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Perspective

Designing Chemical Products Requires More Knowledge of Perception

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Introduction

There are three main types of chemical products. The first, commodities, is developed on the basis of cost: the lowest cost producer tends to dominate the market. The second type, molecular products, is exemplified by pharmaceuticals, discovered and developed quickly. The third type of product, often called ‘‘performance products’’, has added value because of its function. This function frequently is a consequence of the product’s microstructure.

The key step in the design of these products differs widely. For commodity products, the key step is manufacture, because manufacture dominates the final product price. For molecular products, the key step for development is discovery, a step normally based in chemistry. For performance products, the key step is identification of product need, rewritten as quantitative technical specifications.

Identifying the need for a performance product depends on how this need is expressed. When the need can be expressed in physical or chemical terms, performance product design is similar to other product types. When the need is expressed as a consumer attribute, like ‘‘smooth’’, ‘‘clean’’, or ‘‘tender’’, design is complicated by the incomplete understanding of human perception.

Background

To justify these assertions, we remember that the chemical industry has been dominated by the production of commodity chemicals. These chemicals, produced in amounts of over 10,000 tons per year, are made in equipment explicitly developed for that single product. Such dedicated commodity chemical manufacture has, over the past 50 years, been optimized to produce high-purity chemicals as cheaply as possible. This optimization is one reason that the chemical industry has been successful.

Because over 30 million chemicals are known, we can easily forget how few chemicals are actually produced in such large amounts. Some of these are shown in Figure 1. This graph shows the value of the chemical business on the ordinate, and the description of specific compounds on the abscissa. What is impressive about this graph is how quickly it levels off. Only about 50 or so chemicals actually have yearly sales of over a billion dollars. We do not pretend that smaller sales of chemicals are not important: we are routinely startled by chemicals made in very small quantities which sell for several hundred million dollars per year. Our point is that the number of chemicals actually made in dedicated equipment and in large quantities is actually about 50. Demand for these products is growing, but only roughly in proportion to the world’s population.

Nonetheless, significant growth is still occurring in the chemical business. This growth is not in the commodity area but in more valuable products made in smaller amounts. This is evidenced by the jobs taken by new chemical engineering graduates. Thirty years ago, three quarters of those graduates went to work for the commodity chemical businesses, for companies like BASF, Dupont, and Dow. Now, only about one-third of graduates go to work for this type of company. Similarly, 30 years ago, only about 15% of graduating chemical engineers went to work for companies which added major value to the cost of their raw materials in making specialty products. 3M, Pfizer, Intel and Nestle are examples. Today, almost half of new graduates go to such companies.

Product Characteristics

To explore this change in more detail, we must define more carefully what we mean by chemical products. One definition idealizes them as three different types:

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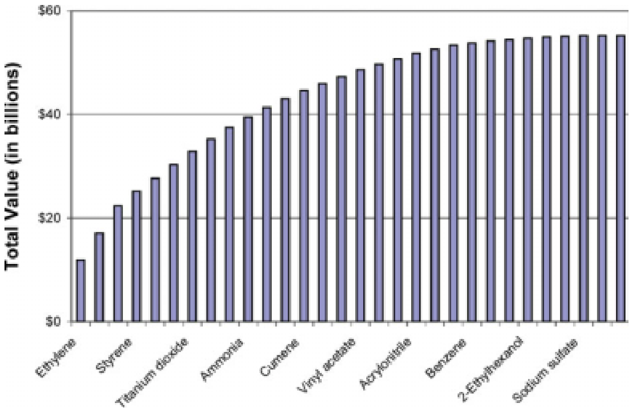

Figure 1. Cumulative value of chemicals.

