On the Role of Microeconomics, Planning, and Finances in Product Design

Miguel J. Bagajewicz

Chemical, Biological and Materials Engineering Dept., University of Oklahoma, Norman T-335, OK 73019

DOI 10.1002/aic.11332

Published online October 16, 2007 in Wiley InterScience (www.interscience.wiley.com).

In this article it is claimed that in order to obtain the right composition, structure, and functionality for a new product, one needs to anticipate what the demand of the product will be and take into account all costs involved (associated manufacturing and supply chain). To obtain the demand, one needs a pricing model, which in turn relies on consumer preferences that are connected to the product composition, structure, and functionality. Thus, a model, including the varying characteristics of the product, the manufacturing capacity and site, the supply chain and ultimately, the markets, is proposed. I use a very simple case of insect repellent to illustrate how the best repellent, identified as the one that consumers will prefer the most, is not the most profitable one and how one can obtain the insect repellent composition that maximizes profit. © 2007 American Institute of Chemical Engineers AIChE J, 53: 3155–3170, 2007 Keywords: optimization, product design

Introduction

Product design has been advocated to be one of the new frontiers opened for chemical engineers.^{1,2} It is claimed that we are moving from a commodity based chemical industry to a high value added and product performance-based one. Some call it a shift in interest,³ with obvious impact in research and education,^{2,4} while others advocate that this is just an expansion of the competency that will still include the commodity supply chain, but will incorporate the new performance-based constraints that a product contributes.^{5–10} Bagajewicz^{11,12} claims that this expansion goes farther than defining product performance and that the definition of a venture associated to a particular product goes all the way from its molecular design, which settles its properties, to all the finance aspects (commercialization, pricing, etc), going through the definition of the manufacturing process and the associated supply chain.

This paradigm "shift" or paradigm "expansion," suggests, arguably implicitly, that process engineering is a mature field, while product design is a relatively virgin filed, at least virgin from the use of tools and methods that the PSE community. One good example of efforts following the suggested path is the article by Wibowo and Ng,¹³ who analyze the issues associated with the fabrication of creams and pastes. There are several papers dealing with refrigerant development,^{14,15} drug development,^{16–18} solvent, and computer aided molecular design in general,^{10,19} all of which are in fact product design after all. Cussler⁶ illustrates some of the differences between the two paradigms (Table 1). To do the comparison he uses the so-called Conceptual Design paradigm developed by Douglas,²⁰ which is very similar to the Onion Model proposed by Smith and Linnhoff.^{21,22} There are, of course, other approaches to process design, like the reducible superstructure approach (best represented by the book of Biegler et al.²³) for which we present our own counterpart version in this article.

The table has a couple of interesting features

(a) Makes product design the center, albeit in the sense of "discovery" of existing commercial molecules, but it also applies to molecular design.

(b) Suggests ad hoc idea generation and selection steps that presumably vary from product to product, for which a systematic search is not available or has to be constructed case by case.² We have seen examples on searches driven by

Correspondence concerning this article should be addressed to M. J. Bagajewicz at bagajewicz@ou.edu.

^{© 2007} American Institute of Chemical Engineers

Table 1. Process Design vs. Product Design
(Following Cussler (Ref. 6))

Process Design	Product Design
Batch versus continuous	Customer need
Input/output	Idea generation
Recycles	Selection
Separation/heat	Manufacture

functionalities (refrigerants, drugs, etc.) like those performed by Camarda and Maranas,²⁴ Sahinidis and Tawarlamani,¹⁵ and also described in Ostrovsky et al.²⁵ and Achenie and Sinha.¹⁹ Recently, Hill³ suggested that the issue is not composition alone anymore but it also involves microstructure.

(c) Some who advocate product design² only call it "chemical" product design, which rules out mechanical and electronic and electromechanical devices, etc. Therefore, it is only a matter of time until this expands to all products. Evans,²⁶ for example, has recently emphasized the upcoming integration between the process industries as providers of commodities and the discrete industries the providers of package goods, devices, appliances, automobiles, etc.

(d) The title of the table suggests that these are opposite and to an extent, excluding activities.

Gani²⁷ has reviewed the challenges of the field point out the "needs for multilevel modeling with emphasis on property models that are suitable for computer-aided applications, flexible solution strategies that are able to solve a large range of chemical product design problems and finally, a systems chemical product design framework with the overall objective to reduce the time and cost to market a new or improved product."

Stephanopoulos⁵ reemphasized the idea of product design and suggested that manufacturing is indeed migrating from being process (commodity)-centric to being product-centric, all this judged by the performance of the companies in the stock market and other associated facts. He suggests that a company should maximize value-added through the supply chain and that while the process centered industry focuses on commodities, the product-centered industry focuses on identification of customer needs as a driving force. He asks if "Process Systems Engineering is prepared to engineer (design and manufacture) products, or someone else should do it?" The question was provocative enough to rise my interest and help showing that this IS very much a problem to be handled with PSE tools, although, as I describe in this article, extending the hands to get help from disciplines that have not been traditionally its partners. In addition, one must wonder if he refers to the role of chemical engineers in all end user products, not only chemical products. This is supported by calls to extend the role of the PSE community into formulations.28

In parallel to this push for extending the borders of chemical process systems engineering to new areas, a new concept of supply chemical chain was recently discussed in detail by Grossmann and Westerberg²⁹ and later by Grossmann³⁰ and in the United States National Academies report by Breslow et al.³¹ The chemical supply chain extends from the molecule level to the whole enterprise. Breslow et al.³¹ suggest that (bold and underlining was added).

"Another important aspect in the modeling and optimization of the chemical supply chain is the description of the dynamics of the information and material flow through the chain. This will require a better understanding of the integration of R&D, process design, process operation, and business logistics. The challenge will be to develop quantitative models that can be used to better coordinate and optimize the chemical enterprise. Progress will be facilitated by new advances in information technology, particularly through advances in the Internet and by new methods and mathematical concepts. Advances in computer technology will play a central role. Fulfilling the goal of effectively integrating the various functions (R&D, design, production, logistics) in the chemical supply chain will help to better meet customer demands, and effectively adapt in the new world of e-commerce. Concepts related to planning, scheduling, and control that have not been widely adopted by chemical engineers should play a prominent role in the modeling part of this problem. Concepts and tools of computer science and operations research will play an even greater role in terms of impacting the implementation of solutions for this problem."

Hill³ presented an overall product design procedure starts similar to that of Cussler.⁶ He identifies the following steps

(a) Identification of consumer "needs."

(b) Translation of the need in a technical target (quantification of the need).

(c) Reduction to a physical prototype, that is, the identification of what substance or set of substances (active ingredients) that could help accomplish the target property.

(d) Testing a physical prototype. Actually manufacture the new product and test it against a variety of relevant criteria.

Hill³ claimed that chemical engineers are involved with steps (c) and (d) but hardly with steps (a) and (b). In addition, he claims that to the process above described, *one needs to add the assessment of the manufacturing process* (this would be step (e)).

Hill³ also argued that mathematical programming approaches, which exist for certain combinations of the above process are not yet available for the case of a structured product, where aside from composition, other physical considerations (texture, microstructure, stability, etc) are not covered.

As it has been pointed out earlier, models that target molecular discovery through mathematical programming based on targeted properties exist. Moreover, attempts to perform molecular discovery through mathematical programming together with process synthesis have been developed.

