

An Introduction to Chemical Product Design

This chapter explains what this book is about and why its subject is important. This is a book about the design of chemical products. In our definition of chemical products, we include four categories. The first, commodity products, is familiar. Second, there are molecular products, which provide a specific benefit. Pharmaceuticals and pesticides are obvious examples. Third, there are products whose microstructure, rather than molecular structure, creates value. Paint and ice cream are examples. The fourth category, chemical products, comprises devices which effect chemical change. An example is the blood oxygenator used in open-heart surgery.

The nature of chemical product design is described in Section 1.1. It emphasizes decisions made before those of chemical process design, a more familiar topic. Chemical product design is a response to major changes in the chemical industry which have occurred in recent decades. These changes, described in Sections 1.2 and 1.3, involve a split in the industry between manufacturers of commodity chemicals and developers of specialty chemicals and other chemical products. The former are best served by process design, and the latter by product design.

The fourth section of this chapter outlines the product design procedure that we will use in the remainder of the book. This procedure is a simplification of those already used in business development. Such a simplification clarifies the basic sequence of ideas involved. Moreover, the simple procedure allows us to consider in considerable detail the technical questions implied in specific products. This technical approach is suitable for those with formal training in engineering and chemistry, and may also be challenging for those whose training is largely in business. Chapters 2–5 give more detail on how to apply this simple design template to chemical products.

Further detail of the different categories of chemical product – commodities, molecular products, microstructured products, and devices – are given in the final section of this chapter. The distinction between these categories is rationalized on the basis of the length scale which is key to their performance and manufacture. We argue that the four-step template described in Section 1.4 can be applied

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usefully to each of these categories of product, but that the emphasis is different in each case. These differences of emphasis are the subject of the second half of the book: in Chapters 6–9 we discuss the key steps, and the most important technical tools, for the design of each category of product.

1.1 What Is Chemical Product Design?

Imagine four chemically based products: an amine for scrubbing acid gases, a pollution-preventing ink, an electrode separator for high-performance batteries, and a ventilator for a well-insulated house.

These four products may seem to have nothing in common. The amine is chemically well defined: a single chemical species capable of selectively reacting with sulfur oxides. The ink is a chemical mixture, which includes both a pigment and a polydisperse polymer “resin.” The electrode separator should provide a safeguard against explosion if the battery accidentally shorts out. The ventilator both provides fresh air and recovers the energy carefully conserved by insulating the house in the first place.

What these products do have in common is the procedure by which they may be designed. In each case, we begin by defining what we need. Next, we think of ideas to meet this need. We then select the best of these ideas. Finally, we decide what the product should look like and how it should be manufactured.

We define chemical product design as this entire procedure. At the start of the procedure, when we are deciding what the product should do, we expect major input from both marketing and research, as well as from science and engineering. By the end of the procedure, when we are focused on the manufacturing process, we expect a reduced role for marketing, and a major effort from engineering. However, we believe that the entire effort is best viewed as a whole, carried out by integrated teams drawn from marketing, research, and engineering.

We can see how product design develops by considering three of the products already mentioned in somewhat more detail. For example, for the pollution-preventing ink, our original need may be to reduce emissions of volatile solvents in the ink by 90%. Our ideas to meet this need include reformulating the polymer resin in the ink in two different ways. First, by using a polydisperse resin of broad molecular weight distribution, we can control the ink rheology and so eliminate the need for volatile solvents in the ink itself. Thus, there will be no emissions during printing. Second, by adding pendant carboxylic acid groups to the resin, we can make the resin not only an effective component of the ink but also an emulsifying agent in dilute base. If we wash the presses with dilute base, we can clean them without volatile solvents and without solvent-soaked shop rags. The manufacture of the new ink will be very similar to that used for the existing ink.

Consider the amine for scrubbing acid gases. Current acid-gas treatment often uses aqueous solutions of amines, such as monoethanol amine. After these solutions absorb acid gases like carbon dioxide and sulfur oxides, they are regenerated by heating. Though this heating gives an efficient regeneration, it can be expensive. The need is for amines that can be more easily regenerated. Our idea

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is to effect the regeneration with changes in pressure. We would absorb the acid gases at high pressure and regenerate the amines at low pressure, where the acid gases just bubble out of solution. In order to achieve this end we have little idea how to proceed, so we are forced to synthesize small amounts of a large number of sterically hindered amines. We will test all candidates to find the best ones. We will then manufacture the winners. Like many high value added chemicals, these will be custom syntheses, made in batch in equipment used for a wide variety of products. This obviates the need for intensive process design in many of the chemical products which we are considering.

