5
Product Development

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5.1
Background

Over the past 20 years, the changing political situation and the advent of new technologies have had a profound impact on societies in the vast majority of countries all over the world. This influence has been manifested, among other things, by the growing demand for totally new products and services. This trend has resulted in mergers, and acquisitions of many businesses at a scale not previously observed. The changes in the organization of the businesses have very deeply influenced the manufacturing and processing industries. The main consequences have been the lowering of profit margins of commodities, growing pressure on the environmental aspects of production and conservation of raw materials, very high costs of the research and development (R&D), significance of low-tonnage and high-added value products, growing importance of the customer-oriented products, reduction of the time between development and bringing the product to the market, shortening of the life cycle of the products, and issues related to intellectual property rights.

All of these factors have caused a visible change in processing industries. It was manifested by the move from process-oriented to product-centered businesses. The consequence of this switch is the emergence of interest in product development.

The activity has been known to the industry for many years. However, its importance and the need for a more systematic approach have only been realized in the last five to eight years.

It is obvious that the driving force for the generation of new chemical products is higher satisfaction of existing needs or fulfillment of new ones. However, it is hard to imagine even a fraction of those needs when realizing that the largest substance database, the Chemical Abstracts Service (CAS), contains around seven million commercially available chemicals, and around 4000 new substances are added each day.

The generalization of the product concept is captured by the multilevel approach proposed by Kotler (1989). The product is composed of core, tangible and augmented parts as presented in Fig. 5.1. The core product assures the minimal fulfillment of

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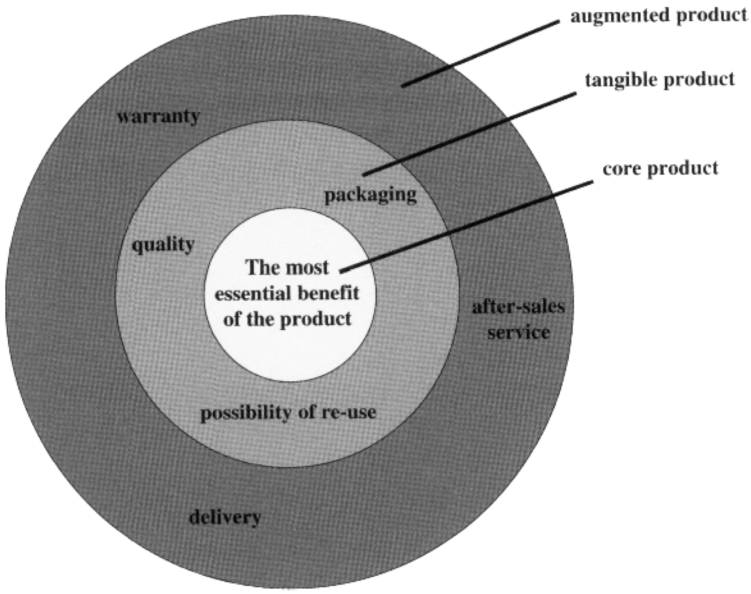

Figure 5.1 The concept of product (Kotler 1989).

the customer's needs. It is a physical component of the product, e.g., paint or adhesive. The tangible and augmented part of the product is composed of physical as well as the immaterial elements, e.g., services.

The activity of CAPE specialists related to product development concentrates on the analysis of the function-property-composition relations (Villadsen 1997; Rowe and Roberts 1998a; Cussler and Moggridge 2001; Gani and O'Connell 2001; Wesseling 2001; Charpentier 2002). However, when looking at Kotler's concept of the product it is clearly visible that such an approach corresponds exclusively to the core product and still there is a lot to be done by the CAPE community with respect to tangible and augmented elements of the product.

The consequence for the process engineer is a need to look not exclusively at the composition or form of the core product but also at its function in a more general context, e.g., chemical sensors in the package that inform about the state of the core product or degradability facilitating the elimination of the product.

The behavior of the product at the market is described by the concept of product life time. The concept introduced by Buzzell (1966) and later much criticized (Dhalla and Yuspeh 1976) is still a good tool for the determination of where the product is in its development path and the consequences for its engineering. The generalized product life time is presented in Fig. 5.2.

The analysis of a product life cycle shows that the involvement of process engineers changes during its duration. The most intensive design activities of process engineers at the product development phase are later replaced by the involvement of the production phase and incremental changes of the product. The last phase, elimi-

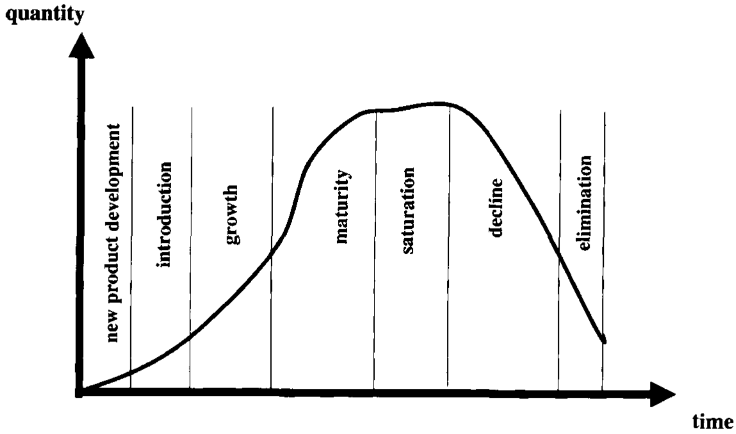

Figure 5.2 Product life cycle (Baker and Hurt 1999).

nation, is also a place where the process engineers have to be involved to ensure the required environmental, legal and technological compromise.

