

Product Design in Price-Competitive Markets: A Case Study of a Skin Moisturizing Lotion

Miguel Bagajewicz, Season Hill, Amanda Robben, Heyde Lopez, Monica Sanders,
Erin Sposato, Curtis Baade, Shamara Manora, and Juliana Hey Coradin

School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK 73019

DOI 10.1002/aic.12242

Published online May 12, 2010 in Wiley Online Library (wileyonlinelibrary.com).

In this article, we apply a recently developed method for product design to the formulation of skin lotions and extend its application to consider price-competitive markets. The method is based on the use of consumer preference functions that are in turn parameters of price-demand relations. These relationships are then embedded in a business model that aims at determining the optimal lotion formulation from the profitability point of view. The model allows to distinguish the formulation that leads to the consumer most preferred skin lotion from the most profitably one in a quantitative fashion. In the latter case, the selling price is also determined simultaneously with the optimal formulation. The example analyzed shows that the consumer most preferred lotion is not profitable, whereas a slightly less preferred lotion is very profitable. We then extend the new product design procedure to consider a competitive environment in which prices of all competitors, change dynamically until equilibrium is established.

© 2010 American Institute of Chemical Engineers AICHE J, 57: 160–177, 2011

Keywords: product design, microeconomics, lotion

Introduction

Product design requires the collaboration of marketing experts and engineers. Although marketing experts identify consumer needs and wants (we call them consumer preferences here), engineers try to advance a formulation that will accomplish some of these needs and wants in a profitable way. 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 (like effectiveness, thickness, smoothness, etc., in the lotion design case), which are expressed in terms of measures that are not sometimes the same as the ones used by engineers to describe the product. For example, effectiveness of a skin moisturizing lotion is usually expressed by a consumer by some measure of reduction of the number of scales produced in a certain period of time, or certain skin feel after a

given time, whereas the engineer, who knows what chemicals are responsible for the dry skin and for desquamation will connect effectiveness to the concentration of these chemicals at certain depths of the skin and then will be able to target the right level of these chemicals in the final product.

As stated, just trying to match all consumer needs and wants to the full extent may not lead to a successful design because often such a product is unprofitable. To address the identification of the right level at which consumer preferences are to be matched, together with the price at which the product ought to be sold so that maximum profit is achieved, a procedure that considers all these elements together was recently developed.¹ The method proposes to use microeconomics models to make the connections between consumer preferences, product price and product structure, composition, and/or functionalities.

Alternative product design procedures, like the one proposed by Cussler and Moggridge² or Seider et al.,³ advocate the identification of consumer needs first using them as targets for the product design considering profitability and consumer response to price later. Bagajewicz's¹ methodology

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

fits into frameworks currently popular for product development, like the Stage-Gate™ Product-Development Process (SGPDP).⁴ For the technology development phase of the SGPDP, the Stage-Gate™ Technology-Development Process (SGTDP) has been proposed,^{4,5} which deals with all the innovation phases. The methodology proposed by Bagajewicz¹ can be used to scope the technology development part of SGPDP. However, it requires considerations and modeling that the SGPDP does afterwards in a sequential manner. Indeed, the product development phase of SGPDP has various phases (concept, feasibility, development, manufacturing, and product marketing). The first two help shape up the product based on consumer needs and wants, consumer surveys, and tests. At this stage, the SGPDP method also suggests to build a business case for each product option. The main assumption is that once the concept and the feasibility have been tested, one product to be refined will emerge. Bagajewicz¹ claims that identifying the product first and determining its marketability/profitability later prevents the design procedure from identifying of the profit-optimal product. He claims that 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, thus preventing making decisions that can later face manufacturing roadblocks (especially cost) or marketing problems (lack of profitability for example). To reinforce the idea, recent case studies suggested answers where the innovation is discouraged from being pursued because the market preferences and consumer behavior towards prices do not anticipate higher profitability.^{6,7} In the SGPDP context, these technologies would continue to be developed until their inferior profitability or eventually, their lack of profitability is discovered at later stages.

Finally, neither Cussler and Moggridge,² Seider et al.,³ the stage-gate procedure,⁸ nor Bagajewicz,¹ discuss connections between the product designed and its ability to be profit-optimal under price competition.

In this article, the model developed by Bagajewicz¹ is applied to the case of designing a moisturizing skin lotion targeting patients with Ichthyosis Vulgaris, a genetic disorder that causes extreme scaly and dry skin and patients with no so severe dry skin disorders, like xerosis. These can be caused by dry air, overexposure to water, and harsh soaps or irritants, among other environmental factors. We also extend the design procedure proposed by Bagajewicz¹ to consider price-competitive markets.

The article is organized as follows: First a brief background on skin and Ichthyosis vulgaris is given. Then, the consumer preference model is presented followed by the determination of the “perfect” product. We then analyze the manufacturing and costs of such lotions and determine its profitability. We then present a simplified business model that allows assessing better price, possible demand, and the composition of the most profitable lotion under noncompetitive and competitive markets.

Relevant Skin Anatomy and Physiology Issues

Skin is composed of three different layers: the epidermis, the dermis, and the subcutaneous layer. The outer most layer is the epidermis, where most of the moisturizing effects

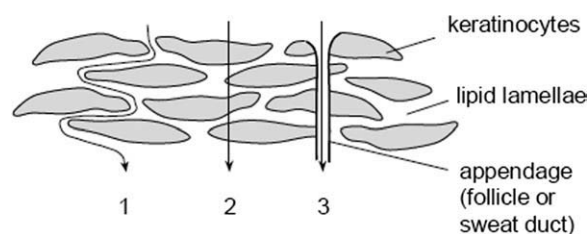


Figure 1. Transdermal transport pathways.¹⁴

takes place. In turn, this layer, is subdivided into several strata. From the inner to the outer layers, they are: Stratum Basale, Stratum Spinosum, Stratum Granulosum, Stratum Lucidum, and Stratum Corneum.⁹ As the cells move through these strata, they die losing their nucleus.

The stratum corneum (SC), the outer most layer is composed of ~20 layers of dead, anucleated cells, called corneocytes, embedded in a lipid matrix. Corneocytes are the protein-rich end products of keratinocyte differentiation, filled with a network of keratin fibers. During terminal differentiation, the plasma membrane of corneocytes is replaced with a tough, insoluble proteinaceous envelope. This layer around the corneocytes, which is called the cornified envelope, consists of cross-linked proteins.¹⁰

The corneocytes have two main roles in the permeability barrier: one role is to function as “spacers,” that is, they force water, microbes, and xenobiotics through the tortuous lipid-enriched extracellular pathway. The other one is their scaffold function for lamellar bilayer organization.¹¹ The corneocytes also contain natural moisturizing factors (NMF), composed by free amino acids and other small water soluble molecules, which are product of filaggrin protein degradation and anerobic metabolism, respectively.¹⁰ The NMF located in the SC are osmotically active and responsible for the absorption and retention of water.

The lipid matrix is mainly composed of ceramides, cholesterol, and free fatty acids (FFA). The lipids form multilayer lipid sheets with alternating strata of hydrophilic polar “heads” of the lipid molecules, aligned toward an aqueous phase, and lipophilic hydrocarbon chains aligned toward the inner of a lipid bilayer. The lamellar sheets are covalently bound to the cornified envelope by ω -hydroxyceramide, forming a lipid envelope that stabilizes the intercellular domain. In the outer desquamating layers of the SC, the well-organized structure is lost.¹⁰

The water content in a normal, healthy SC is around 30%.¹² SC hydration depends on the rates at which water reaches it from the tissue below and the rate at which it leaves the skin surface by evaporation as well as on the ability of retaining water. The small amount of water that travels through the SC, known as transepidermal water loss (TEWL), hydrates its outer layers to maintain its flexibility and provides enough water to allow enzyme reactions that facilitate SC maturation events, together with corneodesmolysis and ultimately desquamation.¹³ There are three routes of percutaneous transport through the startum corneum. These three pathways are illustrated in Figure 1.

Pathway 1 consists of intercellular diffusion through the lipid lamellae, Pathway 2 is transcellular diffusion through the keratinized proteins and the lipid lamellae and finally,

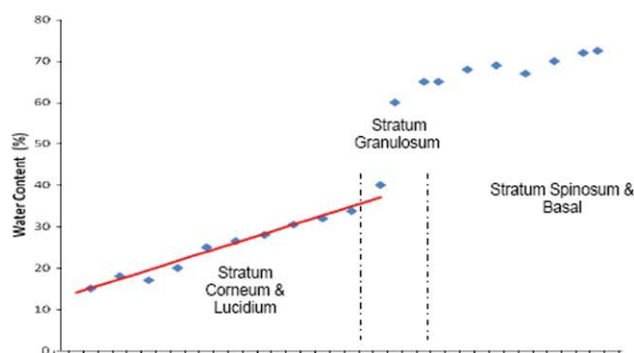


Figure 2. Water profile across human skin.

(Adapted from Ref. 18).¹⁸ [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Pathway 3 is characterized by diffusion through the skin appendages (i.e., hair follicles and sweat ducts). Because of the compactness of the intracellular matrix, transcellular absorption (Pathway 2) is a thermodynamically and kinetically impossible passageway for chemical transport.¹⁵ In addition, more recent experiments show a higher susceptibility for percutaneous absorption to occur via intercellular diffusion through the lipid lamellae.¹⁶ Thus, only the intercellular pathway was examined to determine the transdermal diffusion of the lotion's ingredients into the skin. Models of percutaneous absorption are based on the assumption that the skin is a homogeneous medium with a uniform permeability coefficient.¹⁴ Flynn¹⁵ showed experimentally that water permeability and diffusion depend heavily on the partition coefficient and the molecular weight. Thus, intercellular diffusion can be thought of as a process taking place in a three phase continuum.¹⁴

Water travels through the lipid bilayer primarily along the polar head group regions, which constitute a tortuous diffusion pathway, thereby increasing the distance that a water molecule would have to travel to completely traverse the SC. This "tortuosity" is thought to be an important aspect of the stratum corneum, which would be lost if there was a transcellular pathway.¹⁷ Finally, water acts as a plasticizer on corneocyte proteins giving elastic properties to the cells. Indeed, if deprived of water, dry skin is prone to crack open on mechanical stress. As atmospheric conditions vary enormously, the corneocytes are hydrated from bodily water lost through the barrier.¹³ Therefore, water gradients are established within the different layers of the SC. A typical water concentration profile is shown in Figure 2, where key features are emphasized. In this figure, the widths of these morphological regions are not drawn to scale and the vertical axis is percent water expressed as grams of water per total grams (water plus dry mass) of tissue.

