



# TOOLS FOR CHEMICAL PRODUCT DESIGN

FROM CONSUMER PRODUCTS TO BIOMEDICINE

Edited by  
MARIANO MARTÍN  
MARIO R. EDEN  
NISHANTH G. CHEMMANGATTUVALAPPIL



COMPUTER-AIDED CHEMICAL ENGINEERING, 39

# Contents

List of Contributors

xvii

## Section I

### Basic Concepts and General Tools

- 1. Mathematical Principles of Chemical Product Design and Strategies** 3

*L.Y. Ng, N.G. Chemmangattuvalappil, V.A. Dev, M.R. Eden*

- 1. Introduction 3
- 2. Chemical Product Design Strategies 5
  - 2.1. Initial Efforts 5
  - 2.2. Design of Experiment and Mixture Design of Experiments 5
  - 2.3. Computer-Aided Molecular Design 8
  - 2.4. Molecular Signature Descriptors 13
  - 2.5. Enumeration Approach 14
  - 2.6. Mathematical Programming Approaches 16
  - 2.7. Metaheuristic Approaches 20
  - 2.8. Decomposition-Based Approaches 24
  - 2.9. Multiobjective Chemical Product Design 25
  - 2.10. Chemical Product Design Under Property Prediction Uncertainty 34
- 3. Conclusions and Future Directions 36
- References 37

- 2. Integrated Consumer Preferences and Price/Demand-Driven Product Design: An Alternative to Stage-Gate Procedures** 45

*M. Bagajewicz*

- 1. Introduction 45
- 2. Product Design Integrated Model 46
- 3. Consumer Satisfaction Score 48
- 4. Consumer Preference Model 52
- 5. Manufacturing and Distribution Costs 52
- 6. Price-Demand Consumer Model 53

7. Profit Model and Optimization	55
8. Competitive Markets	56
9. Conclusions	58
References	58
<b>3. VPPD-Lab: The Chemical Product Simulator</b>	<b>61</b>
<i>S. Kalakul, S. Cignitti, L. Zhang, R. Gani</i>	
1. Introduction	61
2. Systematic Framework for Chemical Product Design	62
2.1. Modeling Module	66
2.2. Product Design Module	66
2.3. Product Analysis	75
2.4. New Product Template	76
3. VPPD-Lab Software Implementation	76
4. VPPD-Lab Application Examples	78
4.1. Stability Check of Solvent Mixtures	78
4.2. Design of a Lubricant Blend	79
4.3. Design of a Jet Fuel Blend	83
4.4. Design of an Insect Repellent Lotion	86
5. Conclusion	91
References	92
<b>4. Development of a Multiscale Strategy and Application to Chemical Vapor Deposition</b>	<b>95</b>
<i>L.E.K. Achenie, Y. Sharifi, D.G. Lee</i>	
1. Introduction	95
1.1. Background	95
1.2. Multiscale Modeling	97
2. Global Optimization of the Substrate Geometry in Zinc Sulfide Deposition	100
2.1. Multipoints Arbitrary Shape Design Model	100
2.2. Genetic Algorithms	102
2.3. Multiobjective Optimization	103
2.4. Multiobjective Genetic Algorithms	105
2.5. Implementation of a Genetic Algorithm in Shape Design	106
2.6. Results and Discussion	110
2.7. Summary	113
3. Chemical Vapor Deposition Modeling Using Agent-Based Simulation	113
3.1. Modeling	113
3.2. Agent-Based Modeling in NetLogo	116
3.3. Results and Discussions	116
3.4. Summary	119
4. Conclusions (Overall)	120
References	120

<b>5. Molecular Property Clustering Techniques</b>	125
<i>F. Eljack</i>	
<b>1. Introduction</b>	125
1.1. Molecular Design	125
1.2. Property Prediction and Group Contribution Methods	127
<b>2. Property Integration</b>	128
2.1. Property Integration for Process Design	128
2.2. Property Clusters and Group Contribution Methods	129
<b>3. Visual Molecular Clustering Design Approach</b>	129
3.1. Conservation Rules for Molecular Property Clusters	131
3.2. Graphical Representation of the Molecular Design Problem	132
3.3. Example: Solvent Design	134
<b>4. Algebraic Property Clustering Technique for Molecular Design</b>	140
4.1. Problem Statement	140
4.2. Algebraic Property Clustering Method	140
4.3. Proof of Concept: Algebraic Property Clustering Method	142
<b>5. Conclusions</b>	147
<b>References</b>	147

## Section II

### Molecular Design

<b>6. Computer-Aided Molecular Design and Property Prediction</b>	153
<i>R. Gani, L. Zhang, S. Kalakul, S. Cignitti</i>	
<b>1. Introduction</b>	153
<b>2. Molecular Design: Problem Formulation</b>	156
2.1. Structural Constraints	157
2.2. Property Constraints	159
2.3. Process Model and Other Constraints	167
<b>3. Molecular Design: Solution Methods</b>	167
3.1. Heuristic or Rule-Based Techniques	168
3.2. Mathematical Programming Techniques	168
3.3. Hybrid Techniques	169
<b>4. Computer Aided Product Design: Framework</b>	170
4.1. Step 1: Problem Definition	170
4.2. Step 2: Computer-Aided Molecular Design Constraint Selection	172
4.3. Step 3: Computer-Aided Molecular Design Formulation	173
4.4. Step 4: Solution Strategy	173

