CHEMICAL PRODUCT DESIGN

1. Introduction

Chemical product design is the process by which we choose what product we will make. It precedes chemical process design, which deals with how we plan to make the product chosen. In the past, most of those involved in the chemical industry emphasized process design, because this enterprise was focused on perhaps 50 commodity products. For these commodities, price was the key, and efficient production was the route to low prices. This strategy correctly dominated the efforts of the chemical industry in the twentieth century.

Now the goals of this chemical enterprise have become much broader. These goals include not only the 50 or so commodity chemicals, but several thousand high value added chemicals. Many of these are pharmaceuticals. The broader goals of the chemical industry also include chemical mixtures, often with specific microstructures, like detergents, and coatings. The goals include polymers processed to have characteristics desired in filters or films. These broader goals mean that chemical professionals now participate in a wider variety of business decisions. These include deciding what to make.

In this article, we suggest a four step template by which we can decide which chemical products we want to make. Because of the enormous variety of products which are possible, we should not expect this template to work perfectly in every case. Instead, we offer the template as a mental checklist for organizing our thinking. We ourselves use this checklist again and again as we refine our efforts at product design. The four steps are as follows:

1. *Needs*: We must decide what need our product will fill.
2. *Ideas*: We must generate chemical ideas that could satisfy this need.

3. *Selection*: We must efficiently select the best ideas.
4. *Manufacture*: We must design the process for making our product.

The first three steps of this template are unique to Product Design, but the fourth step includes the more familiar topics of Process Design.

We will give details of each of these four steps in the body of this chapter. Before we give these details, we can gain an overview from quickly applying this template to three possible products: an improved amine for gas scrubbing, a pollution preventing ink, and a battery separator.

Current gas scrubbing often uses aqueous solutions of amine like monoethanol amine to absorb acid gases like carbon dioxide and hydrogen sulphide. Once saturated, or loaded, the resulting solutions are warmed to strip out the absorbed acid gases. Because the solutions are dilute, the warming takes a lot of energy. Thus the need is for an amine that can be more easily regenerated. Ideas to do this could include amines that are used as concentrated solutions, or those that undergo phase transitions and, hence, require a smaller temperature increase than currently dictated. The idea actually selected was to search for a pressure sensitive, hindered amine, one that complexed acid gases at moderate pressure, but released them under partial vacuum. Those involved synthesized and tested several hundred hindered amines to find attractive candidates. They eventually synthesized one of the best in industrially useful quantities. Note that the important steps were the definition of the need and the creation of ideas, even though most of the work was in the chemical synthesis of candidate amines.

The second example, the pollution preventing ink, originates in the use of methylene chloride in printing. This carcinogenic solvent is used to adjust the ink's viscosity and to clean the presses between runs. The need to reduce methylene chloride use led to ideas like using less solvent, capturing and condensing the solvent's vapor, using toluene as a solvent, and modifying the ink's chemistry. Many of these ideas were tried in turn; the one selected eventually was to change the ink's chemistry. In particular, the ink contains a low molecular weight polymeric resin. By changing the molecular weight distribution of the resin, we can make an ink that does not require adding solvent to adjust its viscosity. By adding pendant carboxylic acid groups to the resin, the ink can be washed off the presses with aqueous base: The ink essentially becomes its own soap. Manufacturing the new ink turned out to be very similar to manufacturing the old ink. The key was inventing the new ink chemistry.

The third example, a shutdown battery separator, is used in the high energy batteries in laptop computers and other portable electronic devices. These batteries store chemical energy in an anode and a cathode separated by a microporous polymer sheet. This microporous separator is often a polyolefin made by stretching to form small pores, followed by a careful warming with the film under tension to relax the polymer and freeze the pores in place. Unfortunately, if these batteries short out, they can explode. Thus the need is for a separator that will allow unrestricted ionic transport under normal operating conditions, but which will stop this transport if the current is excessive.

Ideas to meet this need ranged widely, from pedestrian fuses to silly fancies. The idea selected depended on the fact that a shorted battery gets hot. This warmth softens the microporous polymer separator. If the heat treatment in making the separator was changed, then this softening would close the pores in the separator. In developing this product, the engineers involved used their experience in making the original film with pores that always stayed open. In these original efforts, the engineers frequently had failures, when the pores would not stay open. Now, with a new product need, these failures became the key to a success.

In the rest of this article, we will examine in detail this template of needs, ideas, selection, and manufacture. We will illustrate each step with additional examples, but we want to stress the steps independently, rather than to list case studies. Using the template this way, we believe, best illustrates how products are designed.

2. Needs

The first step in designing a chemical product is defining what it is that a successful product should achieve, which is the Needs stage of product design.

Before considering how to define product needs, it is worth thinking about what it is that stimulates product development. We broadly identify two driving forces to product design. The first is the pull of the market, where a market opening is identified and then a product designed to fill this opening. This route is typical for new consumer products. A company will formulate a new soft drink in response to the marketing department identifying a market opportunity. Examples of market pull products are a deodorizing fabric for sports, a needle-free injector for medical applications, and an improved dusting cloth.

The second driving force to product development is technology push. Here the initial stimulant is not a perceived consumer opportunity, but an advance in technology, a new invention looking for an application. For example, during the Cold War there was a major effort to produce strong, lightweight materials for military applications. Having developed these high performance materials, companies began to look for other uses and found squash rackets and golf clubs. These are examples of technology push products.

As a second example, in 1775, shortly after discovering oxygen, Priestly said, “Who can tell but that, in time, this pure air may become a fashionable article in luxury. Hitherto only two mice and myself have the privilege of breathing it”. By 2001, small bottles of oxygen were being marketed as OPUR and used by celebrities. Perhaps this is the slowest technology push product design in history.

The two driving forces of market pull and technology push result in rather different statements of product needs. In the case of a market pull product, we wish to define exactly what the market opportunity is. Product design then identifies an appropriate technology to exploit this opportunity. In the case of a technology push product, it is the other way around: the needs stage involves specifying the new technology and identifying areas of superiority to existing technology. The product design then consists of identifying markets where this new technology can be advantageously exploited.

While the form of the needs specification will vary depending on the spur to product development, the process by which this specification can be established is similar. This topic is what we now discuss.

2.1. Needs Identification. In defining product needs, we first remember that the product is not for ourselves. We must make sure that the needs we define reflect the requirements of those who will ultimately use the product and not simply our own prejudices. This means that needs identification will always begin by asking others what it is that they require: we must find our "customers" and identify their needs. We use the term customers in a loose sense here. We do not necessarily mean those who will buy our product, rather those who will benefit from its chemistry, which may be organizations such as companies or government agencies rather than individuals.

The consensus among marketing organizations is that the best way to get this sort of information is by face-to-face interviews. Fewer than 10 such interviews risk missing significant information, while more than 50 simply leads to duplication. If organizations are involved, we must of course interview individuals within those organizations. It is worth talking separately to several; it is always surprising the degree of disagreement present within a supposedly homogeneous organization.

One group merits particular attention, the "lead users". These are the people most expert in the product and those who will benefit most by its improvement. In the case of a market pull product, the lead users are those who very much depend on existing and competing products. In the case of a technology push product, the lead users are those most responsible for the technological advance that has stimulated the product development.

In addition to individual interviews, test panels and focus groups are sometimes used to help identify needs, particularly for consumer products.