The primary feature of the water gradient is the large discontinuity in the water content at the SC-stratum granulosum interface. This discontinuity starts after the last granular keratinocyte and accounts for ~50% of the water gradient across the epidermis. Thus, the gradient in the SC stretches from 15% at the skin surface to 40% at its innermost layer, compared with 80% within the granular layer, indicating that there is a significant barrier to water loss at the SC-stratum granulosum interface. These data suggest that a barrier to

water loss begins prior to the formation of the SC and is present within the granular layer.¹³ If we consider only to the SC gradient, it can be approximated as a linear gradient in the region between the outside environment and the SC-stratum granular interface.

The osmolytes or natural moisturizing factors (NMF), responsible for water retention capacity of the stratum corneum, are composed primarily of amino acids or their derivatives such as pyrrolidone carboxylic acid (PCA) and urocanic acid (UCA) (products of filaggrin protein degradation), together with lactic acid, urea, citrate, and sugars.¹³ They are present at high concentrations mostly within the corneocytes. However, a fraction of the NMF is also extracellular to the corneocytes, for example, the sugar fraction of NMF is probably derived from the processing of glucosylceramides whereas lactate and urea is largely derived from sweat and anaerobic glycolysis.¹³ The total free amino acid content of the corneocytes is on the order of 2 M, making them very hygroscopic.¹⁹ Thus, corneocytes that retain more water appear more swollen because they possess the highest concentration of these factors.¹³

Typical profiles of the major NMF components were measured in vivo by Caspers et al.²⁰ Figure 3 shows typical normalized profiles for Serine, Glycine, PCA, Arginine, Histidine, Alanine, and UCA. All these NMF components generated from filaggrin decrease in concentration toward the surface of the SC. In turn, because lactate is derived from eccrine sweat, it shows a gradient different from the amino acid derived from NMF components.¹³ Once it is released through sweat glands over the skin surface. Therefore, if we consider that it is not volatile, it cannot be vaporized there. Thus, maximum concentration is found on the skin surface,

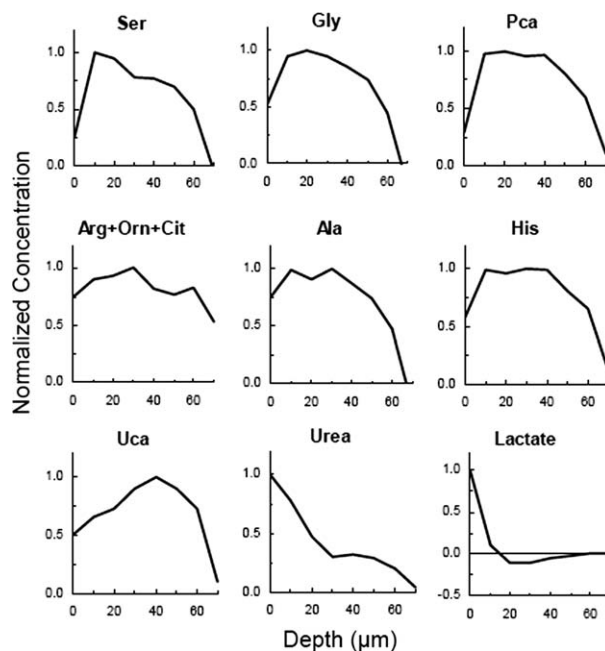


Figure 3. Typical in vivo concentration profiles of NMF and sweat constituents in the stratum corneum.

(Adapted from Ref. 20).²⁰

Table 1. Active Ingredients of Lotions

| Class | Function |
|------------|--|
| Humectants | Attract and bind water |
| Occlusives | Prevent loss of water from skin |
| Exfoliants | Promote dead skin removal |
| Emollients | Fill intercellular spaces on surface of skin |

and not somewhere else inside it as happens with amino acids. The same thing happens with the urea profile.

Influence of weather

There are not many studies that quantitatively measured SC water profiles in relation to skin condition.¹³ However, Warner and Lilly²¹ studied these differences between winter and summer. In summer, the SC water content drops to about 35% in the innermost corneocytes. This profile is largely maintained at over 25–35% water content except at the surface where it drops to 12%. In contrast, in winter, the SC does not maintain the higher water content after the mid-layers of the SC and is finally <10% in the outermost layers.¹³ It is clear that winter dry skin does not have the capacity to retain as much water as the normal-looking skin in summer, highly likely as a result of the reduced barrier lipids, reduced NMF levels, and decreased corneocyte size.

Desquamation

An important process, related to skin dryness that occurs in the SC is desquamation, which is the shedding of dead skin. By shedding a layer of skin everyday, the damaged cells are replaced by healthy cells.

Dry Skin Disorders

When the skin hydration falls below 10%, the skin becomes rough, dry, and develops a fine scale.²² When the skin hydration falls below normal values, the condition called Xerosis develops, which can be a result of a range of factors, including UV light, exposure to surfactants, and changes in the environment. They perturb in different ways the tight control of the various processes leading from profl-

laggrin synthesis to conversion to filaggrin and then to NMF.²³ In turn, Ichthyosis is a family of incurable genetically inherited disorders characterized by severely scaly skin. The most common form of it is ichthyosis vulgaris, which is thought to be caused by a post-transcriptional defect in the expression of proflaggrin, a histidine-rich protein that is proteolytically processed into flaggrin, which is in turn degraded into NMF during differentiation. It accounts for 95% of all ichthyosis cases and affects one in every 250 people in the US.²⁴

The treatment of Ichthyosis vulgaris involves the use of moisturizing lotions to restore the lipid bilayer of the SC, delivery of moisturizing agents to the skin as well as agents that promote desquamation. Moisturizers work in various ways: hydrating the SC directly by increasing the NMF content, or by sealing it off with occlusives (thick, greasy agents). Finally, to promote desquamation and increase water binding, keratolytic agents are used. These include α -hydroxy acids, such as lactic acid, glycolic acid, salicylic acid, urea, and propylene glycol.

Humidifying Lotions

Water alone cannot be used as an effective moisturizer because it forms a thin film that is very quickly lost by evaporation before it has the chance to penetrate into the skin. Thus, three approaches are used to moisturize the SC: (1) humectancy (to help retain water in the skin); (2) occlusion (to reduce water loss from the skin); or (3) emolliency (to mask the rough scaly condition).^{23,25} Finally, exfoliants are added to promote desquamation.

The types of ingredients can be further separated into two main categories: active and inactive ingredients. Active ingredients are the chemicals that help with the main function of the lotion: humidify and help desquamation (the contributors to its effectiveness). Inactive ingredients do not affect the function of the lotion, but they make it possible to use the active ingredients and contribute to some consumer preferences related to the application of the lotion. Table 1 lists the types of ingredients and their purpose. Table 2 lists ingredients and their function. We now describe each active ingredient family of compounds separately.

Table 2. Typical Active Ingredients

| Humectants | Occlusives | Emollients | Exfoliants |
|--|-------------|--|-------------|
| Glycerin (glycerol) | Mineral Oil | Sunflower Oil | Urea |
| Allantoin | Petrolatum | Almond Sweet Oil | Lactic Acid |
| PEG | Ceramide | Macadamia Nut Oil | Malic acid |
| Sodium-2-pyrrolidone carboxylate (PCA) | Beeswax NF | Hazelnut, Oil | |
| Propylene glycol | Dimethicone | Coconut Oil (76%) | |
| Urea | Cholesterol | Aloe Vera Oil | |
| Lactic Acid | Lanolin | Grapeseed Oil | |
| | | Acrylates/c10-30 Alkyl Acrylate Crosspolymer | |
| | | Isopropyl Palmitate | |
| | | Decyl Oleate | |
| | | Palm Oil | |
| | | Castor Oil | |

Table 3. Inactive Ingredients of Lotions

| Class | Function |
|---------------|--|
| Solvent | Contains and Disperses Ingredients |
| Thickeners | Increase viscosity |
| Preservatives | Prevent contamination by microbial organisms |
| Buffers | Adjust pH of moisturizer |
| Emulsifiers | Helps Mix Aqueous and Oil Phases |
| SC Lipids | Lipids naturally found in stratum corneum, help barrier recovery |
| Color | Usually white |
| Fragrance | Provide desirable scent |

Humectants

Humectants can be defined as compounds that will attract moisture to the skin. Some mimic the role of NMF in the SC and some are the same as the NMFs. Humectants widely used in moisturizers are glycerin, propylene glycol, PCA, lactic acid, and urea. Lactic acid belongs to the group of α -hydroxy acids. The water-binding capacity of the sodium salts of lactic acid and PCA appears to be higher than that of glycerin and sorbitol. Urea also has strong osmotic activity.²⁶ The water retained by humectants is primarily body water. The humectancy route can also attract water to the skin from the outside but only under high humidity conditions.²³

Occlusives

Occlusive agents work as a physical barrier, blocking the loss of water from the skin. They form a stable continuous film on the skin surface. Occlusives are composed basically by hydrophobic agents that form a film on the skin which reduces TEWL by preventing evaporation of water from the SC. Some examples are petrolatum, mineral oil, beeswax, lanolins, and oils.¹²

Emollients

Emollient is a word derived from the Latin adjective for soft (“molle,” i.e., soft or smooth). Their purpose is to make the skin smoother. They are mainly composed of lipids that are similar to the intercellular lipids of the skin and are likely refill the damaged lipid matrix. The combinations of fatty acids, ceramide, and cholesterol in the moisturizers help to repair lipid bilayers affected by soaps, solvents, and extreme dry/cold weather conditions by replacing key lipid

Table 5. Concentration Bounds

| Type of Ingredient | Min Concentration | Max Concentration |
|--------------------|-------------------|-------------------|
| Solvent | 65.00% | 75.00% |
| SC-Lipid | 0.00% | 35.00% |
| Emulsifiers | 1.00% | 20.00% |
| Humectants | 0.05% | 15.00% |
| Emollients | 0.05% | 15.00% |
| Preservatives | 0.10% | 10.00% |
| Fragrance | 0.00% | 0.25% |
| Occlusive | 0.10% | 10.00% |
| Thickener | 0.10% | 2.00% |
| Buffer | 0.00% | 2.00% |
| Exfoliants | 0.10% | 1.00% |

components.¹² Examples of widely used emollients are lanolin, glyceril sterates, and glycol palmitate.

Exfoliants

An exfoliant assists in the removal of surface dry, scaly patches from the surface. This process creates a smoother surface composed of cells that are more hydrated than the dry scales that were removed.²⁷ It has been proposed that glycerin aids the digestion of the superficial desmosomes and thereby ameliorate dry flaky skin. Furthermore, α -hydroxy acids, such as lactic acid and glycolic acid, might be useful in moisturizers because of their influence on the flexibility of SC and removal of superficial scales.²⁶

Clearly, a compound may act as both humectant and exfoliant: Urea and lactic acid are two common compounds that have these two different features when applied over the skin. Some oils act as both emollients and occlusives.