After the first 50 or so, the incremental value of a new compound is less than $1B. (USITC, 2003).

commodities, molecular products and performance chemicals (Cussler and Moggridge, 2010). These three types of products have different key characteristics, as suggested in Table 1. The most familiar type, commodities, is dominated by cost because the selling price is often only slightly higher than the cost of the feed stock. Thus, commodity chemical plants become large and specialized: the cost per mass made can be reduced if the equipment becomes larger. The basis of the design of commodity processes is reaction engineering and unit operations—''unit ops''—those mainstream topics of traditional chemical engineering. These topics are discussed in the majority of the articles in this journal.

The risk in commodity chemical operations is no longer in uncertain science or incomplete engineering, which was true 30 years ago. Now the real risk is the dependability of the feedstock. Most commodity chemicals are made either from natural gas or from petroleum; most are likely to be made from those same feedstock's in the foreseeable future (Banholzer et al., 2008).

The second and third types of chemical products may be less familiar. The second type, in the third column of Table 1, involves molecules with molecular weights of 500–700 daltons and with specific and major social benefits. The most obvious examples of these products are pharmaceuticals. The key to production of pharmaceuticals is not their cost but their time to market, that is, the speed of their discovery and production. This speed is often restricted by regulations by the Food and Drug Administration. The first product to market tends to get at least two thirds of the sales of the molecule, at least for the life of the patent. These products are not made in dedicated equipment, but in whatever reactors are available at a specific time. Thus process optimization will be less important than questions of scheduling. After all, because the equipment is not dedicated to any particular product, the question will be, ''When can we get in to make ours?''

The exception to this picture occurs when pharmaceutical companies lose patent protection and must compete with generic manufacturers. Then questions of efficient production become more significant. Profit margins may drop dramatically, because the key is no longer discovery and time to market, but rather cost to produce the active ingredient. Generic pharmaceutical production will be an important part of the chemical business in the future, existing in parallel with discovery-based pharmaceutical operations.

The third type of product centers on those where value is added by processing to make a specific microstructure. The key to these products is their function, the benefits they provide. For example, we do not care why our shoes shine after we have applied polish; we only care that they do shine. It is the shine, not the molecules that produce the shine, that is important. Customers are willing to pay a premium for such a function, be it in a coating, a food, or a cleaner.

The characteristics are these performance products are shown in the fourth column of Table I. While the function of these products is frequently related to their microstructure, the science responsible for this microstructure is fragmented and incomplete. It is fragmented between various disciplines. Those formulating cosmetics do not often talk to those making paint, and those developing foods only rarely discuss problems with those making nonwoven fabrics. In addition, there can be a major split in the design of this type product between those in business, those in engineering, and those in psychology. For example, if we want to know what makes a soy protein-based meat substitute tender, the business people say that the analysis of tenderness belongs in engineering. The engineers say this is not a question of engineering but one of psychology. The psychologists respond that this is not an issue of psychology at all, but one of business. Thus, this important aspect of the design of microstructured products may fall between marketing, engineering and psychology.

Template for Design

At this point, we must begin to ask what the mental route we use to design chemical products. In this discussion, we return to commodity chemical process design because this is the most familiar. One cogent description of such a design process, due to James M. Douglas (1988), is often described as ''the synthesis of material flow''. It is shown on the left of Table 2. Douglas's scheme can be idealized as four steps. In the first step, we decide if we will make product in a

Table 1. Three Types of Products*

	Commodities	Molecules	Performance
Key	Cost	Speed	Function
Basis	Unit Ops	Chemistry	Microstructure
Risk	Feedstock	Discovery	Science

*The traditional chemical industry is based on commodities, but growth is expected to be greater in other areas.