It is of course well known that steps (a) and (b) involve marketing considerations such as anticipated demand, tentative prices, consumer behavior, advertisement costs, possibly contracts, etc. While Hill³ hints that these two steps (a and b) are the steps that generate targets for the rest of the steps, he does not elaborate on all the marketing issues, implying, I presume, that they are taken care somehow on their own. In addition, connections between manufacturing and markets through supply chains like plant location and pricing has also been developed.³²

Regarding marketing, the term coined to describe the process of bringing a new product service to market is new product development (NPD). There is even a Product development and management association (http://www.pdma.org/ about/) that nucleates practitioners around workshops, publications, and conferences. All soft issues concerning new products are covered in the handbook edited by Kahn.³³ The NPD process is conceived as composed of two traits: idea generation, product design, and detail engineering on one side and market research and analysis on the other. These ideas of integration over the whole enterprise linking business decision-making to process and product design have been also substantiated by Ng.³⁴

In this article I propose a modeling scheme for product design, which counterparts what the reducible superstructure approach is for process design. Moreover, I claim that there is no such thing as the differentiation established in Table 1. Rather, I claim, process design is one (important) part of product design. In addition, as it will become apparent in the article, I claim that without considering microeconomics, product design cannot be properly accomplished. The question remains at what point in the cycle, microeconomics needs to be considered. I claim that in some form, it should be included immediately. In the rest of the article, I discuss the different types of products, differentiating between composition, structure, and functionality. Then, the current state of the art is described followed by the proposed model. After the model is presented, I discuss the role of pricing theory, and later review the methodologies already available for integration with finances, supply chain design/operations. A simple example is presented to illustrate some of the novel ideas.

Consumer-Related Properties of Products

One group of products are pure components or mixtures, in various forms (sometimes structured), like creams, pastes, lotions, soaps, food, flame retardants, insect repellents, pesticides, etc, which are either directly consumed by end-users or sold as raw materials for other end-user products. Their characteristic is that they are "used" once. The other group of products is devices, which serve certain functionality and are characterized by the fact that can be used repeatedly. They are in general, mechanical or electronic devices.

Although the boundary between these two groups is not well defined sometimes, both groups have been recognized by Chemical Engineers as excellent opportunities in which they could make a difference, even in cases where there are many other engineering disciplines involved. One example is the hemodialysis device, the fuel cell, or the espresso coffee maker.⁴

One needs to be careful in defining "targets" for the design of these products, especially if language that will be shared by different fields (marketing, economists, and engineering) is to be used. Thus, in defining a product, one cannot at first express its properties and functionalities using engineering-like properties like viscosities, heat capacities, vapor pressures, etc, as well as device functionalities like efficiencies, etc. One needs to identify other "properties," those that make customers "happy" or "satisfied." Thus, for example, soaps and lotions have properties like "creaminess, thickness, and smoothness,"^{2,13} which are related to viscosity and surface tension and if the lotion/soaps/cream is multiphase to the proportion of phases, drop sizes, etc. Foods have all types of "tastes" that can be related to the concentration of substances (sugar, pepper, species, additives in general), and "textures."

I call these "consumer properties" (y), with the understanding that they need to relate through some continuous function $g(\bullet)$ to the engineering-properties (viscosities, densities, composition, membrane area/thickness, etc), denoted by x.

State of the Art and Challenges

There are two types of product design activity

• Product design through combinatorial enumeration and optimization of existing (a-priori defined) alternatives.

• Product "discovery" and design through mixture (or even molecular) design. We now need to add structure design to achieve functionality.

The former makes use of simple enumeration of existing candidates, using certain sorting criteria. One would call this some sort of "selection" process, in contrast with the discovery associated to the design of novel products which have never been synthesized. In the case of products composed of mixtures of components like soaps, margarine, etc., as cited in Hill³ the associated issue is composition and structure.

Discovery is more difficult because it requires that a property prediction scheme be built associated with a set of groups" or atoms and their interconnection pattern that will constitute a molecule or a mixture of molecules. In this case, the synthesis step requires the identification of existing commodities and their proportion in a mixture, and/or a set of reactions that would lead to new molecule(s). Examples of this type of procedure can be found in several articles and books.^{4,35} For example, the "discovery" of new refrigerants can be made targeting high heat of vaporization and low heat capacity; Cussler and Moggridge² do the same for de-icing products. In the case of devices, Seider et al.⁴ discuss the hemodialysis machine or the automotive fuel cell. When "market driven" new products are considered, the target performance is usually set by Marketing. "Technology driven" new products, where properties are first set by discovery on the engineering side. As we shall see later, in both cases, no matter who identifies the consumer "needs," a consumer model to establish the relationship between demand and price taking into account consumer preferences is needed. Finally, Costa et al.⁸ discuss several additional intricacies, including the need of modeling consumer preferences.

Thus, what marketing provides is one and only one instance of consumer properties that corresponds to one state of consumer "satisfaction" and it also figures out (simultaneously or later) what price the consumer would be willing to pay for it. In addition, it targets markets in which the product will be sold. This identification is based on perceived consumer needs and is obtained using various instruments like surveys as well as direct exposure of prototypes to consumers. This type of data gathering has been extensively studied.³⁶

When engineers analyze the desired properties, assuming that they are feasible to achieve, they provide the costs, but they do so by targeting a set of well-known physico-chemical properties (x). Somewhere in this process there is a function x = g(y), that translates consumer properties into desired physicochemical properties. Once the vector of desired properties x = g(y), is known, engineering and R&D provide in return the product structure z and the cost through a function



Figure 1. Current state of the art in product design.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

 $C(\bullet)$, as illustrated in Figure 1. Associated to the product structure, Engineering assesses manufacturing and distribution costs, and even might produce prototypes and test them.

Marketing makes use of several different tools to perform the choices of markets and to determine product composition/structure: product positioning, value pricing, etc. Product positioning³⁷⁻³⁹ requires defining the market, identifying the dimensions (attributes) of the product, sample customers, contrast with the market preferred combination of attributes (ideal product) and determine the "position", i.e., the distance from ideal. The process also includes creating an image or identity of the product in the minds of their target market. In turn, value pricing⁴⁰ is the practice of setting prices based on the value of a product to the customer. It is customary to make graphs of perceived price versus perceived benefit. Although perceived benefit is easy to comprehend, perception of price, instead of straightforward price is used because usually consumers do not compare prices based on the same quantity/volume/mass of product and there are other factors like product presentation, packaging, guarantees, etc. The difference between the latter and the former is the value. This is illustrated in Figure 2.

A product that is in the value equivalent line (45 degree line) has the "right price" from the point of view of the consumer. This technique can eventually capture the relationship between product composition/structure (if one is designing a product) and perceived benefits, as well as determining the perceived price. Unfortunately, the technique does not allow predicting demand so some method to determine it needs to be used.

The scheme presented in Figure 1 suggests an iterative cycle where marketing adjusts its desired consumer properties y until the profitability is maximized. I do not know how many iterations are performed in industry (if any), but even if they are performed to convergence, one has to wonder how these iterations are performed. In other words, given z_i and therefore *Cost* (z_i), how is y_{i+1} obtained? While this is hard to know and may be it is an ad-hoc procedure in each case anyway, what we know is that what Marketing usually wants is to maximize profit, so that is the starting point to build a strategy.

Finally, there are indications that, even when well defined and well-posed, this type of iterative procedure may not be optimal. Indeed, Guillen et al.⁴¹ have looked at a scheme in which production scheduling provides costs of multiple products based on demands provided by marketing, which in turn has its own model to perform pricing, and therefore is able to come up with the corresponding demand (the simple price imesdemand = constant relation was used). The idea is based on the fact that altering the production schedule in multiproduct facilities should (and indeed does) have an effect on the fixed costs per unit used in existing classical pricing models.⁴²⁻⁴⁵ When this model was run iteratively, it was found it sometimes diverges and even when converged, it rendered an inferior solution to the case in which both models are integrated into a single one. We might expect the same behavior for product design, although I am not willing to try because it is actually likely to be easier to deal with the integrated model anyway. What this model also showed is that prices should be viewed as first stage decision variables instead of exogenous parameters (unless the firm is a price-taker).

Regarding integration, Breslow et al.³¹ suggested the need of "integration of several parts of the chemical supply chain," which "will give rise to a number of challenges, such as modeling for molecular dynamics, integration of planning, scheduling and control (including internet based), and integration of measurements, control, and information systems," *but fall short of discussing the full integration with economics management and business.*

Therefore, aiming at the said integration we want to have an **integrated** model that will help making the following decisions simultaneously

- Product structure/composition/functionality
- Market choice
- Product price for each market
- Associated manufacturing method

• Associated supply chain, including plant locations and transportation

- Associated to these decisions, one would get:
- Capital investment and manufacturing costs
- Supply chain costs
- Projected sales (demand) in each market
- Revenues, etc.