Inactive ingredients can vary considerably. Some examples of their purpose/function are shown in Table 3. The corresponding ingredients are shown in Table 4. We discuss most of them later.

FDA Classification

According to the Food and Drug Administration (FDA), cosmetics are defined as, “... articles intended to be applied to the human body for cleansing, beautifying, promoting attractiveness.”²⁸ Skin moisturizers are considered cosmetic products as long as the concentration of ingredients stays below the Cosmetic Ingredient Review (CIR) allowed limits (Table 5), thus removing any jurisdiction of the FDA for the ingredients used.

Table 4. Typical Inactive Ingredients

| Solvent | Thickeners | Preservatives | Buffers | Emulsifiers | Lipids | Colorants | Fragrance |
|---------|-------------------|-----------------------------|-------------|----------------------|-------------------------|------------------|--------------------|
| Water | Sorbitol | Rice Bran Oil | Citric Acid | Sorbitan Monolaurate | γ -Linoleic Acid | TiO ₂ | Hazelnut Fragrance |
| | Glyceryl Stearate | Disodium EDTA | TEA | Cetearyl Alcohol | | | |
| | Oleic Acid | Potassium Sorbate | NaOH | Cetyl Alcohol | | | |
| | Stearic Acid | Vitamin C (L-Ascorbic Acid) | Maleic Acid | | | | |
| | Xanthan Gum | Phenoxyethanol | | | | | |
| | Carbomer | Methylparaben | | | | | |
| | Isostearic Acid | Propylparaben | | | | | |

Table 6. Consumer Properties used in the Consumer Preference Model

| Consumer Properties |
|---------------------|
| Effectiveness |
| Thickness |
| Greasiness |
| Smoothness |
| Creaminess |
| Spreadability |
| Absorption Rate |

Lotion Manufacturing

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.²⁹ The oil-in-water emulsions, which are less sticky on application, predominate in the market and is 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. 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 post-treatment 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.

Consumer Preference Model

We first start with defining the consumer preference score of product i (H_i) as a weighted average of normalized scores of different consumer related “properties” ($y_{i,j}$):

$$H_i = \sum y_{i,j}w_j \quad (1)$$

where w_j are the weights.¹ The scores are typically defined in the range from zero to one. It is important to notice that these are properties defined in plain terms and assessed by consumers by comparison to existing products. In the particular example of lotions, these properties are shown in Table 6. For the purpose of maintaining the analysis simple, some properties are omitted (color, fragrance, etc.). We believe this simplification does not make the example too simple (the features left aside can be manipulated independently for the most part) and most important, it does not interfere with the goals pursued here, which are the illustration of the product design methodology under price competitive and noncompetitive conditions, rather than identifying the right lotion for any particular market. We now discuss each of these in detail, including ways the consumer assesses them.

Approximately, 100 potential consumers were asked to rate the lotions properties outlined in Table 6 using an informal survey. At the end of the survey, the participants were asked to specify the relative importance of each property to them. The results of the relative importance of each property are shown in Table 7. The consumer rated their first preference,

second preference, third preference, etc., on each of the seven properties assessed in this lotion, by distributing 100 possible points among them. The relative importance of each one was then determined using the mean values of the points assigned.

In turn, to establish the preference score for each property, a test the consumer would conduct to rate the property from one extreme to the next (i.e., very thin to very thick, not greasy to very greasy, etc.) was crafted. Next, the consumer rated property (large, small, poor, etc.) is connected to a physical property of the lotion (viscosity, surface tension, concentration of insolubles, etc.), all of them in turn related to the concentrations of all ingredients and drop size. All the consumer preference weights and scores are a reflection of informal surveys conducted by the authors and although they are not scientific they were considered appropriate to illustrate our procedure. We are aware that more elaborate surveys ought to and in fact are made in real product preference assessment. We now illustrate this process for each property.

Because our article is mostly aimed at studying the influence of microeconomics in the decision making, we simplified the connections between properties and variables, picking the most relevant ones. We believe that, even at this level of simplicity, which does not require as much time as a detailed study, one can discover important facts about the product one is designing. Such rapid decision making, especially at early stages of the stage-gate process are of value.

Effectiveness

The effectiveness of a lotion is based on how well the lotion can treat the skin problems associated with Xerosis and Ichthyosis Vulgaris. As previously mentioned, the problems people face with these two conditions include:

- Severely dry skin
- Thickened skin
- Dismantled lipid bilayer

As noted above, the skin hydration layer in the SC, the outer most layer of the skin is normally around 30%.²³ When the skin hydration level falls below 10%, the skin becomes severely dry and chapped.²² Not only is keeping the skin hydration level around 30% important for an esthetically pleasing skin, but when the skin is adequately hydrated the desquamation process remains active, the skin acts as an effective barrier against infection.³⁰ When the desquamation process is hindered, dead skin cells are not renewed from the stratum corneum leading to a build up of dead skin cells, which causes the skin to thicken. The lipid bilayer surrounds hydrophilic cells to retain water within the skin. When the

Table 7. Weights Attributed to Each Consumer Property According to Informal Surveys

| Consumer Property | Weight |
|-------------------|---------|
| Effectiveness | 24.49% |
| Thickness | 10.52% |
| Greasiness | 11.41% |
| Smoothness | 14.55 % |
| Creaminess | 15.08 % |
| Spreadability | 10.18% |
| Absorption rate | 13.76% |

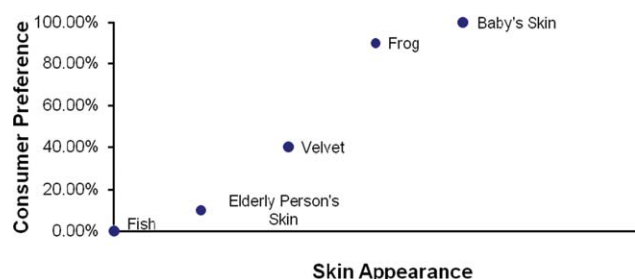


Figure 4. Consumer preference for skin appearance.

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

lipid bilayer is dismantled or ruptured, moisture from the skin is able to escape into the environment by TEWL.²⁵

We consider that the SC's water content gradient remains constant under the same environmental conditions (humidity and temperature). Thus, the water that is kept outside the corneocytes is always the same, no matter if we are discussing a healthy or unhealthy skin, since the amount of water that reaches the SC from the inner layers (and we assume a body water content constant) and the amount of water that leaves the skin surface by evaporation (which we will assume that is in equilibrium with the air humidity) are similar. The difference between a healthy and diseased skin would reside in the presence or absence of NMF. The gradient of water would be the same for both, but the water retention capacity different: "healthy" corneocytes would have the ideal amount of NMF and, then, the ability to "hold" water inside it. On the other hand, a damaged skin would be characterized by depleted NMF and, consequently, less hydration.

Assuming that the ingredients used to "replace" NMF (the active ingredients known as humectants, like glycerin, allantoin, PEG, and sodium PCA) will quickly diffuse through skin and will be quickly absorbed (which is quite common), the only problem, then, is to determine the adequate amount of humectant that need to be added to the SC, the rate being thus of little importance. Also, we are assuming that all we need is a specific amount of NMF, no matter which NMF is chosen. It means that, in a moisturizing lotion, we do not need to replace all the amino acids that are depleted. Instead, the importance resides in adequately

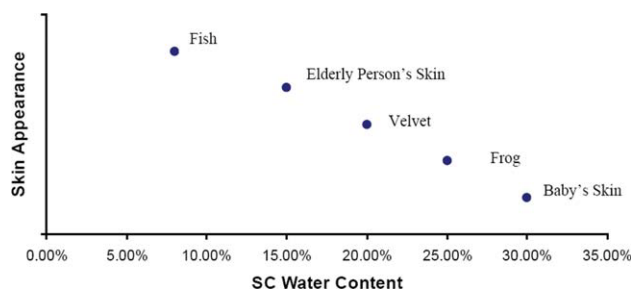


Figure 5. SC water content related to the skin appearance.

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

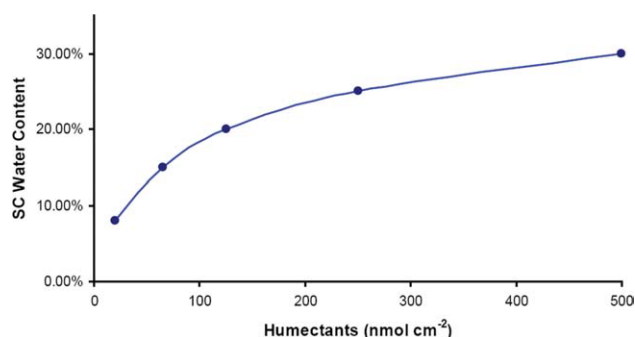


Figure 6. SC water content as a function of humectants applied.

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

replacing quantitatively the NMF, and not necessarily qualitatively. All the matter of effectiveness of a lotion would be to quantify and, then, correctly replace the depleted NMF. We consider this a simplifying assumption that helps us make progress in preliminary studies, one that does not substantially alter results and one that can be expanded later. Besides, targeting each individual NMF would require patient specific ingredients that are not possible in an over the counter lotion. Although water content is not the only property that determines skin appearance, we are assuming this is the most important one in general and in relation to the skin disorders we are treating, in particular. A multivariable analysis ought to be performed, but is not the objective of the article. In addition, to be effective in treating Ichthyosis Vulgaris, a lotion should be able not only to promote hydration but also to help in desquamation process. However, once the main active ingredients added to a lotion promote both hydration and desquamation, we assume the effectiveness of exfoliants and humectants as being the same (and, in fact, the common ingredients associated with these functions—urea and lactate—promote both).

To relate the consumer preference to physical properties, we need first that they describe their "preference." Figure 4 illustrates the results as they are related to effectiveness. In turn, skin appearance can be correlated to the SC water content. As stated above, a typical human SC hydration is between 10% and 30%.³⁰ Then, assuming a linear relation, a fair assumption, we obtain the results of Figure 5.