A third example of product design is house ventilation. Well-insulated houses are energy efficient, costing little to heat, but they may exchange air at less than one tenth of the recommended rate. To get more fresh air, we can open a window, but this sacrifices our efforts at good insulation. The need is for a fresh air exchanger that captures the heat and humidity of our snug house, but exhausts stale air, with smells and carbon dioxide. Our idea is for an exchanger for both heat and water vapor for this energy-efficient house. We can manufacture this in the same way as other low-cost, cross-flow heat exchangers. In this example, our product is a device – not a chemical – that increases health and comfort in the house.

The designs of the ink, the acid-gas absorbant, and the home ventilator are examples of the subject of this book. This subject is different from chemical process design. In process design, we normally begin by knowing what the product is, and what it is for. Most commonly, it is a commodity chemical of carefully defined purity; ethylene and benzene are good examples. This material will be sold into the existing market for such a commodity, so we know the price we can expect. The focus of our process design will be efficient manufacture. We will usually use a continuous process, depending on optimized, dedicated equipment, which has been thoroughly energy integrated. This type of careful process design is essential in order to compete successfully in the commodity chemical business.

The chemical products discussed in this book are different. Their promise stems less from their efficient manufacture, and more from their special functions. They will usually be made in batch, in generic equipment; or will themselves be small pieces of equipment. Process efficiency may be less important than speed to reach the market place. Energy integration may be of secondary value. Indeed, most product design may occur before manufacture is even an issue.

We believe that product design merits increased emphasis because of major changes in the chemical industry. We do not argue that the chemical engineer's concern with process design should disappear. However, we do assert that the topics we study should reflect the chemical industry of today. How this has developed is outlined in the next section.

1.2 Why Chemical Product Design is Important

Chemical product design has become more important because of major changes in the chemical industry. To understand these changes, we will review the history

Table 1.2–1 Growth of textile fibers in 10^6 lb/year
 From 1950 to 1970, synthetic fibers grew about 20% per year. Since then, their growth is 5% per year. (Source: Spitz; US Department of Commerce).

	1948	1969	1989
Cotton, wool	4353	4285	4794
Synthetics	92	3480	8612

of the industry, using as an example the development of synthetic textile fibers. We also need to examine how these changes have affected employment.

1.2–1 CHANGES IN THE CHEMICAL INDUSTRY

From 1950 to 1970 the chemical industry produced ever increasing amounts of synthetic textile fibers, as shown in Table 1.2–1. Over these decades, while the production of natural fibers was about constant, the production of synthetics grew 20% per year. This growth is comparable to that of the software industry today; Du Pont can be seen as the Microsoft of the 1950s. This was a golden age for chemicals.

However, from 1970 to 1990, synthetic textile fibers grew by less than 5% per year, about the same as the growth of the world population. From 1970 to 1990, the industry stayed profitable by using larger and larger facilities. Bigger profits came from consolidating production into bigger plants, designed for greater efficiency in making one particular product. Interest in computer-optimized design was a consequence of this consolidation. Such optimization meant small producers were forced out. For example, the number of companies making vinyl chloride in the USA shrank from twelve in 1964 to only six in 1972 (Spitz, 1988).

More recently, the industry has required new strategies to stay profitable. These strategies often centered on restructuring, which was three times more likely to affect engineers than the general working population. Whether called “restructuring,” “downsizing,” “rightsizing,” or “rationalization,” the strategy meant many mid-career engineers were suddenly looking for new jobs. The Engineering Workforce Commission in the USA now feels that engineers will average seven different jobs per career, a dramatic change from two per career in the recent past (National Science Board, 2003). Middle management, that traditional goal of bright but not brilliant students, is no longer a safe haven. While starting salaries remain high, the envy of other technical professions, these salaries have not increased faster than average wage inflation in 30 years. In this environment, professional organizations like the American Institute of Chemical Engineers now provide more help in job transitions and financial planning. Such organizations can no longer behave only as nineteenth-century-style learned societies.