<b>5. Case Studies</b>	177
5.1. Refrigerant Design	177
5.2. Surfactant Design as Emulsifier for Emulsified Ultraviolet Sunscreen	182
5.3. Other Application Examples	185
<b>6. Future Challenges and Concluding Remarks</b>	186
<b>Appendices</b>	186
Appendix A: List of Marrero and Gani (2001) First-Order Groups	186
Appendix B: Refrigerant Design Computer-Aided Molecular Design Formulation	188
<b>References</b>	193
<b>7. The Incorporation of Safety and Health Aspects as Design Criteria in a Novel Chemical Product Design Framework</b>	197
<i>J.Y. Ten, M.H. Hassim, D.K.S. Ng, N.G. Chemmangattuvalappil</i>	
<b>1. Introduction</b>	197
<b>2. Computer-Aided Molecular Design</b>	199
<b>3. Integration of Inherent Safety and Health in a Computer-Aided Molecular Design Framework</b>	201
3.1. Problem Formulation	201
3.2. Inherent Safety and Occupational Health Indexes Selection	201
3.3. Model Development	206
3.4. Molecular Design	208
3.5. Multiple-Objective Optimization	209
<b>4. Case Study: Solvent Design for Gas Sweetening Process</b>	210
4.1. Case Study: Problem Formulation	211
4.2. Case Study: Fuzzy Optimization	213
<b>5. Conclusions</b>	216
<b>References</b>	218
<b>8. Molecular Design in the Pharmaceutical Industries</b>	221
<i>K. Boone, F. Abedin, M.R. Anwar, K.V. Camarda</i>	
<b>1. Introduction</b>	221
<b>2. General Concepts in Pharmaceutical Product Design</b>	222
<b>3. Design and Development of the Active Pharmaceutical Ingredient</b>	223
3.1. Overview	223
3.2. Ligand Screening	225
3.3. Structure-Based Drug Design	225
3.4. Receptor-Based Approaches	226
3.5. Ligand-Based Approaches	226

4. <b>Pharmaceutical Formulation Design</b>	228
4.1. Overview	228
4.2. CAMD Approaches to Formulation Design	229
4.3. Formulation Design to Minimize the Aggregation of Protein Drugs	231
5. <b>Conclusions</b>	234
<b>References</b>	235
9. <b>Ionic Liquid Product Design</b>	239
<i>A.T. Karunanithi, R. Farahipour</i>	
1. <b>Introduction</b>	239
1.1. Ionic Liquids	239
1.2. Computer-Aided Molecular Design	241
1.3. Computer-Aided Ionic Liquid Design	241
2. <b>CAMD Formulation of the Ionic Liquid Design Problem</b>	242
2.1. Generation of Feasible Ionic Liquid Structures	243
3. <b>Ionic Liquid Property Prediction</b>	246
3.1. Thermodynamic Modeling of Ionic Liquids for CAILD	246
3.2. A New Group Contribution Approach for the Prediction of Activity Coefficients in Systems Involving Ionic Liquids	248
4. <b>Computer-Aided Ionic Liquid Design Solution</b>	249
5. <b>Case Study 1: Design of Ionic Liquids for Polymer Dissolution</b>	250
5.1. Computer-Aided Ionic Liquid Design Problem Formulation and Solution	252
5.2. Results	256
6. <b>Case Study 2: Ionic Liquid Design for Heat Transfer Applications</b>	257
6.1. Thermal Conductivity	257
6.2. Melting Point	259
6.3. Computer-Aided Ionic Liquid Design Problem Formulation and Solution	259
6.4. Results and Analysis	261
7. <b>Summary and Conclusions</b>	263
<b>References</b>	265
10. <b>Integrated Multiobjective Molecular and Process Design: Operational and Computational Frontiers</b>	269
<i>A.I. Papadopoulos, P. Linke, P. Seferlis</i>	
1. <b>Introduction</b>	269
2. <b>Decomposition-Based Approach for the Integrated Molecular and Process Design</b>	276
2.1. Approach Overview	276
2.2. Computer-Aided Molecular Design and Multiobjective Formulation	277
2.3. Classification Using Data Mining	279
2.4. Process Design	281

<b>3. Integration of Molecular and Process Design With Process Operability Decisions</b>	283
3.1. Motivation	283
3.2. Proposed Framework	284
3.3. Application to Organic Rankine Cycles	287
<b>4. Utilization of Advanced Grid and Cloud Computing Resources</b>	294
4.1. Motivation	294
4.2. Existing Infrastructures and Challenges in the Deployment of Computer-Aided Process Engineering Tools	296
4.3. Proposed Software-as-a-Service Architecture	297
4.4. Workflows for Integrated Molecular and Process Design	298
4.5. Implementation of Workflows	301
<b>5. Conclusions</b>	306
<b>References</b>	307
<b>11. The Signature Molecular Descriptor in Molecular Design: Past and Current Applications</b>	315
<i>D.P. Visco, Jr., J.J. Chen</i>	
<b>1. Molecular Descriptors</b>	315
<b>2. Introduction to Signature Molecular Descriptor</b>	316
<b>3. Advantages of Signature</b>	319
3.1. Advantages of Signature: Complete Documentation of Atomic Topography	319
3.2. Advantages of Signature: Canonical Representation of Molecule	320
3.3. Advantages of Signature: Tunable Specificity/Degeneracy	320
3.4. Advantages of Signature: Efficiently Combine Atomic Signatures to Form New Structures	320
<b>4. Applications of Signature</b>	321
4.1. Applications of Signature: QSARs	321
4.2. Applications of Signature: QSAR/QSPR and Molecular Design	322
4.3. Applications of Signature: QSAR/QSPR, Molecular Design, and Experimental Validation	323
4.4. Applications of Signature: QSAR/QSPR and Classification	323
4.5. Applications of Signature: Inclusion in Biological Software	324
4.6. Applications of Signature: Industrial Bioreaction Pathway Design	324
4.7. Applications of Signature: Signature as a 3D Molecular Descriptor	325