In turn, the SC water hydration is related to the lotion concentration of humectants/exfoliants. Three types of water with different molecular mobility can be found: for a water content below 10%, the primary water is tightly bound, presumably to the polar sites of the proteins or to the intercellular regions. When the degree of hydration exceeds 10%, the secondary water is hydrogen-bounded around the protein-bound water, and above 40–50%, the water resembles the bulk liquid. The amount of tightly bound water, which does not seem to have any plasticizing effect, is almost the same in different types of pathological skin, whereas the amount of secondary water, accounting for the elasticity, is much smaller in the SC from psoriatic patients and from elderly persons with xerosis than in normal SC.²⁶ Thus, one could expect that once the correct amount of NMF in a lotion is

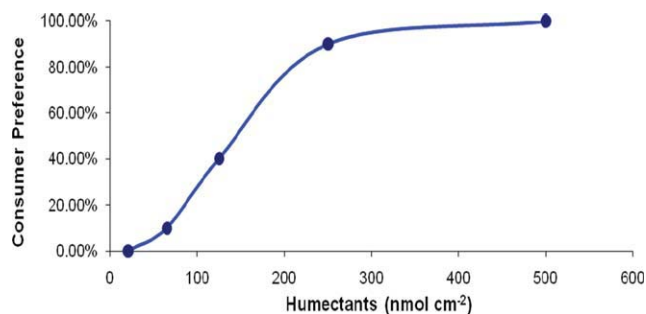


Figure 7. Consumer preference for effectiveness vs. the amount of humectants applied.

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

included, the consumer will be satisfied. Even if more humectant is added, more water cannot be “hold” and the consumer preference will not change.

Nakagawa et al.³¹ found that 500 nmol of NMF applied to 1 cm² of skin is about five-fold the level of NMF in the SC. Assuming that, with this amount, the skin would be fully hydrated (around 30%) and that, if more is added, little is changed, we can correlate the SC water content to the amount of NMF applied on skin. The result is shown in Figure 6. The last step to evaluate effectiveness is to correlate the consumer preference to the amount of NMF applied on the skin. The result obtained is shown in Figure 7. The amount of humectants/exfoliants applied to 1 cm² of skin is then related to their concentration in the lotion. We use a typical value of amount of lotion applied of 2 mg/cm².³²

Thickness

The thickness of a lotion is an important property that can be related to the lotion’s efficiency, stability, and consumer acceptability. For the majority of end users, the thickness of a product is easily recognized but very difficult to define.²⁵ Cussler and Moggridge² explain that the notion of thickness for consumers stems from rubbing the fluid in between two fingers applying preset values of pressure and velocity and measuring the height of the fluid layer. This is related to viscosity, which can be determined by using various relationships between the dispersed phase viscosity and the continuous phase viscosity.

Emulsions contain an emulsifying agent which has two principal functions: to decrease the interfacial tension between oil and water, thereby enabling easier formation of the emulsion; and also to stabilize the dispersed phase against coalescence once it is formed. Emulsions can be either oil-in-water (O/W) type (oil is the dispersed phase) or

water-in-oil (W/O) type (the opposite).³³ In the case of lotions, the insolubles conform the disperse phase (droplets), whereas the continuous phase contains the ingredients that are soluble in aqueous solutions.

To evaluate the consumer preference of thickness, consumers were asked to classify the lotion thickness in comparison with some daily (and well known) fluids. In more elaborate surveys, they may be asked to place a designated amount of fluid on pad of thumb and then rub it between thumb and index finger in a lateral motion. Finally, they are asked to rate how they would prefer a lotion to be. Table 8 shows the viscosities used for comparison and the consumer perception. The result of the normalized consumer preference in comparison with “Thick as ...” is shown in Figure 8. This Figure 8 reveals that consumers prefer a lotion that appears to be neither too thin nor too thick.

Now, it is necessary to relate the consumer preference to the corresponding physical property: viscosity. To establish the correct connection we resort to an explanation given by Cussler and Moggridge.² When one rubs a cream or lotion over a skin, the force per unit area is given by the well known relation

$$\frac{F}{A} = -\eta \frac{dv}{dy} \quad (2)$$

where A is the area of the fingers, η the viscosity, v the fluid velocity, and y the distance normal to the skin. If we approximate the derivative linearly, assuming zero velocity at the skin and velocity v at the cream surface $y = h$, then we write

$$\frac{F}{A} = -\eta \frac{v}{h} \quad (3)$$

The area A is constant and following Cussler and Moggridge² we find that h is proportional to $\eta^{0.5}$. Thus, because the comparison should be done at the same finger velocity v (constant velocity), we can rewrite the equation above in the following way:

$$\text{Thickness} \propto (\text{“assessments of viscous”}) A \frac{\eta v}{\eta^{0.5}} B \eta^{0.5} \quad (4)$$

where A is a proportionality constant and $B = Av$. This means that, in fact, the assessments of “thickness” is proportional to the square root of viscosity.

Since the lotion is an oil-in-water (O/W) emulsion, the determination of the viscosity involves several steps. The

Table 8. Viscosity Consumer Perception and the Fluids Used for Comparison by Consumers

| Viscosity (Poise) | Consumer Perception | As thick as |
|-------------------|---------------------|----------------|
| 3700 | Extremely Thick | Toothpaste |
| 640 | Moderately Thick | Dishwashing |
| 85 | Moderately Thin | Salad Dressing |
| 19 | Extremely Thin | Coffee Cream |



Figure 8. Consumer preference for thickness comparing the lotion to different products.

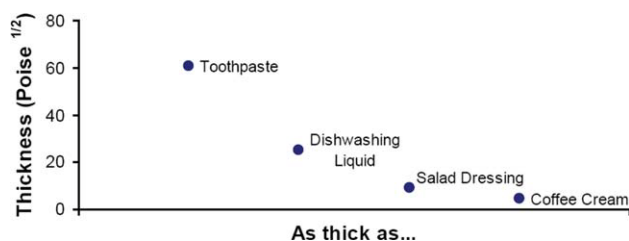


Figure 9. Thickness of different fluids.

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

first step is to list the viscosities of all the ingredients that we intend to use in our lotion and obtain the viscosity of each phase (mixing rules can be used). To determine the overall viscosity of the lotion, the Yaron and Gal-Or equation can be used (retrieved from Pal³³):

$$\eta = 1 + I(\lambda) = 1 + \frac{5.5[4\lambda^7 + 10] - \left(\frac{84}{11}\right)\lambda^2 + \left(\frac{4}{\kappa}\right)(1 - \lambda^7)}{10(1 - \lambda^{10}) - 25\lambda^3(1 - \lambda^4) + \left(\frac{10}{\kappa}\right)(1 - \lambda^3)(1 - \lambda^7)} \quad (5)$$

where η is the overall viscosity of the lotion, λ is the cubic root of the volume fraction (ϕ) of the dispersed (oil) phase, κ is the ratio of the viscosity of the dispersed phase to the viscosity of the continuous (water) phase, and I is a function of λ .

It is important to notice that this volume fraction might be related also to the method of production and dispersion of the oil phase in the aqueous phase. However, most frequently used models do not take into account the droplet size distribution.²⁹ Thus, we assume that the oil droplets are homogenous and equally distributed in the lotion. Overall, for concentrated emulsions, the cell model of Yaron and Gal-Or gives reasonable predictions of relative viscosity over a wide range of κ and ϕ .³³ Also, to optimize the droplet size, we need to deal with the shear forces applied in the production mixing and equipment (e.g., colloid mill). In colloid mills, the shear-rate depends on the rotational speed, rotor radius, and the gap width between the stator and rotor.²⁹ Consequently, they are important for estimating the energy input. On the other hand, once we plan to maximize consumers' preference by varying the concentrations of the compounds, we will assume that the size of the desired droplet is achieved with the equipment we have. Some experi-

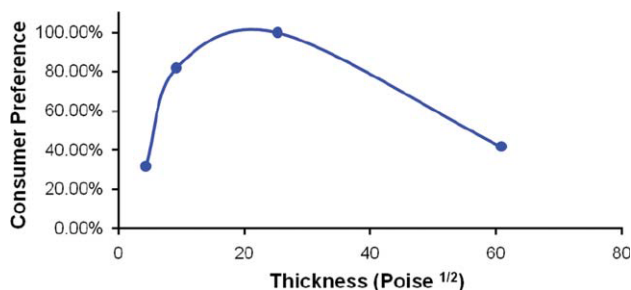


Figure 10. Consumer preference as a function of the thickness of the lotion.

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

Table 9. Concentration of Fatty Oils, Consumer Perception and Comparison Fluids

| Concentration of Oils (% w/w) | Consumer Perception | As grease as... |
|-------------------------------|-----------------------|-----------------|
| 30 | Very Greasy | Grease |
| 20 | Moderately Greasy | Baby Oil |
| 10 | Moderately not-Greasy | Suntan Lotion |
| 5 | Not Greasy | Alcohol |

mental evidence for the droplet size independence of relative viscosity is shown in Pal.³³

Now, the thickness of the fluids used for comparison are shown in Figure 9 and the result of normalized consumers' preference as a function of thickness is shown in Figure 10. Finally, thickness is a function of the ingredients concentration that can be obtained with the above formula.

Greasiness

Greasiness is a property that reflects the oiliness of the skin after a lotion is applied. Fatty oils used as emollients generally consist of glycerides, chemicals that contain glycerols (about 10%), and fatty acids (90%). Greasiness on the skin can be determined by visual and tactile signals. The changes in oil phase components suggested to improve rub-in may increase the greasiness, whereas increasing the water phase may reduce greasiness.³⁴

Oily materials, such as emollients and fatty oils, are esthetically unsatisfactory to consumers and an excessiveness of oils on the skin can lead to swelling and inflammation to the SC. The greasiness of the lotion is easy to measure and can be determined simply by knowing the concentration of insolubles/oils in the lotion.

Consumers were interviewed and asked how greasy they would like a lotion to be. The test was made by comparison with some well-known substances. The concentrations of oils and the consumer perception of it are shown in Table 9. In Figure 11, the consumers preference for different levels of greasiness in comparison to other fluids is shown. There is a maximum: consumers prefer a lotion that is not so greasy as a baby oil, nor so "dry" as alcohol.

To have the consumers preference related to the physical property "concentration of insolubles," we need to know the concentration of insolubles in the fluids used for comparison. This is shown in Figure 12. In Figure 13, the consumer preference is shown as a function of the concentration of



Figure 11. Consumer preference for greasiness comparing the lotion to different products.



Figure 12. Oil concentration of different fluids.

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

insolubles and the plot can be used to predict the consumers' preference based on oil concentration.

Smoothness

The smoothness of a lotion is mainly related to the perception of applying a lotion without feeling granules or other particles. The ideas about smoothness of emulsions come primarily from the sensory characterization of foods. Since the 1980s, the smoothness of liquid and semi-solid food has been shown to be closely (and inversely) related to friction forces.³⁵ Because the skin is a surface itself, it is convenient to analyze and describe it in terms of a surface phenomenon, such as friction. We can state that the greater the friction forces needed to apply a lotion, the smaller the feeling of smoothness. The smoothness, therefore, is inversely proportional to the coefficient of friction (μ):

$$\text{Smoothness} \propto \frac{1}{\mu} \quad (6)$$

However, to evaluate our lotion, we need to correlate the friction coefficient to a range of values of one or more components. Nacht et al.³⁶ and Sivamani et al.³⁷ studied the effect of greasiness of different lotions in the coefficient of friction of skin. From not greasy to very greasy, they proved that increasing the greasiness, there is a decrease on the coefficient of friction, as can be seen in Figure 14.