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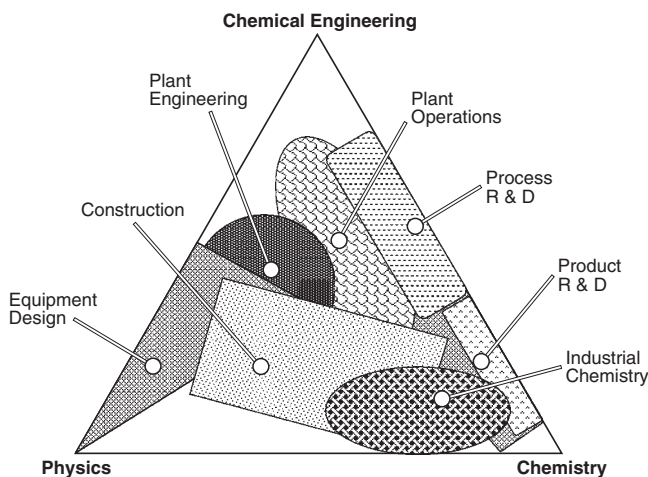


Figure 1.2–1 Skills learned by chemical engineers Traditional skills are a blend of physics, chemistry, and engineering. These are sufficient for chemical product design.

Having exhausted optimization and restructuring as ways to stay profitable, chemical companies now have three remaining options. First, they can leave the chemical business. This option seems reasonable to a surprising number, including some petrochemical businesses. Second, chemical companies can focus exclusively on commodities. This seems a preferred strategy for some private companies, who may be better able to handle the ebb and flow of the profits from a commodity business. It implies a ruthless minimization of research and a concentration on in-house efficiency.

The third strategy open to these chemical companies is to focus their growth on specialty chemicals or high-performance materials. Such chemicals, produced in much smaller volumes than commodities, typically have much higher added value as well. This higher added value means that more research and higher profits are possible. Not surprisingly, many chemical companies are turning their focus to specialty chemicals or high-performance materials.

Interestingly, this new focus has not changed the skills that companies demand from chemists and chemical engineers, though it has changed the jobs that they do. The various subjects which chemical engineers learn can be positioned on the triangular diagram in Figure 1.2–1. The three corners of this plot represent training in physical sciences, in the chemical sciences, and in chemical engineering subjects. Different jobs use these three elements in different proportions, as shown in the figure. There is no surprise in this: plant engineering will demand a greater knowledge of mechanics and a smaller background in chemistry than those involved in research and development. Figure 1.2–1 also suggests national averages. British chemical engineers have more chemical engineering and less chemistry than their counterparts in the USA. Please do not take this diagram too literally; use it instead as a catalyst for thought. We maintain that the basic skills

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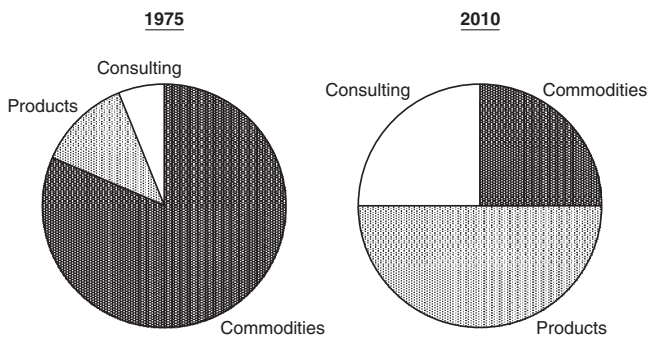


Figure 1.2-2 *Changes in employment* The dominance of commodity chemicals has been eclipsed by efforts on other types of products.

needed by chemical engineers have always been diverse and have not altered dramatically.

1.2-2 CHANGES IN EMPLOYMENT

While changes in the chemical industry may not have changed the skills needed, the focus of chemical companies on specialties and new materials has had a major impact on the jobs which chemists and chemical engineers do. To examine this impact, we compare the jobs taken by recent graduates with those taken by graduates twenty five years ago. Our data for this are fragmentary, taken from records of graduates from the universities of Cambridge and Minnesota. They are probably biased towards large corporations, about whom our university placement offices have better records.

The available data suggest major changes, as shown in Figure 1.2-2. In 1975, three quarters of chemical engineering graduates went to work in the commodity chemicals business. The small number who did not were split between work on products, either design or development; and work in other areas, which for convenience we have labelled “consulting.” This category includes those working directly for consulting firms as well as those carrying out specific tasks like environmental-impact statements.