Example 2A: Nonionic Surfactants. A typical washing powder for clothes cleaning made by a major manufacturer contains $\sim$5% of nonionic surfactants, the remainder being anionic surfactant, mainly linear alkyl sulphonates. Nonionic surfactants are particularly effective for the removal of greasy stains. The company would like to increase their loading to $\sim$10% to improve washing performance. The problem is that nonionic surfactants are sticky liquids, while washing powders must be free flowing granules. Simply increasing the nonionic surfactant loading using current technology results in agglomeration of the powder into a sticky mess. How can the nonionic surfactant loading be increased whilst maintaining the physical properties of the washing powder?

Solution. We must first identify the customers, so that we can ask what is required. It is tempting to think of the customers as those who buy and use the washing powder, but in this case that is not appropriate. They will simply tell you they want an inexpensive product that works well. As a result of numerous interviews with users, the marketing department has already decided that an increase in nonionic surfactant loading is desirable. The relevant people to talk to in this case are within the company, those who are going to have to implement changes in formulation: the engineers who run the powder manufacturing plants. We should aim to talk to 5–10 such people, to give us a good coverage of the issues involved and highlight differences of opinion. A typical interview with a plant engineer might go as follows:

What Do You Do Now? *We blend the anionic detergent and solid additives in an extrusion process. This makes the detergent go white and springy, which we want. We granulate to get the particle size right, and finally spray on nonionics and perfumes.*

What Happens If You Spray on More Nonionic? *It is hopeless. You end up with a big sticky lump of detergent—its not a powder any more.*

What Is Good about What You Do Now? *It gives a high density product—better than spray drying the detergent. It is efficient—we get the solids mixing and physical structuring of the anionic detergent at the same time. Its easy to change the additives at the end for different products just by spraying different amounts.*

What Is Wrong with What You Do Now? *Nothing. We make five different brands this way. Have done for years. They clean people's clothes OK. I do not see the problem. Why do marketing want something new anyhow?*

Where Do You Get Your Materials From? *We buy them from a subcontractor—a specialist manufacturer. They supply the anionic detergent—it's a yellow sticky paste when we get it—and the nonionic—it's a thick liquid. Solids come from another company and perfume from a third. The formulation chemists tell us what to put in and then we have to find it. We always like to have at least two suppliers of each material.*

This interview starts to show us the needs—how any solution must fit into the existing process. It also tells us other people to talk to—the formulation chemists and the subcontractors who supply the detergents. We will then get a fuller picture of what is needed. Our next task will be to organize these interviews into a list of more coherent and specific needs.

2.2. Interpretation of Needs. The needs recorded from the information gathering just described will be a hotchpotch of conflicting and incomplete statements, of varying relevance and practicality. Our task is to organize these needs as groups and to edit them into a cogent list. We will drop some stated needs, either because they appear impractical or are beyond our company's expertise.

It is also useful to rank the needs, for example, as essential, desirable and useful. The essential needs are those without which the product cannot succeed. We will aim to achieve as many desirable needs as possible, particularly if competitor products fail to do so. We are unlikely to design explicitly for the useful needs, although we will keep in mind that it will be a bonus if our product can fulfill these, too.

The way in which needs are grouped and organized will depend on the product being considered. It will usually be an easy task if we aim to improve an existing product. The more innovative the proposal product, the harder it is to satisfactorily define the needs. We may need to modify the needs statement later as our ideas take shape. It may also be useful to return to the customers, perhaps a different group, to further explore our marked list of needs.

Example 2B: A Fishy Business. Fish farming is now a major international business. One company supplies food for salmon and other farmed species to markets in Scotland, Norway, and Chile. They wish to improve the performance of their product in order to secure these growing markets. A group of engineering consultants has been hired to recommend improvements. The current product consists of cylindrical pellets made by extrusion of a mixture of fish meal, fish oil and wheat. An interview with a fish farmer might go as follows:

What Do You Do Now? *We use a water cannon to spray the pellets over the fish pens. We feed once a day.*

What Is Good About the Current Product? *It's really easy to deliver—the water cannon is no work. The fish love it. They grow really fast.*

What Is Bad About It? *It is oily. You always get an oil film. This seems a waste and is not good for the fish. I also worry about the oil breeding fungi, which gets into the gills of the fish. The big fish always get to the top first and eat most of the food. We would like to give more to the smaller fish.*

Where Do You Buy Your Food From? *We get 70% from your company and 30% is local waste. The waste is not so good; it is messy and the fish will not eat it all—they seem to prefer food with oil in. But it is cheap.*

Interpret these needs into a form useful for product specification.

Solution. We can easily classify the needs inferred from this interview.

Essential

Good nutritional value.
Mechanical strength.
Fast dispersion to get food to smaller fish.

Desirable

Inexpensive.
Good oil retention.

Useful

Ease of manufacture using current process.
Hygienic appearance.

We are now ready to continue development.

2.3. Quantification of Needs. Our aim now is to convert our qualitative list of needs into specifications, including as much quantitative and chemical detail as possible. In doing this, it is useful to consider three steps:

1. Write complete chemical reactions for any chemistry involved.
2. Make mass and energy balances important to the product's use.
3. Estimate the rates of any important changes that occur during the product's use.

Having produced a set of ideal product specifications in as much detail as possible, we should examine these carefully. Being a result of individuals' wish lists, they will often be entirely impractical involving huge flows, enormous concentrations or massive costs. If this is the case, we must revise our specifications to be more realistic. This may lead us to abandon the project altogether. If the only way of meeting customer requirements is to break a law of thermodynamics, we should stop product development now. This type of critical examination is sometimes known as a "chicken test" after a Canadian method for testing aero engines for their capacity to fly through flocks of geese. We are asking ourselves if the project is obviously unrealistic, before committing large resources to it.

Table 1. **Heats of Combustion of Alternative Fuels (kJ)**[a]

Fuel	per mol	per g	per cm^3
H_2	286	143	0.013 (at 1 atm)
CH_3OH	726	23	18
$Li \rightarrow Li^{+} + e^{-}$	293	42	23
octane	5470	48	34
toluene	3910	43	37

[a] The comparison shown is sometimes obscured by the way data are presented.

Setting specifications often involves estimating physical properties of the final product. These estimates depend on two types of knowledge. First, they depend on the so-called "structure–property relations", which relate macroscopic properties like scratch resistance or creaminess to chemical and physical structure at much smaller size scales. Most obviously, this may be molecular structures, which dominate properties like drug efficacy or product acidity. Surprisingly often, "structure–property relations" involve structures of nanometer or micrometer size. Meat tenderness, paint "hiding power", and polymer transparency are examples where such microstructure are key.

The second type of knowledge useful for setting specifications involves qualitative generalizations of physical properties. These generalizations are often obscured by differences between results per mole, per volume, and per mass. As an illustration, consider the alternative fuels shown in Table 1. On a molar basis, octane is the most powerful fuel listed; on a mass basis, hydrogen is; on a volume basis, toluene is the choice. Because we sensibly describe chemical reactions with stoichiometry, generalizations like this are often obscured. This type of judgment is a key to setting product specifications.