The first phase of the product life cycle, new product development (NPD), is a type of activity where process engineers have always been active. However, the structural changes of many industries, as mentioned at the beginning of this chapter, imposed a need for more comprehensive participation of the process engineers in NPD. The involvement of process engineers will be easier to structure by analyzing the theories of new product development. Saren (1984) has introduced four types of NPD: departmental stage model, activity-based approach, decision stage model and conversion process. The activity-based approach developed by Booz, Allen and Hamilton (1982) seems to be the most adequate for the illustration of the involvement of process engineers in product development. The modification of activity-based model presented by Ulrich and Eppinger (2000) is the starting point for the analysis of the methods and tools to be used by process engineers in NPD.

The generic activity-based model of product development is composed of the phases presented in Fig. 5.3.

Chemical product development is a process composed of the definition phase and product design, as presented in Fig. 5.3. The very essence of the product development is the identification of how the needs could be satisfied by the chemical and physical interaction of the substances and the chemical composition and structure of those substances.

It means the determination of the needed (expected) function of the product, translation of the required function (adhesiveness, chemical impact, smell, taste, elasticity, etc.) into the properties like viscosity, density, color, smell, microstructure, etc., and finally the identification of the single chemical component (its molecular structure) or mixture possessing those properties. In the definition phase a specialized business strategy and market research tools are used. Business strategy tools are applied in the planning phase to outline what should be produced and for whom.

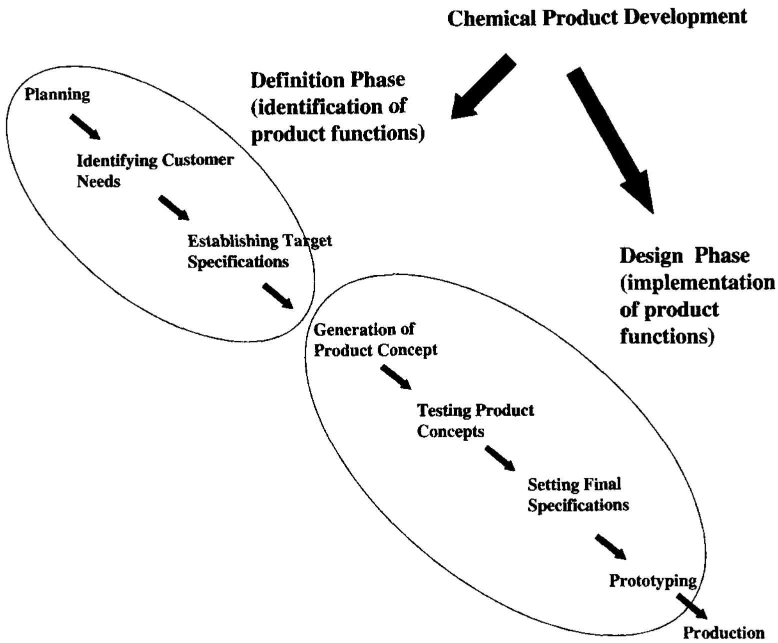

Figure 5.3 Chemical product development (Ulrich and Eppinger 2000).

Market research tools are used to identify the needs and requirements concerning the pre-defined class of the products and the market segment.

In the CAPE community, product development was traditionally reduced to product design and, due to the character of the chemical industry, product design was equivalent to formulation. Formulation is defined as the blending/mixing and processing of ingredients in order to obtain a product characterized by the precisely determined properties (specifications). The main design problem in formulation is finding the relation between the composition and structure of the mixture as well as the type and conditions of processing it and the required final properties of the product.

The great variety of products is a source of the fundamental difficulties in the generalization of the product formulation. Usually the know-how in formulation is restricted to a narrow class of the products (e.g., specialized soaps or rubbers). Knowledge of formulation for one type of the product is not easily transferable to the other types of products. The high specialization and the very complicated physical and chemical phenomena related to the processing of the ingredients, as well as their interactions, resulted in characteristic development of methods and tools used in formulation and more generally in product design.

There are three main classes of methods applicable to product design:

- experimental design
- knowledge-based methods
- computer-aided molecular design.

Historically, the oldest method of product design was experimental design that evolved into sophisticated statistical methods, capable of handling very complicated mixing and processing problems. The interest of the CAPE community has been recently attracted to the statistical analysis of processes that can lead to the identification of new products. The attractiveness of experimental design has been strongly limited by the considerable costs and time needed for the realization of the experiments and the subsequent analysis of data. The trends for limiting the cost and time of development, the existence of a huge amount of data, and information related to the development of new products and stored by the companies were the main factors promoting the application of knowledge-based methods. The common feature of these methods is the use of historic data and information and the generation, on this basis, of new knowledge applicable to the actual product design problems. The proposed methods and tools are: rule-based systems, neural networks, genetic algorithms, case-based reasoning systems, TRIZ, and data mining.

The last group of methods is related to computer-based molecular design. This approach has been dynamically developing over recent years. An important contribution of the CAPE community in this field was recently reported by Achenie, Gani, and Venkatasubramanian (2003).

There are two approaches to product design (Fig. 5.4). Product design can be formulated as a forward problem if the design starts from the given structure of a molecule or composition of the material, and aims at determining the properties of this material. The second approach, considering design as a reverse problem, starts with the given properties of a material and finds the molecular composition fulfilling the requirements. Experimental methods are an example of the forward problem formulation. The knowledge-based methods as well as computer-based design could be used in forward or reverse problem formulation.

This chapter is limited to the description of experimental and knowledge-based methods. It covers the last 10 years and does not include the review of computer-based molecular design. The relatively new subjects to the CAPE community, such as quality function deployment, case-based reasoning and TRIZ method, are described in more details. The application of other methods and tools is reviewed in the context of the designed product type, i.e., catalysts, dyes, rubbers, etc.