Thus, the newly proposed paradigm for product design suggests a structure like the one given in Figure 3.

Some elements addressing how one could address all these decision making process is described by Pekny⁴⁶ who explores the role of different algorithm architectures in large



Figure 2. Value pricing scheme.



Figure 3. Proposed product design model.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

scale engineering problems. In addition, one important conclusion should be made:

Process Design, which is mistakenly associated to the design of production facilities of commodities only, is an integral part of product design. Product design cannot exist without process design. So, there is no antagonism of any sort and distinctions as those of Table 1, should only be made when the limits of the design exercise are restricted.

The task, then, is to construct an integrated model that will contain several building blocks: A supply chain model, a process synthesis model (or process optimization if the process exists and it will be adapted, or process retrofit model if changes to existing plants are to be considered), a planning and scheduling tool if the new product will be part of a family of products manufactured in multiple sites, a consumer satisfaction and pricing model, and some algorithm that will connect product structure/properties/functionalities to the other models. Of all these, the first three are fairly well known. Of the last two, several concepts from microeconomics can be borrowed and used for the consumer pricing model but the algorithm making the aforementioned connections needs to be built almost ad-hoc for every case. I am nonetheless providing some framework on how it could be attempted in conjunction with the pricing model.

Model Mathematical Structure

The integrated two stage stochastic model proposed is as follows. Let w_1 be a variable vector containing first stage variables, such as manufacturing capacity, plant locations, warehouses, transportation means, customer zones, etc. Let w_2 be the set of second stage vector of variables, such as production levels, demands, advertising expenses, etc., and let π be the price (assumed a first stage variable for simplicity). Finally, using the scenario approach, let p_s be the probability of scenario s; let q the scenario independent parameters, which are costs of plant equipment and plant construction, parameters needed to calculate the product properties (assumed certain for the time being), etc.; finally, let t_s be the scenario dependent parameters of the model, like future demand constraints, the consumer budget (Y), the weights in the consumer model, etc, the prices of the raw materials and

the utilities, etc. Then we want to maximize the Expected Profit as shown below

$$\begin{array}{l} \underset{z,p}{Max} \sum_{s} p_{s} NPVR_{s} - Fixed \ Capital \ Investment \\ s.t. \\ NPVR_{s} = Sales_{s} - Manufacturing \ Costs_{s} \\ - \ Supply \ Chain \ Costs_{s} - Marketing \ Costs_{s} \\ Sales_{s} = Sales \ (z, \pi, w_{1}, w_{2s}; q, t_{s}) \\ Fixed \ Capital \ Investment = Fixed \ Capital \ Investment \\ (z, w_{1}, ;q) \\ Manufacturing \ Costs_{s} = Manufacturing \ Costs \\ (z, w_{1}, w_{2s}; q, t_{s}) \\ Supply \ Chain \ Costs_{s} = Supply \ Chain \ Costs \\ \end{array}$$

(1)

 $(z, w_1, w_{2s}; q, t_s)$

Marketing $Costs_s = Marketing Costs (z, w_1, w_{2s}; q, t_s)$

We called it two stage model because it 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.⁴⁷

We have thus reduced the problem of product design to determining the functional relation of all these function with the product composition/structure/functionality z. Indeed, the model should "discover" or "design" a new molecule/mixture/structure by adequately varying z, which contains structural molecular parameters (groups, or other information like connectivity indices), concentrations of compounds in mixtures, phases, structure, etc., or it optimizes continuous parameters of a known mixture. Everything, first stage and second stage costs, as well as second stage sales are thus dependant on the molecular, microscopic design, or the structure/functionality chosen. This is the smallest scale. Then there is the manufacturing scale, where the appropriate technology to produce the chemicals/devices is selected, the investment level is determined, etc. In the next scale, one has the supply chain costs (plant location, transportation issues, etc.). Finally, the Marketing scale includes sales and marketing costs, including advertising.

Process synthesis (flowsheeting) is mature enough to provide means to obtain a flowsheet, and therefore the corresponding fixed capital investment as well as manufacturing costs associated to any product described by z for any scenario. The same can be said for methodologies to design supply chains: they are well-known and directly usable. Although I make the assumption here that superstructure-like methods should be able to capture the manufacturing structure, I recognize that in some cases they may be too hard to formulate. This might be the case for the manufacturing of complex composite materials, thin films, etc. or when molecular discovery is part of the design, which requires the reaction synthesis path to be added, even in the case of methodologies used in specialty chemicals, agrochemicals, food, pharmaceutical, bio, and related industries. In particular, pharmaceutical and biomedical devices are intertwined with complex networks of HMO's, insurance companies, etc., that

AIChE Journal December 2007 Vol. 53, No. 12 Published on behalf of the AIChE DOI 10.1002/aic 3159

makes the case rather cumbersome to model. I intentionally leave this angle of the problem unexplored in this article so I can advance the concepts surrounding the modeling of the consumer behavior, which I feel are currently missing altogether from the PSE product design literature.

Advertising, and costs associated to sales directly are standard, albeit not simple sometimes. Finally, the sales function Sales, is simply given by the product of price p and demand d_s . The demand vector for scenario s, can be determined using pricing models. This is then, the object of the following section, where we establish the role f z in the relationship pricedemand, which we borrow from microeconomics theory.

Having stated what the concept of the model is, I now present one version of the consumer pricing model and the consumer preference parameter. Later, I concentrate on illustrating the calculation of the consumer preference parameter and how the consumer pricing model alters the design of the product. The example was chosen in such a way that manufacturing is not an issue (it is just mixing) and supply chain is oversimplified. I am certain that many other products will exhibit strong manufacturing and supply chain contributions, which I leave for future articles to illustrate. At the end of the article I come back to discuss additional issues, like advertising, uncertainty, financial risk, budgeting, contracts, etc., to simply indicate how they fit in the above presented scheme.

Pricing Model

We assume first that there is an established market for the new product and that what we are looking is for (profitable) substitutes. The question is what price will be the right one to attract the optimal number of customers and the new demand associated to it, for a given new product.

We begin with posing the consumer optimization problem. In classical microeconomics, this is posed as follows^{43,45}: Consider two products, with demands d_1 (for the new product) and d_2 (for the existing products). Then the consumer maximizes his utility (satisfaction) $u(d_1, d_2)$ subject to a budget limitation, that is:

$$\begin{array}{c}
 \text{Max } u(d_1, d_2) \\
 s.t. \\
 p_1 d_1 + p_2 d_2 \leq Y
\end{array}$$
(2)

where p_1 is the new product's selling price, and p_2 the competitor's product price. A typical utility function is concave and has constant elasticity of substitution, which is a term used to describe the shift from one product to another under price shifts and is defined as follows:

$$\sigma_{\rm ES} = -\frac{\partial \left(\frac{d_1}{d_2}\right) \left(\frac{p_1}{p_2}\right)}{\partial \left(\frac{p_1}{p_2}\right) \left(\frac{d_1}{d_2}\right)} = -\frac{\partial \ln \left(\frac{d_1}{d_2}\right)}{\partial \ln \left(\frac{p_1}{p_2}\right)} \tag{3}$$

To understand this, consider a certain level of consumption of the two products d_1 and d_2 and consider a relative increase in $\left(\frac{p_1}{p_2}\right)$ of k%. Then, the assumption (rooted in observations) is that the relative change in the ratio $\left(\frac{d_1}{d_2}\right)$ is $k\sigma_{\rm ES}\%$. A few 3160

utility functions that satisfy this property have been proposed. One well-known function is the Cobb-Douglas utility $u(d_1, d_2) = d_1^{\alpha} d_2^{\beta}$, which has $\sigma_{\rm ES} = -1$. Because utility functions are concave, that is, marginal utility decreases with consumption, α and β are smaller than one. When $\alpha + \beta = 1$ the utility doubles when both d_1 and d_2 double. Conversely, when $\alpha + \beta < 1$, utility increases by a factor smaller than two when both d_1 and d_2 double, which means there is so called decreasing returns to scale, which is standard. The Cobb-Douglas utility has some problems. For example, it is zero when only one product is consumed, which is not true. In addition, the solution to consumer utility maximization is:

$$p_1 d_1 = \frac{\alpha}{\beta} p_2 d_2 \tag{4}$$

or alternatively

$$p_1 d_1 = \frac{\alpha Y}{(\alpha + \beta)} \tag{5}$$

which says that revenues p_1d_1 are constant, no matter what one does with prices. If production costs are proportional to d_1 , then maximization of profit (understood in its simplest form as revenues minus costs) will suggest $d_1 = 0$ and $p_1 \rightarrow \infty$.

