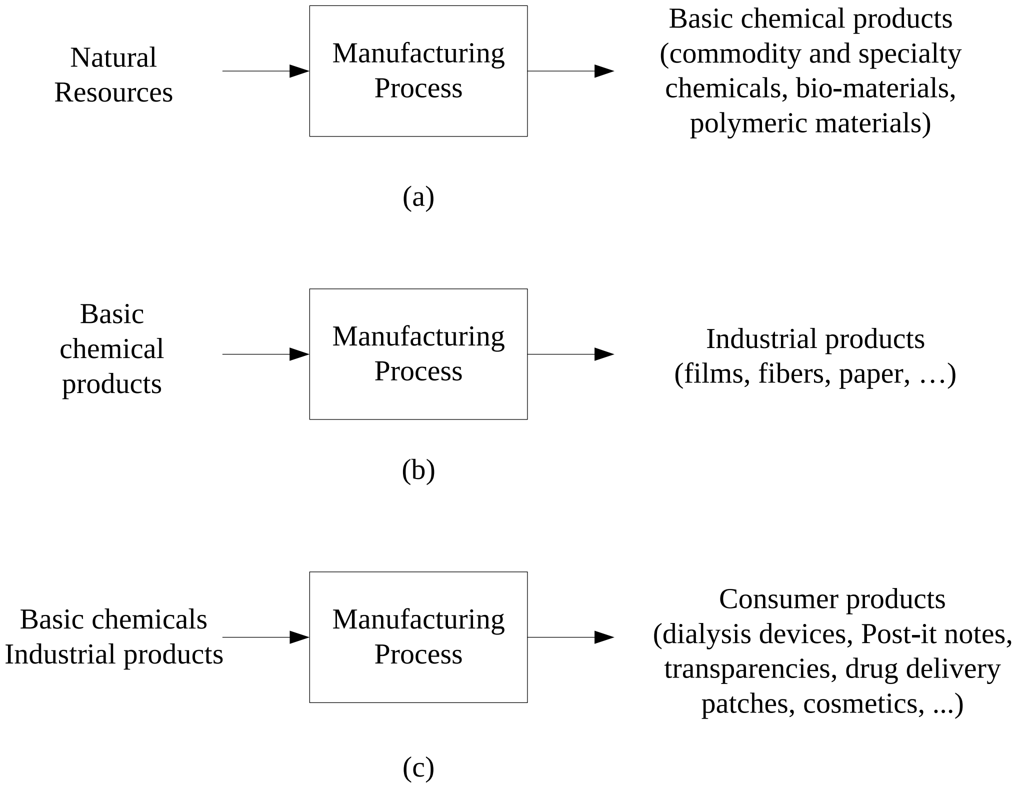
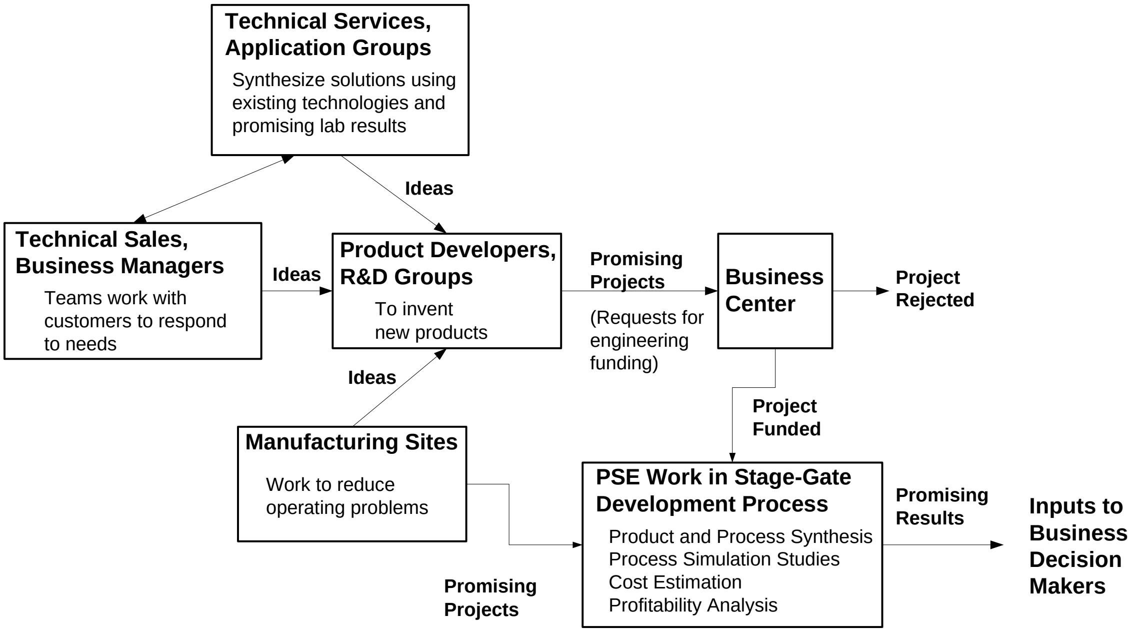