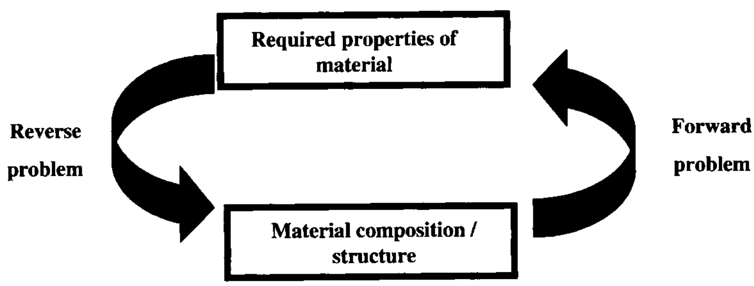

Figure 5.4 Forward and reverse formulation of the product design problem.

5.2 Definition Phase

Identification of consumer needs is a field where market research is given the last word. Often the comments found in process engineering literature about the "identification of the consumer voice by the use of questionnaire" are misleading and in fact quite different questions should be asked. Although direct contact with the customer is not a core speciality of process engineers, a basic knowledge of the methods and the applicable tools is very important. Attention should be focused on two types of tools. The first group is composed of the tools enabling not only identification of the actually expressed requirements but also their translation into engineering characteristics of the materials. The second group focuses on the identification of future needs, which are not yet foreseen by the great majority of consumers. Both activities are aimed at positioning the future product with respect to customers, competitors, and regulators.

5.2.1 Translation of the Requirements into the Parameters

The capturing of the requirements of a new product is composed of information gathering, information transformation, and finally generation of the requirements. The specialized techniques are the domain of market research and many noteable books exist dealing with the subject, e.g., Bruce and Cooper (2000). There are several methods and tools related with the quantification of the product attributes expressed by the customers and their translation into the engineering variables of the product. The most common are: conjoint analysis and quality function deployment.

Conjoint analysis is used to determine the desired level of the product attributes and their influence on various business decisions. It enables fixing of the tradeoffs between the requirements. The detailed description is presented in Baker and Hurt (1999). Quality function deployment is a more popular method enabling determination of the engineering variable values of the product, identification of the attributes and variables to be improved, and positioning of the product with respect to the competitors.

Quality Function Deployment

The quality function deployment (QFD) method enables the conversion of the needs of the customers into the product design variables (ReVelle et al. 1998). QFD is composed of four steps:

- identification of the attributes essential for the consumer when evaluating the product, and determination of the relative importance of the attributes;
- determination of connections between the attributes identified by the consumer and design variables;

- estimation of the target values of the design variables satisfying the needs of the consumers;
- assessment of the degree of satisfaction with the existing products (designs).

QFD is realized by the tool called House of Quality (Hauser and Clausing 1988), presented in Fig. 5.5.

The basic form of House of Quality is used not only for the translation of the customer needs into the product design requirements but is also applied to the systematic identification of product features. This evaluation could be based on the assessment of the competitiveness of the given product with regard to the other products on the market or by the identification of tradeoffs using a correlation matrix.

An application of the House of Quality for the chocolate couverture is given by Viaene and Januszewska (1999) (Fig. 5.6).

The analysis, conducted by the use of the questionnaires, has revealed that the most important characteristics applied by the customers in the evaluation of the chocolate couverture are: flavor, appearance, and texture. Those attributes were introduced into the "what" part of House of Quality (Fig. 5.6). There are the parameters of the couverture that are measured by the instrumental analysis (acidity level, sugar content, fat content, hardness, particle size, adhesiveness). Moreover there is a group of sensory variables: color intensity, color brightness, texture on surface, texture on snap, melting in hand, aroma, acidity, bitterness, cocoa body, fruitiness, sweetness, smokiness, first bite, oily mouth coating, aftertaste, adhesiveness, smoothness, melting in mouth. Both variables determined by the instrumental anal-

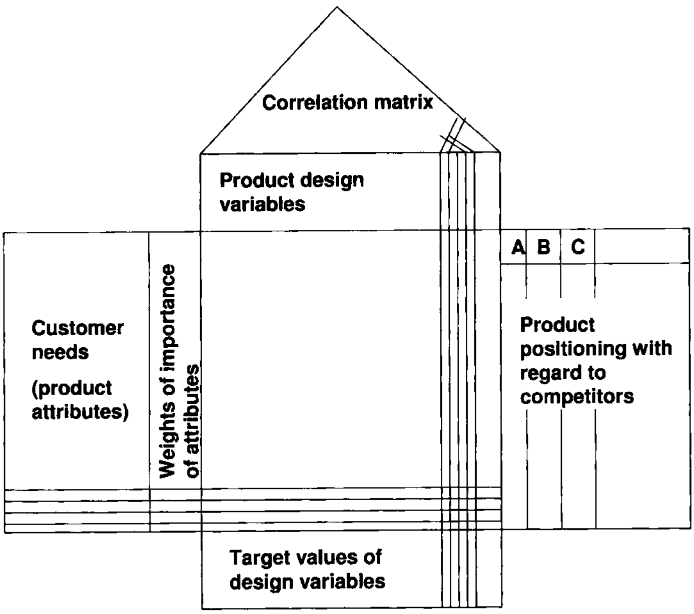

Figure 5.5 The House of Quality.

