TOOLS FOR CHEMICAL PRODUCT DESIGN
FROM CONSUMER PRODUCTS TO BIOMEDICINE

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1. INTRODUCTION

Product design requires the collaboration of marketing experts, economists, and engineers, and has been advocated to be one of the new frontiers opened for chemical engineers (Westerberg and Subrahmanian, 2000; Cussler and Morridge, 2001). Hill (2004) and Stephanopoulos (2003) argued that this renewed interest in products has obvious impact on research and education (Seider et al., 2004; Cussler, 2003), while others advocate that this is just an expansion of the competency that will include the commodity supply chain, and will incorporate the new performance-based constraints of a product (Joback and Stephanopoulos, 1995; Bagajewicz, 2005; Costa et al., 2006a,b; Ng et al., 2006; Siddhaye et al., 2000, 2004; among many others).

Typically, while marketing experts identify consumer “needs and wants” and economists provide means to assess costs and profit, engineers try to advance a product structure/formulation that will achieve the product functionality that targets some of these needs and wants in some optimal way (in the current western economy, it is usually maximum profit). In other words, the needs and wants are not always fully met by the products marketed to these consumers. These needs and wants are usually expressed using consumer-related properties, in terms of properties defined in plain language that are not many times the same as the ones used by engineers to describe the product.
Product design procedures, like the one proposed in the area of process systems engineering by Cussler and Moggridge (2001) or Seider et al. (2004), are the ones that insist on the identification of consumer wants and needs first using them as targets for the product design, while considering consumer response to price as well as optimality (profit or other objective) later. Similarly, the Stage-Gate™ Product Development Process (SGPDP) (Cooper, 2001, 2002, 2005) proceeds in a similar manner by using so-called phases sequentially (first concept, then feasibility, development, manufacturing, and finally product marketing). The first two help shape up the product based on consumer needs and wants using market surveys and tests. At this point, the SGPDP method also suggests building a business case for each product option. The main assumption is that once the concept and the feasibility have been tested, then one product, which could be later refined, emerges.

The claim made in this chapter is that identifying the product first and determining its impact on economics of a company (or other societal areas) later prevents the design of achieving an optimal product. Instead, simultaneously treating product quality (measured by consumer preferences), behavior against price, as well as manufacturing costs, is the right way to identify such profit-optimal product structure (composition, form, functionalities, effectiveness, etc.), and prevents making decisions that can later face manufacturing roadblocks (especially cost) or marketing problems (lack of or smaller profitability or other societal impacts). To reinforce the idea, recent case studies (Street et al., 2008; Heflin et al., 2009) suggested answers where the innovation is discouraged because the market preferences and consumer behavior towards prices do not anticipate higher profitability.

Then, the main idea is not to develop the best product as seen by the study of consumer needs and wants, but the optimal one, eventually (or not) balancing the wants and needs with the costs (company cost and/or societal costs), as well as projected revenues. The most obvious objective in our current western economic system is profit, and we will use it here without loss of generality. When and if one wants to add societal objectives, those ought to be treated as constraints or “costs.” Otherwise, if profit is confronted with societal objectives, the problems become multiobjective. By contrast, we claim that in the SGPDP context, the (many times) wrong product would continue to be developed until the lack of optimality (profitability or other) is discovered at later stages.

2. PRODUCT DESIGN INTEGRATED MODEL

We consider the following to be the key elements:

- Product identification: type and functionality. This requires identifying consumer needs and wants first, as in SGPDP. We keep in mind that there are products that can be introduced in the market without them being wants
and/or not even perceived needs, generating artificially, so to speak, new wants and needs that did not exist before. Examples of this artificial generation of needs and wants abound.

- Identification of product attributes: These are typically the functionalities that are given value by consumers. For example, in the specific case of skin lotions (Bagajewicz et al., 2011), an example we use frequently in this chapter, one would identify its effectiveness, thickness, smoothness, color, creaminess, scent, etc. In devices such as cars, one talks about power, acceleration, comfort, accessories, etc. In medical devices, one talks about its accuracy, its false positives/false negative. We claim that such a list can be made for every product!