<b>5. Computer-Aided Molecular Design: Signature Case Studies</b>	325
5.1. CAMD: Signature Case Study: Virtual High Throughput Screening	325
5.2. CAMD: Signature Case Study: Reactant, Product, and Reaction Pathway Design	330
5.3. CAMD: Signature Case Study: Ideal Structure Similarity Searching	334
<b>6. Conclusion</b>	338
<b>References</b>	338

## Section III

### Customer Products

#### 12. Integrated Process and Product Design Optimization 347

*F.P. Bernardo*

<b>1. Introduction</b>	347
<b>2. Conceptual Model</b>	348
2.1. Decomposition of the Property Function for Product Operational Properties	351
2.2. Basic Formulation of Product Design Problems	353
<b>3. Optimization Formulations for Product/Process Design</b>	357
3.1. Two-Stage Approach to Invert the Property Function	359
3.2. Integrated Product/Process Design	360
3.3. Computational Implementation	361
<b>4. Examples</b>	362
4.1. Perfumes	362
4.2. A Cosmetic Emulsion	363
4.3. Formulation of a Pharmaceutical Ointment	367
<b>5. Conclusions</b>	370
<b>References</b>	370

#### 13. Tools for Formulated Product Design 373

*M. Martín, A. Martínez*

<b>1. Introduction: Formulated Products and Raw Materials</b>	373
<b>2. Mathematical Formulations</b>	374
2.1. Pooling Problem	374
2.2. Chemical Process Design	377
<b>3. Cases of Study</b>	380
3.1. Formulated Product Design: Laundry Detergents	380
3.2. Formulated Raw Materials: Algae Design	386
<b>4. Conclusions</b>	390
<b>References</b>	390



<b>14. Simulation-Based Food Process Design</b>	<b>393</b>
<i>T.E. Moxon, S. Bakalis</i>	
1. Introduction	393
2. Stomach	396
2.1. Gastric Emptying Rate	397
2.2. Gastric Secretions	399
2.3. Gastric Breakup	401
3. Small Intestine	404
3.1. Mass Transfer Phenomena	404
4. Conclusion	411
References	412
<b>15. A Structured Approach for Product-Driven Process Synthesis in Foods Manufacture</b>	<b>417</b>
<i>C. Almeida-Rivera, P. Bongers, E. Zondervan</i>	
1. Introduction	417
2. Process Synthesis in the Food Industry	420
3. A Product-Driven Process Synthesis Approach	422
3.1. Generalities	422
3.2. Structure of the Methodology	424
4. Case Study: Synthesis of Ice Cream by Cold Extrusion	429
4.1. Framing Level	429
4.2. Consumer Wants and Product Function	432
4.3. Input–Output Level	437
4.4. Task Network	437
4.5. Equipment Selection and Design	438
5. Conclusions	438
References	439
<b>16. Managing Risk in the Design of Product and Closed-Loop Supply Chain Structure</b>	<b>443</b>
<i>L.J. Zeballos, C.A. Méndez</i>	
1. Introduction	443
2. Literature Review	445
3. Problem Description	446
4. Problem Formulation	447
5. Example	452
6. Results	452
6.1. Sensitivity Analysis Study	456
7. Conclusions	461
Appendix A	461
Appendix B	465
Acknowledgments	473
References	473

<b>17. Optimization of Blending-Based Products</b>	475
<i>N.A. Yunus, Z.A. Manan</i>	
1. Introduction	475
2. Designing Liquid Blended Products	475
3. Solution Approach: Optimization	477
4. A Case Study: Gasoline Blends	478
4.1. Problem Definition	478
4.2. Problem Formulation	479
4.3. Solution Strategy	480
4.4. Results and Discussion	482
5. Conclusions	485
References	485
<b>18. Decomposition-Based Optimization of Tailor-Made Green Diesel Blends</b>	487
<i>L.Y. Phoon, H. Hashim, R. Mat, A.A. Mustaffa</i>	
1. Introduction	487
2. Tailor-Made Green Diesel Blend Design Algorithm	488
2.1. Phase 1: Problem Formulation	488
2.2. Phase 2: Decomposition-Based Computer-Aided Optimization	492
2.3. Phase 3: Fuel Enhancement	495
2.4. Phase 4: Experimental Validation	496
3. Application	496
3.1. Phase 1, Task 1.1: Problem Definition of Tailor-Made Green Diesel Blends	496
3.2. Phase 1, Task 1.2: The Property Models	497
3.3. Phase 2, Task 2.1: The Feasible Blends Candidates	499
3.4. Phase 2, Task 2.2: The Feasible Blends	500
3.5. Phase 2, Task 2.3: The Optimum Green Diesel Blends	501
3.6. Phase 3, Task 3.1: The Fuel Additives	501
4. Results and Discussions	503
5. Conclusions	504
Acknowledgments	504
References	505