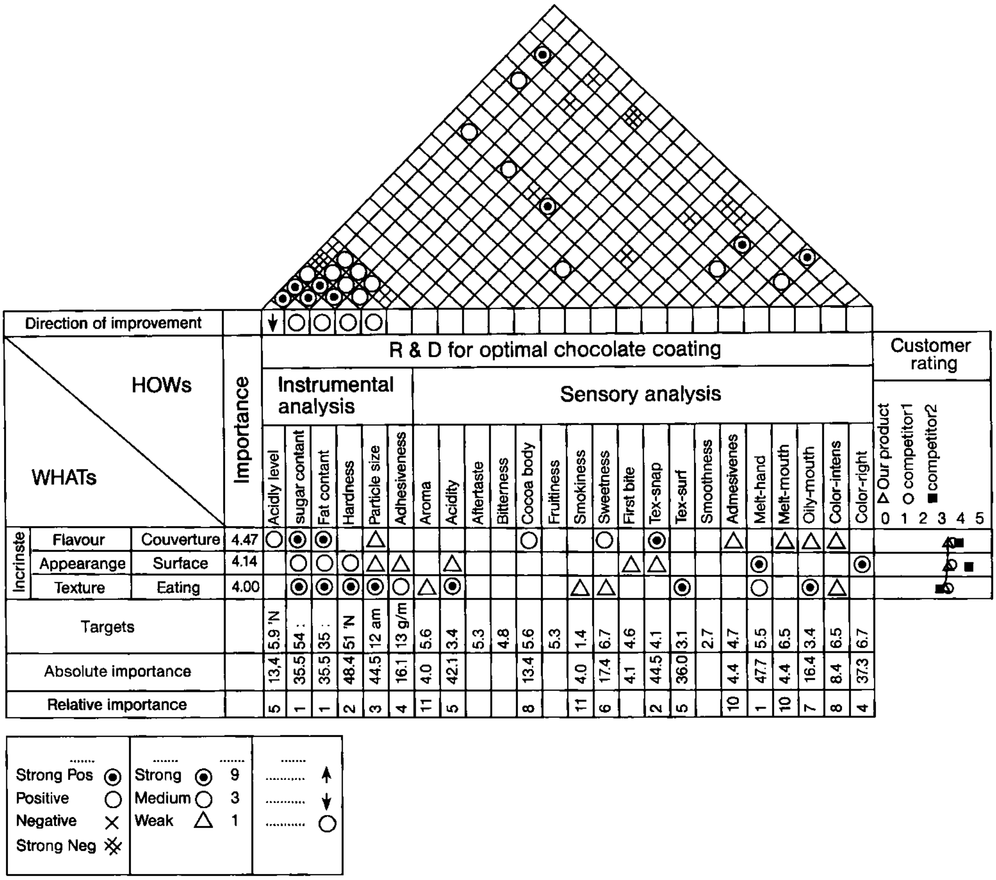

Figure 5.6 House of Quality for the chocolate couverture (Viaene and Januszewska 1999).

ysis and sensory analysis are introduced into the "how" part. There were several samples evaluated by the customers. Every sample had the different values of the variables related to the instrumental and sensory analyses. In the next step the relation between the attributes proposed by the customers and the variables from the "how" part are determined using the statistical analysis of the results of the questionnaire. The relations between the attributes and the variables are expressed as strong positive, positive, neutral, negative, strong negative. They are symbolically introduced into the central part of the House of Quality. Next, based on the importance of the attributes given by the customers and the technical knowledge obtained from the analysis of the relations between the attributes and variables, the target values for the variables are determined and introduced at the bottom of the House. The roof of the House represents the interrelations between the design variables. It allows the study of the tradeoffs between them. On the right side of the House, the positioning of the given product with respect to the products of the competitors is given. It allows for the identification of the weakest attributes of "our" product with respect to the competitors. The detailed information on the application of QFD to the product development is given in ReVelle et al. (1998).

5.2.2
Forecasting Methods for New Product

The forecasting of new products is an activity where the various methods are applied, e.g., expert judgment; brainstorming, one-to-one interviews with customers and salespeople, surveys of customers, idea generation, etc. The complete review is given by members of TFAM working group (2004). The methods of the new product forecasting could be divided as market and product-oriented. The market-oriented methods deal with the information collected from the analysis of the consumers' behavior, their needs and economic factors related to the existing products. They use complicated statistical tools, mostly penetration models, however new approaches emerge, e.g., chaos theory (Phillips and Kim 1996). The market-oriented methods of new products forecasting are mainly the domain of market analysts.

However, the obtained results are not encouraging as the estimations of the sales of the new products have errors reaching 50–60% (Kahn 2002).

5.2.2.1
Idea Generation

The phase of idea generation is a key point for engineers interested in the enhancement of their creativity. There are two major groups of methods supporting idea generation: intuitive and analytical. The most common, unstructured intuitive methods applied to the engineering problems are explained below.

Brainstorming

Brainstorming is the most popular creativity enhancement method. Originally introduced by Osborn (1953), it is based on four rules: (1) evaluation of ideas must be done later; (2) the quantity of the generated ideas is most important; (3) encouragement of strange and "wild" proposals, (4) improvement and combination of the generated ideas is welcomed. There are many types of brainstorming: stop and go, Gordon-Little variation, trigger method, etc. The detailed description is given in Proctor (2002).

Synectics

The objective of the method developed by Gordon (1961) is to look at the problem from a different perspective (to make familiar strange and vice versa). To achieve it, a set of four analogies (personal, direct, symbolic and fantastic) and metaphors is used. The detailed description of the method is presented in Proctor (2002).

Lateral Thinking

Lateral thining is the group of methods introduced by De Bono in 1970 based on the unconventional perception of the problem. The main factors enabling the lateral thinking are: identification of the dominant ideas, searching for new ways of looking at the problem, relaxation of the rigid thinking process, and the use of chance to encourage the emergence of the other ideas.

The most common analytical methods applied to the engineering problems are as follows.

Morphological Analysis

This method was introduced by Zwicky in 1948. It is based on the combination of the attributes of the product or process (like properties, functions, etc.) with the elements of the product or the process. It can generate all possible combinations of the attributes, however, its applicability is practically limited to three-dimensional analysis of the attributes. There exist many variations of the method, such as attribute listing and SCIMTAR (Proctor 2002).