More recently, the distribution of jobs has become completely different. The largest group of chemical engineering graduates, in Minnesota’s case more than half, now work primarily on products. This includes students who work on materials, on coatings, on adhesives, and on specialty chemicals. The number who work in commodity chemicals has dropped so that it is now less than a quarter of new graduates. The number who work in consulting has risen dramatically, as commodity chemical businesses outsource many of the functions which they used to do in house. For example, in one case, a commodity chemical company has taken its process engineering group from 1500 persons to fewer than 50. This is not a business cycle; this is a change in the way in which that company expects

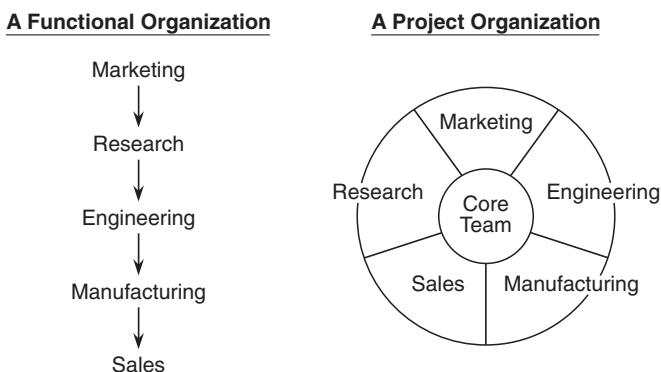


Figure 1.3-1 Two limiting types of corporate organization The project organization is believed to give greater speed and synergy but greater management complexity.

to do business: they will buy the process engineering they need from consultants. This is why the number of people involved in consulting has risen.

The emergence of products as a focus for chemical engineers implies changes in what chemical engineers do. In the past, we chemical engineers could limit our thinking to reaction engineering and unit operations, waiting for the marketing division to tell us what chemicals needed to be made, and in what amounts. Such intellectual isolation is no longer possible. Now we can expect to be involved in teams, a consequence of a new corporate culture.

I.3 Changes in Corporate Culture

At the same time, there have been changes in corporate culture, in the ways in which companies do business. These are consequences of the changes in the chemical industry discussed in the previous section, and they are at least as important, because they alter the ways chemical engineers work. Two major changes are especially important: the way in which corporations organize their product design, and the ways in which corporate strategy affects jobs. Each is discussed below.

I.3-1 CORPORATE ORGANIZATION

The organization of product development is most easily discussed by comparison of two limiting cases: organization by function, and organization by project. These are shown schematically in Figure 1.3-1. Both can be effective.

In a functional organization, different divisions have different responsibilities: marketing, research and development, engineering, legal affairs, and so on. Product development proceeds by each division doing its job, and then passing its results on to the next division. The result is like chemical reactions in series, as suggested by Figure 1.3-1. This organization is especially associated with large, established industrial companies which have major capital investments

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in manufacturing. For example, the marketing department of an automobile company could discover that consumers want better climate control, i.e. better heating and air-conditioning. Marketing would report their results to research, who would develop the electronic controls required for this goal. Engineering would extend the research results so that the new controls could be manufactured cheaply and efficiently. Throughout the process of product design, the development is sequential: marketing talks largely to research, only rarely to engineering. Such a functional organization can be effective, but it is almost always slow.

A common alternative is a project organization. In a project organization, a core team is formed from the different divisions. The team will normally include representatives from marketing, research and development, engineering, production, etc. These core team members will have complete responsibility – and a good deal of resources – to design and develop the target product. They will be judged not by their immediate functional supervisors, but rather by a panel of senior managers well versed in the company's long-term strategy. Functional supervisors still have the job of making the divisions run smoothly. Such divided management can be chaotic and inefficient. As Figure 1.3–1 suggests, it is like parallel chemical reactions, with a good chance of synergy between functions. Above all, this form of product development is fast, and fast product development is believed to maximize profits, so that project management is currently the organization urged by most business consultants.

1.3–2 CORPORATE STRATEGY

Superimposed on its organization, a corporation will have strategic forces driving product development. Again, the driving forces are most easily described in terms of two limiting cases. First, corporations which look towards their markets for inspiration are said to be “market-pull.” Corporations which emphasize extending their technology are said to be “technology-push.” Examples of market-pull companies are common. W K Kellogg, the makers of breakfast cereal, are interested in new products from grain. They constantly assess the market for consumer wishes for new cereals or new grain-based snack foods. Honeywell make home thermostats, a major product because a significant fraction of the world's energy consumption goes for domestic heating. Honeywell are interested in any new products for home comfort that can complement their thermostats. Patagonia, makers of technical mountain-climbing equipment, now also make raincoats. They are pushing to expand their market: many more people need raincoats than ice axes.