- Consumer preferences: Establish a quantitative measure of how much a consumer prefers a product (regardless of its price) given the attributes. This is where we depart slightly from what economists call “hedonic value” and “hedonic pricing,” started by studies like those on “revealed preference theory” pioneered by Samuelson (1938) and continued through time (see Baltas and Freeman, 2001). In all these cases, the underlying idea is that the consumer makes choices that are influenced by (1) perceived preference of one product versus others, (2) price(s), and (3) budget. In other words, when price and affordability are not considered, consumers will almost always declare preference for the product that has their best-perceived quality, but when price and budget are included, the choice is different. Thus, consider cars: asked what car would one like, one may, for example, choose a fancy sport car; when budget is considered, the choices are based on the car type and model they can afford (accessible range of prices), and within that range, preferences play a role, so many times, one “pays for quality.”

- Consumer buying behavior: A price demand relationship that incorporates the consumer preferences.

- Optimization: A procedure that is capable of identifying the attributes that achieve the “right” product to manufacture given a certain criteria [we use the maximization of profit here, but it could be as stated above any other (set of) criteria].

Fig. 2.1 shows the linkage between the components. Consumer preferences, prices, demands, and budget feed the consumer model as parameters. The optimization variables are the product structure/composition/design, which, in turn, are used to compute the cost. Both the cost and the consumer model are then used to evaluate the profit. An optimization procedure, be it mathematical programming, stochastic procedures, genetic algorithms, or other ad hoc procedures, can be used to find the optimal product. In a model that is more amenable to readers that prefer mathematical programming schemes, one can summarize (and generalize) the scheme of Fig. 2.1 by maximizing net present value as a function of all marketing decisions made together with the product structure.
3. CONSUMER SATISFACTION SCORE

We first start with defining the consumer satisfaction score of product candidate, \( i \) \((H_i)\), as a function of certain parameters \((r_{i,j})\) and normalized scores of different consumer-related “properties” \((y_{i,j})\):

\[
H_i = f(r_{i,j}, y_{i,j})
\]  

(2.1)

We believe that satisfaction (and later preferences) ought to be established without incorporating prices in the analysis first, and then use relative preferences in a price/demand model of choice. Until now, we used the simplest form for satisfaction, a linear one, as follows:

\[
H_i = \sum w_{i,j} y_{i,j}
\]  

(2.2)

where \(w_{i,j}\) are weights (Bagajewicz, 2007). The weights represent how much a specific attribute contributes to the overall satisfaction. To determine those, one needs to perform marketing surveys on products without factoring the price. In turn, the scores, defined in the range from zero to one together with the weights, determine an overall score, \(H_i\), in the range from zero to one.

Consumer properties are defined in plain terms that the product user defines in plain language. In the case of a few published examples, these properties are shown in Table 2.1. In turn, these consumer properties have to be expressed in terms of engineering properties \((x_{i,k})\).

In unpublished work performed by several groups of undergraduate chemical engineering students, we have tested these ideas for a variety of products, using their corresponding attributes, later connected to engineering properties: hospital oxygen generators (ease of use, noise, appearance, maintenance frequency, reliability, durability, etc.), carbohydrate vaccines

\[\text{FIGURE 2.1 Integrated product design procedure.}\]
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<td>Absorption rate</td>
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<td>Color</td>
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**Associated Engineering—Manipulated Properties**

- Composition
- Dose
- Material and radius particles
- Composition
- Grape
- Barrel type and burn
- Time
- Etc.
- Sensor(s) type (MV)
- Geometry
- Materials

**Engineering Properties Used for Assessment**

- Diffusivities
- Viscosity
- Surface tension
- Density
- Release time duration
- | Size
- Weight
(efficacy, side effects, delivery method, etc.), cholesterol inhibitor (efficacy, side effects, etc.), vodka (clarity, aroma, sensation, aftertaste), roach killers (durability, speed, odor, toxicity, etc.), automotive hydrophobic coating (texture, frequency of application, water retention, application method), flame retardants (retardancy time, number of applications, odor, setting time, biodegradability, toxicity), osteoarthritis alleviation treatment (frequency, pain upon application, etc.), cartilage tissue repair method seeding chondrocytes (long-term outcome, invasiveness, recovery time), anticavity toothpaste (effectiveness, thickness, cooling effect, abrasiveness, sweetness, foaminess, creaminess, etc.), new refrigerants (safety, global warming potential, ozone depletion impact, compatibility with existing system, stability, explosion potential, etc.), and polymer composite gasoline tank (weight, gasoline diffusion, potential spillage, emission tests, strength upon impact, rupture), each one presenting its own set of challenges, but adhering to the same concepts.