Analogies

Analogies is a group of methods with case-based reasoning as the most useful for engineering applications. They exploit the similarities between the features of the existing problems and the features of the problems or design known from the past. A good survey of case-based methods is given by Leake (1996). The special class of analogy-based methods is an approach exploiting biomimetics, i.e., analogies with living systems (French 1994).

TRIZ

TRIZ is a popular method of systematic creativity support introduced by Altshuller in 1984.

There are many books that describe TRIZ (theory of inventive problem solving), e.g., Savransky (2000), Salamatov (1999). However, the book by Mann D. (2002) seems to be the best introduction.

The main findings of TRIZ are:

- All innovations start with the application of a small number of inventive principles.
- Trends exist in the evolution of technologies.
- The best solutions transform the harmful effects into useful ones.
- The best solutions remove the conflicts existing in the system.

Those findings are translated into the basic principles of TRIZ.

Contradictions

There are two types of contradictions. A technical contradiction takes place when there are two parameters of the system in conflict, i.e., the improvement in the value of one parameter lessens the value of the other one. The technical contradictions are solved by applying a contradiction matrix. A physical contradiction takes place when the parameter should simultaneously have two different values. The physical contradictions are removed applying the principles of separation in time and space.

Ideality

There is a tendency in the evolution of the systems that they always change towards the state where all benefits of their function are realized at no cost or harm.

Functionality

Every system has its main useful function and all its elements have to fulfill this function. Otherwise they are under-used and could be a source of conflict. The notion of functionality allows for the generalization of various aspects of the system functioning resulting in the possibility of transferring know-how between the various fields (technical, medical, biological, etc.).

Use of Resources

Any physical element of the system or phenomena accompanying its functioning has to be used to maximize the system functionality. The application of the basic principles is realized as shown in Fig. 5.7. It is based on the translation of the actual problem into the general one (identified by Altshuller), finding the general solution to this problem (also identified by Altshuller), and then transforming it into the solution of the actual problem.

The basic principles are implemented in several tools (inventive principles, S-fields, contradiction matrix, separation principles, knowledge effects, trends, etc.) (Mann 2002).

An example of application of the modified TRIZ to product design, is given by Nakagawa (1999). The problem was the insufficient quality of the porous polymer sheet. The reason was a foam ratio in the process of forming a polymer sheet that was too low. The gas dissolved in the molten polymer was escaping during the process through the surface of the sheet, which resulted in the creation of small, unequally distributed bubbles. The application of USTI resulted in several alternatives for concerning the material itself as well as its manufacturing. The proposed solution dealing directly with the polymer composition was the addition of the solid powder to the molten polymer to act as seeds for the bubbles.

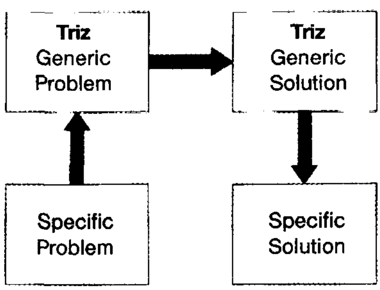

Figure 5.7 The general principle of application of TRIZ (Mann 2002).

5.2.2.2
Creativity Templates

The analysis of the market by interviewing the customers and salespeople can lead to incrementally innovative products. However, as was shown by Goldenberg and Mazursky (2002), it will not introduce a breakthrough product earlier than the competition. The reason is that the saturation of the market with the new-needs-aware customers is so low that their identification by the market research is practically impossible early on in the process. There are practically very few customers able to express the new breakthrough need in terms of the existing products. With time the awareness of the consumers grows and it becomes easier to reach new-needs-aware persons, but the competitors have the same chance as well and the competitive advantage of our product diminishes (Fig. 5.8). Goldenberg and Mazursky (2002) have suggested an introduction of creativity templates to generate new products. This idea was inspired by the TRIZ method (Orloff 2003). The first step consists of listing the attributes of the existing product. Next the attributes are manipulated

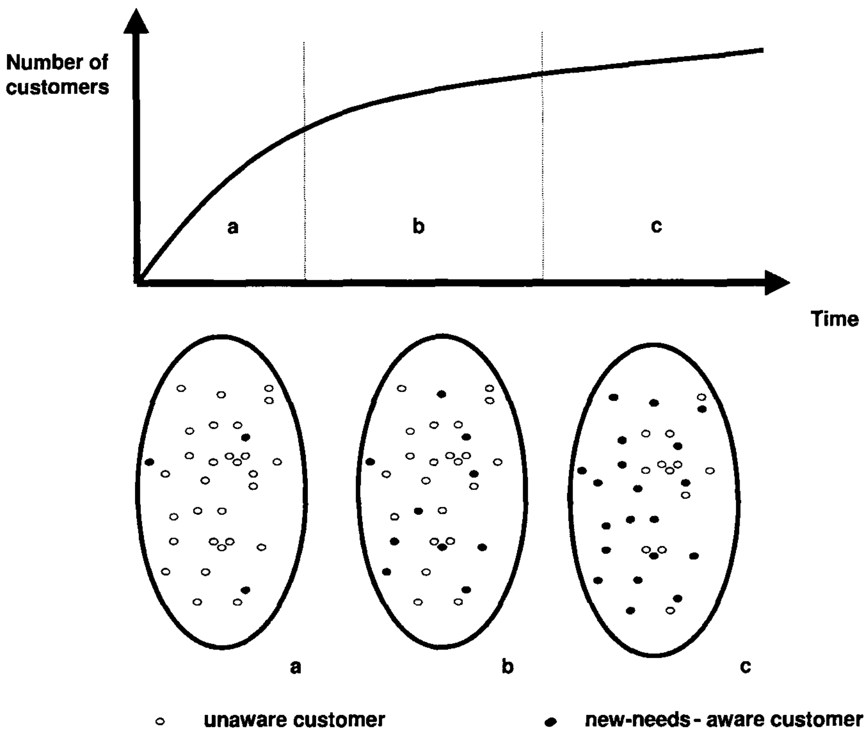

Figure 5.8 The change of the new-needs awareness of customers with time. (a) Early period of the need recognition-very few aware consumers. (b) Mature period of the need recognition-aware consumers are numerous. (c) Saturation period of the awareness-the need is obvious for the considerable majority of the customers.

using one or more templates (subtraction of the attributes, their multiplication, division, task unification or attribute dependency change). The examples of the method application are given in Goldenberg et al. (2003).