There are many alternatives to the Cobbs-Douglas utility. One that is additive is the Constant Elasticity of Substitution (CES) utility: $u(d_1, d_2) = (d_1^{\rho} + d_2^{\rho})^{1/\rho}$, for which $\sigma_{\text{ES}} = 1/(\rho$ - 1). Note that this function is linear in d_i when the demand for the other good is zero. The function is concave for ρ smaller than one, which provides diminishing marginal utility as the demand increases. Finally, the solution to consumer utility maximization is:

$$p_1 d_1^{1-\rho} = p_2 d_2^{1-\rho} \tag{6}$$

or alternatively

$$p_1 d_1 = p_2 (Y - p_1 d_1)^{1-\rho} d_1^{\rho} \tag{7}$$

which says that revenues p_1d_1 are zero for $d_1 = Y/p_1$, and goes through a maximum. Profit maximization occurs when $p_2(Y - p_1d_1)^{1-\rho} d_1^{\rho} - Kd_1$ is maximum at some point between $d_1 = 0$ and $d_1 = Y/p_1$ (K is the production cost per unit). Other utilities can be found in standard books of microeconomics and pricing theory and using them does not alter the proposed model, as long as they are not inconsistent, like the case of the Cobb-Douglas utility above illustrated.

So far, we discussed these utilities without mentioning the difference in quality between products. In fact, the emphasis has been put in the reaction of consumers to prices. In the case of the Cobbs-Douglas utility, one can think of α and β as related to the respective products' quality. Indeed, given equal prices $(p_1 = p_2)$, we get $d_1 = \frac{\alpha}{R} d_2$ and therefore $\frac{\alpha}{R}$ can be understood as the consumers making choices according to preferences not related to prices. But we have already seen all the problems this utility presents. In the case of CES utility, we have the phenomenon that when prices are equal, demands are equal irrespective of the value of ρ .

To overcome the problems presented by the CES utility, we construct the utility based on functions of demand, which

DOI 10.1002/aic Published on behalf of the AIChE

we could call "satisfaction functions," that is, we could write $u(d_1, d_2) = (h_1^{\rho} + h_2^{\rho})^{1/\rho}$, where $h_i = h_i(d_i)$. Thus, elasticity of substitution is constants with respect to x_1 and x_2 , which makes sense. We propose the following:

$$h_1 = \alpha d_1 \tag{8}$$

$$h_2 = \beta d_2 \tag{9}$$

In these expressions, β is a measure of how much more the consumer prefers product 2 over product 1; it compares the "wants and needs." In turn, α represents how much the consumer is aware of the superiority of the product. This idea comes from Hedonic theory.^{48–50}

To illustrate the role of β , we consider $\alpha = 1$, that is, consumer's perfect knowledge of both products. Then consuming k units of product 1, gives the same utility (satisfaction) as consuming k/β units of product 2. For $\beta = 0.5$ one needs twice as many units to achieve the same utility level. Conversely, if the consumers have the same preference for each product, that is they are indifferent, then $\beta = 1$, and only half of the people know about the new product, then consuming k units of product 2. For $\alpha = 0.5$ one unit of product 1 gives the same utility by consuming αk units of product 2. For $\alpha = 0.5$ one unit of product 1 give the population the same utility as half unit of product 2. This, however, does not work the same way for small increments around a given point where both demands are different from zero, in other words, the same utility is not achieved in the simple manner described above. Indeed, setting du = 0 renders:

$$\Delta d_2 = \left(\frac{\alpha}{\beta}\right)^{\rho} \left[\frac{d_2}{d_1}\right]^{1-\rho} \Delta d_1 \tag{10}$$

which says that the same utility is achieved by a substitution of product 2 by product 1 in a manner that is dependent of the level of consumption (d_1 and d_2).

Under these conditions, the solution to consumer utility maximization is given by the following implicit equation for d_1

$$\Phi(d_1) = p_1 d_1 - \left(\frac{\alpha}{\beta}\right)^{\rho} p_2 \left[\frac{Y - p_1 d_1}{p_2}\right]^{1-\rho} d_1^{\rho} = 0$$
(11)

The above function has several properties. Among others: (a) it predicts $d_1 = d_2$ when the prices are equal and when $\alpha/\beta = 1$, (b) it predicts a monotone decreasing value of d_1 with p_1 , which makes sense, and most important (c) it predicts a monotone decreasing value of d_1 with β (the larger β is the worse product 1 compares), (d) for the same prices ($p_1 = p_2$), same type of products ($\beta = 1$) one obtains $d_1 = \alpha^{\frac{\rho}{1-\rho}}d_2$, which indicates that the market is split unevenly when consumers are not totally aware of the new product, and (e) its elasticity of substitution is still constant. Indeed,

$$\sigma_{\rm ES} = \frac{1}{1 - \rho} \tag{12}$$

Although the above utility function was chosen because of its appealing structure (elasticity of substitution), we recognize the need to choose the appropriate utility for each product, an exercise that should originate in marketing surveys. While there are many objections one can make to the use above utility function, the concepts advanced will not change if a new utility is proposed; only some expressions will. Thus, we will accept this form, to advance the point we are trying to make about the need to incorporate the consumer behavior.

There are of course, other utility functions that lead to different relationships between price and demand. In addition, there are other pricing methods that do not rely on the consumer utility maximization. For example, cost-plus pricing is a method commonly used by firms. The common thread in all forms of common pricing is that the price is determined by the cost of the product plus an additional amount to represent profit. Different forms vary in the way the surplus is calculated. In this option, even though the price is fixed, some price-demand relationship is still needed.

Regardless of the type of function used, its determination for a new product would be challenging and often not necessarily very accurate. While overcoming challenges is part of progress I worry about overcoming uncertainties, which I believe can be handled using two stage stochastic frameworks as we discuss in more detail later.

Thus, changing the product leads to changes in β and therefore this influences sales. I discuss now a consumer preference model that can be used to obtain the inferiority function β .

Consumer Preference Model

I suggested¹² that the consumer preference coefficient β is given by the ratio the competition preference function (H_2) to the new product preference function (H_1):

$$\beta = H_2/H_1 \tag{13}$$

Thus, if the preference for product 2 is half of that for product 1, $\beta = 0.5$. In turn the consumer preference function is proposed to be constructed as follows:

$$H_i = \sum_j \omega_{i,j} y_{i,j} \tag{14}$$

In this expression the property scores $y_{i,j}$ of characteristics are the contribution of property *j* to the preference function of product *i* (like for example effectiveness, durability, feel, form, scent, and toxicity of an insect repellent, which is our example presented below). These scale from zero to one. In turn, $w_{i,j}$ are weights, satisfying $\sum_{j} \omega_{i,j} = 1$, which determine the importance of each product attribute and is determined solely by surveys.³⁶

These consumer related or "marketing" properties (consumer-properties as defined above) are properties that a regular consumer or surveyor can relate to and do not use any engineering jargon. The task of engineers is to connect these properties to physical properties or functionalities and ultimately to product composition or functionality or structure. This connection is the essence of our theory of product design. We now illustrate this briefly through an example.

Example

Consider an insect repellent to compete with an emerging competitor of the current market leader, a DEET-based repellent. It was decided that the basic active ingredient would be

AIChE Journal December 2007 Vol. 53, No. 12 Published on behalf of the AIChE DOI 10.1002/aic 3161

Picaridin, the same as the emerging competitor. Four ingredients were chosen to contribute to these characteristics: picaridin, ethanol, aloe, and fragrance. This example was chosen for its simplicity and because it illustrates well the relationships between product structure, profitability, and consumer preferences. The optimization model is in this case is very simple. First, manufacturing is reduced to a set of mixing tanks and we assume that the ingredients are bought. We also make some simplifying assumptions about the supply chain: We assume that the US divided into several regions, we consider one distribution center in each region and we assume one fixed location for the manufacturing plant. Finally, we choose only one type of consumer: middle age, camping families.