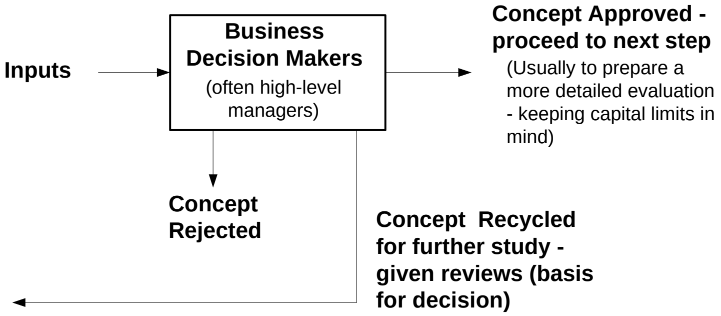
Figure 1 Manufacture of chemical products

Business Decision-Making

As new chemical products are conceived, companies in the chemical industry, and many other commercial and governmental organizations, have *Business Decision Makers (BDMs)*, typically within high-level management. These persons receive inputs from the many sources shown in Figure 2a. The inputs, or proposals, often originate from the ideas of *Technical Sales Groups*, often known as *Business Managers*, whose teams work with current customers, seeking to learn about customer needs. Inputs also originate from the ideas of *Technical Service Groups* (also known as *Application Groups*), who interact closely with *Technical Sales Groups*, working to synthesize solutions using existing technologies and promising laboratory results. Often these ideas are fed to *Product Development Groups* (also known as *Research and Development* (*R&D*) *Groups*), who work to invent new products and technologies. Their most promising ideas and concepts are sent usually to a *Business Center* in a request for a budget to carry out an engineering study. When approved, product and process systems engineering work is undertaken to carry out product and process synthesis, process simulation studies, cost estimation, and profitability analyses. As promising results are obtained, these are the basis for proposals, or inputs, to the *BDMs*. In recent years, especially for product design, five product and process engineering steps are carried out in a sequence that has become known as the *Stage-Gate* product development process (Cooper, 2001, 2002). After each step, as discussed in the next section, a *Real-Win-Worth* (*RWW*) evaluation is carried out, and when promising the results are forwarded as inputs to the *BDMs* for approval.



(a) Input sources



(b) Decisions

Figure 2. Business decision making

Another source of inputs for *BDMs* originate at the *Manufacturing Sites*, which often work to resolve operating problems, leading to ideas for variations on existing products, retrofits, or even new processing methods. Often these ideas are fed to the *Product Development* groups, with engineering studies undertaken, as described above. Here, also, the most promising results provide inputs to the *BDMs*.

Finally, it is important to note that most business areas have a group of financial analysts who carry out detailed economic analyses, including sensitivity and uncertainty analyses, to accompany inputs to the *BDMs*.

Figure 2b shows the inputs processed by the *BDMs*, with decisions issued in three principal categories: (1) the concept is approved with the authors of the proposals authorized to proceed to the next step of the Stage-Gate process, (2) the concept is recycled for further study, given reviews that are the basis for the decision, and (3) the concept is rejected. Note, however, that rejected proposals are often not entirely rejected. In many cases, research and development managers find some combination of time, equipment, and motivated employees able to rework the proposal with a "new look."