Thus, in general, we write:

$$y_{i,j} = f(x_{i,j})$$  \hspace{1cm} (2.3)

where $x_{i,j}$ are engineering properties. Thus, we can finally define a product using the aforementioned manipulated properties.

We now present a procedure to determine this relationship for the case of the humidifying skin lotion (Bagajewicz et al., 2011). We first note that in this case, the composition is the manipulated variable, and all other properties are the result of this choice. Composition is described in this case by humectants (bind water), occlusives (prevent loss of water), exfoliants (dead skin removal), emollients (fillers of intercellular space), perfumes, and many other inactive ingredients (solvents, thickeners, preservatives, buffers, emulsifiers, colorants, etc.) that help achieve the desired degree of satisfaction through the manipulation of viscosity, density, diffusivity, and surface tension (Bagajewicz et al., 2011). To illustrate the connections between manipulated variables and satisfaction, we show how the consumer preference for effectiveness (the ability to humidify the stratum corneum) is related by consumers to skin appearance. To establish the preference score, one needs to poll a certain number of potential customers of the targeted market segment. Thus, in our example, the effectiveness is rated (Fig. 2.2A) and connected to the skin water content (Fig. 2.2B) and later to the presence of humectants in the skin (Fig. 2.2C). The resulting connection between preference and amount of humectants in the skin is seen in Fig. 2.2D. Thus, the amount of humectants per lotion application can later be defined in terms of the lotion composition of humectant compounds.

Similar connections can be made for other properties. For example, for thickness, consumers are asked to rank how different mixtures flow (ketchup, mayonnaise, cream, etc.), and connections are made to the resulting viscosity
FIGURE 2.2  (A) Preference versus skin appearance, (B) skin appearance versus water content, (C) water content versus humectants, (D) preference versus humectants content.
obtained by the composition (thickness is proportional to the square root of viscosity). In turn, for greasiness, consumers are asked to rank several different products (grease, baby oil, suntan lotion, alcohol) regarding their perceived feeling of greasiness and connections are made to the fatty oil contents. Smoothness is related to greasiness and thickness (it is a metadescriptor, a descriptor composed of other descriptors); so is creaminess. Finally, spreadability identifies the ease of a fluid to displace another fluid on a given surface. Consumers are asked to rate their satisfaction to this product attribute by comparing to other substances (glue, syrup, detergent, ketchup, oil, water). This is connected to surface tension. Absorption rate, related to the ease or speed with which a product disappears on application, is related to diffusivity in the stratum corneum. We omit for reasons of space connections and derived engineering properties for other products in the above table. They are described in the associated papers.

We now turn our attention to the weights in Eq. (2.2). To establish these, there are several marketing survey techniques that we omit discussing here in detail. In the simplest form, without loss of generality, one could ask several consumers to rate the product properties outlined in Table 2.1 as most important, second importance, third importance and so on, and then use this information to obtain the weights.

4. CONSUMER PREFERENCE MODEL

We now turn into the determination of consumer preference score to quantify how much a consumer prefers one product, $i$, over another product, $j$. This is done by defining:

$$\beta_{i,j} = f(H_i, H_j)$$

Without loss of generality of the product design procedure, we used $\beta_{i,j} = \frac{H_i}{H_j}$ so far. Thus, for example, $\beta_{i,j} = 1$ indicates that there is indifference, $\beta_{i,j} = 0.5$ indicates that product $i$ provides the consumer twice the satisfaction of product $j$, and $\beta_{i,j} = 0$ that product $j$ does not satisfy consumers at all (i.e., $H_j = 0$), which is an extreme that is hardly found in practice. Finally, $\beta_{i,j} > 1$ would indicate that product $j$ is better than product $i$ for the consumer.

5. MANUFACTURING AND DISTRIBUTION COSTS

In our example, lotions are emulsions that can be either oil-in-water or water-in-oil. The choice is mainly dictated by practical considerations, such as ease of application and consumer perception (Wibowo and Ng, 2001). The oil-in-water emulsions, which are less sticky on application, predominate in the market and are the choice for our study. Emulsifying agents are used to stabilize the oil-in-water mixture. The most common type of emulsifier are
surfactants, which decrease the interfacial tension between the two phases. The actual manufacturing procedure is simple and consists of mixing the oil and water phases together. The following steps show how the lotion is made:

1. Heat and mix the aqueous and oil phases separately.
2. Combine both phases into one batch.
3. Perform posttreatment modifications (i.e., decrease drop size using a sonificator, followed by a colloid mill and homogenizer). As we shall see later, drop size plays a role in some properties.