Table 2. Process vs. Product Design*

Process Design	Product Design
1. Batch vs. continuous	1. Customer need
2. Input/output	2. Idea generation
3. Recycles	3. Selection
4. Separation/heat	4. Manufacture

*The traditional question of how to make a product must be expanded to the issue of what product to make.

batch or a continuous mode. Because for commodities, the production costs will be cheaper continuously, the answer almost always is to operate in a continuous mode. The second step is to draw an input/output diagram, called a "flow chart." Such a chart suggests how different chemicals will be fed to the process and how different products will come out of it. Third, because we will rarely use stoichiometric feeds which react completely, any streams coming out of our continuous reactors will be mixtures of reagents, products and byproducts. We will want to separate the reagents and recycle them back to the reactor. We will want to remove any byproducts to produce purified product streams. These recycles will be added to our flowchart. Finally, in the fourth step, we will want to detail the separation processes. Most frequently, for commodities, we will separate by distillation. In the fourth step, we also will develop the heat integration which makes our process still more efficient. In commodity process design, we will often support this four-step template with detailed calculations of molecular structure-property relations (Wei, 2007). This four-step template is an excellent way to begin commodity chemical process design.

The design of other types of chemical products is quite different, as shown on the righthand side of Table 2 (Ulrich and Eppinnger, 2007; Cussler and Moggridge, 2010). The general template still has four steps. In the first step, we must define a customer need: what do the customers actually want? We normally will want to convert this need into quantitative specifications, a step which takes us beyond marketing and moves us firmly into engineering. In our second product design step, we will generate ideas to meet this need. Typically we will need a lot of ideas—perhaps around one hundred. We will need to sort and screen these ideas to reduce this number to four or five, which is normally the maximum on which we can afford to make detailed calculations. The third step in our design template is to select the best of this small group of four or so ideas. This selection is difficult, because it usually involves not only quantitative engineering but also more qualitative criteria. In other words, the selection depends not only on unit operations and recycles but also on risk assessment. Finally, in the fourth step of the product design sequence, we must decide on the manufacturing that we will use (Wesselingh et al., 2007). Notice that this manufacturing includes all of the steps in the process design sequence. However, because the amounts involved are different, we will often make different choices for manufacture. For example, for molecular products, we'll often use batch reactors.

Most Difficult Design Step

We want to use this product design template as effectively as possible. In every case, the steps of a particular design will vary in difficulty. The way in which they vary depends strongly on the type of chemical product involved. Thus, we want to identify which steps are likely to give us the most trouble, which part of the design template will be the most difficult.

What we believe to be the most difficult steps are summarized in Table 3. Commodity chemicals are dominated by cost, and cost is dominated by manufacture. Thus the hard step for most commodity chemicals is the fourth one in Table 2. It is that step which is the focus of efforts on chemical process design. It is that step which is traditionally covered in chemical engineering. However, that step is likely to be less important in the chemical industry's future growth.

Table 3. The Most Difficult Design Step*

	Commodities	Devices	Molecules	Performance
Key	Cost	Convenience	Speed	Function
Basis	Unit Ops	Unit Ops	Chemistry	Microstructure
Hard Step	Manufacture	Selection	Selection	Needs

*The difficult step is "selection" for devices and pharmaceuticals. It is "needs" for performance products.

At the same time, we believe there is a subset of commodity chemicals where cost is not the dominant variable. This is for chemical devices, that is, small chemical plants which produce small amounts of the desirable chemical. In this case, cost is no longer the only variable, because the convenience of use may also be important. One good example is home oxygen supply, which supplies oxygen-enriched air at the home of an emphysema patient. It is the selection between the alternatives of oxygen cylinders, oxygen selective membranes, and oxygen selective pressure swing absorption that is the difficult step of the design.

The results for molecular products are more complex. As explained previously, the key to a molecular product, especially a pharmaceutical, is its discovery, followed by the speed with which a successful molecule can be brought to market. The key in this discovery is almost always in chemistry or microbiology, and not in engineering. However, once the target molecule is identified, engineering becomes important. The development engineer will need to choose between varieties of techniques which the chemist will have discovered are effective. For example, he must choose percent conversion in each reaction. He must select the solvents used for any extraction. He must insure adequate supplies for FDA-mandated clinical trials. As for chemical devices, the key step in design of molecular products is selection.