Stimulating Idea Generation and Product Design

To stimulate idea generation and product design, increasingly, *BDMs* have instituted new corporate policies that include:

> <u>Fifteen Percent Rule</u> (3M), in which employees are allowed 15% of their time to work on projects of their own choosing.
>
> <u>Tech Forums</u>, which are organizational structures that encourage technical exchange in specific areas, including physics, life sciences, product design, and intellectual property.
>
> <u>Stretch Goals</u> to stretch the pace of innovation. For example, at 3M, a goal is set at 50% of annual sales to be comprised of products introduced over the last four years. A second goal is for 10% of annual sales to be comprised of products introduced over the last year.
>
> <u>Process Innovation Technology Centers</u>, in which chemical engineers and material scientists help researchers scale-up bench-scale concepts. Areas for development and scale-up include coating, drying, and inspection and measurement.
>
> <u>Six Sigma</u>, in which design strategies are utilized to increase quality control.

These approaches are discussed by Gundling (2000) and Coe (2000). Brief discussions are provided also by Seider et al. (2004).

Corporate Alliances

In recent years, the more profitable companies are focusing on specialty and industrial chemicals with only a handful of companies remaining that focus on a full range of diversified chemical products. As a result, few single companies remain having the technical skills and manufacturing resources to produce complex products alone. For example, when designing a new fuel cell, a design team may determine that company X is well-suited to manufacture a new porous anode and cathode, company Y is best for the manufacture of a new co-polymer (for thin films), and company Z is best to assemble the fuel cells comprised of the specialty and industrial chemicals from X and Y. This challenges design teams and BDMs to arrange for consortia of companies to collaborate in product design and manufacture.

Stated differently, as product design proceeds, decisions are needed regarding how deep the designing company can penetrate into the "food chain." In a typical scenario for fuel cells, the company may plan to develop a new porous anode during the first year, followed by a process to produce the polymer during the second year, and acquire a company with a fuel-cell assembly line during the third year.

New PSE Concepts in Design Courses

Over the past decade, the role of process systems engineering (PSE) concepts (such as process synthesis, process simulation, cost estimation, and profitability analysis) in process design courses has become well defined. More recently, with more emphasis being placed on product design, the Stage-Gate product development process was introduced by Robert G. Cooper (2001, 2002 – www.prod-dev.com). This five-step process is illustrated in Figure 3 and is discussed briefly below.