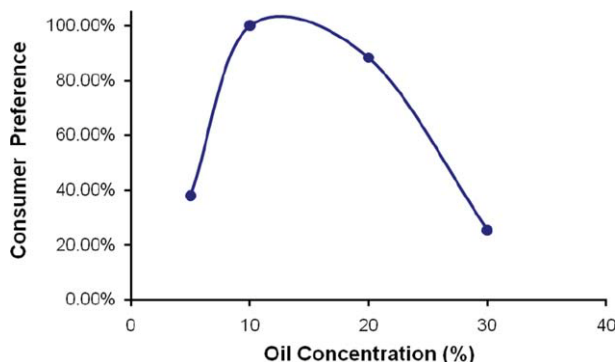


Figure 13. Consumer preference as a function of oil concentration.

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

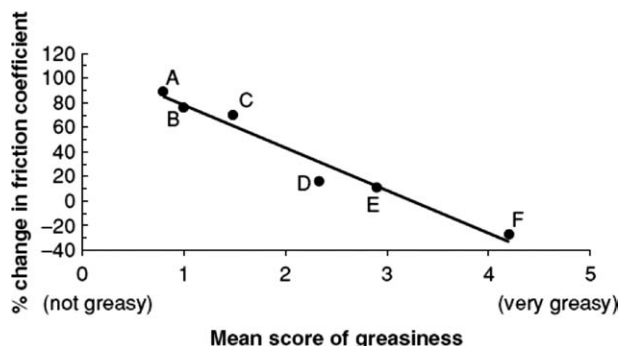


Figure 14. Change in coefficient of friction vs. greasiness.

(Adapted from Ref. 36).³⁶

Summarizing, smoothness depends directly on the greasiness or oiliness of the lotion and inversely on the coefficient of friction of the skin. A mean value of 0.4 can be assumed, as reported by Sivamani et al.³⁷ Thus, using Nacht et al.³⁶ plot (Figure 14), assuming a greasiness of 0%, 5%, 10%, 20%, and 30% for numbers 0, 1, 2, 3, and 4 in the plot above, respectively, we can write:

$$\begin{aligned} \% \text{ Change in coefficient of friction} \\ = -0.0472 * \text{Greasiness} + 1.0606. \quad (7) \end{aligned}$$

The values of greasiness used for comparison are shown in Table 10. In Table 11, there are the different rates used for interviewing consumers. It is worth noticing that, once we deal with smoothness of application of a lotion, the comparison "as smooth as" is related to consumers' perception of the surface over that they are applying the lotion. Friction coefficients depends on surfaces interactions and must always be related to two surfaces. In our case, it is the skin and the lotion. The consumer preference as a function of the feeling of different surfaces "as smooth as ..." is shown in Figure 15. As expected, the smoother the feeling of application, the bigger the consumers' preference. The smoothness

Table 10. The Smoothness as a Function of Coefficient of Friction

| Greasiness (%) | Percentual change in coefficient of friction | "New" coefficient of friction* | Smoothness |
|----------------|--|--------------------------------|------------|
| 30 | -0.3554 | 0.25784 | 1.93918 |
| 20 | 0.1166 | 0.44664 | 1.11947 |
| 10 | 0.5886 | 0.63544 | 0.78685 |
| 5 | 0.8246 | 0.72984 | 0.68508 |

Table 11. Consumer Perception of Smoothness

| Smoothness | Consumer Perception | As smooth as... |
|------------|---------------------|-----------------|
| 1.93918 | Very Smooth | Baby's Skin |
| 1.11947 | Moderately Smooth | Cotton |
| 0.78685 | Moderately Rough | Carpet |
| 0.68508 | Very Rough | Lizard |

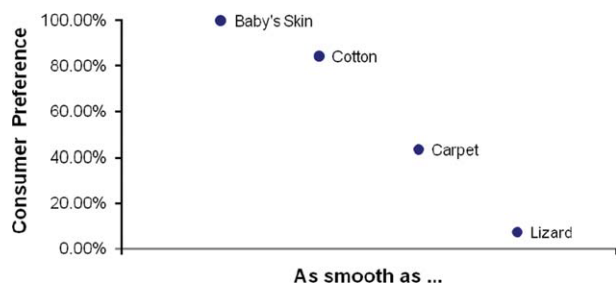


Figure 15. Consumer preference for smoothness comparing the skin to different surfaces.

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

of the surfaces used for comparison is plotted in Figure 16. Finally, Figure 17 can be used to predict consumers' preference as a function of smoothness of the lotion. As we can see from Table 10, this smoothness is related to greasiness.

Creaminess

The creaminess of a lotion can be regarded as a metadescriptor, that is, a composite of other independent descriptors³⁸ and has been mainly associated to smoothness and thickness by Kokini et al.³⁹ as follows:

$$\text{Creaminess} = (\text{Thickness})^d \times (\text{Smoothness})^b. \quad (8)$$

The studies of the creaminess of oil in water emulsion systems has been primarily related to viscosity and to a lesser degree the volume fraction of oil.⁴⁰ These ideas came from the sensory descriptions of food creaminess, like the work of Janohj et al.,³⁸ who evaluate the sensory properties of a yogurt. As stated by the same authors, the size of the oil droplets has not been found to affect the sensory perception of creaminess significantly. Akhtar et al.⁴⁰ were the first to suggest that the creaminess perception appeared to be more enhanced by a higher viscosity than by a higher volume fraction of oil. Akhtar et al.,⁴¹ while studying butter fat-in-water emulsions, proved that creaminess and thickness were strongly correlated and attributed to samples of higher viscosity. Kokini and Cussler³⁵ suggested that the creaminess of some semi-solid foods can be evaluated by the following expression:

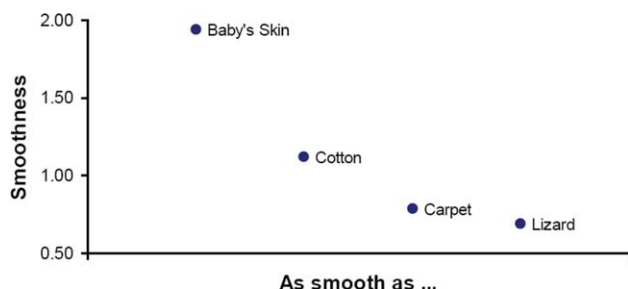


Figure 16. Smoothness of different products.

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

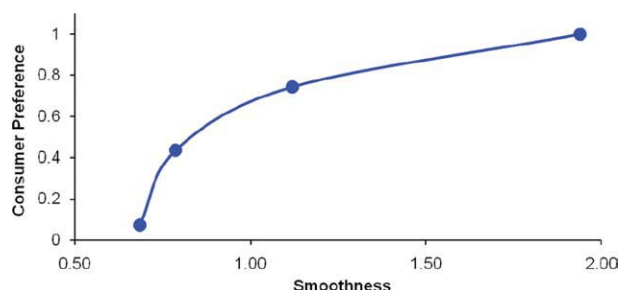


Figure 17. Consumer preference as a function of smoothness.

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

$$\text{Creaminess} = [(\text{Thickness})^{0.54} \times (\text{Smoothness})^{0.84}]. \quad (9)$$

We adapt this function to the case of our lotion, as has been suggested by Cussler and Moggridge.²

Creaminess as perceived by the consumers can be assessed, for example, by asking them to swirl one of their finger in a container of lotion and then rate the creaminess. Also, it can be evaluated by asking consumers to compare the creaminess of different materials and then rate how they would like a lotion to be. The results of consumers' preferences in comparison ("As creamy as ...") to different foods are shown in Figure 18. The creaminess of these foods used for comparison is shown in Figure 19. Finally, the consumer preference as a function of creaminess is shown in Figure 20.

Spreadability

Spreadability can be categorized as another dimension of wetting called spreading wetting and is a property that identifies the ease of a fluid to displace another fluid on a given surface. In the consumer's point of view, spreadability can also be defined as "Slip," which expresses how the product glides across the skin. As explained by Barton,³⁴ a moisturizer for skin will require a degree of slip to prevent putting a dry skin under undue stress application. Esters are among the best sources of slip in a formulation, but mineral oils and silicones are also important Barton.³⁴

Spreading wetting can be differentiated if the spreading occurs spontaneously or not.⁴² For spreading to occur



Figure 18. Consumer preference for creaminess comparing the lotion to different foods.

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

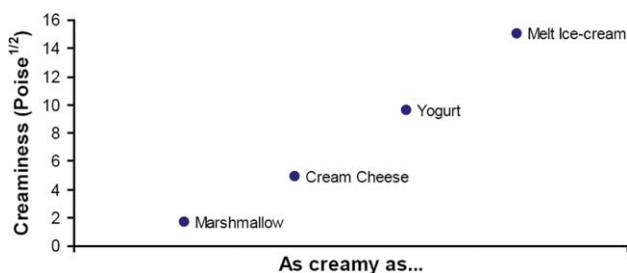


Figure 19. Rate of creaminess of the foods used for comparison.

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

spontaneously, the surface free energy has to decrease throughout the spreading of a fluid. Thus, spontaneity and free energy are connected. In turn, the surface free energy is given by:

$$\Delta G_w = -A[\gamma_{SA} - (\gamma_{SL} + \gamma_{LA})] \quad (10)$$

where ΔG is the total decrease in surface free energy due to spreading wetting, A is the interface area, and γ is the surface tension of the skin-air interface (SA), skin-lotion interface (SL), and the lotion-air interface (LA). Thus, the more negative is ΔG the higher the tendency to spread will be. So, the spreading coefficient, $S_{L/S}$, which is related to $-\Delta G$ can be rewritten using Young's equation as follows:

$$S_{L/S} = \gamma_{LA}(\cos \theta - 1). \quad (11)$$

Because $(\cos \theta - 1)$ is always negative $S_{L/S}$ is always negative. It means that the cohesive force is greater than the adhesive force and the formation of liquid lenses occurs.²⁵

Table 12 describes the correlation made between the spreading coefficient and the contact angle. It is important to notice that, as can be seen in Eq. 11, the spreading coefficient depends both on the surface tension and contact angle. The surface tension of our lotion is a function of the composition. Thus, we assess consumer preferences just as a function of the contact angle (which, in turn, is also a function of composition) and compare the relative spreading capabilities. Finally, once the lotion's surface tension is found, one

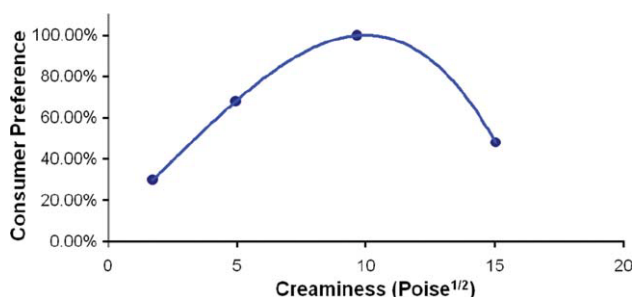


Figure 20. Consumer preference as a function of creaminess.