6. PRICE—DEMAND CONSUMER MODEL

To determine demand as a function of price, we use the constant elasticity of substitution demand model presented by Bagajewicz (2007)

\[
p_1 d_1 = \left( \frac{\alpha}{\beta} \right)^\rho p_2 \left[ \frac{Y - p_1 d_1}{p_2} \right]^{1-\rho} d_1^\rho \tag{2.5}
\]

\[
d_2 = \frac{Y - p_1 d_1}{p_2} \tag{2.6}
\]

where \( \beta \) is the previously defined preference score and \( \alpha \) is the level of awareness of the new product (zero when consumers are not aware of the new product and one when they are fully aware), \( p_1 \) and \( p_2 \) the new product and the competition prices, \( d_1 \) and \( d_2 \) the corresponding demands, \( Y \) the total budget of the consumers, and \( \rho \) is a parameter related to the elasticity. Without loss of generality, we use \( \rho = 0.75 \) and consider \( \alpha = 1 \).

We realize that the market in this case has a maximum demand (\( D \)) given by the number of people that would actually seek moisturizing lotions in the market in question. Thus, Eq. (2.5) can only be used if the market is unsaturated, i.e., when \( d_1 + d_2 < D \). In a saturated market, consumers have enough budget to buy either product, and the demand will be driven by preferences, not preferences and budget anymore. In such case, maximizing consumer utility, (Bagajewicz, 2007) renders:

\[
D = d_1 + d_2 \tag{2.7}
\]

\[
d_1 = \frac{D}{1 + \gamma} \tag{2.8}
\]

\[
\gamma = \left( \frac{\alpha}{\beta} \right)^{\frac{\rho}{1-\rho}} \tag{2.9}
\]

Thus, the way we establish demand as a function of the rest of the parameters (\( \alpha, \beta, \gamma, D \) and \( \rho \)) by obtaining \( d_1 \) and \( d_2 \) using Eqs. (2.5) and (2.6). If these do not satisfy \( d_1 + d_2 < D \), then we use (7) through (9).
For our example of the skin lotion, the market was determined by looking at what areas of the US have signs and symptoms of xerosis and ichthyosis vulgaris that are the worst (see Bagajewicz et al., 2011 for more details). Also, for the example in question, a fixed capital investment, working capital, and total capital investment were determined as a function of total manufacturing capacity. The demand as a function of price was calculated for different values of $b$ and is shown in Fig. 2.3 (we used $D = 500,000$ bottles/month). It can be inferred that for prices less than $10, the consumer budget is not a limiting factor. At prices around $10, we reach the maximum demand we could have for our product, and it will not increase for lower prices.

Then the total product cost for each value of $b$ was computed by looking at what ingredients can match the selected value of $b$ at minimum cost. They vary from $7.5/bottle for $b = 0.97$ to $8.00/bottle for $b = 1.11$. The competitor’s lotion cost is $9.40/bottle.

One can also consider the possibility of multiple competitors; in such case, one can reformulate the consumer utility function and perform its maximization subject to the budget constraint, assuming $\alpha = 1$, one gets (Street et al., 2008):

$$d_j = \beta_j^{\rho/(1-\rho)} \left( \frac{p_1}{p_j} \right)^{1/(1-\rho)} d_1 \quad j \neq 1$$

(2.10)
where \((\beta_{j,1} = H_j/H_1)\), which, with the help of the (active) budget constraint

\[
\sum_j p_j d_j = Y
\]  

(2.11)

provides the different demands as a function of all prices. Both equations are solved for different process, \(p_1\), and if the sum of the demands is larger than the natural maximum demand \(D\) (in our case, the total number of households that could use some carpet deodorizer), then the demands are no longer driven by the consumer budget and are only driven by preferences in which case the consumer preference function is maximized subject to the demand constraint \((\sum_i d_i = D)\). Using this model, Street et al. (2008), showed that a proposed carpet disinfectant/deodorizer that is superior to others is not worth pursuing.