The final step in quantification of needs is to specify a benchmark, which is an existing or idealized product against which we can measure the performance of our development. If we cannot beat the benchmark, the product is not worth developing. In some cases, when an innovative new product is being contemplated, no obvious benchmark will be available. We may be able to envisage an idealized benchmark by analogy with similar products. Sometimes, however, we must do without the security of a benchmark for comparison.

Example 2C: Water Purification for a Family. The WHO estimates that 1.7 billion people do not have access to a clean water supply (12,000 children per year die from diarrhoeal diseases—the world's biggest cause of child death). In the absence of major civil engineering projects, the point of demand is the family unit. A large non governmental organization has decided to design a water purification unit suitable for use by individual families in third world countries. Interviews with governmental and nongovernmental agencies working in such countries, and most importantly the lead users, usually the mother, reveal the following list of needs:

Essential

Supply a family with safe drinking water.
Inexpensive.

Desirable

Rural focus.

Simple to operate.

Useful

Environmentally sustainable.

Assess these needs, quantifying where possible.

Solution. The first question is how much water we need to purify. A person requires about 5 L of drinking water per day and typically uses ~50 L for cooking, cleaning, and washing. A household might be 10 people. So a minimum reasonable requirement would be 100 L/day, up to 500 L/day being desirable. A 5-year lifetime will be desirable, so a total lifetime throughout of 200,000 L will be necessary.

What do we need to remove? Waterbourne diseases are the greatest threat—we must remove protozoa, bacteria, and viruses. Toxic materials are also sometimes a problem, but it is probably not useful to focus on these—the variety is very great, the problem usually local and a better solution is often preventing discharge. So we will focus on disease organisms. There are WHO guidelines for microbial removal and it would be useful to have these in mind, but to see these high standards as an absolute requirement might be a mistake. After all, an affordable but slightly less effective device will be more useful than one which no one can buy.

Getting the cost right will be critical. What is affordable is clearly variable, but we must be aware that we are considering some of the poorest people in the world. We might hope for some support from aid agencies, but ideally a device affordable by the users without aid is best. Interviews in Nepal have revealed that a cost of >$10–15, with a annual running cost of $3–5, will be beyond the reach of most of the rural population. This requirement is clearly stringent and one we may not be able to meet and should not be seen as an absolute limitation: What we are really saying is the cheaper the better, this limit being the target.

The rural focus means that the device must operate in the absence of a power supply. Any consumable should be locally available. The product must be easy to explain and to use by those with little experience of technology.

Environmental sustainability is a rather vague need. It is best rephrased as the need to avoid the consumption of source local resources or the production of damaging waste.

So our final needs list will be

Remove viruses, bacteria, and protozoa from 100 L/day.

Total lifetime at least 200,000 L.

Equipment as cheap as possible, ideally $10–15; annual operating cost under $5.

Operate in the absence of power, using locally available materials.

Simple to operate.

No consumption of source resources or discharge of toxic waste.

Chlorination is a sound benchmark, whis is simple, cheap, and well established, but has problems in terms of supply, use, and discharge of chemicals. Our device must be more attractive than local chlorination if it is to succeed.

We have now completed the Needs stage of product design. We have produced a ranked list of what our product needs to achieve and put this into quantitative and scientific terms as far as possible. We have also made a check that our aims are not wholly unreasonable and ideally we have a benchmark by which to judge the success of our product development. Up to this point, we have consciously avoided trying to think of solutions for our product needs. We want to define what we wish to achieve without prejudice caused by a preconception of what the product will look like. If we do already have an idea of the product's nature, we should try to keep it out of our considerations until the end of the Needs stage. Only now that we have well-established criteria for the success of any product should we begin to develop ideas for the product itself.

3. Ideas

Once we have chosen specifications for our target product, we need some good product ideas. In principle, we only need one idea, the one that we will manufacture. In practice, product development requires up to 100 ideas in order to find one truly worth pursuing. In these paragraphs, we describe how we get these ideas, how we organize them, and how we choose our best candidates for further effort.

3.1. Idea Generation. To get our 100 or so product ideas, we will depend on people more than publications. The most important people are those on the team responsible for developing the specific product. We will normally assemble this team for free-ranging discussions that aim at generating possible answers. How to run such "brainstorming" discussions is carefully described in the literature, and so is not detailed here. We mention only that these discussions should initially be noncritical, and that all participants should be treated as equals. Discussions of new chemical products are sometimes curtailed for reasons as trivial as that the boss' spouse disagrees with some of the ideas suggested.

In addition to depending on the product team, we should pay special attention to customers who already are using existing, similar products. Some of these customers, called "lead users" in the business literature, may have already adapted our existing products for their own uses. These lead users often have excellent suggestions. Other human sources—consultants, private inventors, and the like—are often less useful. Literature has widely ranging value. Patents and trade information from competitors is often more useful than archival literature. Other methods for ideas use forms of chemical synthesis, as detailed elsewhere. Still, in most cases, the key is most often the product development team.

3.2. Ideas Sorting. We now have our 100 or so ideas of widely varying quality. We must somehow sort through these ideas to locate the best five or so for further developments. Evaluating all to the same degree will normally take more resources than we will ever have, and will take much longer than we will even want. Thus we must find fast ways to find the best ideas.

We suggest proceeding with two stages. First, without quantification, we should try to sort the ideas on completely qualitative grounds, reducing the number to perhaps twenty. Later, with a bare minimum of quantification, we should try to screen the surviving ideas, aiming to get just the five or so we think are best. For the present, we will talk about how to get from 100 to 20; later, we will describe ways to go from 20 to 5.

To reduce the number of ideas to 20, we just make a list of all the ideas. We can then easily remove redundancy. Often this redundancy will occur because some ideas are special cases of others. For example, in a discussion of better barriers for landfills, one idea could be "The barrier should capture mercury."

A second idea might be "The barrier should adsorb all heavy metals except calcium."

The first idea is just a special case of the second.

In addition to removing redundancy, we want to drop ideas that are obvious folly. In doing so, we should be cautious, because some silly ideas may contain dreams. Sometimes, we can benefit from keeping a separate list of these flawed dreams, just to serve as a stimulus to later development. Normally, the efforts to remove redundancy and folly will still leave us up to 70 ideas.

To reduce the number of ideas further, we should try to organize them into categories, in a type of outline. How this should be done depends on the ideas generated: There seems to be no general strategy. Once this outline is made, it may expose gaps, which may imply repeating the brainstorming. More often, we will find that large groups of ideas will be inconsistent with our organisation's objectives or its strengths. These groups of ideas can be dropped, a major simplification. These last steps commonly cut the number of ideas to meet our target of twenty. One note of caution, however, many of our best ideas will often cluster under a single heading. Because we do not want to overspecialize too soon, we should consider choosing at least one idea beyond this cluster for the next stage of product development.

Example 3A: Multilayered Polymer Films for Secure Documents. Counterfeiting documents is big business. In the United States alone, >$250 million of counterfeit currency is recovered each year. To reduce this problem, some nations have gone to composite polymer films produced by multilayer extrusion as an alternative to paper for printing money. Australia has led the way. Their experience suggests that small denomination bills circulate so rapidly that paper bills wear out in <1 year, but large denomination bills circulate much more slowly. Because composite polymer bills last four times longer, their higher cost—twice that of paper—can be recovered in a couple of years.

Our company hopes to build on our experience in multilayer extrusion to make new films for all types of secure documents. We are part of a project team charged with identifying these documents. What should we recommend?