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

Table 12. Spreading Capability and Consumer Perception as a Function of the Contact Angle

| Contact Angle | Spreading Capability | Consumer Perception | As spreadable as... |
|---------------|----------------------|---------------------|---------------------|
| 180° | 0.00% | No Spreading | Glue |
| 150° | 6.70% | Little Spreading | Syrup |
| 120° | 25.00% | Some Spreading | PeptoBismol |
| 90° | 50.00% | Fair Spreading | Liquid Detergent |
| 60° | 75.00% | Large Spreading | Ketchup |
| 30° | 93.30% | Strong Spreading | Vegetable Oil |
| 0° | 100.00% | 100% Spreading | Water |

can also find the contact between the lotion and the skin and then predict the spreadability.

The contact angle between the lotion and the skin can be predicted using Young's equation for the contact between a liquid and a solid surface, as follows:

$$\cos \theta = \frac{\gamma_{SA} - \gamma_{LS}}{\gamma_{LA}} \quad (12)$$

where γ_{SA} represents the surface tension of the skin-air interface (and we will assume a mean value of 27 dyne/cm, taken from Kyat et al.⁴³), γ_{LS} is the interfacial tension between the lotion and the skin, and γ_{LA} is the surface tension of the lotion-air interface.

Knowing the surfaces tension of all the compounds (we estimated them using Escobedo and Mansoori⁴⁴), we can predict the surface tension of the emulsion. However, we still do not have the interfacial tension between the skin and the lotion. The last one can be approximate by:

$$\gamma_{LS} = \gamma_{SA} + \gamma_{LA} - 2(\gamma_{SA}\gamma_{LA})^{1/2}. \quad (13)$$

Figure 21 shows the results of the survey. Participants were asked to compare a lotion spreadability to that of different well-known substances (glue, syrup, PeptoBismol, liquid detergent, ketchup, vegetable oil, and water) and then rate their preferences. This property could also be assessed, for example, by asking consumers to take a designated amount of lotion, measure the distance the fluid travels in a period of time, and then rate it based on preferences.

To evaluate and relate the consumer preference to contact angle, we need first to relate the substances used for comparison with the contact angle. This is shown in Figure 22.

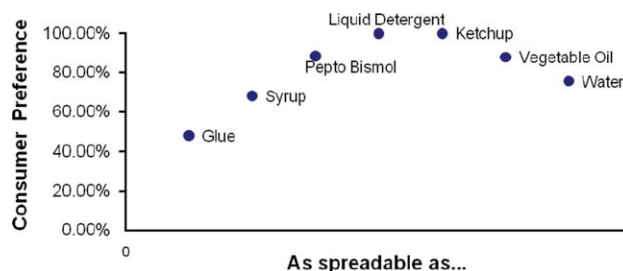


Figure 21. Consumer preference for spreadability comparing the lotion to different products.

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

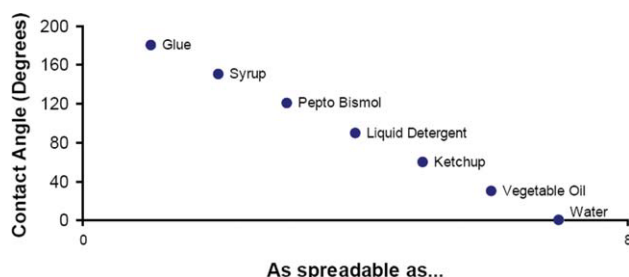


Figure 22. Contact angle of different substances used for comparison.

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

Finally, we can predict the consumer's preference as a function of the contact angle with the plot of Figure 23.

Absorption rate

Absorption rate is the property described by Barton³⁴ as rub-in. It is related to the ease or speed with which a product disappears on application. The absorption rate for the lotion is reflective of the steady state diffusion time necessary for percutaneous absorption to occur. According to the diffusion correlation proposed by Ho,¹⁴ the absorption rate (t_{sc}) of the lotion is a function of the mass flux of chemicals into the bloodstream (m_{sc}) and the amount of mass transferred per unit area (Q_{sc}). The mass flux of the lotion's ingredients through the epidermis can be determined using the solution of the diffusion equation proposed by Ho¹⁴ and the time to "steady state." The result is given by:

$$t_{sc}^* \approx 0.45 \frac{L_{sc}^2 R_{sc}}{D_{sc}} \quad (14)$$

where L_{sc} is the depth of SC, D_{sc} the effective diffusivity, and R_{sc} the retardation factor. Thus, the steady-state time is inversely proportional to the diffusion coefficient, which depends on the chemical characteristics of the compounds present in the lotion. Knowing this diffusion coefficient and the retardation factor of all the compounds of our lotion, we are then able to calculate the time necessary for complete rub-in.

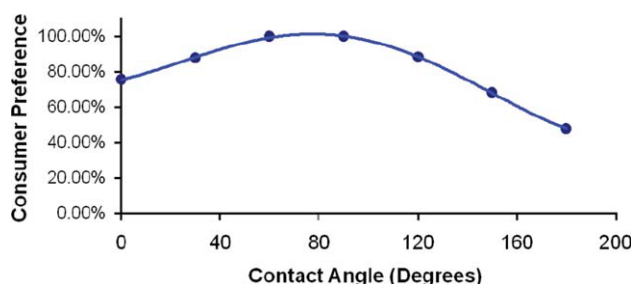


Figure 23. Consumer preference of spreadability as a function of the contact angle.

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

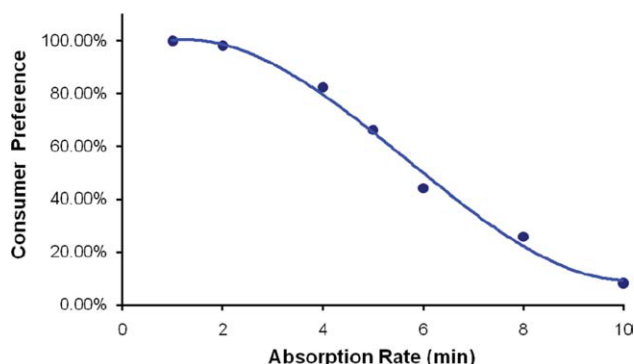


Figure 24. Consumer preference as a function of the time to reach steady state.

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

We show the consumer preferences obtained through our survey in Figure 24. A lotion that takes no time to a little over 2 min to absorb is the most preferred.

The Best Lotion

We retrieved the "Super Moisturizing Lotion" from the Cosmetic and Toiletry Formulations Database⁴⁵ and used it as a starting/reference point. Then, using all the information provided earlier, we were able to vary in a certain range the concentration of each ingredient, to find the composition that would give the largest preference to consumers. The optimized formulations were obtained by iterative numerical method using Microsoft Excel Solver. Table 13 shows the composition of the best lotion, regardless of price when using the same ingredients. We found a preference of 78.7% and 80.3% for the original and optimized formulation, respectively.

Different compounds were added to the model to try to identify a lotion with a better preference. The result for these enlarged list of ingredients is shown in Table 14. Even varying the ingredients, it was not possible to achieve more than 82% preference in this case. In some cases, the product that gives 100% preference is possible, like the carpet deodorizers designed with this same methodology by Street et al.,⁵ but not in this case.

Competition

We now looked at one competitor (Table 15). A preference of 79.96% was achieved for this competitor.

Business Model

To determine demand as a function of price, we use the constant elasticity of substitution demand model presented by Bagajewicz.¹

$$p_1 d_1 = \left(\frac{\alpha}{\beta} \right)^\rho p_2 \left[\frac{Y - p_1 d_1}{p_2} \right]^{1-\rho} d_1^\rho \quad (15)$$

$$d_2 = \frac{Y - p_1 d_1}{p_2} \quad (16)$$

Table 13. Composition of Original and Optimized Formulation of Our Lotion

| Ingredient | Function | Reference Formulation | Optimized Formulation |
|--|----------------------------|-----------------------|-----------------------|
| Deionized Water | Solvent | 74.50% | 65.00% |
| glycerin (glycerol) | Humectant | 5.00% | 0.00% |
| Sodium PCA (50%) | Humectant | 3.00% | 5.00% |
| Mineral Oil | Occlusive | 3.00% | 3.04% |
| Isopropyl Myristate | Emollient | 2.00% | 0.00% |
| Hydrogenated Polyisobutene (polysynlane) | Emollient | 4.00% | 6.65% |
| Xanthan Gum | Thickner | 0.50% | 2.00% |
| Cetyl Alcohol | Emulsifier | 2.00% | 6.90% |
| Sorbitan Palmitate | Emulsifier | 1.20% | 0.00% |
| Polysorbate 40 | Emulsifier | 3.80% | 10.53% |
| Titanium Dioxide | Cosmetic Pigment | 0.00% | 0.88% |
| Citric Acid | pH adjuster | q.s | q.s |
| Other components | Preservative/dye/fragrance | q.s. | q.s |
| Total Sum | — | 99.00% | 100.00% |
| Consumer Preference | — | 78.7% | 80.3% |

where β is the ratio of the competitor's preference score to the new lotion score (H_2/H_1) measuring how much more the consumer prefers Product 2 over Product 1, α is the level of awareness of the new product (0 when consumers are not aware of the new product and 1 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 ρ is a parameter related to the elasticity. We use $\rho = 0.75$ and consider $\alpha = 1$ for simplicity and without loss of generality.

As an example, the β value for the lotion of Table 14 (82% of consumer preference for Lotion 1, $H_1 = 0.82$) related to competitor's lotion preference (80% preference, $H_2 = 0.8$), would be $H_2/H_1 = 0.97$. If the preference for competitor's product were half of that of our product, β would be equal to 0.5. At first, one could think that the smaller the β value, the more profitable would be the new product. We will show that this is not necessarily correct.

We realize that the market in this case has a maximum demand (D) given by the number of people who would actually seek moisturizing lotions in the market in question. Thus, Eq. 15 can only be used if the market is unsaturated, that is, 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 utility¹ renders:

$$D = d_1 + d_2 \quad (17)$$

$$d_1 = \frac{D}{1 + \gamma} \quad (18)$$

$$\gamma = \left(\frac{\alpha}{\beta} \right)^{\frac{\rho}{\rho-1}}. \quad (19)$$

Thus, the way we establish demand as a function of the rest of the parameters (α , β , Y , D , and ρ) by obtaining d_1 and d_2 using Eqs. 15 and 16. If these do not satisfy $d_1 + d_2 < D$, then we use (17) through (19).