For performance products, the result is different again. As explained before, performance products are dominated by their function and this function comes from product microstructure. However, function is a badly defined variable, especially for consumer products (Meilgaard et al., 2007). What makes skin smooth? What makes cookies fresh? What makes room air comfortable? In these cases, we will have explicit product goals phrased in terms of consumer assessments which have no exact scientific definition. We will not be able to write product specifications without refining the assessments. It is this conversion from needs to specifications which is the difficult step in performance product design.

How the "Needs" Step Limits Performance Products

Performance products can be difficult to develop because the science of human perception is incomplete. In this assertion, we do not refer to neural processing of external stimuli, which has been carefully studied. Rather, we are uncertain how different products produce these stimuli. We can

Table 4. How Perception Occurs*

	Stimuli	Sensation	Perception
Vision	Spectra	Wavelength	Color
Sound	Vibrations	Intensity	Tone
Touch	Foods, Clothes	Force	Texture
Taste, Smell	Chemicals	Flux	Flavor, Odor

*Sight and sound are understood, but touch, taste and smell are not.

explore this further by considering how perception occurs, as summarized in Table 4. The best understood perception is vision (Hunt, 2004). There, the stimulus is of a particular spectrum of colors, a distribution of wavelengths. We perceive this distribution as an average over three types of receptors in the eye, which are sometimes approximated as being responsive to green, yellow, and red light. This integrated average is our perception of color. Notice that the spectrum of a new product does not have to be the same as the benchmark to generate the same color; only the integrated average does.

There is a vivid example of this in every hardware store (see cover). Imagine we want to paint our bedroom the specific color of yellow that van Gogh used so successfully to show cafes in the south of France. We could of course paint our room using the same pigments in van Gogh's paintings, which are known. However, using those pigments would both be toxic and expensive. Instead, we simply toddle off to the hardware store to match the yellow in van Gogh's pictures against one of the small color chips available in the store. The colors available in the store are not made with the same pigments used by van Gogh; they do not give off the same spectrum of light as van Gogh's pigments do. They do give the same integrated average over the same three receptors in our eye, and so they give the same perception of color. Such an understanding of perception is available not only for color vision but also for sound.

Such an understanding of perception is not available for touch, taste or smell. To be sure, the last few years have produced major advances in the molecular biology of smell but not in the simulation of smell. In other words, many details of the chemical changes involved when neural receptors are challenged with specific molecules are now understood; but the way in which chemical challenges diffuse to and competitively react with the receptors remains a mystery. However, while the chemical senses seem for the moment incomplete, the sense of touch also has remained out of reach. For example, the attribute "creamy" is highly desirable in food and cosmetics, but despite a century of focused scientific work, no one knows what "creamy" is (Bourne, 2002).

How Touch Might be Specified

We feel that developing a theory of touch would be an important step in product design, and we believe that many of the tools needed for this effort are already known. What seems incomplete is an integrated picture of how this perception of surroundings occurs. How such a theory of perception might be developed is the subject of the last part of this article. We will consider three attributes in particular: the softness of foams, measured with the fingers; the thickness of liquids, measured with the tongue; and the manageability of hair, measured by a variety of techniques.

We begin with softness, for which results are shown in Figure 2. To get these results, we presented an untrained panel of 12 persons with 13 samples of rubber with widely varying stiffness. We measured the spring constant of the rubbers using a ARES rheometer (Rheometric Scientific, Newark DE). We asked each of the members of the panel to rank the relative softness of the 13 samples (Moskowitz et al., 2005). The data are obtained by ratio scaling. In this technique, each person chooses one rubber as a standard and evaluates the relative softness of the other samples: "Sample B is twice as soft as sample A, but sample C is three times less soft than sample A." We found their assessments agreed with each other with an R^2 of greater than 0.96. The geometric averages of these assessments of "softness" vs. the spring constant show an R^2 of 0.86.