Examples of technology-push companies are less common but can nonetheless be found among everyday names. W L Gore makes Goretex, that breathable film basic to high-quality raincoats. But Gore do not make raincoats: instead, they have used their basic material to make medical products, including arterial transplants. Exxon-Mobil has used its knowledge of petrochemical reactions to develop a series of new metallocene catalysts for polyolefins. Astra-Zeneca has used its experience with injectable therapeutics to develop delivery systems for

different drugs. Interestingly, both “market-pull” and “technology-push” companies can use the same product design procedure. This procedure is described next.

I.4 The Product Design Procedure

Product design is a major topic both in disciplines like sales and marketing, and in technical professions such as mechanical engineering. Not surprisingly, schemes for this design procedure vary widely. Many are complex, especially with respect to the role of management. Many have features that seem specific to the particular subdiscipline that they represent.

The product design procedure used in this book is a simplification and generalization of those used in these other areas. It depends on four steps:

- (1) *Needs*. What needs should the product fulfill?
- (2) *Ideas*. What different products could satisfy these needs?
- (3) *Selection*. Which ideas are the most promising?
- (4) *Manufacture*. How can we make the product in commercial quantities?

The characteristics of this approach are discussed in the rest of this section. We shall see as we go along that the application of this template to the case of chemical products leads to several new and characteristic features of the design process.

I.4–I HOW THE PROCEDURE ORGANIZES THIS BOOK

These four steps are the key to the organization of the first half of this book. Assessment of needs, the subject of Chapter 2, includes deciding on a standard for comparison – a benchmark – and on converting the qualitative needs to quantitative specifications. The benchmark chosen may be an existing product or an ideal. Needs must be as well defined as possible, and framed in technical terms, so that any specifications are definitive.

Finding ideas that might meet these needs is the next step in product design. Normally, we will wish to search for a large number of these ideas by all reasonable means. This search, the subject of Chapter 3, may include brainstorming by individuals and teams and synthesizing tangent compounds by combinatorial chemistry. Once these numerous ideas are identified, they must be screened using objective and subjective judgments, also described in Chapter 3.

At this point, we should have reduced the large number of fragmentary ideas for products to a short list of promising candidates. Typically, this reduction will be about a factor of twenty: if we start with a hundred ideas, we should have about five survivors. We must now select the best one or two for further design and development. If the characteristics of each of the surviving ideas were directly comparable, this would be easy. They normally are not. For example, we might be sure that one idea will work well but be expensive; a competing idea might be

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cheap but we may be unsure if it will work. Deciding between these ideas includes risk management, as described in Chapter 4.

Finally, we must manufacture the product, and estimate the costs involved. Parenthetically, this fourth step could correctly be called “process design.” We have not done so because we found our descriptions then seemed more complicated than necessary. These manufacturing efforts, described in Chapter 5, are different from those expected for commodity chemicals, where we expect to use dedicated, optimized equipment which operates continuously. Here, we will normally use generic equipment, run in batch for a variety of specialty products.

This is different to traditional chemical engineering – and is exciting.

1.4–2 LIMITATIONS OF THE PROCEDURE

The four-step procedure outlined above is controversial. We should review the controversies now, so that we are prepared for exceptions and diversions in the practice of product design. The controversies cluster around three criticisms: that the procedure is not general, that management and not technology is the key, and that chemical product design is part of process design. Each controversy merits discussion; they are tackled below.

First, is the four-step procedure as outlined general? It is clearly a major simplification. Many business texts argue that such a procedure is universally applicable for any product in any industry. These texts are frequently written by business consultants eager to make money by applying their own standard template to specific problems. At the same time, many professional product developers argue that this or any procedure cannot represent the peculiarities of their own industry; that only those with particular interests can hope to be effective. While there is clearly some truth in this argument, these product developers may be like those who have denied that correlations of heat transfer could be used for food products because they were based on measurements for petrochemicals.

We believe that both sides of the debate have their merits. The four-step procedure used here is unquestionably an approximation. Certain techniques introduced in particular steps of the procedure can have value at other stages. For example, risk management, introduced in the selection step in Chapter 4, may have value in screening product ideas, explored in Chapter 3. It is unlikely that real product design will always be a simple sequential procedure as we suggest; iteration between stages is almost certain to be necessary. Still, we must begin somewhere, and the current procedure has been for us a sound and creative start. We suggest trying it; any necessary modifications quickly become obvious in specific cases. A framework in which the subject may be understood is an aid to learning in chemical product design just as an analogous template has been successfully applied for years in process design.

The second controversy is the claim that management, not technology, is key to product design. An irritating feature of most business books on product design is the extreme emphasis on the central role of management. The implication is that technology is always available if only the managers do their job properly