Solution. Our team quickly identified >200 possible products in one of the fastest, most straightforward efforts that our company has seen. After the redundancy and folly is removed, the ideas can be organized under the four headings shown in Table 2. Because this list is so broad and often so vague, it should be further edited to represent our company's strengths.

3.3. Idea Screening. We must now reduce our 20 surviving idea down to a still smaller number, normally 5 or fewer. We will still not have the

Table 2. **Possible Products Based on Multilayered Films**

I. Minor Improvements in Existing Products
   These improve or modify the existing paper document.
   A. Currency
      1. Paper currency with irremovable polymer strip.
      2. Machine-readable currency to tell denomination or lifetime.
   B. Passports and Corporate Identification
      1. Identification page of a passport made of multilayered polymer.
      2. Fingerprints added with optical ink.
   C. Credit Cards
      Polymer patch that takes signature.
   D. Surface Treatments
      1. Antidestructive.
         a. Multilayer polymer window that diffracts light.
         b. Polymer lamination.
      2. Antigraffiti coating.
      3. Miscellaneous.
         a. Fluorescent patches.
         b. Antibacterial agents.
         c. Waterproof coatings.

II. Change in Substrate
   These replace the paper with a polymer composite.
   A. Synthetic Polymers
      1. Currency, stock certificates, and Traveler's checks.
         a. Synthetic plastic currency stamped with optical ink.
         b. Polymer currency with different colours for the different denominations using dyed injected polymers.
         c. Metal coins that have a polymer core.
      2. Identification cards.
         a. Polymer passports.
         b. Polymer social security card.
         c. Oriented polymer paper.
         d. Polymer currency with layers of different orientation.
      3. Memorabilia like baseball cards made of polymer.
   B. Optically Unique Synthetic Polymers
      1. Currency, stock certificates and traveller's cheques.
         a. Polymer films with a multi-layer window.
         b. Polymer films with different thickness to induce colour.
         c. Polymer films with partial burnouts to generate patches of colour.
         d. Machine readable strips for use in vending machines.
      2. Credit Cards made with a homogenous polymer backing.
      3. Identification Cards, including driver's licences.
         a. Cards.
         b. Cards that change colours with light.
         c. Cards with burn out patches that change colour with light.
   C. Combinations of Synthetic and Optically Unique Polymers

III. Adhesive Additions
   These products use adhesive to attach them to existing documents.
   A. Currency
   B. Documents
      1. Multilayer optical films to authenticate legal documents.
      2. Multilayer films to replace notary stamps.
   C. Identification
      1. Multilayer optical polymer films adhered to passports.
      2. Multilayer optical polymer films adhered to student IDs with school logo.

Table 2 (*Continued*)

- D. Credit Cards
  1. Multilayer optical polymer films placed on credit cards.
- E. Checks
  1. Multilayer optical polymer films with adhesive backing used on checks.

IV. Environmentally Benign Products
This smaller set of ideas involves recycling, and is partially redundant.
- A. Secure Products from Recycled Plastic
- B. Secure Products with Later Uses
  Polymer currency that can be recycled into other products.

resources to make more detailed calculations for the 20 survivors, so we need approximate but quantitative tools that let us continue the screening, but on a still more rational basis.

One commonly effective method for this screening is to choose five or fewer key attributes shared by most of the surviving ideas. These attributes will include factors like scientific maturity, ease of engineering, risk of failure, and cost. We should choose factors that are different for different products. For example, even if safety is the most important product attribute, we gain nothing by choosing safety if all our potential products are equally safe.

Once these key attributes are chosen, we need to assign weighting factors to each. Normally, we will normalize these weighting factors, assuming values that sum to 1. Note that this implies that all products that we are still considering are capable of satisfying all attributes at least to a limited extent. If there is one attribute which is truly essential, we should drop all ideas that cannot satisfy this constraint, and continue our evaluation for the survivors.

On the basis of these attributes and their weighting factors, we now score all of our ideas relative to a convenient benchmark. We find it convenient to assign the benchmark scores of 5, and then to choose scores from each new product between one (poor) and 10 (excellent). We then calculate an average weighted score for each product. The potential products with the highest scores are those that we choose for further development. This screening method is partially illustrated by the following example.

Example 3B: Lab-on-a-Chip. This example is of a technology push project. Developments in the microelectronics industry have resulted in the fabrication of very small devices becoming standard practice. Channels down to 100 μm can be cut, with flow control devices and separation stages on a comparable scale, which means that it is possible to produce miniature chemical plants on a scale of a few centimetres. While the potential of such devices as detectors or reactors is large, few commercial products have yet been produced. Prototypes for deoxyribonucleic acid (DNA) sequencing, blood testing and a handful of other applications have been made. A company holding patents in nanofabrication is looking at the best areas in which to launch its technology in the marketplace. The following needs have been established:

Table 3. **Grouping of Selected Ideas for Lab-on-a-Chip**

Detectors/Analysers

- A. Medical/Laboratory
  1. Compact analytical instrument.
  2. Drug development.
  3. Screening of blood/vaccines/food/water supplies for infectious agents.
  4. Diagnosis of disease, eg, acquired immune deficiency syndrome (AIDS), hepatitis, cancers, and Alzheimer's disease
- B. Industrial
  1. Chemical plant on-line testing.
  2. Effluent testing (chemical plant/sewage plant).
- C. Commercial End User
  1. Air pollution detector (smoke/CO/H_2S).
  2. Food testing (nut/GM/rot/animal products).
  3. Accurate breathalyzer.
  4. Blood sugar testing for athletes/diabetics.
  5. Home pregnancy tests.
  6. Check blood–iron levels for anaemics.
  7. Allergy testing at restaurants.
  8. Alerting asthma.
  9. Check pollution levels for surfers.
- D. Regulatory/Police Use
  1. DNA analysis and fingerprinting (spit, urine, hair).
  2. Drug detection—sniffer chip.

Producers

- E. Medical
  1. Hormone production.
  2. Making insulin.
  3. Wasp sting remedy.
  4. Timed production and dose of drugs, especially for the elderly.
  5. On-the-spot antidotes for biocides or rabies etc.
  6. Production of drugs with very short shelf life in, eg, first aid kit.
  7. Internal surgery—nutrients for tissue growth.
- F. Industrial
  1. Production of speciality chemicals as/when needed.
  2. Chips to spin fibres—tiny spinnerettes for polymers.
  3. Manufacture of dangerous chemicals in small quantities (eg, phosgene/hydrogen cyanide).
- G. Commercial
  1. Make-up manufacture.
  2. Night-clubs—smoke/foam production.

Combined Detectors and Producers

- H. Commercial End User
  1. Suncream detector and applicator.
  2. Variable strength deodorant—alter strength.
  3. Air freshener—variable strength.
  4. Worktop coating that tests and releases antibacterial agent.

Cleaners/Removers

- I. Medical
  1. Minidialysis—remove alcohol from system to sober up quickly.
  2. Artery cleaner.
- J. Industrial
  1. Critters-on-a-chip—detect, map and digest environmental pollutants.
  2. Cleaning water supplies via ion exchange.
  3. Fouling/corrosion detection/remediation.
- K. Commercial
  1. Stain removal for washing—seek out and remove dirt.