5.2.2.3
Product-oriented Methods

The product-oriented methods could be of special interest for the CAPE community. They concentrate mainly on the technical aspect of the product and try to forecast future trends of the technology development. The most common method is technology/product roadmapping (Petrick and Echols 2004). An example of a roadmap for technology/product planning is presented by Phaal et al. (2004).

The forecasting of technological trends and products based on the use of TRIZ is presented by Mann (2003). He cited the generic trends of technology evolution:

- systems with increasing benefits and decreasing cost and harm;
- increased dynamization within systems;
- increased space segmentation;
- increased surface segmentation;
- increased controllability;
- increased complexity followed by reduced complexity;
- use of all available physical dimensions within a system;
- decreased number of energy conversions;
- increased rhythm coordination;
- increased action coordination.

Mann (2003) also presented the application of trends to the forecasting of the product development.

5.3
Product Design

The concept of design is very difficult to define due to the fact that design activity could lead to extremely diverse products and consequently a broad spectrum of activities is possible.

A survey of chemical product design could be performed from the following various perspectives:

- classes of the products (e.g., basic chemicals, specialty chemicals, pharmaceuticals, crop protection, consumer products);
- development phases of the project:
  - development of the product concepts (determination of its form, features and draft specifications);
  - detailed design (identification of the complete specification and corresponding composition and structure);
  - product testing;
  - final design;

  - The specificity of the product development has to be taken into account, e.g., pharmaceuticals the steps involved are discovery, initial tests, clinical trials, legal approval;
- degree of innovativeness: new class of products, derivatives of the existing group of products, incrementally improved and breakthrough of new products;
- used tools, etc.

The next subchapter focuses on the methods and tools used in chemical product design.

5.3.1
Experimental Design

Experimental design is one of the oldest engineering product design methods. Traditionally, it can be divided into the studies of the influence of process variables (temperature, pressure, etc.) and analysis of the properties of the materials by changing their composition. The first type of experiment is called experimental process design and the second is mixture design. There is also a third type called combined experimental design, when the characteristic of the materials is studied as a function of mixture composition and process conditions.

5.3.1.1
Planned Experimental Design

The mixture design experiments are carried out to precisely determine the composition of the components. The usual experimental mixture design deals with three to ten components. The existence of the various types of the component constraints (relational constraints, constraints resulting from the interaction of components) is typical for the mixture design. The studied attribute (taste, viscosity, stability, etc.) is recorded for every experiment. Depending on the number of components and the specific composition constraints, a precise number of experiments are conducted according to the selected experimentation plan. *A priori* determined compositions and experimentally obtained values of the attributes are used for obtaining linear, cubic or higher-order regression equations. A good introduction to mixture design is given by Eriksson et al. (1998).

The most popular fields of application of mixture design are pharmaceuticals, food products, polymers and paints. A few of the most typical are:

- *Blending:* Olive oils were blended to ensure the best sensory quality. There were eighteen experiments carried out to find the optimal composition, according to eight sensory criteria, of four olive oil mixtures (Vojnovic et al. 1995).
- *Formulation:* A mixture of dispersants was designed for use in oil spill cleanup. In order to evaluate a mixture of three different dispersants, ten experiments were performed consisting of the measurement of the effectiveness of oil dispersion (percentage of oil removed from the water surface) as a function of the dispersant mixture composition (Brandvik 1998).

- *Pharmaceutical formulation:* The objective was to find the optimal composition of the tablet coating ensuring the required release rate of the active ingredient from inside of the tablet. The coating was composed of three components and the release rate was determined by the measurements of the diffusion coefficient in 13 experiments with different mixture compositions (Bodea and Leucuta 1997).

The combined experimental design is an active field of research allowing for the prediction of the product properties not only as a function of the composition but also of processing mode. The application fields are the same as for the mixture design:

- *Blending:* In a process consisting of the blending of three different flours, the product attribute was baking quality. Sixty-six experiments were performed to identify the polynomial that correlates the composition of the flour mixture and mixing time with the baking quality of bread (Naes et al. 1999).
- *Pharmaceutical formulation:* The studied property of the material was its viscosity as a function of its composition (active substance: tolfenamic acid, block copolymer, ethanol and buffer) and one process variable (Cafaggi et al. 2003).

Mixture design is a very well-established method within product design. However, changes in the business environment, as mentioned at the beginning of this chapter, have caused long time periods and relatively high costs, which are the main factors limiting the attractiveness of experimental mixture design.

5.3.1.2
High-Throughput Experimentation

The estimated number of inorganic compounds is around 10^9 (only for materials composed of five elements). The number of drug-like structures is projected to be as high as 10^{63} (Cawse 2002). Consequently, new methods of research are needed to identify, with relatively high probability, new promising materials in such a huge space. High-throughput experimentation (HTE) is used to tackle the problems where the parameter space is too large to be handled efficiently using conventional approaches. HTE consists of the use of miniaturized laboratory equipment, robotics, screening apparata and computers.

The main field of HTE application is the determination of the composition of drugs, multifunctional materials, coatings, and catalysts as well as the determination of their formulation. A good introduction to the subject is given by Cawse (2002). The main problems related to the application of CAPE to HTE consist of handling the complexity resulting from the amount of data and highly complicated phenomena under consideration. As a consequence, the research interest concentrates on the design of databases, data mining, integration and representation, conversion of data to knowledge, experimental control systems, and decision-supporting systems to facilitate "hit-to-lead" process aiming at the maximization of the number of the successful designs.