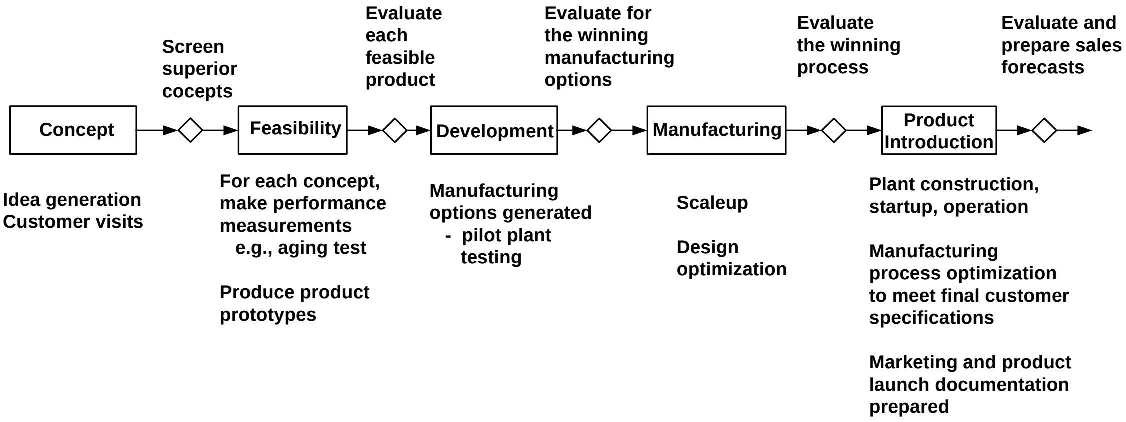


Figure 3. Stage-Gate product development process

Stage-Gate Product Development Process

As shown in Figure 3, each of the steps in the product development process is followed by a gate at which a *Real-Win-Worth (RWW)* evaluation is carried out, with positive results presented to the *BDMs* who provide approval to proceed to the next step. In the *Real* evaluation, the extent of reality is assessed for a potential product. The *Win* evaluation assesses the competitiveness of the product with competitors in the market place (and the ability of the customer's manufacturing facility to accept the product, when applicable). Finally, the *Worth* evaluation assesses the anticipated financial reward of the new product. Next, let's examine the five Stage-Gate steps and the *RWW* evaluation at each step. Notice that the latter becomes more quantitative as the Stage-Gate process proceeds. Also, notice that the steps differ somewhat with the type of chemical product.

Step 1 – Concept

This is one of the most creative steps in which ideas are generated, keeping in mind customer needs. In this step, customer requests are translated into product requirements. Through an iterative process, the requirements are reviewed with the customers and refined as necessary. Product concepts are generated to achieve these requirements. Then, for the best concepts, the *RWW* evaluation is applied. The *Real* analysis evaluates whether the perceived needs for the concept are technically realistic and whether the business opportunity is potentially realistic, given limited information at this stage. Under *Win* analysis, at this point, usually just patent information is available to address potential competition in the marketplace. For *Worth* analysis, only crude estimates of costs and profitability are possible at this stage. Inputs to the *BDMs* consist of the superior concepts, which they screen for acceptability.

Step 2 - Feasibility

In this step, for each accepted concept, a rigorous feasibility study is undertaken. Usually this involves laboratory experimentation, with performance measurements made that correspond to the anticipated product performance. For example, an aging test may be devised to assess the product durability. Again, the *RWW* analysis is applied to those products identified as feasible. In this gate, the *Real* analysis confirms that feasibility specifications are met. The *Win* analysis begins to assess the ability of the customer to utilize the feasible product (often in manufacturing facilities). Finally, the *Worth* analysis is refined after feasibility is confirmed. Given more promising inputs, the *BDMs* screen the feasible products.

Step 3 – Development

This step involves generation of the manufacturing options; that is, process synthesis for basic and industrial chemicals, and synthesis of the assembly line for configured consumer products. Often, these options are screened using process simulation and pilot-plant testing. In this case, the most promising processing concepts are evaluated using *RWW* analysis. Under *Real* analysis, the assessment focuses on workability of existing processing techniques. Here, a process that involves a complex separation of solid species might be given a low *Real* evaluation. Under *Win* analysis, the manufacturing process might be compared with others to judge its comparative ease of construction and operation. Under *Worth* analysis, as the manufacturing steps are identified, more meaningful cost estimates may be possible. Once again, the *BDMs* evaluate the most promising results, accepting those that meet higher criteria.

Step 4 – Manufacturing

This step involves the final design. The manufacturing process is scaled-up and optimized when appropriate. Again, the *RWW* analysis becomes more critical. Under *Real* analysis, the assumptions of scale-up must be carefully assessed. Under *Win* analysis, a more carefully conducted comparison of potential operability and controllability with other processes would be assessed. Under *Worth* analysis, the cost estimates should be refined using more detailed methods and databases, enabling a more quantitative assessment. And, consequently, the *BDMs* assessment should be more critical, given that approval leads to the construction of the manufacturing plant.

Step 5 – Product Introduction

This step involves construction of the manufacturing plant, start-up, and operation, with emphasis on quality control. To achieve the product specifications, the process is optimized. Marketing and product launch documents are prepared. In the *RWW* analysis, under the *Real* analysis, the realities of the anticipated channels to the market are evaluated. At this point, the *Win* analysis focuses the ease of control and operation as compared with other manufacturing alternatives. Finally, the *Worth* analysis involves sales forecasts for the new product. Preferably, these sales forecasts include firm commitments by buyers. When the *BDMs* approve these inputs, operation of the plant proceeds as planned.