Essential

Use of current technology for a more cost effective product or a completely new product.

Quick to market—relies on using existing technology.

Desirable

Use company's technology to its full potential.

Useful

Environmentally benign.

Easily marketable.

Explore ideas for devices that could be produced using existing technology.

Solution. After brainstorming, the design team came up with 73 ideas; this list was reduced to 39 by the removal of redundancy, folly, and excessive requirements. The remaining ideas were then organised as shown in Table 3.

We must reduce this list to a handful for detailed consideration in the Selection stage. This reduction can be done in two stages. First, one major identified need is using technology to ensure a swift entry into the market, which is desirable both for the usual reason that the first product into a market usually takes the lion's share of sales, even in the absence of other competitive advantages. Also, in this particular case, the product being considered is intended not just as a device in its own right, but also as an exemplar of the many other potential applications of the company's nanotechnology—a flagship for the company's future. It is doubly important to minimize the risk of technological failure or delay. The company's technology is currently not developed in the areas of detection and separations. The whole categories of E, F, G, H, and I are therefore rejected not because they are inherently bad ideas, but because they will not provide the most risk-free and speedy route to a successful first product. We may well return to these ideas in future years.

To achieve an initial screening of the remaining 21 ideas we use the criteria developed in the Needs section. We very crudely assess each idea on three criteria: market size; maturity, and reliability of technology; likely time to market. Only those ideas that look promising and all three of these vital criteria will be considered further. An example screening of the first four ideas is shown in Table 4. Of these only the first is taken forward to the Selection stage, as are B1, C1, D1 and J3.

Table 4. **Screening of Four Ideas for Lab-on-a-Chip**

	Market size	Technology	Time
compact analytical instrument	++	+	+
drug development	++	+	−
screening of liquids for infectious agents	+	+	−
diagnosis of disease	++	−	−

4. Selection

With a handful of good ideas remaining, we must next choose from these the best one to take forward for product development. Because all the remaining ideas are promising, this decision involves considerably more effort than we put into cutting the number of ideas down in the screening just described under Ideas. As far as possible, we must quantify how each idea will measure up to the criteria we set for a successful product at the Needs stage. This quantification will involve making estimates based on chemistry and engineering, and perhaps doing some simple experiments. At the same time, we still wish to develop our product as quickly as possible and do not want to put resources into exploring products we will end up rejecting. The key to success in the Selection stage is to make reliable choices with minimal effort.

4.1. Assessment. The Needs stage provided a list of criteria by which to judge the success of our product development. We emphasized the importance of quantifying the needs as far as possible. This approach will now show its value. The first step in selecting between the remaining ideas is to estimate how each will perform relative to our criteria. In order to do this, we must gather more information about each idea. This process will involve firming up exactly how each idea will work; we may need to do some simple experiments to achieve this, we will certainly need to explore the literature some more. As we generate more detailed information on each idea, the idea itself will change and become clearer. Thus there is an iteration between the Ideas and Selection stages—as we explore an idea in more detail, the idea evolves and new ideas may emerge. Thus, although we present product design as a linear four step procedure, we understand that this is a simplification.

4.2. Comparison. Having made an assessment of each idea against each criterion, we must now make an overall comparison among the ideas. In some cases, particularly where the identified needs are primarily technical, this will be easy once good estimates of performance are available. In other cases, subjective judgements will be necessary, either in comparing unlike criteria or inherent in the criteria themselves. In such cases, we often proceed by drawing up a decision matrix in the same way as was described for screening at the Ideas stage. Previously, we were interested in eliminating the weak ideas and the emphasis was on making quick decisions. Now, we are considering strong ideas and the emphasis must be on making a good decision. While the methodology of the decision matrix remains the same, we must now put a lot more effort in to evaluating each idea against each criterion. We should recognize that the decision matrix is a highly imperfect tool for making a complex decision where numerous subjective and objective criteria are involved. We believe it has value because it ensures that all important factors are explicitly examined and because it allows more detailed research to be conducted where the decision remains inconclusive. Also, for the technically trained, the decision matrix is a useful way of ensuring that subjective factors, such as the feel, look or taste of a product, are not overlooked in favor of the more objective factors that, we can calculate and feel more comfortable with.

Example 4A: Selecting a Polymer Film that Stops Ultraviolet (UV) Light. On summer days, cars get hot because UV sunlight passes through the windows and is absorbed by the car's interior. Because our company has considerable expertise in thin film technology, we are interested in making a film which could be attached to these windows, and which would block light. Such a defect-free film should have four key properties

1. It should be transparent to visible light.
2. It should block 99% of UV light.
3. It should be 70–150-μm thick, but cost less than current competitors.
4. It should be easy to apply.

These properties derive partially from a competitive benchmark, a clear plastic film with a vapor-deposited metal coating. This benchmark, available in a variety of colours, costs \$8–12 m^2.

After idea generation, sorting and screening, we came up with two alternative products. One is a multilayered polymer composite with an internal UV-absorbing layer and an adhesive backing. The second, more imaginative product is also a multilayered film, but the internal layer has a slight electrical conductivity. When no current is flowing through this conducting layer, it is opaque; but when a current is flowing, it becomes transparent.

Which product should be developed further?

Solution. After considerable discussions, our project team decides on four attributes for evaluating these products: cost, engineering, ease of application, and aesthetics. "Cost" should include manufacturing and development expenses. The attribute "engineering" reflects the ease of manufacturing the product. Ease of application includes the effort of installation and maintenance required by the customer. Aesthetics includes both quality and market appeal.

Using these criteria, our project team comes up with the selection matrix shown in Table 5. The UV absorbing polymer is cheap and easily made with our existing technology, but the product is not otherwise much different to the benchmark. The conducting polymer is costly, hard to make, and difficult to install. While it is superior aesthetically, it ranks below the benchmark that it is designed to replace. We should make the product which builds on our current skills, if we decide to make any product at all.

4.3. Getting Close to a Decision.

At this point we should have a good indication of which idea looks the most promising in terms of fulfilling the needs defined in the first stage of product development. However, before proceeding with the development of this idea, we pause to consider two important factors, which so far have been largely overlooked: intellectual property and risk.

Table 5. **Selecting a UV Barrier Film**

Attribute	Attribute importance	Benchmark product	UV absorber with adhesive backing	Electrically activated absorber
cost	0.25	5	7	2
engineering	0.25	5	9	2
ease of applications	0.25	5	5	3
aesthetics	0.25	5	5	9
score		5	6.5	4.0

Intellectual property is a complex area and should be referred to an expert. The important point here is to make sure that the ownership of the intellectual property is clear before large resources are invested. Often the profitability of a product (notably a pharmaceutical) depends on the exclusive license granted by patent protection. In such cases we must ensure there is at least a good prospect of obtaining such protection before proceeding. In all cases, we must at least ensure that our activities will not be restricted by any intellectual property held by others.

In assessing how well our product ideas measure up to the criteria set by the defined needs, we have largely ignored the issue of risk. However, the ideas we are choosing among may range from minor developments to an existing product to risky and untested new technology. We need to factor this into our decision. Risk may take three forms: the product may not work; the product may take a long time to develop; and external problems may occur because of local politics, fashion or a changing economic situation. The first of these, product function, should be unlikely; by this stage we should have eliminated product ideas that are likely to fail. The second, development time, is largely a technical issue that we should be able to make a good stab at predicting. It can often be translated into a financial risk—the longer a development programme is likely to be, the greater the uncertainty in cost and the larger the return must be. The third, external problems, is the hardest to estimate, and ultimately comes down to a matter of judgment.