The successful application of HTE to products design are numerous, e.g., homogeneous and heterogeneous catalysts (Murphy et al. 2003). The review of HTE applications to materials design is presented by McFarland and Weinberg (1999). A few examples given below focus on CAPE-related problems in THE.

- *Catalyst design:* Caruthers et al. (2003) have outlined a procedure for the more comprehensive use of data from HTE in catalyst design. The final objective of the presented research is to achieve a balance between the speed of the data generation and abilities of their transformation into knowledge. The proposed process of "knowledge extraction" consists of planning HTE in a way that allows for the discrimination of the models of catalytic reaction models, determination of the kinetic constants and relating them to the catalyst microstructure. The proposed forward modeling is realized by the application of the rules capturing the human expertise, neural network (NN), and genetic algorithm (GA). The proposed system is not yet fully automatic.
- *Pharmaceuticals design:* The acute problem facing the pharmaceutical industry is growing discrepancy between the R&D investment and a number of newly registered drugs (Anonymous 2004). The declining number of new drugs is due, among other factors, to the concentration of efforts in HTE technology on the generation of active pharmaceutical ingredients (API) – selectivity and potency at the target are the mainly studied features – and neglect of the studies of the API form (salt, polymorphic, hydrates, solvates, etc.). Those forms determine the properties of the API, such as solubility, stability, biocompatibility, etc. Those properties, on the other hand, determine the metabolism, toxicity, and formulation design of the pharmaceuticals. A comprehensive description of the problem is presented by Gardner et al. (2004).

An interesting application of CAPE tools to HTE is the use of case-based reasoning for identifying the required conditions for protein crystallization (Jurisica et al. 2001).

5.3.2
Knowledge-based Tools

5.3.2.1
Case-based Reasoning

Case-based reasoning (CBR) consists of solving new problems using the solutions of old problems. The central notion of CBR is a case. The main role of a case is to record a single past event where a problem was solved. A case is represented as a pair: problem and solution. Several cases are collected in a set to build a case library (case base). The library of cases must roughly cover the set of problems that may arise in the considered domain of the application. The set of cases in the case library generates two different spaces (a problem space, involving only problem descriptions of the individual cases), and a solution space built by solutions of those problems. There are five steps in CBR: (1) introduction of a new problem, (2) retrieval of the most similar cases, (3) adaptation of the most similar solutions, (4) validation of the current solution, and (5) system learning by adding the verified solution to the database of cases. The retrieval is a basic operation of CBR. The current problem is defined by a list of the parameters with their values, e.g., names of additives, their amount, material processing, etc. This description is positioned in the problem space. During the retrieval step, the current problem is matched against the problems stored in the case base. The matching is realized by the calculation of the similarity function. The similarity function can be visually defined as a distance between the current problem and the past one in the problem space. The most similar problem and its solution are retrieved to create a starting point for finding the solution of the current problem. In most cases, the solution of the retrieved problem could not be accepted as the solution to the current one as even small differences between problems may require significant modification of the solution. An adjustment of the parameters of the retrieved solution to be conformed to the current problem is called adaptation. The adaptation often requires additional knowledge, which can be represented by the rules or equations. The received solution and the current problem together form the new case that is incorporated in the case base during the learning step. In such a way, the CBR system evolves into a better reasoner as its capability is improved by extending stored experience. CBR is beneficial when the problems are not completely understood and a reliable model can not be built. Moreover, the problem may not be completely defined before starting to search possible solutions. The approach proposes solutions quickly so it can considerably accelerate the design process. Introductions to CBR are given in Watson (1997) and Aamodt and Plaza (1994).

The method has been used in various applications: formulation of tablets, plastics, rubber and agrochemicals. The examples described in the literature that deal with the tablet formulation concentrate on the selection of the tablets ingredients and their composition. Typically the tablet is composed of:

- filler (to ensure that the tablet is large enough to be handled);
- binder (to facilitate granulation);
- lubricant (to facilitate manufacturing);
- disintegrant (to ensure an easy intake of the drug after the swallowing);
- surfactant (to guarantee dissolution of the drug);
- active component (to perform the treatment).

The proposed system (Craw et al. 1998) is aimed at the retrieval as well as adaptation. The potentially interesting formulation is adapted by the application of the rule-based system. It allows one to determine the most adequate ingredients by the elimination of the various conflicts and constraints related to the simultaneous presence of some of them in a tablet. The adaptation is realized using the voting mechanism consisting of the selection of the most frequently used ingredients among the retrieved cases. The supplementary rules ensuring, for example, stability of the system, are used. An additional feature is adaptation of ingredients quantity by the application of two methods (average quantity from the retrieved cases or the best match). The adaptation phase realized by the application of the hybrid algorithm combining induction and instance-based learning was introduced by Wiratunga et al. (2002). An interesting improvement of the cases retrieval has been proposed by Craw and Jarmulak (2001). The application of the genetic algorithm has been proposed for handling the growing case base as well as to capture the changing approach to the principles of formulation. The growing case base contains new knowledge that should be handled differently and the changes of the principles of formulation reflect the modifications in company politics.

The application of CBR to the design of the closed rubber cells was presented by Herbeaux and Mille (1999). The paper deals with the determination of composition of the rubber as well as the operating parameters for the extrusion and vulcanization phase. The main function of the proposed CBR system is the retrieval of the cases and not their adaptation.

The design of tires was presented by Bandini et al. (2004). The problem consisted of determining the recipe for the manufacturing tread (elastomers, silica, carbon black, accelerants, etc.) as well as determination of the conditions for compound mixing and vulcanization. The chemical formulation of the product depends on the desired properties of the tire. The desired properties are determined as a function of the car set-up, weather, type of road, etc. The problems dealing with the vulcanization and tuning of the product have been solved using the CBR system. The rest of the activities related to the tire design are obtained using rule-based systems.