Then, we want to choose the product composition and the optimal price to maximize the Profit¹¹ for which we use a net present value. This has been investigated and discussed in detail by Bagajewicz.^{51,52} The level of demand that the model chooses determines the associated FCI. In a simplified manner, for just one product a deterministic model is as follows: Let *x* be the composition of the product, *p* its price and df_t the discount factor for the time period *t*. Then,

s.t.

$$\begin{split} NPV &= \text{Revenues} - \text{Manufacturing Costs} \\ &- \text{Fixed Capital Investment} \\ \text{Revenues} &= \sum_t df_t \left(\text{Demand}^* p \right) \\ \text{Demand} &= \text{Demand} \left(x, p \right) \\ \text{Fixed Capital Investment} &= \text{Fixed Capital Investment} \\ & (\text{Demand}) \\ \text{Manufacturing Costs} &= \text{Manufacturing Costs} \\ & (\text{Demand, } x) \\ \text{Transportation Costs} &= \text{Transportation Costs} \left(\text{Demand} \right) \end{split}$$

We omit for the moment complications like many markets, different products and process for these markets, time varying parameters, the role of advertising, etc.

This scheme has been also applied to a variety of products: Skin replacement products, 53 skin lotions, 54 wine making, 55 novel biomedical devices. 56

Consumer properties

Six important consumer properties characteristics of the repellent were chosen: effectiveness, durability, stickiness, form, scent, and toxicity.⁵⁷ We now show how to relate those to concentration.

Effectiveness. A common experiment performed on repellents is the "mosquitoes in a box" test. In this test, a known mosquito population is placed inside a long rectangular box. One side of the box is treated with the repellent of interest and at the end of a certain amount of time, the number of mosquitoes on the repellent side of the box is counted. Fifty percent of the mosquito population on the repellent side would prove the repellent was ineffective and would correspond to a utility of zero. Zero mosquitoes on the repellent

3162 DOI 10.1002/aic Published on behalf of the AIChE

side would prove the repellent was completely effective and would correspond to a utility of 100. We now present one result of such experiment (Figure 4) where all data presented comes from informal surveys of small number of persons, performed only to advance the concept and should not to be used to make conclusions.

Figure 4a shows a graph that relates the consumer preference score of effectiveness to the common person/consumer measurable property (% of mosquitoes). The first graph comes from hypothetical observation (abscissa) and survey of consumers (ordinate). What is important here is the trend.





[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 4b relates the measured quantity of mosquitoes to % picaridin. This second graph is also experimental in this case. The third graph (Figure 4c) provides the relationship sought $y_{\text{eff}} = y_{\text{eff}}(x)$.

Durability. Durability is defined as the length of time that one dose of repellent remains effective. We assume that a great repellent, one that would have a score of 100%, would last 12 h or more, and would be best explained by a linear relationship with slope 100/12 (%/h). Next, the repellent durability (time) needs to be related to some physical property of the repellent. This physical property is the composition of the overall liquid mixture. For simplicity, we chose to model the situation like follows: (a) There is a vapor layer of composition c_{is} immediately close to the liquid that is in equilibrium with the liquid composition, that is, $c_{is} = p_{is} / RT = x_i P_i^0(T) \gamma_i / PRT$, (b) the rate of removal of the mixture from the layer is assumed to be given by a natural convection mass transfer coefficient (although a more elaborate diffusion model can be constructed), that is: $N = h \sum c_{is}$, and (c) replenishment of the vapor phase to reach equilibrium is considered instantaneous. Therefore, one can write $\frac{dm_i}{dt} = -AN_i = -Ac_{is}N$, and $M = \sum m_i$, where A is the area; so after substitution one obtains a differential equation for the mass of each component in the liquid as a function of composition, which can be integrated numerically using $m_i = m_i^0$ at t = 0. For the mass transfer coefficient we have used a correlation for forced convection turbulent mass transfer on a flat plate $(k_{\rho}^* = 0.0365 N_{\text{Re},L}^{0.8} \frac{D}{L})$. We understand this model can be enhanced substantially, but we chose to keep it simple and only for the purpose of being able to advance the conceptual approach we are presenting. Results, which illustrate the concept, are shown in Figure 5 including the final durability score.

Stickiness. The first step in relating utility to stickiness was assigning qualitative descriptions to levels of stickiness preference (Figure 6a), which comes directly from consumer surveys. Then, we relate these levels of stickiness to some measurable physical property through a "Paper Test" (Figure 6b). To perform this test, a person applies repellent of a specific formulation to the underside of his arm and places a two-inch-by-two-inch piece of paper on the applied area. The thickest piece of paper that sticks to the applied area and does not fall off determines the stickiness of the repellent. Thickness of paper, or basis weight, is measured by the weight of 500 sheets of that type of paper. For example, a full sheet of 50-pound paper would weigh 1/500 of 50 pounds, or one tenth of a pound. The next step is to relate this consumer test to a physical property of the repellent formula. Ethanol and picaridin are nonsticky, so only aloe can be related to the feel consumer test. For simplicity, we assumed each contributes independently of the other. All results are shown in Figure 6.

Scent. To construct the scent utility function, the consumer determines how satisfying each fragrance scent strength would be to them. In addition, alcohol also contributes to scent but negatively. Thus, for we compute the total scent score using the weighted average of two preference scores:

$$Y_{i,\text{scent}} = \frac{Y_{i,\text{ethanol}} x_{i,\text{ethanol}} + Y_{i,\text{fragrance}} x_{i,\text{fragrance}}}{x_{i,\text{ethanol}} + x_{i,\text{fragrance}}}$$
(15)

AIChE Journal Dece

```
December 2007 Vol. 53, No. 12
```





[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 7 shows the results: The first two figures show the scores for fragrance and ethanol as a function of consumer perception. The most preferred point is where the repellent has only a trace scent, and it decreases for any change in strength. Ethanol, in turn, has an increasing negative effect for the whole range. A linear relationship between concentration and scent power is used for both species (100% corresponding to overpowering and 0% to none).

Form. There are two forms of repellent available to consumers-lotion or spray. The most important physical property

Published on behalf of the AIChE DOI 10.1002/aic 3163



Figure 6. Stickiness score versus aloe concentration: (a) stickiness score versus stickiness perception level; (b) paper basis weight versus stickiness perception level; (c) stickiness (paper weight) versus % aloe; (d) stickiness preference score versus % aloe.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

to ascertain this form is the mixture viscosity (surface tension would address droplet size) because it determines if the product will be flowing free enough to be a spray. If it is too thick, it will be a gel or lotion. Liquids with a kinematic viscosity over 75 centistokes will be too thick to be sprayed by a finger pump, a typical packaging for insect repellent. The values for dynamic viscosity are known or estimated for each of the materials. For any mixture, the resulting dynamic mixture viscosity is calculated with the Grunberg and Nissan method⁵⁸ and converted to kinematic viscosity.

The form score is derived from consumer preferences. For example, if z% of consumers prefer spray repellent over the lotion form, a repellent in spray form would have "100% score" to z% of consumers, but smaller, 50% in our case, to the other (1 - z)%. Thus, a spray repellent would have an overall consumer preference score of $z_{cs} = z + 0.5*(1 - z)$. Conversely, a repellent in lotion form would have a score of $z_{cl} = (1 - z) + 0.5z$. Finally, the relationship between viscosity and utility can be expressed with an "If ... then...." statement giving the utility for any mixture viscosity, i.e. "If kinematic viscosity is less than 75 centistokes, utility is z_{cl} ."

Toxicity. The major benefit of a picaridin-based repellent is the decreased health risk compared to DEET-based repellents. A consumer preference score should be based on the danger to health that is associated with each component. As the risk increases, consumer happiness will decrease; this is modeled as a linear relationship. The risk associated with each component is derived from the National Fire Protection Association (NFPA) Health Hazard rating, often found on Material Safety Data Sheets (MSDS). The NFPA ratings are as follows for each material: DEET-2; picaridin-1; ethanol-1. Results are shown in Figure 8. A linear relationship is used to describe the NFPA toxicity score as the concentration of each.