Nevertheless, at this point, we should at least think hard about what factors could compromise the success of the product. In thinking about risk, one needs to consider both the probability of an event and the seriousness of its consequences. It is often useful to do this by drawing up a table giving total risk as a product of probability and consequence. Just as when using decision matrices, the numbers should not be treated with excessive reverence—the procedure is really a means of ensuring all factors are carefully considered.

Having identified the risks involved in our favored product, we have three possible responses. We might decide an idea, while attractive, is too risky to merit time and effort. This realization might lead us to select a different idea of smaller potential, or to abandon the project altogether. It is essential that we carefully consider this latter option before proceeding to the manufacturing stage, when large amounts of money must be invested. Most practitioners of product design will say that the most common mistake is to abandon projects too late. Alternatively, we may decide simply to accept the risks and to proceed. This minimizes the time to product launch and is often the appropriate strategy if financial risks can be offset against the advantage of getting to market earlier. Proceeding in spite of risk is particularly apt where we hold a patent. We should be more circumspect in dealing with risks of a safety or environmental nature. Third, we may decide to do a little more research, perhaps including an experimental programme, before committing resources to product manufacture, which is closer to the traditional approach of prototyping: It will often result in a better product, but also in a longer (and more expensive) development period.

Example 4B: Moderate Scale Oxygen Production. Oxygen, one of the largest commodity chemicals, is often made at the site where it is needed. The traditional manufacturing method, dating from Von Linde's 1905 process, is cryogenic distillation. This technique is extremely effective, but requires a large capital investment, and so is most suitable for large scale. In the last few decades, pressure swing absorption has been developed to produce oxygen at smaller scales, capturing this part of the market from distillation. For example, pressure swing adsorption units not much larger than a beer can are commercially available to produce oxygen enriched air for patients with emphysema.

As a manufacturer of distillation equipment, we are considering new technologies for making 85% oxygen at a rate of 6000 scfh. Our current technology, based on high capacity trays, is not economic at this small scale. As alternatives, we are interested either in structured packing or in hollow fibre membranes. The structured packing, which recently came off patent, consists of metal guides, mounted crossways, looking like stacks of stainless steel venetian blinds. It is an established technology now supported by both the original manufacturers and new entrants.

Hollow fiber membranes are much more speculative. Selective membranes are commercially used to produce nitrogen enriched air. Selective membranes, which retain a nitrogen enriched waste and permeate an oxygen enriched product are not commercially attractive at this scale. Porous, nonselective membranes are not used to effect selectivity but to control a condensate flow moving countercurrently to the vapor, in a configuration like that of a shell-and-tube heat exchanger. Such membranes are completely untried, though academic reports promise productivity increases of several orders of magnitude. It is the porous, nonselective membranes used as a form of structured packing which are then focused here.

Which if any technology merits development?

Solution. The cryogenic distillation of air involves three major types of equipment: compressors, heat exchangers, and distillation columns. The compressors are the biggest capital expense, perhaps one-half of the total; and the heat exchangers are another 30%. Thus we could conclude that distillation design is not important anyway. However, the compressors and heat exchangers will be standard to any distillation process, and margins for a commodity like oxygen will always be small. Thus cutting the size of the distillation columns could be a significant gain.

To examine the effect of column size in more detail, we compare equipment capacity and cost for trays, structured packing, and membranes in Table 6. The first column of figures in this table gives the relative cost of the three internals. In the past, structured packing has been expensive; but with patents expiring, costs have dropped significantly. Membrane costs are a complete guess: while

Table 6. **Cost Estimates for Different Distillation Internals**

Column internals	Cost per column volume	Column capacity	Column size	Column cost
Sieve trays	1	1	1	1
Structured packing	2	3	1/3	2/3
Nonselective membranes	10	50	1/50	1/5

Table 7. **Risks for Alternative Distillation Internals**

Structured packing	Probability	Consequence	Risk
competition from other manufacturers	0.9	0.3	0.27
performance failures	0.1	0.5	0.05
nonselective membranes competition from other manufacturers	0.1	0.5	0.05
performance failures	0.7	0.7	0.49

in principle there is no reason that membranes should be more expensive than trays, we expect that they will need frequent replacement.

The other columns in the table give the capacity, the size, and the column cost. The capacity of the membranes is extremely high, a consequence of the fact that membrane units are largely unaffected by flooding. The result is that the cost of the membrane-based column is potentially much less than those of the other internals.

The difficulty with the membrane alternative is that it is so risky. To understand the origin of this risk, we can compare structured packing with membranes using the risk estimates in Table 7. Structured packing is going to work. If we have any trouble, we know that we have not assembled it correctly, and we can imitate existing products to overcome these shortcomings. However, the expiration of patents in this area means that many competitors are now scrambling for new business. Thus the risk for structured packing comes from the marketplace, not from the technology.

As Table 7 shows, the risk for membranes has a different origin. There is no current competition. Even if competitors appear, they are unlikely to have more experience than we, so we will not have any implicit disadvantages. At the same time, we may have major difficulty in achieving the performance that we expect from the literature. If we do have trouble with membrane performance, we have little experience of how to fix this, so the consequences will be major.

In this situation, our selection is unclear. We can do nothing, accepting that the market for our trays may get smaller in the future. We can decide that we are efficient manufacturers, and enter the competitive structured packing market, recognising both the risk and the fact that we cannot do much to reduce it. Finally, we can gamble on the membrane market, trying through further technical development to reduce the probability of performance failures from the current value of 0.7 to a reasonable goal of 0.2. Then—and only then—membranes may make sense as an alternative to structured packing.

5. Product Manufacture

By this stage, we have decided which chemical product we want to manufacture. We have identified a customer and that customer's product needs. We have generated ideas to fill that need, and we have selected the best idea. We are ready to decide how we will make the product.

5.1. Preparation. The very wide range of chemical products possible means that we will need to consider a wide range of manufacturing methods.

Table 8. **Different Chemical Products are Manufactured Differently**

	Commodity chemicals	High value chemicals	Microstructured products
key factor	cost of product	speed of manufacture	function, from microstructure
examples	ethylene, ammonia	penicillin, viagra	paint, detergent
amount made	$>10^7$ kg/year^{-1}	$<10^4$ kg/year^{-1}	$<10^6$ kg/year^{-1}
typical molecular weight	100	600	>100; often $>10^4$
phase during synthesis	gas	dilute liquid solution	concentrated solution or melt
chemical reactor	dedicated, continuous, plug flow	generic, batch, stirred tank	ranges widely
common separation	distillation, absorption	extraction, adsorption	often not required

To provide some initial guidance for manufacture, we find it useful to think of four types of products. The first type is devices, especially for medical applications. Examples include the artificial kidney and the osmotic pump for drug delivery. The manufacture of many devices depends on mechanical engineering more than on chemistry and chemical engineering. We do not discuss devices, because this topic is thoroughly described elsewhere.