## Section IV

### Design of Structured Products

<b>19. Strategies for Structured Particulate Systems Design</b>	509
<i>C. Amador, L. Martin de Juan</i>	
1. Relevance of Structured Particle Products in Industry	509
2. Scales of Structured Particle Product	511

2.1.	Spray-Dried Detergent Particles	512
2.2.	Spray-Dried Milk Powder	514
<b>3.</b>	<b>Supramolecular Structure</b>	515
3.1.	Crystalline and Amorphous Structure Phase Composition	515
3.2.	Water Activity ( $a_w$ )	521
3.3.	Thermal Phase Transitions	523
3.4.	Mechanical Properties, Viscoplasticity, and Rheology	527
3.5.	Particle Size Distribution (PSD)	529
<b>4.</b>	<b>Particle Structure</b>	532
4.1.	Volume Fraction and Size Distribution of the Domains That Constitute the Particle Structure	535
4.2.	Spatial Distribution of the Domains that Constitute the Particle Structure	538
4.3.	Porosity and Pore Size Distribution	540
4.4.	Specific Surface Area	541
4.5.	Surface Energy	542
4.6.	Surface Forces	542
4.7.	Surface Roughness	543
4.8.	Formation of Particle Structure During Drying	544
4.9.	Modeling of Particle Structure During Drying	546
<b>5.</b>	<b>Mesostructure</b>	549
5.1.	Size and Shape Distribution of Each of the Different Particulate Components	550
5.2.	Contact Points	555
5.3.	Particle Spatial Distribution	557
5.4.	Liquid Spatial Distribution	559
5.5.	Particle Packing	560
5.6.	Permeability and Wetting	561
5.7.	Bulk Flow Properties	562
5.8.	Compaction Curves: Elastic and Plastic Deformation of Particle Systems	565
5.9.	Particle Attrition	566
<b>6.</b>	<b>The Grand Challenge on Structured Particle Product Design: An Integrated Approach</b>	569
6.1.	Modeling Approach on Structured Particle Product Design	570
	<b>References</b>	572

## Section V Biomedicine

<b>20.</b>	<b>Computational Tools for the Study of Biomolecules</b>	583
	<i>P.G. Jambrina, J. Aldegunde</i>	
<b>1.</b>	<b>Introduction</b>	583
1.1.	The Ideal Scenario: Quantum Mechanical Treatment	584

2.	<b>Energy Calculations for Molecules</b>	587
2.1.	Ab-Initio Methods	587
2.2.	Density Functional Theory (DFT)	597
2.3.	Semiempirical Methods	603
2.4.	Force Fields	607
2.5.	Hybrid Methods: Quantum Mechanics/Molecular Mechanics	618
2.6.	Beyond Atomistic Simulations: Coarse-Grained Methods	624
3.	<b>Preparing a Molecular Dynamics Simulation</b>	625
3.1.	Experimental (Crystal) Structures	626
3.2.	Homology Modeling	629
3.3.	Docking	630
4.	<b>Dynamics Simulations</b>	631
4.1.	Purely Quantum Mechanical Techniques	631
4.2.	Classical Trajectories	632
4.3.	Nonadiabatic Processes	633
4.4.	Canonical Molecular Dynamics Simulations	634
4.5.	Enhanced Sampling Methods	637
5.	<b>Conclusions</b>	641
	<b>Acknowledgments</b>	642
	<b>References</b>	642
21.	<b>Walk-In Brain: Virtual Reality Environment for Immersive Exploration and Simulation of Brain Metabolism and Function</b>	649
	<i>G. Hartung, A. Alaraj, A. Linninger</i>	
1.	<b>Summary</b>	649
2.	<b>Medical Images</b>	651
2.1.	Overview	651
2.2.	Three-Dimensional Brain Imaging Modalities	652
2.3.	Extracting Vectorized Data	652
2.4.	Calculations of Physiological Metrics	653
3.	<b>Virtual Patient Simulation</b>	653
3.1.	Overview	653
3.2.	Simulating Patient-Specific Structures in Three Dimensions	654
3.3.	Modification and Re-Simulation of Structures	655
4.	<b>Immersive Virtual Reality Environment</b>	655
4.1.	Overview	655
4.2.	Design of Virtual Reality Environment	656
4.3.	Subject-to-Subject Automated Recognition of Points of Interest	656
4.4.	Manipulation of Original Structures with the Addition of Medical Devices	657
5.	<b>Conclusion</b>	657
	<b>References</b>	658
	<b>Index</b>	659

# Integrated Consumer Preferences and Price/Demand–Driven Product Design: An Alternative to Stage-Gate Procedures

M. Bagajewicz

*University of Oklahoma, Norman, OK, United States*

*E-mail: bagajewicz@ou.edu*

## 1. INTRODUCTION

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

Typically, while marketing experts identify consumer “needs and wants” and economists provide means to assess costs and profit, engineers try to advance a product structure/formulation that will achieve the product functionality that targets some of these needs and wants in some optimal way (in the current western economy, it is usually maximum profit). In other words, the needs and wants are not always fully met by the products marketed to these consumers. These needs and wants are usually expressed using consumer-related properties, in terms of properties defined in plain language that are not many times the same as the ones used by engineers to describe the product.