7. PROFIT MODEL AND OPTIMIZATION

In a very general form, one can pose the problem one of maximizing of expected profit, using a two-stage stochastic model

\[
\text{Max} \sum_s pr_s \text{NPVR}_s - \text{Fixed Capital Investment}
\]

\[
s.t. \quad \text{NPVR}_s = \text{Sales}_s - \text{Manufacturing Costs}_s - \text{Supply Chain Costs}_s - \text{Marketing Costs}_s
\]

where \(pr_s\) is the probability of scenario \(s\), which includes consumer budgets, total demands, and even preferences! The model has “here and now” decisions (first-stage variables) and “wait and see” or recourse decisions (second-stage variables). The former are decided upfront, and the latter are taken in response to certain scenario materializing as illustrated by Barbaro and Bagajewicz (2004). We also treated uncertainty in wine manufacturing (Whitnack et al., 2009).

Instead of formalizing everything in a large numerical method, we realize that the problem can be nicely decomposed: if the value of \(\beta\) is fixed, one can calculate the net present worth (NPW) for all products that have that value of \(\beta\). In principle, there might be more than one product corresponding to each value of \(\beta\), a situation we believe is infrequent.

For our illustrating example, with the cost computed and demand, one can now compute the profit (NPW) for a 10-year lifespan as a function of price for different values of \(\beta\) (Fig. 2.4). The “best lotion” (82% preference, \(\beta = 0.97\)), is not the most profitable one, while a lotion with 80% of consumer preference would be more profitable, with a selling price between $9 and $10.
8. COMPETITIVE MARKETS

Once our product is introduced to the existing market, some of the market will leave their current suppliers to use our product instead. This essentially takes the demand away from our competitors, decreasing their cash flow. The competitors can respond to the introduction of our product in four ways to earn some of their demand back:

1. change their amount of advertising
2. change their composition
3. change their production costs
4. change their price

The first one, change in their amount of advertising, would affect the awareness function ($\alpha$). The second competitor’s response, changing their composition, affects directly $\beta$. If the competitor changes his product in such a way that he will attract more of the market, our NPW will be also affected. We do not discuss these here either. The third action the competitor can take in response to our product is to minimize their manufacturing costs. This would not directly affect our product. The last action the competitor can take is to change their sales price to gain back some of the market. The new price the competitor is described by the function as follows:

$$p_2 = p_{2,0} - \gamma(p_{2,0} - C_2) \left( \beta \frac{d_{2,0} - d_2}{d_{2,0}} \right)^{\alpha_1/\alpha_2}$$  \hspace{1cm} (2.12)
where $p_{2,0}$ is the competitor’s original price, $\gamma$ is a proportionality constant (we use $\gamma = 0.28$), $C_2$ is the competitor’s manufacturing cost per bottle, $\beta$ is the usual relative preference, $d_2$ is the new demand for the competitor’s product, $d_{2,0}$ is the original demand of the competitor’s product, and $\alpha_i$ is the respective awareness of the products (we assumed them to be equal to one). Thus, the new price is adjusted by multiplying the difference in cost and old price ($p_{2,0} - C_2$) by a function of the relative demand drop. After this is done, a new equilibrium is achieved and a new cycle is started. To assess this process, we built a discrete dynamic model that considers monthly price adjustments over a 10-year horizon. Finally, for the cases we looked at, the maximum demand $D$ was never surpassed. The NPW was then calculated as a function of the initial price. Fig. 2.5 shows the NPW for each beta, indicating that a product of similar quality than the competition is now the most profitable, with the best starting price being $8. In Fig. 2.6, we plot both prices and show them reaching equilibrium within 1.5 years. In all cases, equilibrium is achieved within a 2-year period. All prices converged to the same equilibrium, regardless of the starting price.
9. CONCLUSIONS

This chapter presents an alternative approach to product design. We claim that one needs to use an integrated model, which looks over a time horizon and determines, simultaneously, the product. In several cases, we found that the best product is not necessarily the most profitable one. However, a product with slightly less of consumers’ preference is more profitable.

We finished applying different strategies to predict selling price and demand in a competitive market, looking for the maximization of profit. We found that the equilibrium price in a competitive market depends on the preference and total product cost, but not on the starting selling price.

REFERENCES