The other types of chemical products can be roughly classified as shown in Table 8. The first type, commodity chemicals, made in amounts $>10^7$ kg/year^{-1}, normally have molecular weights <100. As a result, their manufacture uses gaseous reagents, supported catalysts, and purification via distillation. This manufacture always has product cost as its primary focus. Commodity chemicals were the source of chemical industry growth in the last one-half century.

The two other types of chemical products shown in Table 8 are much harder to describe. The more obvious type, 10 thousand high value added chemicals, are exemplified by drugs. These compounds have molecular weights typically in the range of 500−700 Da. Their chemical structure is normally well defined, one of many available isomers. The finished products are crystalline, of exceptionally high purity.

Once a high value added product is identified, it is normally manufactured as quickly as possible, because the first manufacturer will usually command two-thirds of the market. This need for purity and speed, plus the small amounts to be manufactured, dictate the use of dilute solutions and generic equipment. Manufacture is more like gourmet cooking than like petroleum refining.

The third type of chemical product, which is the most heterogeneous, often has a useful microstructure. This large group of products includes most "specialty chemicals". Manufacturing ranges widely, and product properties are often a function of product history. For example, polymer properties are affected by molecular weight distribution, and paint quality changes if the paint is frozen. The process engineering required is normally a compromise between the first two types.

At the end of the Selection stage, we had sufficient information to convince ourselves that we had selected the best idea and that it had a high probability of success. Inevitably, there will have been gaps in our knowledge of the details of exactly how the product would work. In order to make the product, we not only need to be confident that the product can be made to work, but we must also establish in detail exactly how it is going to fulfil our aims. Before going further, we must fill in this missing information. This missing information may be obtained by literature searches, by consulting experts and by conducting experiments. It may be tedious, time consuming and expensive. That is why we put it off until after we had decided to proceed with product development. We do not wish to put this level of effort into more than one product idea or into an idea we later abandon if we can possibly avoid it.

Example 5A: Corrosion Resistant Paints. For many years, marine paints have contained high concentrations of hexavalent chromium to reduce corrosion. The advantage of such a paint is that it is "self-healing": When the paint is scratched, an electrochemical cell is established between the newly exposed metal and the chromium ions which, after an intricate series of chemical steps, results in the exposed metal being coated with a layer of pentavalent chromium gel. This new "self-healed" layer provides considerable protection against further corrosion. Unfortunately, even without being scratched, these marine paints also leach chromium into the water, causing considerable damage to marine life.

Efforts to replace chromium have been unsuccessful, but they have spurred development of a wide variety of paints with the potential to reduce corrosion. Most obviously, these have centred on the development of new polymers. Epoxy-based resins have been particularly successful. However, these still provide less protection than desired.

One method to further improve epoxies is to incorporate flakes of clay or mica into the resin. If these inorganic materials are exfoliated and pretreated so that they are wet by the resin, they can offer dramatically enhanced corrosion protection. However, the improvements reported vary widely, probably because the effect of the flakes depends dramatically on their alignment. If they are aligned randomly, the effect of flakes on corrosion is minor, a reduction of perhaps 10%. If the same flakes are aligned parallel to the surface, then the effect is predicted and observed to be much larger, a reduction of at least a factor of 10—over 1000%. Such a corrosion resistant paint is an example of a microstructured product, a product whose performance is dictated not so much by its chemical composition as by its microstructure, in this case the aspect ratio and alignment of the flakes. A patent search shows no significant conflicts, though patents exist for flake filled plastic bottles. Curiously, there are a large number of patents and publications that mention human skin, which has a similar geometry of impermeable protein flakes.

How should we study corrosion resistance in paints with aligned flakes?

Solution. Answering this question requires a method of evaluating corrosion and a technique for aligning flakes. The standard method of evaluating corrosion is microscopic evaluation of metal coupons after exposure to a salt fog. While this method is well established and reliable, it is tedious, effective for a final evaluation but not for a preliminary screening. As a result, we decide to defer using the salt fog and just to put cooled coupons into boiling 0.1 N sodium chloride solution. We will examine them microscopically.

Aligning flakes can be done in at least three ways. First and most directly, we can use a suspension of flakes in a mixture of polymer and solvent. Such a solution—a lacquer—is spread onto the metal coupons; and evaporation of the solvent aligns the flakes. However, the solvents used are often chlorinated, so their evaporation is environmentally abusive. Second, we can spread a hot melt of polymer containing flakes over a metal coupon, using the shear to align the flakes. However, applying such a shear dependent coating to an entire ship will be extremely tedious.

The third method of aligning flakes is the most attractive alternative, but the one about which the least is known. It uses a water borne latex containing suspended flakes. If the flakes are mica, they are larger than the latex droplets; if the flakes are clay, they are smaller. We should plan experiments with both sizes of flakes to measure the alignment induced by the fusion of the latex droplets into a film.

5.2. Final Product Specification. Before designing the processing route, we need to produce a final specification for the product we have decided to make. We should by now have obtained all the information required to do this. For a typical chemical product, we need to define the physical structure, the chemical composition, the chemical reactions that occur during the product's operation and the thermodynamics of the product (including the microstructure). Clearly which of these dominates depends on the type of product being made, and this was the purpose of considering this in the preparation step just outlined.

The key to a product is often how it responds to a change, which may involve dissolution (or precipitation) in a solvent, response to a temperature or other physical change, or a chemical reaction (pH change being the most common initiator). It is important to specify these chemical changes carefully as well as the nature of the product itself.

Example 5B: A Self-Warming Baby Milk Bottle. A baby milk manufacturer wishes to market a self-warming bottle for feeding babies in the absence of a easily accessible power supply. It has been decided to achieve this by using a double skinned bottle, the inner space being filled by a material which will undergo an exothermic reaction.

Set final specifications for such a product.

Solution. We must first think what to use for the exothermic reaction. Obviously, it is much better if it can be regenerable. A quick literature search reveals the crystallization of sodium acetate trihydrate from water to be ideal. This crystallization can be triggered in a variety of ways, the liquid phase is stable in the absence of triggering, and can be regenerated by putting the empty bottle in boiling water. Recent advances in triggering make the reaction much more reliable and also allow regeneration by microwave heating, ideal for a baby's bottle. The maximum temperature reached is $\sim 50^\circ C$, hot enough to get the milk to the required $37^\circ C$, but without posing any safety hazard. We need to determine two things for our final specification: the mass of sodium acetate solution required and the characteristic time for warming. First, we look at the overall heat balance

$$\left[\begin{pmatrix}\text{mass of}\\ \text{sodium acetate}\end{pmatrix} + \begin{pmatrix}\text{mass of}\\ \text{milk}\end{pmatrix}\right] C_p(T_{\text{final}} - T_{\text{initial}}) = -\begin{pmatrix}\text{mass of}\\ \text{sodium acetate}\end{pmatrix} \Delta H_{\text{rxn}}$$

The enthalpy of reaction ΔH_{rxn} is -125 kJ kg^{-1}, and the heat capacities C_P for both milk and sodium acetate are assumed to be 4.2 kJ kg^{-1} K^{-1}. To heat 0.4 kg of milk from a T_{initial} of 15°C to a T_{final} of 37°C, we need 1.13 kg of sodium acetate. This result is quite high, but not impractical.