Template for Product and Process Design

In our textbook, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation* (Seider et al., 2004), a template for teaching product and process design is introduced. This template was reviewed in our recent manuscript (Seider et al., 2003). Herein, space is not available to reproduce this review or even the template, which resides in a figure that requires one full page. Rather, this section addresses the relationship of this template to the Stage-Gate product development process. Beginning with a potential design opportunity, the template shows the step, *Create and Assess the Primitive Problem,* which involves identifying needs, generating ideas, interviewing customers, setting specifications, surveying the literature (especially patents), and carrying out marketing and business studies. Then, if necessary, a step is carried out to *Find Chemicals or Chemical Mixtures that Have the Desired Properties and Performance.* These two steps correspond to the *Concept* step in the Stage-Gate process.

When a process is necessary to manufacture the chemicals, the *Process Creation* and *Development of Base Case* steps in the template correspond closely to the *Feasibility* and *Development* steps in the Stage-Gate process. Note that pilot-plant testing and preparation of a simulation model are included under *Development of Base Case.* Note also that the methods of *Detailed Process Synthesis* and *Plantwide Controllability Assessment* also correspond to the *Development* step.

Finally, the *Detailed Design, Equipment Sizing, and Optimization* step in the template corresponds, in part, to the *Manufacturing* step in the Stage-Gate process. However, for the design of industrial and configured consumer products, special considerations are required for equipment sizing in the *Product Design* step.

Quantitative Analyses in Product Design

Until recently, much of the emphasis in chemical engineering design courses focused on the manufacture of commodity chemicals. Using heuristic and algorithmic methods of process synthesis, as well as process simulators and formal optimization methods, quantitative analyses have been actively employed. The recent shift toward the design of chemical products has made it more difficult to identify design problems suitable for quantitative analysis, in general, and for seniors in chemical engineering, more specifically. This section discusses several kinds of product design problems that are well suited for quantitative analysis by chemical engineering seniors.

Molecular Structure Design

In the *Concept* stage of product and process design, for those primitive designs in which desired properties and performance are specified, it is often necessary to identify chemicals and chemical mixtures to meet the specifications. As discussed by Seider et al. (2004), examples include: (1) thin polymer films to protect electronic devices, having a high glass-transition temperature and low water solubility, (2) refrigerants that boil and condense at desired temperatures and low pressures, while not reacting with ozone in the earth's stratosphere, (3) environmentally friendly solvents for cleaning, for example, to remove ink pigments, and for separations, as in liquid-liquid extraction, (4) low-viscosity lubricants, (5) proteins for pharmaceuticals that have the desired therapeutic effects, (6) solutes for hand warmers that remain supersaturated at normal temperatures, solidifying at low temperatures when activated, and (7) ceramics having high tensile strength and low viscosity for processing. Often design problems are formulated in which the molecular structure is manipulated, using optimization methods, to achieve the desired properties. For this purpose, methods of property estimation are needed, which often include group contribution methods, and increasingly, molecular simulation (using molecular dynamics and Monte-Carlo methods).

As an example, consider the search for a polymer film to protect an electronic device (Seider et al., 2004). Given that the device will operate at temperatures below 50°C, a glass transition temperature, T_g, at 100°C is specified. Since a fairly dense layer having small water absorption is needed, a density, ρ, of 1.5 g/cm^3 with solubility, W, of 0.005 gH_2O/g polymer are specified. In the initial solution (Derringer and Markham, 1985), polymer repeat units were created involving seven molecular groups: $-CH_2-$, $-CO-$, $-COO-$, $-O-$, $-CONH-$, $-CHOH-$, and $-CHCl-$. Using group contribution methods to estimate these properties, the optimization problem:

$$\min_{\text{w.r.t. } \underline{n}} \left(\frac{\rho-\rho^{\text{spec}}}{\rho^{\text{spec}}}\right)^2 + \left(\frac{T_g-T_g^{\text{spec}}}{T_g^{\text{spec}}}\right)^2 + \left(\frac{W-W^{\text{spec}}}{W^{\text{spec}}}\right)^2$$

where $\underline{n}$ is a vector of group numbers, is solved using GAMS to yield the polymer repeat unit, $-((CH_2)_3(CHCl)_6)-$ (Seider et al., 2004).