Product design procedures, like the one proposed in the area of process systems engineering by [Cussler and Moggridge \(2001\)](#) or [Seider et al. \(2004\)](#), are the ones that insist on the identification of consumer wants and needs first using them as targets for the product design, while considering consumer response to price as well as optimality (profit or other objective) later. Similarly, the Stage-Gate™ Product Development Process (SGPDP) ([Cooper, 2001, 2002, 2005](#)) proceeds in a similar manner by using so-called phases sequentially (first concept, then feasibility, development, manufacturing, and finally product marketing). The first two help shape up the product based on consumer needs and wants using market surveys and tests. At this point, the SGPDP method also suggests building a business case for each product option. The main assumption is that once the concept and the feasibility have been tested, then one product, which could be later refined, emerges.

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

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

## 2. PRODUCT DESIGN INTEGRATED MODEL

We consider the following to be the key elements:

- Product identification: type and functionality. This requires identifying consumer needs and wants first, as in SGPDP. We keep in mind that there are products that can be introduced in the market without them being wants

and/or not even perceived needs, generating artificially, so to speak, new wants and needs that did not exist before. Examples of this artificial generation of needs and wants abound.

- Identification of product attributes: These are typically the functionalities that are given value by consumers. For example, in the specific case of skin lotions (Bagajewicz et al., 2011), an example we use frequently in this chapter, one would identify its effectiveness, thickness, smoothness, color, creaminess, scent, etc. In devices such as cars, one talks about power, acceleration, comfort, accessories, etc. In medical devices, one talks about its accuracy, its false positives/false negative. We claim that such a list can be made for every product!
- Consumer preferences: Establish a quantitative measure of how much a consumer prefers a product (regardless of its price) given the attributes. This is where we depart slightly from what economists call “hedonic value” and “hedonic pricing,” started by studies like those on “revealed preference theory” pioneered by Samuelson (1938) and continued through time (see Baltas and Freeman, 2001). In all these cases, the underlying idea is that the consumer makes choices that are influenced by (1) perceived preference of one product versus others, (2) price(s), and (3) budget. In other words, when price and affordability are not considered, consumers will almost always declare preference for the product that has their best-perceived quality, but when price and budget are included, the choice is different. Thus, consider cars: asked what car would one like, one may, for example, choose a fancy sport car; when budget is considered, the choices are based on the car type and model they can afford (accessible range of prices), and within that range, preferences play a role, so many times, one “pays for quality.”
- Consumer buying behavior: A price demand relationship that incorporates the consumer preferences.
- Optimization: A procedure that is capable of identifying the attributes that achieve the “right” product to manufacture given a certain criteria [we use the maximization of profit here, but it could be as stated above any other (set of) criteria].

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

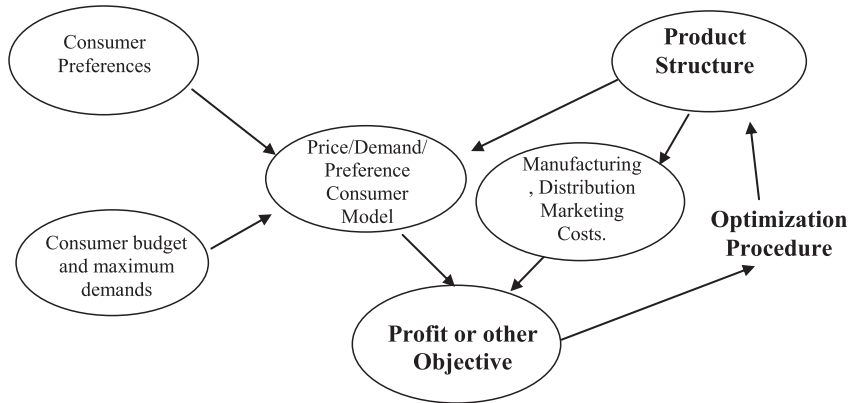


FIGURE 2.1 Integrated product design procedure.

### 3. CONSUMER SATISFACTION SCORE

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

$$H_i = f(r_{i,j}, y_{i,j}) \quad (2.1)$$

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

$$H_i = \sum w_{i,j} y_{i,j} \quad (2.2)$$

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

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

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



TABLE 2.1 Consumer Properties of Selected Products					
Skin Lotion (Bagajewicz et al., 2011)	Carpet Deodorizer (Street et al., 2008)	Insect Repellent (Bagajewicz, 2007)	Wine (Whitnack et al., 2009)	Saliva Diagnostic Kit (Heflin et al., 2009)	Wine Nose (Linehan et al., 2011)
<b>Properties</b>					
Effectiveness	Disinfecting power, odor elimination power	Effectiveness, durability	Acidity	Sensitivity	Accuracy
Thickness	Scent type	Feel	Sweetness	False negative rate	Size
Greasiness	Scent intensity	Form	Bitterness	False positive rate	Weight
Smoothness	Fragrance duration	Toxicity	Clarity	Patient discomfort	
Creaminess	Toxicity	Scent	Color		
Spreadability			Brightness		
Absorption rate			Bouquet		
Color			Body/texture		
Scent			Finish/aftertaste		
<b>Associated Engineering—Manipulated Properties</b>					
• Composition	• Composition • Dose • Material and radius particles	• Composition	• Grape • Barrel type and burn • Time • Etc.		Sensor(s) type (MV) Geometry Materials
<b>Engineering Properties Used for Assessment</b>					
• Diffusivities • Viscosity • Surface tension • Density	Release time duration				• Size • Weight