Next we must look at the rate of heat transfer:

$$-\frac{d}{dt}(\Delta T) = \frac{UA}{C_p}\left(\frac{1}{M_{\text{milk}}} + \frac{1}{M_{\text{acetate}}}\right)\Delta T$$

where U is the overall heat transfer coefficient from acetate to milk, around 50 W m^{-2} K^{-1}; ΔT is the difference between the temperature of the acetate and that of the milk; M_{milk} and M_{acetate} are the masses of milk and sodium acetate, respectively; and A is the surface area between milk and acetate.

We want to find this interfacial area A. To do so we integrate the above equation, giving

$$\frac{\Delta T}{\Delta T_0} = \exp\left\{-\frac{UAt}{C_p}\left(\frac{1}{M_{\text{milk}}} + \frac{1}{M_{\text{acetate}}}\right)\right\}$$

where ΔT_0 is the initial temperature difference between the room temperature milk, at perhaps 15°C, and the acetate, at ~50°C after its rapid crystallisation. We want the milk to reach 37°C after perhaps five minutes, so we should use ~1.5 kg of sodium acetate, giving a final temperature of 43°C. The milk will be at 37°C when $\Delta T = 7$°C, and so

$$\frac{7}{35} = \exp\left\{-\frac{50 \times A \times 300 \times \left(1 + \frac{0.4}{1.5}\right)}{4.2 \times 10^3 \times 0.4}\right\}$$
$$A = 140 \text{ cm}^2$$

Thus the final specification is a double skinned bottle, containing 1.5 kg of sodium acetate in the core surrounded by 0.4 kg of milk, with an interfacial area between the sodium acetate and the milk of at least 140 cm^2.

5.3. The Manufacturing Process. Finally, we must specify the process by which we will achieve the specifications we have just set. This is where chemical product design and traditional process design finally merge. It is worth noting that there are significant differences of emphasis in the process design for a chemical product as compared to commodity chemicals. In commodity chemical manufacture, minimizing cost and maximizing efficiency are usually the goal. Economies of scale, continuous processing and good heat integration are normally required. In the case of products, we are usually producing much smaller quantities of a higher value material. The emphasis tends to be on speed, rather than optimization, and batch processing in standard or shared units is the norm. Also, chemical products usually involve larger, more delicate molecules or solid materials. Separations therefore tend to focus on extraction, adsorption and crystallisation, rather than the distillations which typify commodity manufacture.

The details of the process design will of course vary as widely as the nature of the products we have been discussing. This was highlighted in Table 8, where different categories of chemical products were summarized. Here, we simply give one example of how a chemical product might be manufactured. This example highlights both the similarity to traditional process design and the different emphasis required in producing in small volumes large delicate molecules of high value.

Example 5C: Key Manufacturing Steps in Hormone Replacement Therapy. To relieve the symptoms of the menopause, women are often given estrogens prepared from a variety of natural sources. One such preparation is an extract of the urine of pregnant mares. While other domesticated animals will excrete similar hormone mixtures in their urine, horses are preferred because they evolved in the desert, where water is in short supply. As a result, the physiology of horses aims to limit water loss: their faeces are much drier than, for example, those of cows; and their urine is more concentrated.

Our company is interested in a generic equivalent to this extract because it sells well and because the patents for its production have long since expired. These patents suggest one possible recovery route of the estrogens is by extraction with hexanol. The active materials in the hexanol extract are concentrated by evaporating some of the hexanol. Hexane is then added to the hexanol concentrate, so that the active estrogens can be easily back extracted into water. The result is an aqueous solution not that different to the starting urine, but with a much higher concentration of active estrogens. According to the patents, this concentrate is then purified by washing with various solvents and dried to a powder. The powder is the crude product.

What steps of this preparation are likely to be critical to its manufacture?

Solution. The manufacture of drugs typically involves a reactor and a separation sequence, just like other chemical syntheses. When the drugs are obtained from natural sources, the reactor is a plant, an animal, or a microorganism. Here, the horse is the reactor, and the urine processing is the separation sequence. Such separation sequences tend to involve four steps, sometimes called a RIPP sequence, after the first letter of each of the four steps. The first, "R" step, Removal of Insolubles, is normally a filtration or centrifugation. In this case, a filtration will remove straw and other suspended solids from the urine. The second, "I" step, Isolation, concentrates the active material, most often by extraction. For Premarin, this step is the hexanol extraction and the hexane-driven back extraction. The third, "P" step, is Purification, most often based on chromatography but in this case accomplished by solvent washing. The fourth step, Polishing, normally includes crystallizations and drying. For this case, the product is a mixture of estrogens and, hence, cannot be crystallized. It is dried.

We are interested in which step in this RIPP sequence will be most important for manufacturing. In most cases, this surprisingly turns out to be the Isolation step, not the Purification step. Isolation tends to dominate the cost of the product. As evidence of this, we note that, a plot of the logithrim of the product cost versus the logarithm of the concentration entering the separation sequence is linear, with a slope of (-1), over a range of 10 orders of magnitude in feed concentration. Thus if one product has a feed concentration ten times smaller than a second product, then we should expect its price to be 10 times higher.

For the case considered here, this implies that the hexane–hexanol extraction steps will be the key to the cost-effective production of a generic form of this drug.

6. Conclusion

During the twentieth century, the chemical industry focused on commodity chemicals, especially those derived from petroleum. Profits depended on the efficient, large-scale production of a small number of these chemicals. In recent decades the emphasis shifted toward the manufacture of higher added value products. These chemical products are designed and manufactured to achieve a specific effect, in which the crucial element is a chemical or a chemical transformation. The effectiveness of the product allows it to be sold at a premium price, often under patent protection. In contrast, the traditional commodity products are specified chemically, and sold into a highly competitive global market for a wide range of uses. For chemical products, function is key. For commodities, price is key.

These differences between chemical products and commodities imply important differences in the way they are designed. Because chemical products are defined by function, the design procedure must start earlier: We cannot decide how to make something until we have decided what to make. A chemist or engineer involved in chemical product design must expect to participate in the identification of market needs, the generation of possible solutions and the selection of a product, in addition to the manufacturing decisions, which have been the traditional role of the engineer. This holistic approach to design is in sharp contrast to traditional process design, in which a specification is dictated to the chemist or engineer who then optimizes a process. Product design involves participation at a much earlier stage of product development, usually in a multidisciplinary team.

Since high value added chemical products are normally produced in low volume, they are typically manufactured by batch processing, often in campaigns in generic equipment used for many different products. As a result, much traditional process design becomes irrelevant. Heat integration is harder if several different products are to be made in batch in the same vessel. Control will often be rudimentary. Because margins are high, process optimisation is less of an issue. Instead, time to market is critical. Because products usually have a short lifetime, being first in the marketplace represents a major advantage. Product design therefore tends to focus on speed, not optimization.

Process design is a well-established subject and very effective heuristics exist to aid practitioners. As chemical product design increases in importance, it needs similar heuristics. As we have outlined, there are significant differences in design of chemical products and design of processes for commodity manufacture. For this reason, a simple mapping of conventional process design onto product design is unlikely to be effective. In this chapter, we have outlined heuristics for tackling the design of chemical products. Chemical products are of course immensely varied, ranging from dialysis machines, through herbicides, to ice cream. Inevitably no design scheme offers a panacea. Nonetheless we now have a heuristic available to provide an intellectual framework within which we can start thinking.

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G. D. Moggridge
University of Cambridge
E. L. Cussler
University of Minnesota