Optimization problems of this type can be solved using the basic features of GAMS without the need to learn the methods of constrained optimization. Given limited time in a design course, it is also possible to circumvent the optimization techniques by having the students use the group contribution methods to check whether specified polymer repeat units have the desired properties.

Process Synthesis and Simulation of Batch Processes

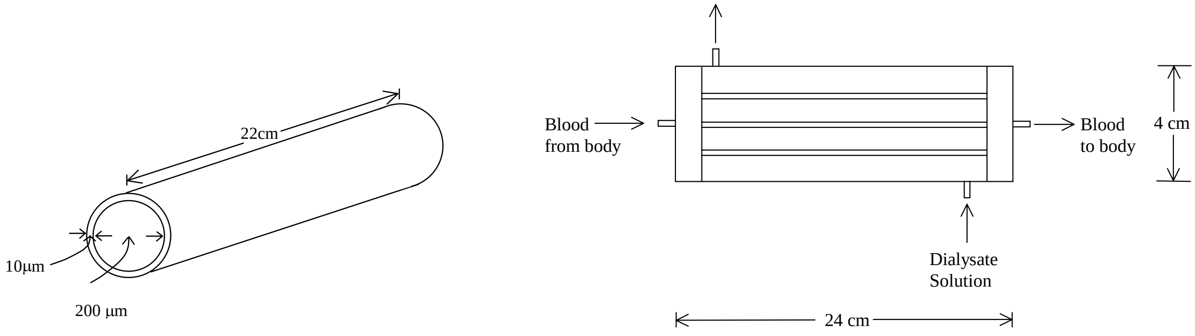
In the *Feasibility* and *Development* stages of product and process design, the scale of production of a specialty chemical often leads to selection of batch operating modes. This is often the case for pharmaceuticals, such as tissue plasminogen activator (tPA), which is manufactured in quantities on the order of 80 kg/yr. After process synthesis, as illustrated for the design of a tPA process by Seider et al. (2004), an initial process flowsheet has been formulated with a recipe of batch operations. Batch process simulators, like BATCH PLUS (Aspen Tech) and SUPERPRO DESIGNER (Intelligen, Inc.), when given this flowsheet and a recipe of operations for each equipment item, carry out material and energy balances and prepare an operating schedule; that is, a Gantt chart. With equipment sizes and costs estimated (as well as profitability analyses) usually using other software (e.g., Aspen IPE), the designs can be adjusted to reduce the cycle time, by eliminating bottlenecks, and to improve an economic objective function.

Using the tPA process as an example, Seider et al. (2004) show that the process synthesis and simulation strategies can be taught using approaches that closely parallel those for the design of commodity chemical processes, such as that for the hydrodealkylation of toluene. This treatment does not involve the formal optimization of the equipment sizes or operating parameters, although for more comprehensive coverage in a design course, it is possible to focus on optimal sequences and schedules for batch operation.

Configured Consumer Products

When the primitive design problem, developed in the *Concept* stage, leads to a configured industrial or consumer product, much of the design activity is centered on the three-dimensional structure of the product. Typical chemically related, industrial and consumer products include hemodialysis devices, solar desalination units, hand warmers, multilayer polymer mirrors, integrated circuits, germ-killing surfaces, automotive fuel cells, insect repelling wristbands, disposable diapers, ink-jet cartridges, transparencies for overhead projectors, sticky wall hangers, and espresso coffee machines, among many others. In many cases, the product must be configured for ease of use and to meet existing standards, as well as to be easily manufactured. Increasingly, when determining the product configuration, distributed-parameter models, involving ordinary and partial differential equations, are being created. Simple discretization algorithms are often used to obtain solutions, as well as finite-element packages, like FEMLAB and FLUENT.

Hemodialysis Device. As an example, consider the design of a hemodialysis device, a disposable, sterilized module that sells for under $10.00. Note that an existing product, the C-DAK 400 artificial kidney contains 10,000 hollow fibers/unit, as shown schematically in Figure 4, with 60,000,000 units sold annually.



