CHEMICAL PRODUCT DESIGN

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Summary

The chemical industry has since the middle of the 20th century focused on process design, the major goal being the more efficient production of a relatively small range of commodity chemicals. The industry was dominated by petrochemicals. In recent decades, higher value added, smaller volume products have become increasingly important. Chemical products depend for their performance on both molecular structure and microstructure; examples are pharmaceuticals, agrochemicals, food products, paints and detergents. The key to such products is improvement in performance rather than minimization of cost. This means that the appropriate design strategies are different. We suggest a four stage template for the generation of new products to meet customer needs. The four stages are the identification of customer needs, the generation of ideas to fulfill these needs, the selection of the best idea and the manufacture of the product. This last stage incorporates traditional process design, but is de-emphasized, due to the high value and low volume of chemical products relative to commodity chemicals. These four steps provide a heuristic for approaching the design of a broad range of chemical products.

1. Introduction

Chemical product design is the procedure by which we choose which product we will make and how we will make it. Around the beginning of the 20th century, this was the key step in the chemical enterprise because many of the products to be made were undefined. Around the middle of the 20^{th} century, chemical product design had been replaced by chemical process design, because the most lucrative products had been identified and the key issue had become the cost of producing those products. Now, as the chemical enterprise sets much broader goals, chemical product design has once again become important.

There are three groups of chemical products. First, there are the fifty or so commodity chemicals that are produced in dedicated equipment and at very large scale. Ethylene, oxygen, and sulfuric acid are examples. The second group is the several thousand high value added chemicals produced in much smaller batches and in generic chemical equipment. Many of these groups are pharmaceuticals. The third group of chemical products consists of chemical mixtures, often with specific microstructures which are not necessarily in thermodynamic equilibrium. Detergents, coatings and copolymers are examples.

In this chapter we suggest a general strategy for designing molecular products and microstructured chemical mixtures. This product design procedure comes before the more conventional chemical process design. In product design, we decide which product we will make; in process design, we explore how we will make it. Chemical product design is the larger topic, and includes process design in a final step.

It has been argued by several authors that the chemical industry has recently undergone rapid changes which increase the importance of product design; some of these authors also suggest appropriate courses of action for industry or education.

In the following sections we will suggest a four-step template by which we can explore which chemical product we want to make. Over many years, other fields, notably mechanical engineering, have developed methodologies for design, on which this template builds. Because of the enormous variety of products possible, we should expect this template only to provide a guide for our thinking. We should expect it to be modified in many particular cases. Still, we think the template can be an effective aid for organizing our thinking.

The four steps in this general template are as follows:

1. Needs: We must decide what need our product would fill.
2. Ideas: We must generate ideas that satisfy this need.
3. Selection. We must efficiently select the best ideas for manufacture.
4. Manufacture. We must make the product.

While the design of commodity chemicals centers on the fourth steps, the design of new molecules and of particular microstructures requires all four steps. Details of each of these steps are given in the sections that follow. These ideas are developed by the authors in more detail in their book “Chemical Product Design”.

2. Needs

Chemical product design begins with defining a need for a specific product. This first step in product design can come from one of two stimuli. The most common stimulus, especially in established markets, is the pull of the market where. In this case, a gap is identified in a known market, which a new product could fill. This stimulus is typical for many consumer products. For example, a company which manufactures hospital supplies may decide there is a new market for surgical scrubs which contain a controlled-released bacteriacide, improving sterilization in the operating room.

The second stimulus for new product development comes from the search for applications of a new technology. This is less common in industry but is the norm for universities trying to develop products. Here the stimulus is not the pursuit of a consumer opportunity but a new invention looking for an application. One example is Gortex films where a nanoporous wire insulating material was used to make improved sports equipment.

The two different stimuli of market pull and technology push often result in different statements of product needs. In the case of market pull, we seek to quantitatively define exactly what the market opportunity is. We will then search for the appropriate technology. When the stimulus is technology push, we seek a market niche where our technology has a potential advantage. Many studies of product development suggest that market pull is about five times more likely to be successful than technology push.

The next steps in the identification of a product need are interpretation of this need and quantification of it. We will discuss these three steps in the following paragraphs.

The first point in identifying needs is to remember that the product is not for us. We must make sure that the needs that we identify are in fact the needs of our customers. This means we have to decide who our customers are. We use the term customers in a loose sense here. We do not necessarily mean those who buy our product, but rather those who will benefit from its development. These beneficiaries may be organizations, including government agencies or private companies. They will only sometimes be individuals.

We will normally need to talk to our customers in face-to-face interviews. Business literature suggests that fewer than ten such interviews miss significant information and more than fifty interviews leads to duplication. In our interviews, we should pay particular attention to “lead users” who will benefit most from any product development. In many cases, these lead users will have already adapted and improved our product for their own specific goals. These product improvements merit our special attention.

We next turn to the interpretation of consumer needs. After all, our interviews will just be a tangle of incomplete and conflicting information, much of which will be irrelevant. Our task will be to organize this tangle into a cogent list. We will drop some stated needs because they are redundant or impractical or beyond what our organization can do. We will also rank the needs as, for example, imperative, important and attractive.

We must plan to get almost the entire imperative group and proportionally fewer of the other groups. Once we have this ranking, we will frequently return to our various customers and ask if our ranking makes sense. This return will require judgment: we may decide to ignore what some of the customers are telling us, but we certainly will want to do so consciously.