To explain this correlation, we first assume that what is actually assessed is the deformation of the fingers, probably with Merkel or Ruffini receptors (Wolfe et al., 2006). What is perceived may be the vertical displacement with a given force or the force required for a given displacement. In either case, the perception of softness will be proportional to

$$softness \propto \frac{1}{k_{flesh}} + \frac{1}{k_{rubber}}$$

where the k's are the Hookian spring constants of the material involved. Thus, a plot of perceived "softness" should vary linearly with the reciprocal of the rubber's spring constant, as shown in Figure 2. This correlation lets us predict softness for other rubbers.

We next turn to the description of foods in the mouth. To simplify this description, we consider only viscous liquids, because their physical properties are much easier to specify than multiphased foods like meat or ice cream. We first realize that the description of these foods is complicated by a large number of synonyms and antonyms, which are used to detail our perceptions (Bourne, 2002). These perceptions, often summarized as "mouthfeel," are exemplified by the descriptors of viscosity, which include "thick" "thin," "viscous," and "smooth." Again, the data are by ratio scalings carried out by 6–20 untrained persons. Figure 3 shows that assessments of "thinness" vs. "thickness" are closely

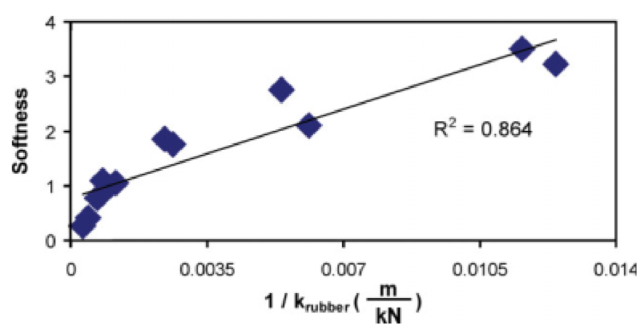

Figure 2. Softness for different foams.

The assessed softness varies with the reciprocal of the foam's spring constant.

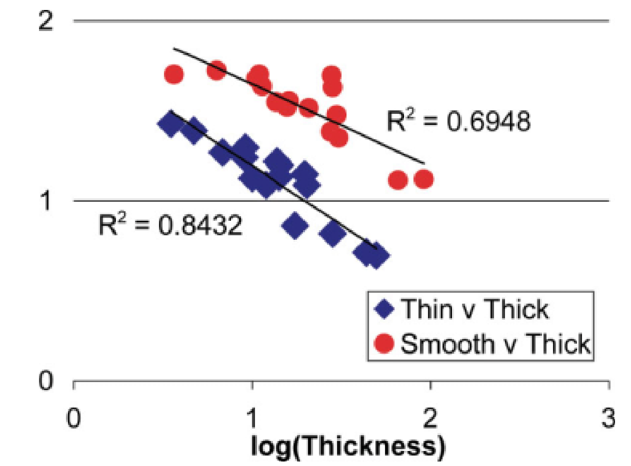

Figure 3. Vocabulary of mouthfeel.

Some words are synonyms or antonyms, and can be removed without loss.

correlated and inversely related (Kokini et al., 1977). Perceptions of "viscous" and "thickness" are similarly correlated, but the corresponding graph now has a positive slope. Perceptions of "smoothness" and "thickness" are also related, although the R^2 in this case is smaller than in the previous examples. "Smoothness" may involve additional physical factors other than that of shear.

We can carry these ideas further by looking at the perceptions of "thickness" vs. the predicted strain on the tongue, as shown in Figure 4. This figure, which includes data from a variety of sources and conditions, shows that a close relationship between "thickness" and physical strain. In fact, the data by deMartine (1975) are assessments with the fingers, whereas the data by Cutler et al. (1983), and by Kokini et al. (1977), refer to assessments in the mouth. The calculation of strain on the tongue requires assessments of tongue velocity and normal force. Because the data of Cutler do not include measurements of these velocities and forces, we have interpolated Kokini's data. Because the three data sets appear to overlap closely, Figure 4 implies that we do not need to duplicate the rheology of a liquid in the mouth to duplicate its thickness. We simply need to develop fluids