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

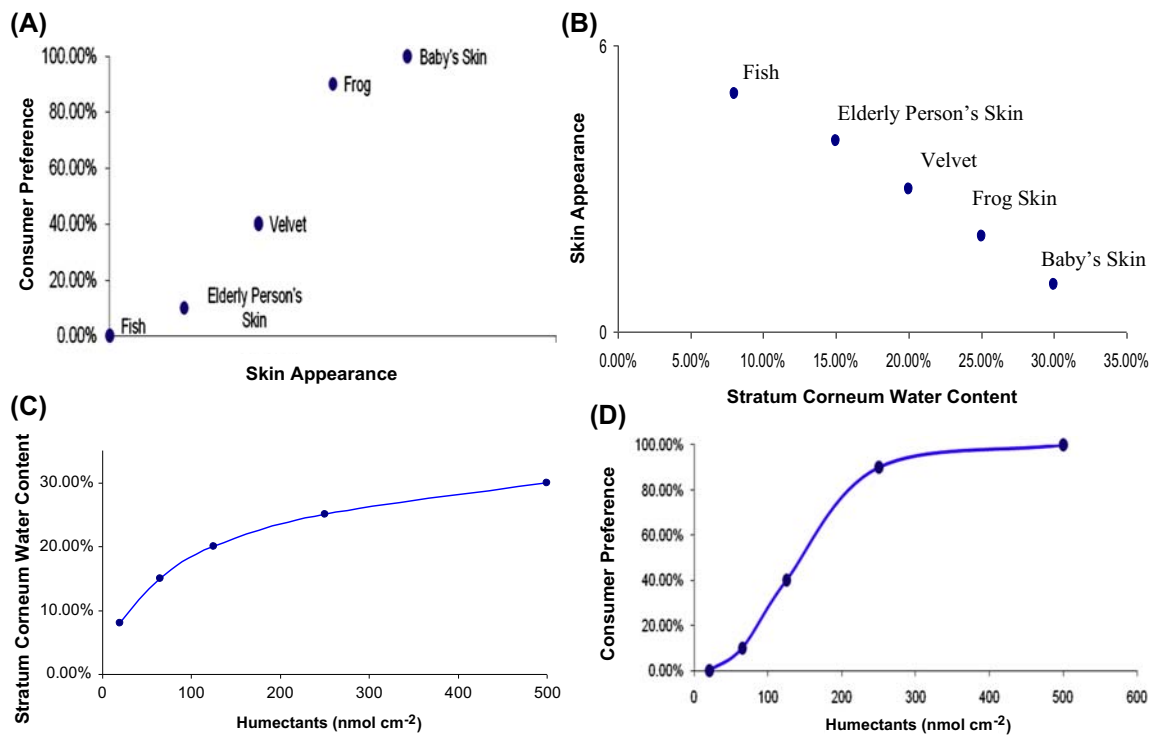
Thus, in general, we write:

$$y_{i,j} = f(x_{i,j}) \quad (2.3)$$

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

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

Similar connections can be made for other properties. For example, for thickness, consumers are asked to rank how different mixtures flow (ketchup, mayonnaise, cream, etc.), and connections are made to the resulting viscosity



**FIGURE 2.2** (A) Preference versus skin appearance, (B) skin appearance versus water content, (C) water content versus humectants, (D) preference versus humectants content.

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

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

#### 4. CONSUMER PREFERENCE MODEL

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

$$\beta_{i,j} = f(H_i, H_j) \quad (2.4)$$

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

#### 5. MANUFACTURING AND DISTRIBUTION COSTS

In our example, lotions are emulsions that can be either oil-in-water or water-in-oil. The choice is mainly dictated by practical considerations, such as ease of application and consumer perception (Wibowo and Ng, 2001). The oil-in-water emulsions, which are less sticky on application, predominate in the market and are the choice for our study. Emulsifying agents are used to stabilize the oil-in-water mixture. The most common type of emulsifier are

surfactants, which decrease the interfacial tension between the two phases. The actual manufacturing procedure is simple and consists of mixing the oil and water phases together. The following steps show how the lotion is made:

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

## 6. PRICE–DEMAND CONSUMER MODEL

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

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

$$d_2 = \frac{Y - p_1 d_1}{p_2} \quad (2.6)$$

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

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

$$D = d_1 + d_2 \quad (2.7)$$

$$d_1 = \frac{D}{1 + \gamma} \quad (2.8)$$

$$\gamma = \left(\frac{\alpha}{\beta}\right)^{\frac{\rho}{\rho-1}} \quad (2.9)$$

Thus, the way we establish demand as a function of the rest of the parameters ( $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $D$  and  $\rho$ ) by obtaining  $d_1$  and  $d_2$  using Eqs. (2.5) and (2.6). If these do not satisfy  $d_1 + d_2 < D$ , then we use (7) through (9).