Weights. These are given in Table 2 and were again obtained using an informal survey of a small number of people.

The best product

When consumer preference (H_1) was maximized, which is equivalent to seeking the minimum of β (because H_2 is fixed), the result suggested a product that is 98.21% picaridin, 1.79% ethanol, 0% aloe, and 0% fragrance with a β value of 0.524. This makes sense because of the weights



Figure 7. Scent preference score from fragrance and ethanol: (a) fragrance preference versus scent power perception; (b) ethanol scent preference score versus scent power; (c) scent preference versus % fragrance; (d) scent preference versus % ethanol.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

used. Such a product is not profitable as it will be shown in the next section.

The most profitable product

The competitor sales price is \$90 and has a formulation of 7% picaridin, 30% ethanol, and the rest water. We used a value of $\rho = 0.76$ and a value of $\alpha = 0.9$, that is, almost perfect knowledge of the new product. Figure 9 shows NPV curves as a function of the proposed price for the new product. We see that the optimal value of beta for this market with the aforementioned weights is $\beta = 0.67$, which gives an NPV of almost 12,000,000. This value of β corresponds to a concentration of 40% picaridin, 58% ethanol, 1% aloe, and 1% fragrance (these last two having reached their imposed lower limit). Interestingly, the curve for $\beta = 0.76$ shows a peak at \$90 (same price as the competition) with an NPV of around 10,700,000 (the corresponding concentration is 30% picaridin, 63% ethanol, 3.3% aloe, and 3.3% fragrance. Lower values of β (0.61 and 0.59) show remarkable lower profit. For values of β lower than 0.59, the NPV is smaller and does not achieve a maximum in the range of prices chosen, showing increasing monotonicity and crossing from negative to positive NPV's at

larger prices. We consider large prices unrealistic and we expect the above consumer model to break down when prices are so different. This will be object of future work. Larger values of β result also in a lower profit anyway.

Multiple Markets

We also investigated the effect of dealing with different markets. We assumed the plant located in Little Rock, AR and the markets corresponding to Table 3. The corresponding composition is 23.8% picaridin, 0% aloe, 65% alcohol, and 11.2% fragrance. We programmed the model in excel and used solver, so the results may not be globally optimal, but are very useful to illustrate the intricacies of the results. The optimal price is \$90, that is, the same as the competition (Figure 10). This is not surprising because most of the values of β are close to one (Table 4). When ROI was maximized, the result is different (Figure 11). The composition is rather different, 26% picaridin, 0% aloe, 65% alcohol, and 9% fragrance and the suggested price is \$108. The values of β are similar to the previous case, but the capital investment is much smaller (around \$1 million vs. \$1.35 million for maximum NPV). Finally, the discontinuities in all graphs stem

AIChE Journal December 2007 Vol. 53, No. 12 Published on behalf of the AIChE DOI 10.1002/aic 3165



Figure 8. Toxicity score versus ethanol and picaridin concentration: (a) toxicity score versus Toxicity; (b) NFPA toxicity versus NFPA toxicity description; (c) NFPA toxicity description versus % ethanol + picaridin; (d) consumer preference toxicity score versus % thanols + picaridin.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

from the fact that when a market had revenues smaller than transportation costs, the market was eliminated. For example, at \$108, Eugene is responsible for the discontinuity.

Unresolved/Unexplored Issues

We now explore some issues that have been left aside in the above example but are important to discuss. They will be addressed in future work.





[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Awareness function

The function α is usually a function of time. It can be assumed to be of sigmoidal form, with the public starting at $\alpha = 0$ or a slightly larger value if there is some element that makes the public instantly aware, like being suddenly present in some store shelves, passing through a growth period reaching a saturation level of some sort. The curve is affected by advertising, which in turn, has a cost. Figure 12 shows two such curves.

Advertising

To effectively advertise a product, service, or good, the following concerns must be addressed and determined. These concerns include: (a) the size of the total advertising budget,

Table 2.	Weights	of the	Preference	Function
----------	---------	--------	------------	----------

Characteristic	Weight
Effectiveness	0.29
Durability	0.24
Feel	0.19
Form	0.14
Toxicity	0.09
Scent	0.05

	December 2007	Vol. 53	, No. 12	AIChE Journ	ıal
--	---------------	---------	----------	-------------	-----

Table 3. Weight Factors for Many Markets

		Weighted Averages					
Market	Effectiveness	Durability	Feel	Form	Toxicity	Scent	
Pittsburg	0.286	0.238	0.190	0.143	0.095	0.048	
Phoenix	0.238	0.286	0.190	0.143	0.095	0.048	
Eugene	0.190	0.238	0.286	0.143	0.095	0.048	
Denver	0.143	0.190	0.238	0.286	0.095	0.048	
Salt Lake City	0.143	0.095	0.048	0.286	0.238	0.190	
Lubbock	0.095	0.143	0.190	0.238	0.286	0.048	
Kansas City	0.048	0.095	0.143	0.190	0.238	0.286	
Sacramento	0.095	0.143	0.238	0.190	0.286	0.048	
Indianapolis	0.190	0.143	0.095	0.048	0.286	0.238	
Jacksonville	0.238	0.190	0.143	0.095	0.048	0.286	
Albany	0.143	0.190	0.286	0.238	0.095	0.048	
Billings	0.095	0.048	0.286	0.238	0.190	0.143	
Baton Rouge	0.048	0.286	0.238	0.190	0.143	0.095	
St Paul	0.238	0.190	0.048	0.095	0.143	0.286	
Memphis	0.143	0.190	0.048	0.095	0.286	0.238	
Charlotte	0.048	0.095	0.286	0.238	0.143	0.190	

(b) the allocation of this budget to marketing areas, (c) the allocation of the individual market area budgets among media, (d) the timing of advertising, (e) the theme of the campaign and, (f) the effort to be invested in a campaign. Figure 13 depicts the basic advertising trend for a generic product, service, or good. During the beginning of advertising, there is a linear trend between the advertising rate and sales of the product. Once the product begins to gain popularity, the sales reach a threshold, and the trend between sales and advertising rate is no longer linear. Soon, the product will begin to saturate the market and the product reaches its height in popularity. At this point, with an increased advertising rate, the product begins to oversaturate the market. As a result, sales begin to decline (see Rao⁵⁹).

The relationship between sales and advertising efforts can also be modeled through the influence of advertising on the awareness and superiority functions (α and β). It might also affect the consumer's budget (Y). Finally, the level of advertising needed should be suggested by the model because advertising increases the aforementioned parameters, but also increases marketing costs.



Figure 10. Profit as a function of quality and price, many markets.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Superiority function

The function β is also subject to change in time and be affected by advertisement. We envision a natural decay through time, which sometimes has to do with technological advances, and which advertising can partially prevent.

Time horizon

With the model parameters (α, β, ρ, Y) naturally changing with time the right model should include the time horizon.

Pricing

Pricing of certain products is subject to several types of discount structures that need to be incorporated. In addition, one should think of incorporating in the model the possibility of picking different prices for different times.

Profit function

As we have explored measuring profit through NPV and ROI, there are other measures or restrictions one might want to use like the cash position of the company, the share holder value strategy, liquidity ratios, etc. A recent paper by Prof.