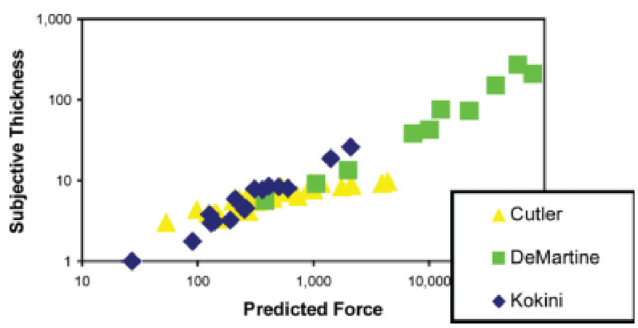

Figure 4. "Thickness" as a function of shear force on the tongue.

These results allow duplicating thickness without duplicating rheology.

Table 5. Descriptors for a Shampoo

Consumer Attributes	Physical Properties
• Manageable	• Shear-thinning polymers
• Texturize before drying	• Moisturizing agents
• Dries fast	• Adjustable water content
• Makes hair smooth	• High surface ion exchange
• Avoids greasiness	• Add emollient natural product
• Nourishs scalp	• Oil in Water Emulsion
• Prevents hair breakage	• Rapid oil uptake (diffusion)
• Cleans easily	• Mostly water-soluble ingredients

which cause the same strain on the mouth, even though these fluids may have a different stress vs. strain rate curve. This is a powerful guide to ingredient substitution.

Of course these examples are considerably simpler than those normally encountered in product development. To make this point specifically, we list properties for a conditioning shampoo in Table 5. The lefthand column in this table lists the attributes that consumers want in a shampoo: their hair must be manageable; it must dry fast; it must be smooth. In the righthand column of the table, we list the physical properties which we can manipulate to get these consumer attributes.

Obtaining these properties implies a balance between adhesion and shear. At rest, we seek polymers which form bonds between hairs. At rest, we want strong bonds caused by nonionic interactions. During combing, we want weak interactions, with small friction. In other words, we seek polymers that form bonds between fibers which drop off dramatically with fiber separation. Thus, we seek a nonionic polymer solution which will easily spread onto the hair (low-static contact angle), retain moisture, and create capillary attraction thanks to Van der Waals interactions. The polymer should have a thixotropic behavior that leads to a progressive decrease in the viscosity when the material is strained, followed by the recovery of its rheological properties after a period of rest.

One possible polymer is guar gum, which consists of linear chains of mannose units linked by 1,4-β glycosidic bonds. Every second mannose monomer carries a galactose residue by the 1,6-α glycosidic bonds. Nonsubstituted guar is nonionic, hydrates in cold water, and behaves pseudoplastically. Under stress, the fluid transforms from a gel to a viscous liquid. Shampoos most preferred by customers show a minimum in apparent viscosity at a shear of 500 Pa. This apparently corresponds to a compromise between forces needed to hold the hair in place and forces needed to allow it to be combed. Thus, we catch glimpses of our perception of hair.

Conclusions

This article begins with the argument that the chemical industry is most likely to grow not by depending on traditional commodities, but by introducing new products with higher added value. Some of these products will be chemical devices, essentially small chemical plants whose value depends not only on cost but also on convenience. Some of these new products will be pharmaceuticals which, once they are discovered, require process designs to produce small amounts quickly and larger amounts inexpensively.

However, it is the third type of performance product, which includes microstructures, that offers the greatest opportunity for growth in the chemical business. These performance products can have value far beyond the cost of their ingredients. They often gain value from the empirically developed details of their processing. The design of these products is strongly influenced by the translation of the consumer needs, often expressed in vague descriptors, into physical and chemical specifications. Developing these specifications is inefficient because there is no existing theory for human perception. We have suggested in this article how such a theory of perception can begin to be developed.

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