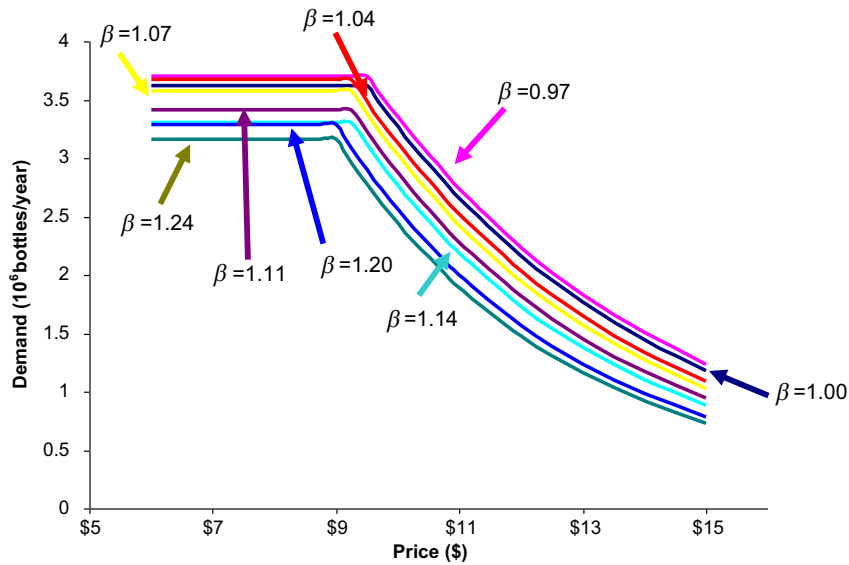


FIGURE 2.3 Demand as a function of prices and preference for lotions.

For our example of the skin lotion, the market was determined by looking at what areas of the US have signs and symptoms of xerosis and ichthyosis vulgaris that are the worst (see Bagajewicz et al., 2011 for more details). Also, for the example in question, a fixed capital investment, working capital, and total capital investment were determined as a function of total manufacturing capacity. The demand as a function of price was calculated for different values of  $\beta$  and is shown in Fig. 2.3 (we used  $D = 500,000$  bottles/month). It can be inferred that for prices less than \$10, the consumer budget is not a limiting factor. At prices around \$10, we reach the maximum demand we could have for our product, and it will not increase for lower prices.

Then the total product cost for each value of  $\beta$  was computed by looking at what ingredients can match the selected value of  $\beta$  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.

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

$$d_j = \beta_{j,1}^{\rho/(1-\rho)} \left( \frac{p_1}{p_j} \right)^{1/(1-\rho)} d_1 \quad j \neq 1 \quad (2.10)$$

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

$$\sum_j p_j d_j = Y \quad (2.11)$$

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

## 7. PROFIT MODEL AND OPTIMIZATION

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

$$\underset{z,p}{\text{Max}} \sum_s pr_s \text{ NPVR}_s - \text{Fixed Capital Investment}$$

*s.t.*

$$\begin{aligned} \text{NPVR}_s &= \text{Sales}_s - \text{Manufacturing Costs}_s - \text{Supply Chain Costs}_s \\ &\quad - \text{Marketing Costs}_s \end{aligned}$$

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

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

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

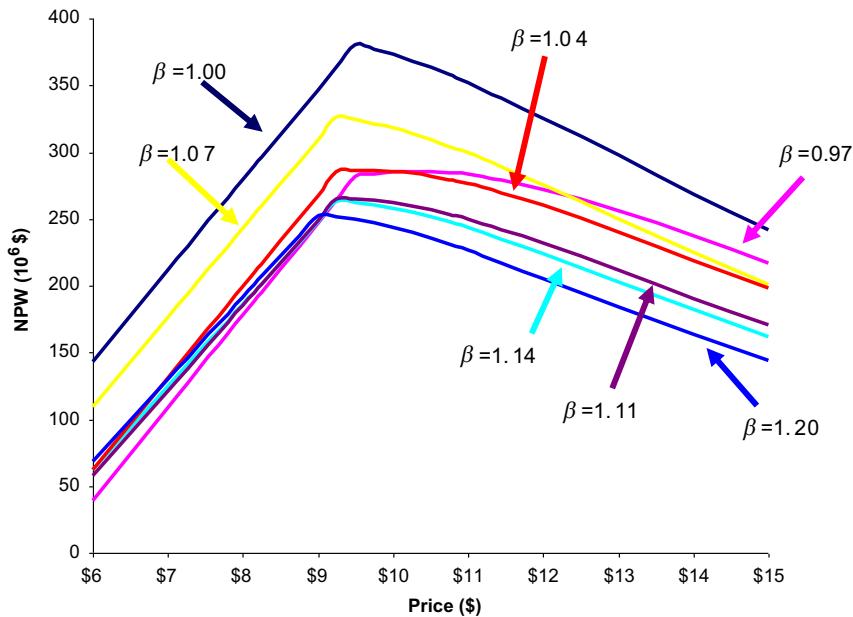


FIGURE 2.4 Net present worth as a function of price for different preferences.

## 8. COMPETITIVE MARKETS

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

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

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

$$p_2 = p_{2,0} - \gamma(p_{2,0} - C_2) \left( \beta \frac{d_{2,0} - d_2}{d_{2,0}} \right)^{\alpha_1/\alpha_2} \quad (2.12)$$



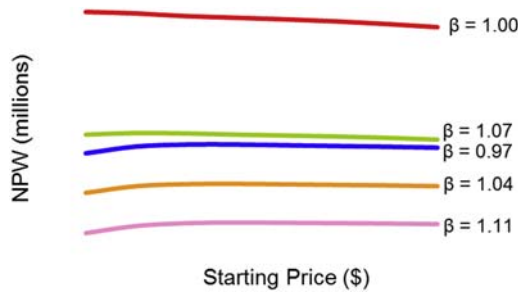


FIGURE 2.5 Net present worth as a function of price and preference.