$1 a \beta \alpha \gamma \gamma$	Table 4.	Values	of	ß	for	Different	Market
--	----------	--------	----	---	-----	-----------	--------

Market	β (Best ROI)	β (Best NPV)
Pittsburg	0.798	0.829
Phoenix	0.784	0.816
Eugene	0.855	0.885
Denver	0.901	0.924
Salt Lake City	1.014	1.022
Lubbock	0.974	0.990
Kansas City	1.091	1.095
Sacramento	0.979	0.997
Indianapolis	0.999	1.014
Jacksonville	0.907	0.931
Albany	0.906	0.931
Billings	1.059	1.071
Baton Rouge	0.890	0.915
St. Paul	0.914	0.934
Memphis	0.970	0.985
Charlotte	1.049	1.061

AIChE Journal Decen

Published on behalf of the AIChE

3167



Figure 11. ROI as a function of quality and price, many markets.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Umeda discusses some of the connections between project decisions and corporate strategies.⁶⁰

Supply chain issues

The examples above do not include illustrations about the intricacies and effect on the product design as well as the choice of markets that are associated to the design and costs of the supply chain. Models such as the one proposed by Tsiakis et al.⁶¹ need to be used. Lavaja et al.^{32,62} explored some of these issues and showed that in the context of multiple markets and multiple prices a new commodity can give rise to more than one manufacturing location. Inventory levels are also usually ignored at the planning stages. They play, however, an important role in managing financial risk.⁶³

Budgeting

Cash management is of paramount importance to determine the real profitability of a project. In most chemical engineering models cash flow is calculated assuming one set of conditions, which are kept the same for the life of the project. Even textbooks of recent update, like Peters et al.⁶⁴ continue to use this type of assumptions. Recently some work has started to depart from this formulation, proposing to follow the cash flow throughout time in more detail.^{32,62,65–67}





[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]



Advertising Rate / Year

Figure 13. Sales as a function of advertising.

Adding cash flow balance constraints allow to determine when and what portion of proceeds is returned as pure profit to the investors or to the company's general account, what portion is used to finance expansions (if an when this is more advantageous than fresh capital investment). One can consider the use of short term market instruments such as treasury bonds, etc, as it is suggested in cash management models.⁶⁸ Finally, capital investment limits may change the solution.

Contracts

Contracts play an important role in defining the shape of the enterprise. Regular or option contracts help determine and manage the financial risks.^{47,63,69}

Competition

The model outlined above considers a static competitor, which does not react to the new market. In reality, one needs to assume a dynamic condition and has to include the competitor model, that is, a model that will determine the competitor's price (or competitors' prices). Although an extensive review can be made of several models (perfect competition, monopoly, oligopoly, etc), we leave this matter unexplored in this article.

Uncertainties and financial risk

Many parameters of the model are uncertain, truly uncertain, like α , β , ρ , *Y*. Moreover, the uncertainties behind β can be related to uncertainties in the weights that define the consumer preference function as well as the consumer perception of each of the function scores (*y*). There are, in general two alternative routes, one is that of building full blown two (or multi)-stage stochastic programming models for expected profit maximization^{70,71} and financial risk,⁴⁷ the dynamic programming approach.⁷² We prefer the former approach. In addition, to deal with financial risk, we proposed to use the framework advanced by Barbaro and Bagajewicz⁴⁷ and the risk averse curve selection proposed by Aseeri and Bagajewicz.⁶⁹

Computational issues

As stated earlier, many products may be associated with complex industry structures (like pharmaceutical drugs) which would make the models too complex to solve. We envision that these models could be complex MINLP's not more complex than the ones we are currently solving is several synthesis problems with multiperiod structure. We point out, however, that at least in the case of the design of one product as opposed to multiple products, a nice decomposition scheme is possible. In fact it has been applied in this article. Indeed, one can actually enumerate the product consumer preference (through the parameter β), by selecting different discrete values, which leads to a nice decomposition: With β fixed, one can solve for the product structure by minimizing its manufacturing cost. This would be equivalent to applying the current proposed methodology of meeting consumer "needs." With the costs defined, one can assess the NPW easily without the need for any optimization, unless the supply chain is to be designed, but this problem is also known as solvable to a great extent. When multiple products are designed, one needs to repeat this scheme for values of the parameter β corresponding to the different products. This is still doable.

Conclusions

The basic message that this article conveys is that pricing and microeconomics, as well as with supply chain, process synthesis and finances are needed when one wants to design new products. A framework was developed in which all the elements of new product commercialization, namely, the product composition/structure/functionality, the manufacturing investment and costs, the associated supply chain and the consumer behavior with respect to price product and price are taken into account in a model that determines all the parameters of the subsystems involved, form the product structure to the choice of markets and the price of the product in each market.

The timing to construct such a model after the first ideas of a new product are laid out is also arguable. Some would argue that it is not practical to do so too early in the design, especially because of the effort (and associated cost) involved. Because one cannot only target consumer "needs" and how to meet them, but also needs to worry about profitability, I argue that the analysis suggested in this article needs to be conducted, whether quantitatively as we propose, or in some other heuristic form.

Acknowledgment

Kamila Sobeslavová also helped in the preparation of this manuscript.

Literature Cited

- 1. Westerberg AW, Subrahmanian E. Product design. *Comput Chem Eng.* 2000;24:959–966.
- 2. Cussler EL, Moggridge GD. Chemical Product Design, 1st ed. Cambridge University Press, 2001.
- 3. Hill M. Product and process design for structured products. *AIChE* J. 2004;8:1656–1661.
- Seider WD, Seader JD, Lewin DR. Product and Process Design Principles. New York: Wiley, 2004.

- Stephanopoulos G. Invention and innovation in a product-centered chemical industry: general trends and a case study. In AIChE Conference, 55th Institute Lecture, San Francisco, November 2003.
- Cussler EL. Chemical product design and engineering (Plenary Talk). In AIChE Annual Conference, Paper 430a, San Francisco, November 2003.
- Cussler EL, Moggridge GD. Chemical product design. In FOCAPD Conference, Princeton, USA, July 2004.
- Costa R, Moggridge GD, Saraiva P. Chemical product engineering: a future paradigm. Chemical Engineering Process. April 10–13, 2006.
- Costa R, Moggridge GD, Saraiva P. Chemical product engineering: an emerging paradigm within chemical engineering. *AIChE J*. 2006;52:1976–1986.
- Ng K, Gani R, Dahm-Johansen K. Chemical Product Design: Towards a Perspective Through Case Studies. Computer Aided Chemical Engineering Series 23. Amsterdam: Elsevier, 2006.
- Bagajewicz M. Integration of process systems engineering and business decision making tools: financial risk management and other emerging procedures. In: Galan M, del Valle EM, editors. *Chemical Engineering Trends and Developments*. pp. 323–377. Chichester, U.K.: Wiley, 2005.
- 12. Bagajewicz MJ. On the integration of process and product design with microeconomics and finances. In Enpromer 2005, 2nd Mercosur Congress on Chemical Engineering, 4th Mercosur Congress on Process Systems Engineering, Rio de Janeiro, Brazil, August 2005.
- Wibowo C, Ng KM. Product-oriented process synthesis and development: Creams and pastes. AIChE J. 2001;47:2746–2767.
- 14. Joback K, Stephanopoulos G. Searching spaces of discrete solutions: the design of molecules possessing desired physical properties. *Adv Chem Eng.* 1995;21:257–311.
- Sahinidis NV, Tawarlamani M. Applications of global optimization to process molecular design. *Comput Chem Eng.* 2000;24:2157–2169.
- Siddhaye S, Camarda KV, Topp E, Southard MZ. Design of novel pharmaceutical products via combinatorial optimization. *Comput Chem Eng.* 2000;24:701–704.
- 17. Siddhaye S, Camarda KV, Southard MZ, Topp E. Pharmaceutical product design using combinatorial optimization. *Comput Chem Eng.* 2004;28:425–434.
- 18. Kier LB, Hall LH. Molecular Connectivity in Chemistry and Drug Research. New York: Academic Press, 1986.
- Achenie LEK, Sinha M. Interval global optimization in solvent design. *Reliable Comput.* 2003;9:317–338.
- Douglas JM. Conceptual Design of Chemical Processes. New York: McGraw Hill, 1988.
- Smith R, Linnhoff B. The design of separators in the context of overall processes. *Trans IChemE ChERD*. 1988;66:195.
- 22. Smith R. Chemical Process Design. New York: McGraw Hill, 1995.
- 23. Biegler LT, Grossmann IE, Westerberg AW. Systematic Methods of Chemical Process Design. New Jersey: Prentice Hall, 1997.
- Camarda KV, Maranas CD. Optimization in polymer design using connectivity indices. *Ind Eng Chem Res.* 1999;38:1884–1892.
- Ostrovsky G, Sinha M, Achenie LEK. On the solution of mixed-integer nonlinear programming models for computer aided molecular design. *Comput Chem.* 2002;26:645–660.
- Evans L. Achieving operational excellence with information technology. In AICHE Spring Meeting, New Orleans, March 2003.
- Gani R. Chemical product design: challenges and opportunities. Comput Chem Eng. 2004;28:2441–2457.
- Cordiner JL. Challenges for the PSE community in formulations. Comput Chem Eng. 2004;29:83–92.
- Grossmann IE, Westerberg AW. Research challenges in process systems engineering. AIChE J. 2000;46:1700–1703.
- 30. Grossmann IE. Challenges in the new millennium: product discovery and design, enterprise and supply chain optimization, global life cycle assessment. In PSE 2003, 8th International Symposium on Process Systems Engineering, China, 2003.
- 31. Breslow R, Tirrell MV, (co-chairs) Barton JK, Barteau MA, Bertozzi CR, Brown RA, Gast, AP, Grossmann IE, Meyer JM, Murray RW, Reider PJ, Roush WR, Shuler ML, Siirola JJ, Whitesides GM, Wolnyes PG, Zare RN. Beyond the molecular frontier. challenges for chemistry and chemical engineering. In Committee on challenges for the chemical sciences in the 21st century, The United States National Academies Press, 2003.