(a) Single tube

(b) Complete module

Figure 4. Hemodialysis device

In the design procedure, which is provided in detail by Seider et al. (2004), a design configuration is postulated, including the blood flow rate (200 ml/min) and the dialysate flow rate (500 ml/min). Then, the mass-transfer coefficients for transfer of urea across the membrane and the pressure drop are estimated. Subsequently, the mass-transfer model (ODEs) for urea concentration in the bloodstream as a function of time is solved. As necessary, the design is adjusted until the urea nitrogen level (BUN) in the bloodstream is reduced from 100 to 30 mg/dL in four hours.

<u>CVD of Polysilicon</u>. Another design involves the chemical vapor deposition (CVD) of polysilicon in integrated circuit (IC) manufacture. For example, an IC transistor involves the generation of a topography in which a gate straddles a doped region of the substrate, in between the source and drain. Together, the topography performs the function of a switch. Here, the gate is a portion of the overall structure that is made from amorphous silicon (referred to as polysilicon), set down onto the original silicon substrate often by the rapid-thermal, chemical, vapor-deposition (RTCVD) process, involving parallel electrodes at low pressure. In one process, it is desired to deposit a 500 Å film on an 8-cm wafer, which sits on top of the lower electrode (Armaou and Christofides, 1999; Christofides, 2001), as shown in Figure 5.

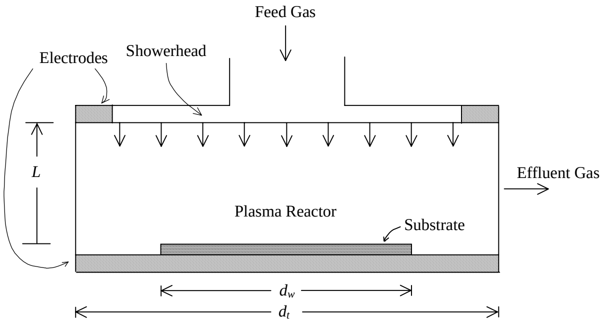


Figure 5. Plasma-enhanced CVD reactor

The reactor is fed with 10% SiH_4 (silane) in He at 1 torr through a showerhead. An RF power source, at 13.56 MHz frequency, is used to generate a plasma (chemically reactive mixture of ions, electrons, and radicals) at 500 K, which is transported by convection and diffusion to the surface of the wafer where they react and deposit amorphous silicon. In product design, the objective is to examine this and other configurations for this reactor, to assure that a uniform thin film, containing few impurities, is obtained. As shown by Seider et al. (2004), the Navier-Stokes equations with species mass balances for SiH_4, SiH_3, and SiH_2 are formulated. These can be solved using FEMLAB to determine the film thickness, with the design adjusted as necessary to achieve more uniform thicknesses.

<u>Espresso Machine Design</u>. To improve the quality, particularly the taste, of coffee, Espresso is prepared in a machine that injects high-pressure steam (20 atm) through a cake of ground coffee. In a conventional machine, shown in Figure 6, the user manually loads ground coffee into a metal filter cup, locks the cup under the steam head, and then opens the steam heater.

Figure 6. Conventional Espresso machine

A product design problem of current interest involves identifying all of the sources of variance in the quality of the coffee produced using the conventional machine, and improving the design to reduce the variance in the quality. For this purpose, product design strategies using Six-Sigma methodology to identify the most significant sources of variance, and integrated design and control methods to attenuate them, are considered by Lewin et al. (2004).

Young Faculty Perspectives

When projecting the nature of design courses over the next decade, it is important to recognize gradual changes in the composition of chemical engineering faculties. With the recent advances in experimental synthesis methods at the nano- or meso-scale, a large fraction of young faculty have recently completed doctoral research on structured materials, protein structures, …, and similar applied chemistry, physics, and biology projects. It follows that these young faculty are more interested in the design of configured consumer products such as biochemical sensors, integrated circuits, multilayer polymer mirrors, and the like, rather than the design of commodity chemical processes. This provides added incentives for developing new approaches for teaching product design.

Conclusions

In this paper, some of the latest approaches for teaching product design have been presented, focusing on the integration of product and process design strategies in chemical engineering design courses at the senior level.

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