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

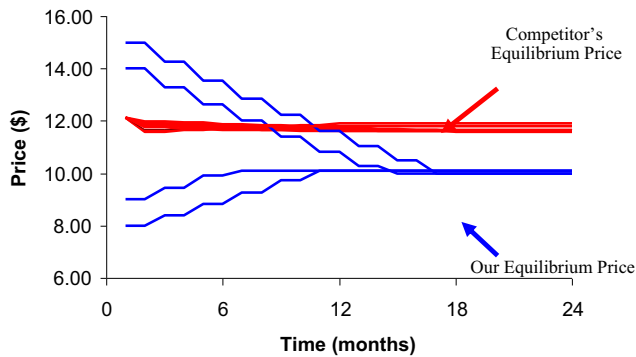


FIGURE 2.6 Our and competitor’s selling price as a function of time for different starting prices ( $\beta = 1.00$ ).

## 9. CONCLUSIONS

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

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

## REFERENCES

- Bagajewicz, M., 2005. Integration of process systems engineering and business decision making tools: financial risk management and other emerging procedures. In: Galan, M., Martin del Valle, E. (Eds.), *Chemical Engineering Trends and Developments*. John Wiley, Chichester, England.
- Bagajewicz, M., 2007. On the role of microeconomics, multi-scale planning and finances in product design. *AIChE Journal* 53 (12), 3155–3170.
- Bagajewicz, M., Hill, S., Robben, A., Lopez, H., Sanders, M., Sposato, E., Baade, C., Manora, S., Coradin, J.H., 2011. Product design in price-competitive markets: a case study of a skin moisturizing lotion. *AIChE Journal* 57 (1), 160–177.
- Baltas, G., Freeman, J., 2001. Hedonic price methods and the structure of high-technology industrial markets: an empirical analysis. *Industrial Marketing Management* 30, 599–607.
- Barbaro, A.F., Bagajewicz, M., 2004. Managing financial risk in planning under uncertainty. *AIChE Journal* 50 (5), 963–989.
- Cooper, R.G., 2001. *Winning at New Products: Accelerating the Process from Idea to Finish*, third ed. Perseus Publ., Cambridge, Mass.
- Cooper, R.G., 2002. *Product Leadership: Creating and Launching Superior New Products*. Perseus Publ., Cambridge, Mass.
- Cooper, R.G., 2005. *Product Leadership: Creating and Launching Superior New Products*, second ed. Basic Books, Cambridge, Mass.
- Costa, R., Moggridge, G.D., Saraiva, P., April 2006a. Chemical product engineering: a future paradigm. *CEP* 10–13.
- Costa, R., Moggridge, G.D., Saraiva, P., 2006b. Chemical product engineering: an emerging paradigm within chemical engineering. *AIChE Journal* 52 (6), 1976–1986.
- Cussler, E.L., November, 2003. Chemical product design and engineering. (plenary talk). In: *AIChE Annual Conference*. San Francisco, Paper 430a.
- Cussler, E.L., Moggridge, G.D., 2001. *Chemical Product Design*. Cambridge University Press.
- Heflin, L., Walsh, S., Bagajewicz, M., 2009. Design of medical diagnostics products: a case-study of a saliva diagnosis kit. *Computers and Chemical Engineering* 33 (5), 1067–1076.
- Hill, M., 2004. Product and process design for structured products. *AIChE Journal* 8 (50), 1656–1661.
- Joback, K., Stephanopoulos, G., 1995. Searching spaces of discrete solutions: the design of molecules possessing desired physical properties. *Advances in Chemical Engineering* 21, 257–311.

- Linehan, S., Nizami, S.N., Bagajewicz, M., 2001. Design of monitoring instruments for wine fermentation using microeconomics and consumer preferences. *Chemical Engineering Communications* 198 (2), 255–272 (2011).
- Ng, K., Gani, R., Dahm-Johansen, K., 2006. Chemical Product Design: Towards a Perspective Through Case Studies. In: *Computer Aided Chemical Engineering Series*, vol. 23. Elsevier.
- Samuelson, P., 1938. A note on the pure theory of consumers' behaviour. *Economica* 5 (17), 61–71.
- Seider, W.D., Seader, J.D., Lewin, D.R., 2004. *Product and Process Design Principles*. John Wiley, New York.
- Siddhaye, S., Camarda, K.V., Topp, E., Southard, M.Z., 2000. Design of novel pharmaceutical products via combinatorial optimization. *Computers and Chemical Engineering* 24, 701–704.
- Siddhaye, S., Camarda, K.V., Southard, M.Z., Topp, E., 2004. Pharmaceutical product design using combinatorial optimization. *Computers and Chemical Engineering* 28, 425–434.
- Stephanopoulos, G., November 2003. Invention and innovation in a product-centered chemical industry: general trends and a case study. In: *AIChE Conference. 55th Institute Lecture*. San Francisco.
- Street, C., Woody, J., Ardila, J., Bagajewicz, M., 2008. Product design: a case study of slow release carpet deodorizers/disinfectants. *Industrial and Engineering Chemistry Research* 47 (4), 1192–1200.
- Whitnack, C., Heller, A., Frow, M.T., Kerr, S., Bagajewicz, M., 2009. Financial risk management in the design of products under uncertainty. *Computers and Chemical Engineering* 33 (No 5), 1056–1066.
- Wibowo, C., Ng, K.M., 2001. Product-oriented process synthesis and development: creams and pastes. *AIChE Journal* 47 (12), 2746–2767.
- Westerberg, A.W., Subrahmanian, E., 2000. Product design. *Computers and Chemical Engineering* 24, 959–966.