- 32. Lavaja J, Adler A, Jones J, Pham T, Smart K, Splinter D, Steele M, Bagajewicz M. Financial risk management for new products: considerations of plant location, pricing and budgeting. In Proceedings of the AIChE Annual Meeting, Austin, Texas, 2004.
- Kahn KB. PDMA Handbook of New Product Development, 2nd ed. New York: Wiley, 2004.
- Ng K. MOPSD: a framework linking business decision-making to product and process design. *Comput Chem Eng.* 2004;29:51–56.
- Achenie L, Venkatasubramanian V, Gani R. Computer Aided Molecular Design: Theory and Practice. Amsterdam: Elsevier Science, 2002.
- 36. Moskowitz HR. Consumer Testing and Evaluation of Personal Care Products. New York: Marcel Dekker, 1996.
- Trout J. "Positioning" is a game people play in today's me-too market place. *Ind Market*. 1969;54:51–55.
- 38. Ries A, Trout J. *Positioning, The Battle for your Mind.* New York: Warner Books, McGraw-Hill, 1981.
- Trout J, Rivkin S. The New Positioning: The Latest on the World #1 Business Strategy. New York: McGraw Hill, 1996.
- Marn MV, Roegner EV, Zawada CC. *The Price Advantage*. NJ: Wiley, 2004.
- Guillén G, Bagajewicz M, Sequeira SE, Espuña A, Puigjaner L. Management of pricing policies and financial risk as a key element for short term scheduling optimization. *Ind Eng Chem Res.* 2005;44:557–575.
- 42. Dorward N. The Price Decision: Economic Theory and Business Practice. London: Harper & Row, 1987.
- Varian H. Microeconomic Analysis. New York: W.W. Norton & Company, 1992.
- 44. Mas-Collel A, Whinston M, Green J. *Microeconomics Theory*. Oxford: University Press, 1995.
- Hirshleifer J, Hirshleifer D. Price Theory and Applications. New Jersey: Prentice Hall, 1998.
- Pekny J. Algorithm architectures to support large-scale process systems engineering applications involving combinatorics, uncertainty, and risk management. *Comput Chem Eng.* 2002;26:239–267.
- Barbaro AF, Bagajewicz M. Managing financial risk in planning under uncertainty. AIChE J. 2004;50:963–989.
- Rosen S. Hedonic prices and implicit markets: product differentiation in pure competition. J Polit Econ. 1974;82:34–55.
- Epple D. Hedonic prices and implicit markets: estimating demand and supply functions for differentiated products. J Polit Econ. 1987;95:59–80.
- Kahn S, Lang K. Efficient estimation of structural hedonic systems. Int Econ Rev. 1988;29:157–166.
- Bagajewicz M. Effect of pricing, advertisement and competition in multi-site capacity planning. In Proceedings of the ESCAPE 2005, Barcelona, Spain, May 2005.
- 52. Bagajewicz M. Integration of process systems engineering and business decision making tools: financial risk management and other emerging procedures. In: Galan M, del Valle EM, editors. *Chemical Engineering Trends and Developments*. pp. 323–377. Chichester, U.K.: Wiley, 2005.
- 53. Tang H, Azzarello J, Ashaye T, Fairbanks B, Hargis M, Williams P, Shaw B, Klink I, Sikavitsas V, Bagajewicz M. Modeling of the FDA approval process: connections between financial risk, early de-

cision making and future pricing. In Proceedings of the AIChE Annual Meeting, Austin, Texas, 2004.

- Bagajewicz M, Lopez H, Sposato E. Use of pricing and consumer satisfaction measures in consumer product design. In AIChE Annual Meeting, Cincinnati, November 2005.
- Bagajewicz M, Kerr S, Frow M. Engineering wine. In AIChE Annual Meeting, San Francisco, November 2006.
- 56. Bagajewicz M, Froude V, Burdett E, Shreve M, Clemente-Harl E, Martin M, Sikavitsas V. Risk management in the development of novel biomedical devices and vaccines. In AIChE Annual Meeting, San Francisco, November 2006.
- Ashley E, Doman S. Insect Repellent Design: Researching Alternatives to DEET. University of Oklahoma Chemical Engineering Advance Design Class Project (Available upon request to the author), 2006.
- 58. Reid RC, Prausnitz JM, Sherwood TK. *The Properties of Gases and Liquids*, 4th ed. New York: McGraw Hill, 1987.
- 59. Rao AG. *Quantitative Theories in Advertisement*. New York: Wiley, 1970.
- Umeda T. A conceptual framework for the process system synthesis and design congruent with corporate strategy. *Ind Eng Chem Res.* 2004;43:3827–3837.
- Tsiakis P, Shah N, Pantelides CC. Design of multi-echelon supply chain networks under demand uncertainty. *Ind Eng Chem Res.* 2001;40:3585–3604.
- 62. Lavaja J, Adler A, Jones J, Pham T, Smart K, Splinter D, Steele M, Bagajewicz M. Financial risk management for investment planning of new commodities considering plant location and budgeting. *Ind Eng Chem Res.* 2006;45:7582–7591.
- Barbaro AF, Bagajewicz M. Use of inventory and option contracts to hedge financial risk in planning under uncertainty. *AIChE J*. 2004;50:990–998.
- 64. Peters MS, Timmerhaus KD, West RE. Plant Design and Economics for Chemical Engineers, 5th ed. New York: McGraw Hill, 2003.
- Romero J, Badell M, Bagajewicz M, Puigjaner L. Integrating budgeting models into scheduling and planning models for the chemical batch industry. *Ind Eng Chem Res.* 2003;42:6125–6134.
- Badell M, Romero J, Huertas R, Puigjaner L. Planning, scheduling and budgeting value-added chains. *Comput Chem Eng.* 2004;28:45–61.
- 67. Powell S, Hodge S, Spencer N, Godwin J, Bagajewicz M. Simultaneous modeling of location, advertisement and competition in investment/capacity planning with risk management. In Proceedings of the AIChE Annual Meeting, Austin, Texas, 2004.
- 68. Orgler YE. Cash Management. California: Wadsworth, 1970.
- Aseeri A, Bagajewicz M. New measures and procedures to manage financial risk with applications to the planning of gas commercialization in Asia. *Comput Chem Eng.* 2004;28:2791–2821.
- Eppen GD, Martin RK, Schrage L. A scenario approach to capacity planning. Oper Res. 1989;37:517–527.
- Ahmed S, Sahinidis NV. Robust process planning under uncertainty. Ind Eng Chem Res. 1998;37:1883–1892.
- Cheng L, Subrahmanian E, Westerberg AW. Design and planning under uncertainty: issues on problem formulation and solution. *Comput Chem Eng.* 2003;27:781–801.

Manuscript received Dec. 28, 2006, and revision received Aug. 6, 2007.