For our example, the market was determined by looking at what areas of the United States have signs and symptoms of xerosis and ichthyosis vulgaris that are the worse. The

Table 14. New Composition Proposed

| Ingredient | Function | New Formulation |
|-------------------------|------------------|-----------------|
| Deionized Water | Solvent | 75.15% |
| Allantoin | Humectant | 1.13% |
| Sorbitol | Humectant | 3.87% |
| Dimethicone | Occlusive | 1.00% |
| Macadamia Nut Oil | Emollient | 0.05% |
| Xanthan Gum | Thickner | 1.97% |
| Potassium sorbate | Preservative | 0.10% |
| Citric Acid | pH ajustor | 0.00% |
| Polysorbate 40 | Emulsifier | 0.25% |
| Sorbitan Monolaurate | Emulsifier | 16.33% |
| γ -linoleic acid | SC lipid | 0.00% |
| Titanium Dioxide | Cosmetic Pigment | 0.15% |
| Helzenut Oil | Fragrance | 0.00% |
| Total Sum | — | 100% |
| Consumer Preference | — | 82% |

Table 15. Competitors Ingredients and Compositions

| Ingredient | Function | Fraction* |
|--|-------------------|-----------|
| Deionized Water | Solvent | 70.84% |
| Acrylates/c10–30 alkyl acrylate crosspolymer | Rheology Modifier | 0.60% |
| Mica/titanium dioxide | Cosmetic Pigment | 3.00% |
| Allantoin | Conditioner | 0.20% |
| Propylene Glycol | Humectant | 3.00% |
| Mmethylparaben | Preservative | 0.15% |
| Dilaureth-4 phosphate | Emulsifier | 3.00% |
| Cetyl Alcohol | Emulsifier | 2.00% |
| Mineral Oil | Emollient | 10.30% |
| Decyl Oleate | Emollient | 6.20% |
| Propylparaben | Preservative | 0.05% |
| Triethanolamine | Neutralizer | 0.36% |
| Fragrance (mint and honey) | Fragrance | 0.10% |
| Methyldibromo Glutaronitrile/Phenoxyethanol | Preservative | 0.20% |
| Total Mixture Value | — | 100.000% |
| Consumer Preference | — | 80% |

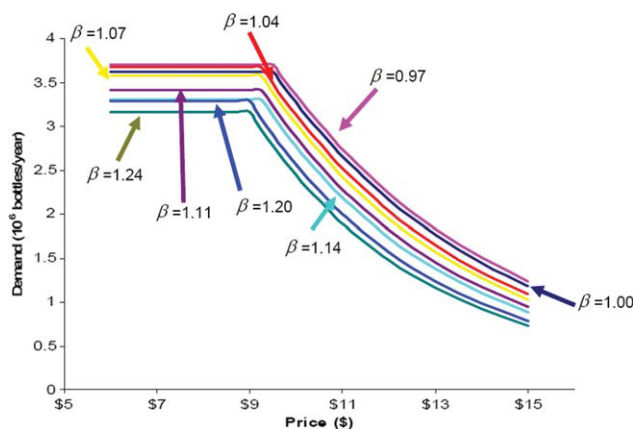


Figure 25. Demand as a function of prices and preference.

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

Northwest U.S. and the Southwest U.S. are the two targeted markets, characterized by dry cold and hot climates, respectively. The total population of the NW and SW U.S. was determined from census records (~91 millions). As ichthyosis vulgaris is a non life-threatening genetic disease, this market should stay constant (as the birth and death rates of the individuals are relatively constant). Approximately 15,000, or 0.4%, are born with ichthyosis vulgaris every year (US Census Bureau). On the other hand, 15% of the population suffers from xerosis. Together these two skin conditions account for 15.4% of the population. Nevertheless, we assumed that 3% of the people suffering from these two conditions will not seek treatment by a moisturizing lotion. Thus, the total target population was 12.4% of the western U.S. (91 million people). Of this population, each person buys a total of three 16 oz bottles of lotion each year at an average price of \$10.00.

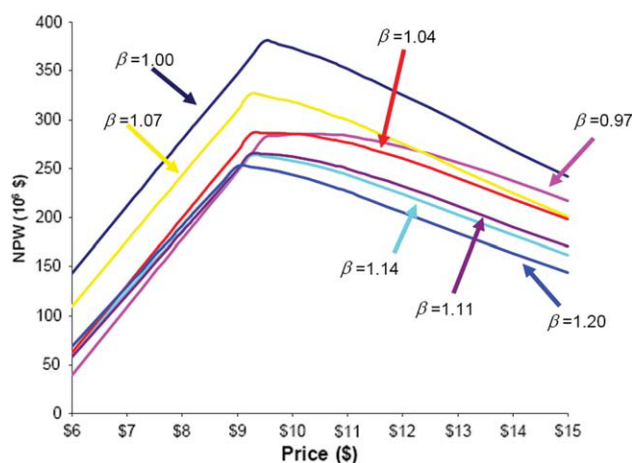


Figure 26. NPW as a function of price for different preferences.

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

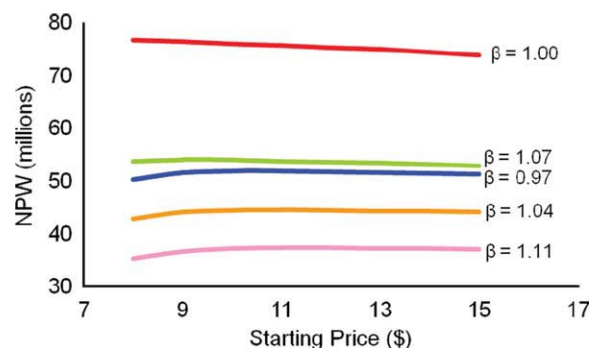


Figure 27. NPW as a function of price and preference.

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

The estimated fixed capital investment (FCI) is around \$4.15 million, plus \$0.73 million for working capital (WC), totalizing almost \$4.9 million of total capital investment (TCI). These values are estimated for the demand of the most preferred lotion. Although the equipment size does vary slightly with the concentration of the ingredients, it is assumed that the cost of the tanks will have a negligible change. Because of this, the equipment cost was calculated based off the max preference solution and not changed for the more profitable lotion. Thus, we will assume the same TCI for all cases.

The demand as a function of price was calculated for different values of β , and is shown in Figure 25 (we used $D = 500,000$ bottles/month). It can be inferred that for prices $< \$10$ 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 β was computed by looking at what ingredients can match the selected value of β at minimum cost. They vary from \$7.5/bottle for $\beta = 0.97$ to \$8.00/bottle for $\beta = 1.11$. The competitor's lotion cost is \$9.40/bottle.

With the cost computed and demand, one can now compute the profit (Net Present Worth—NPW) for a 10 years lifespan as a function of price for different values of β (Figure 26). 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 \$9.00 and \$10.00.

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 competitor's, 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.

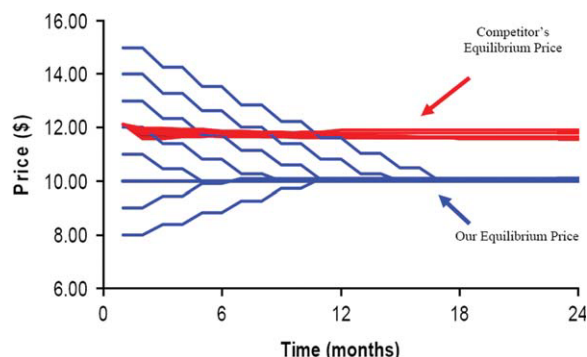


Figure 28. Our and competitor's selling price as a function of time for different starting prices.

$\beta = 1.00$. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The first one, change in their amount of advertising, would affect the awareness function (α). We do not discuss changes in the amount of advertising here.

The second competitor's response, change in their composition, affects directly β , once this is related to the preference, which in turn is related to the composition. 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 affect directly 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 below

$$p_2 = p_{2,0} - \gamma(p_{2,0} - C_2) \left(\beta \frac{d_{20} - d_2}{d_{20}} \right)^{\alpha_1/\alpha_2} \quad (20)$$

where $p_{2,0}$ is the competitor's original price, γ is a proportionality constant (we use $\gamma = 0.28$), C_2 is the competitor's manufacturing cost per bottle, β is the relative preference of the competitor's product divided by the preference of our product, d_2 is the new demand for the competitor's product, $d_{2,0}$ is the original demand of the

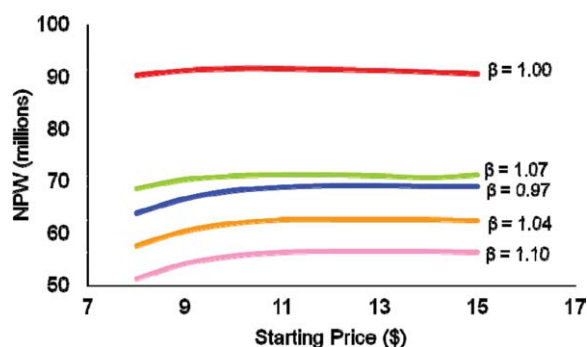


Figure 29. NPW vs. starting price for perfect information.

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

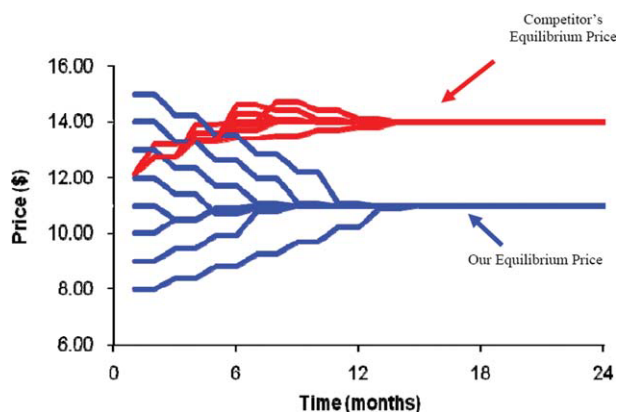


Figure 30. Selling price vs. time for perfect information and various starting prices.

$\beta = 1.00$. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

competitor's product, and α 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. This relative drop is adjusted by the difference in quality: thus if their product is of inferior quality ($\beta < 1$) the adjustment is smaller. In addition, if the awareness of the consumer towards their product is larger than towards ours ($\alpha_1/\alpha_2 < 1$), then the adjustment is also smaller. After this is done, a new equilibrium is achieved and at this point, our company has to change our price to achieve the equilibrium for the market.