Finally, we need to change our qualitative list of needs into quantitative specifications. This is the point where science and engineering become much more important than market research and brand identification. Technically trained individuals must be involved in product development. This is especially important because those in marketing may not understand the limitations of science. For example, they may not understand that it is impossible to get more energy out of a device than goes into it.

We find it useful at this stage to have a mental checklist, which ensures that we are considering all aspects of the science that is involved. One possible checklist would be to consider the three following steps:

1. Write complete reactions for all chemical changes involved. We must pay particular attention to the necessary reagents and byproducts. For example, if one byproduct is toxic, we want to remember that we will need to dispose of it safely.
2. Make complete mass and energy balances, both for the product's manufacture and for the product's use. These balances check that our new product is not in conflict with any scientific laws.
3. Estimate the rates of any important changes during the product manufacture or use. These rate estimates explore what time constraints our eventual product must meet.

We will want our list of product specifications to be as detailed and complete as we can make it. In doing so, we will find ourselves making many estimates, some of which will really just be guesses. The key is not to become obsessed with guessing correctly (although it would be nice if we could). The key is to remember that any estimate implies some risk that we may later want to try to reduce.

Setting these quantitative specifications involves estimating the properties of the final product. These estimates will depend on generalizations about physical and chemical properties. They will emphasize the so-called "structure-property relations," that relate macroscopic properties to microscopic or molecular structures.

The structure-property relations are a goal of materials science that has only partly been realized even after centuries of efforts. The most obvious success is the prediction of the properties of gases: we have no difficulty estimating the viscosity of air. We have some trouble estimating the properties of liquids, but liquid properties turn out to be remarkably constant; for example, the densities of almost all liquids fall within a factor of two. Estimates of the properties of solids, especially their electronic properties, are a topic where enormous progress has been made in the last few decades. The real mystery remains the properties of the solid-liquid mixtures that are central to microstructured products. This major interdisciplinary area remains an active focus for research. We illustrate these ideas with the following example. It will be clear from this example that any template can only be approximate and must be adapted to the specific case being considered. Our template suggests lists of important parameters which need to be considered; which are more significant depends on the specifics of the case. For example, we have suggested a checklist of three items in formulating specifications: in the following example only the energy balance is relevant.

2.1. Example: Using Offshore Wind Energy

Compelling evidence of the existence and magnitude of global warming caused by carbon dioxide emissions has resulted in increasing interest in the use of renewable forms of energy, particularly in Europe. This has been crystallized into policy by the Kyoto Treaty. The U.K. government has committed itself to a target of 10 percent renewable energy generation by 2010. One promising renewable energy source is wind power. In recent years, several large scale wind farms have been constructed offshore in the U.K. and more are being planned. Currently the majority of wind power is supplied directly to the National Grid. A significant drawback of wind generated electricity is its intermittency. Wind farms generally operate at only about 25 percent of their theoretical maximum output, due to the unpredictability of wind. More seriously, the value of the electricity which is generated is reduced because supply must be guaranteed, necessitating the provision of back-up capacity. Inevitably, this problem will become more significant as the fraction of installed generating capacity provided by wind farms increases.

One method of mitigating this problem, while still moving towards the government's renewable target, is to use some of the wind power generated for an application other than direct supply to the National Grid. Such an application might be the generation of a chemical, water purification, or waste treatment, which could operate intermittently without difficulty.

As a benchmark, consider Scroby Sands, a state-of-the-art wind farm off the Norfolk coast, consisting of 30 Vesta 2.0 turbines (height 68 m, diameter 28 m, 2 MW maximum output); taking into account the intermittency of wind, this results in approximately 15 MW of generated power on average. This could supply up to 40,000 households with electricity, approximately half the population of nearby Great Yarmouth.

On average, electricity sells for 0.04 euros/kWh, while offshore wind generated electricity costs 0.06 euros/kWh to generate. Offshore turbines have a design lifetime of 20 years. Capital costs take around 6 months operation to recover. Wind farms can be monitored remotely and require maintenance every six months or so, typically 40 hours per year per turbine.

Whilst wind power currently looks uneconomic, the more so due to its inherently low value compared to more stable supplies, its installation is being driven by political and environmental considerations, combined with predicted price increases in competing technologies, due to diminishing fossil fuel reserves and inversing carbon taxes.

What needs most to be satisfied by such an alternative application? There are a number of constraints, provided by the Kyoto accord, government policy and the nature of wind generation. In considering our needs, we should be careful to separate these constraints from our needs, which should be a statement of what we aim to achieve with our product. We might formulate the following list of needs (Table 1):

Rank	**Need**	**Comments**	**Quantification**
Essential	Uses intermittent source	Power output inherently variable. Ideal application will make full use of energy available and not suffer from enforced down time.	Significant fraction of 15 MW average capacity utilized, with 60 MW peak. Ideal would be to use fluctuating excess, while leaving perhaps 8 MW baseline for sale to National Grid.
Essential	Economically viable	Minimum is to compete with average electricity price. In reality "green" electricity is likely to carry a premium price due to consumer demand and political pressure.	0.08 euros/kwh value should guarantee competitiveness with direct supply to National Grid.
Desirable	Lifetime	The proposed solution should match the lifetime of the wind turbines, both in terms of market for the product and plant lifetime. Ideally service requirements would also be matched.	20 year lifetime.
Useful	Aesthetics and environmental impact	Much of the marketability of wind farms comes from their perceived environmental benefits. Offshore wind farms avoid the aesthetic problems of land-based ones.	No undermining of "green", clean and beautiful image.

Table 1: Needs for Offshore Wind Generation

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Degrees Held:
1991 PhD in Chemistry, University of Cambridge
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