We built a discrete dynamic model that considers monthly price adjustments over a 10-year horizon. Our prices at odd months were calculated by maximizing profit in the next month using Eq. 15 whereas the competitor's price was set using Eq. 20 ensuring that no more than 5% price change was applied. In other words, if Eq. 20 predicts a change larger than 5%, we limit it to 5%. 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. Figure 27 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 Figure 28, we plot both prices and show them reaching equilibrium within 1.5 years. Similar price vs. time profiles were obtained for other values of β . In all cases, equilibrium is achieved within a 2-year-period. All prices converged to the same equilibrium, regardless of the starting price.

We now assume that the competitor uses the same consumer model (Eq. 15) and has somehow arrived at the same values of the parameters (perfect information). Thus, a dynamic model was constructed in which each product new price for the following month is calculated using the same model. Figure 29 illustrates that again, the lotion with a $\beta = 1.00$ was the most profitable with \$10 as starting price. Figure 30 shows the price evolution indicating that market equilibrium is achieved also in around 1.5 years.

The case of imperfect information was broken into two sub cases: The first of which being when the competition calculated a β for our product to be larger than the actual

real value we calculated, and the second of which they use a smaller value of β than the actual real value.

We also assume that the competitor uses other parameter values ($D' = 600,000$ bottles/month and $Y' = \$3,600,000$). In the first sub case, $\beta' = \beta \pm 0.1$. The results indicate that the best answer is again $\beta = 1$ and the starting price is \$10/bottle as in the previous case, so we omit the figures.

Conclusions

We developed a model to predict consumer preference for skin moisturizing lotions. Following a recent developed methodology,¹ 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. Also, we showed that in this specific case study, a lotion that would render 100% preference to consumers is not possible, and no more than 82% of preference was achieved.

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.

Literature Cited

1. Bagajewicz M. On the role of microeconomics, multi-scale planning and finances in product design. *AIChE J.* 2007;53:3155–3170.
2. Cussler EL, Moggridge GD. *Chemical Product Design*. Cambridge University Press, 2001.
3. Seider WD, Seader JD, Lewin DR. *Product and Process Design Principles*. New York: John Wiley, 2004.
4. Cooper RG. *Winning at New Products: Accelerating the Process from Idea to Finish*, 3rd ed. Cambridge, Mass.: Perseus Publ, 2001.
5. Cooper RG. *Product Leadership: Creating and Launching Superior New Products*. Cambridge, Mass.: Perseus Publ, 2002.
6. Street C, Woody J, Ardila J, Bagajewicz M. Product design: a case study of slow release carpet deodorizers/disinfectants. *Ind Eng Chem Res.* 2008;47:1192–1200.
7. Heflin L, Walsh S, Bagajewicz M. Design of medical diagnostics products: a case-study of a saliva diagnosis kit. *Comput Chem Eng.* 2009;33:1067–1076.
8. Cooper RG. *Product Leadership: Creating and Launching Superior New Products*, 2nd ed. Cambridge, Mass.: Basic Books, 2005.
9. Eucerin. *The Epidermis*. Available at: http://www.eucerin.co.uk/skin/skincell_2.html. Accessed February 13, 2008.
10. van der Valk PGM, Kucharekova M, Tupker RA. Transepidermal water loss and its relation to barrier function and skin irritation. In: Fluhr J, Elsner P, Berardesca E, Maibach HI, editors. *Bioengineering of the Skin: Water and the Stratum Corneum*. Boca Raton: CRC Press, 2004:97–104.
11. Elias PM, Feingold KR. Permeability barrier homeostasis. In: Elias PM, Feingold KR, editors. *Skin Barrier*. New York: Taylor & Francis Group, 2006:337–362.
12. Marino C. *Skin Physiology, Irritants, Dry Skin and Moisturizers*. Report Number 56–2-2001 for Safety and Health Assessment and Research for Prevention Program. Available at the Washington State Department of Labor and Industries website: http://www.lni.wa.gov/Safety/Research/Dermatitis/files/skin_phys.pdf.
13. Rawlings AV. Sources and role of stratum corneum hydration. In: Elias PM, Feingold KR, editors. *Skin Barrier*. New York: Taylor & Francis Group, 2006:399–425.
14. Ho C. *Geoscience Approach to Modeling Chemical Transport Through the Skin*. SNL GeoBio LDRD (2002). Available at: <http://www.sandia.gov/geobio/>. Accessed February 13, 2008.
15. Flynn GL. *Physicochemical Determinants of Skin Absorption*. Paper presented at: Workshop on Principles of Route-to-Route Extrapolation for Risk Assessment, March 19–21, 1990; Hilton Head, SC, 93–127.
16. Amsden BG, Goosen MFA. Transdermal delivery of peptide and protein drugs: an overview. *AIChE J.* 1995;41:1972–1997.
17. Wertz PW, Michniak BB. *Hydration and lipids*. In: Fluhr J, Elsner P, Berardesca E, Maibach HI, editors. *Bioengineering of the Skin: Water and the Stratum Corneum*. Boca Raton: CRC Press, 2004:359–368.
18. Warner RR, Myers BS, Taylor DA. Electron probe analysis of human skin: determination of the water concentration profile. *J Invest Dermatol.* 1988;90:218–224.
19. Scott IR, Harding CR. Filaggrin breakdown to water binding compounds during development of the rat stratum corneum is controlled by the water activity of the environment. *Dev Biol.* 1986;115:84–92.
20. Caspers PJ, Lucassen GW, Carter EA, Bruining HA, Puppels GL. Semiquantitative in vivo concentration profiles of NMF and swat constituents in the stratum corneum of the thenar as determined by Raman spectroscopy. *J Invest Dermatol.* 2001;116:434–442.
21. Warner RR, Lilly NA. Correlation of water content with ultrastructure in the stratum corneum. In: Elsner P, Berardesca E, Maibach HI, editors. *Bioengineering of the Skin: Water and the Stratum corneum*. Boca Raton: CRC Press Inc, 1994:3–12.
22. Melton J. *Introduction to the Skin*. 1996. Available at the Loyola University Dermatology Medical Education Website: <http://www.meddean.luc.edu/lumen/MedEd/medicine/dermatology/melton/skinlsn/skinlsn.htm>.
23. Rawlings AV, Harding CR, Walskinson A, Scott IR. Dry and xerotic skin conditions. In: Leyde JJ, Rawlings AV, editors. *Skin Moisturization*. New York: Marcel Dekker, Inc, 2002:119–144.
24. DiGiovanna J, Robinson-Boston L. Ichthyosis: etiology, diagnosis, and management. *Am J Clin Dermatol.* 2003;4:81–95.
25. Knowlton J, Pearce S. *The Handbook of Cosmetic Science and Technology*. Oxford: Elsevier Advanced Technology, 1993.
26. Loden M. Hydration and moisturizers. In: Fluhr J, Elsner P, Berardesca E, Maibach HI, editors. *Bioengineering of the Skin: Water and the Stratum Corneum*. Boca Raton: CRC Press, 2004:295–306.
27. The Skin Sciences Institute. *Skin Care: A Practical Guide to Skin Care Products and Ingredients*. Available at: <http://www.netwellness.org/healthtopics/skincare/brochure.pdf>. Accessed January 25, 2008.
28. Food and Drug Administration. *Is it Cosmetic, a Drug, or Both? (Or Is It Soap?)*. Available at: <http://www.cfsan.fda.gov/~dms/cos-218.html>. Accessed February 13, 2008.
29. Wibowo C, Ng KM. Product-oriented process synthesis and development: creams and pastes. *AIChE J.* 2004;47:2746–2767.
30. Rawlings AV, Harding CR. Moisturization and skin barrier function. *Dermatol Therapy.* 2004;17:43–48.
31. Nakagawa N, Sakai S, Matsumoto M, Yamada K, Nagano M, Yuki T, Sumida Y, Uchiwa H. Relationship between NMF (Lactate and Potassium) content and the physical properties of the stratum corneum in healthy subjects. *J Invest Dermatol.* 2004;122:755–763.
32. Rawlings AV, Matts PJ. Stratum corneum moisturization at the molecular level: an update in relation to the dry skin cycle. *Progr Dermatol.* 2005;124:1099–1110.
33. Pal R. Evaluation of theoretical viscosity models for concentrated emulsions at low capillary numbers. *Chem Eng J.* 2001;81:15–21.
34. Barton S. *Formulation of skin moisturizers*. In: Leyden JJ, Rawlings AV, editors. *Skin Moisturization*. New York: Marcel Dekker, Inc, 2002:547–584.
35. Kokini JL, Cussler EL. Predicting the texture of liquid and melting semi-solid foods. *J Food Sci.* 1983;48:1221–1225.
36. Nacht S, Close J, Yeung D, Gans EH. Skin friction coefficient: changes induced by skin hydration and emollient application and correlation with perceived skin feel. *J Soc Cosmetic Chem.* 1981;32:55–65.
37. Sivamani RK, Godman J, Gitis NV, Maibach HI. Coefficient of friction: tribological studies in man—an overview. *Skin Res Technol.* 2003;9:227–234.
38. Janhoj T, Petersen CB, Frost MB, Ipsen R. Sensory and rheological characterization of low-fat stirred yogurt. *J Text Studies.* 2006;37:276–299.
39. Kokini JL, Kadane J, Cussler EL. Liquid texture perceived in the mouth. *J Text Studies.* 1977;8:195.
40. Akhtar M, Stenzel J, Murray B, Dickinson E. Factors affecting the perception of creaminess of oil-in-water emulsions. *Food Hydrocolloids.* 2005;19:521–526.

41. Akhtar M, Murray BS, Dickinson E. Perception of creaminess of model oil-in-water dairy emulsions: influence of the shear-thinning nature of a viscosity-controlling hydrocolloid. *Food Hydrocolloids*. 2005;20:839–847.
42. Rosen M. *Surfactants and Interfacial Phenomena*, 2nd ed. New York: John Wiley & Sons, Inc, 1989.
43. Khyat AE, Mavon A, Leduc M, Agache P, Humbert P. Skin critical surface tension: a way to assess the skin wettability quantitatively. *Skin Res Technol*. 1996;2:91–96.
44. Escobedo J, Mansoori GA. Surface tension prediction for pure fluids. *AIChE J*. 1996;42:1425–1433.
45. Flick EW. *Cosmetic and Toiletry Formulations*, 2nd ed. Noyes: William Andrew Publishing, Knovel Library website, 2001. Available at: <http://knovel.com/knovel2/Toc.jsp>. Accessed February 13, 2008.

Manuscript received Apr. 9, 2009, revision received July 11, 2009, and final revision received Feb. 26, 2010.