The design of lubricating oils was introduced by Shi et al. (1997). The main problem tackled in the paper was the formulation of an additive that was combined with the oil to create a lubricating agent. The applied CBR system starts with the input information such as the base oil type, viscosity, and constraints of use. The adaptation phase is realized using a rule-based system.

5.3.2.2
Neural Networks

Neural networks (NNs) are well-established techniques in CAPE (see Fausett 1994). The application of NNs to product development covers several types of products. Below a few of the most common applications have been presented.

Fuel Additives

The use of NN for product design has been illustrated by Sundaram et al. (2001) for fuel additives. Fuel additives have been used as combustion modifiers, antioxidants, inhibitors of corrosion, deposit controllers, etc. The role of the deposit controllers is to limit the formation of the deposit on the intake valve and combustion chamber. Due to the high cost of the experiments, additive design has focused on use of the mathematical tools. The authors proposed a hybrid approach combining modeling and NNs. The results obtained from modeling have been used to train the neural net and then compared with the experimental results. Such an approach enabled the tuning of the model, allowing for the prediction of the build-up of the deposit as a function of the composition of the additives.

Rubber Mixture

Borosy (1999) has proposed the application of NNs for the formulation of rubber mixtures. The Internet was used for the purpose of direct (what are the properties of the mixture when the composition is given) and indirect modeling (what should be the composition to ensure the required properties of the mixture). A maximum of 32 variables were needed to describe the mixture composition and processing conditions, and nine variables to capture the characteristics of the product. Adaptively learning NNs have been trained to map the relations between the input and output.

Dyes

Chen et al. (1998) have proposed a combination of NNs and experimental design to formulate a pigment composed of six components. It was a case of solving the direct product design problem. The pigment quality was determined by comparison with three color indices. The proposed approach was limited exclusively to the determination of the pigment composition and did not consider the complicated heating policy in the processing phase.

Greaves and Gasteiger (2001) have applied NNs to predict the molecular surface of acid, reactive, and direct dyes. The mapping of the three-dimensional molecular surfaces into a Kohonen network, enabling the prediction of substantivity, was an example of the direct formulation of the product design problem.

Pharmaceuticals

NN applications concentrate on finding the relation between the composition of the tablet and the required release time, prediction of the physicochemical properties of the substances based on their molecular composition, and formulation of the special purpose tablets (e.g., fast disintegrating).

Takayama et al. (2003) have presented an application of NNs to direct and reverse problems of product design. Two examples of NN application have been given. In the first case, the objective was determination of the optimal composition ensuring the required release of the active substance from the tablet. The tablet was composed of the active substance, two gel-forming materials and disintegrant. The second example dealt with the determination of the optimal composition of the mixture of ketoprofen hydrogels composed of two gel bases, two penetration enhancers, and two solvents. The objective function was the required rate of penetration of active substance and skin irritation.

Türkoglu et al. (2004) have presented the application of NN to the formulation of the tablets composed of the coated pellets. The objective was to identify the formulation ensuring the required disintegration in the gastrointestinal fluid. Four properties of six-component tablets were studied to identify the required composition.

Based on molecular structure, Taskinen and Yliruusi (2003) have presented a survey of NN applications to the direct prediction of the 24 physicochemical properties essential in drug design.

Sunada and Bi (2002) reported their research on the formulation of the rapidly disintegrating tablets. The objective was to achieve fast disintegration in the oral cavity without drinking water. Four-component tablets that formed powder characterized by nine properties were studied. The applied processing method was wet compression.

Refrigerants

Sözen et al. (2004) have studied the prediction of the specific volume of refrigerant/absorbent couples as a function of the system composition, pressure, and temperature using NN. The objective was to determine the properties of the couples ensuring zero ozone depletion, thermal resistance, high evaporation heat at low pressure, low specific volume of vapor, low solidification and high critical temperatures. A similar study was done by Chouai et al. (2002). They determined the thermodynamic properties of three refrigerants.

Polymer Composites

The application of NN to the formulation of the polymer composites has been reviewed by Zhang and Fredrich (2003). They gave a comprehensive overview of the NN application to the estimation of fatigue life, design of unidirectional and laminate composites, assessment of wear of composites, and processing optimization.

There are some examples of NN applications in the design of other products, e.g., food (Jimenez-Marquez et al. 2003), catalysts (Liu et al. 2001), ceramic materials (Sebastia et al. 2003), and lubricants (Konno et al. 2002).

5.3.2.3
Genetic Algorithms

Genetic algorithms (GAs) are gaining a lot of attention in CAPE. A classic book on genetic algorithms was written by Goldberg (1989). This very promising tool of artificial intelligence has been used to design polymers (Venkatasubramanian et al. 1996; Venkatasubramanian et al. 1995), catalysts (McLeod et al. 1997; Corma et al. 2003), and rubber (Lakshminarayanan et al. 2000; Ghosh et al. 2000). Very often GAs are combined with first-principles modeling and other artificial intelligence methods.

The most common hybrid system is NN-GA. They are used for catalyst design (Huang et al. 2003; Rodemerck et al. 2004; Caruthers 2003) and fuel additive design (Ghosh et al. 2000).

5.3.2.4
Rule-based Systems

Nowadays the "classical" rule-based systems are relatively seldom encountered as tools for the support of the product design. The review of such systems has been presented, e.g., by Rowe and Roberts (1998b). However, there are several examples of hybrid systems for design of:

- materials: rule-based and case-based system (Netten and Vingerhoeds 1997), and rule-based and genetic algorithms (Kim et al. 1999);
- cosmetics: rule-based and first principles (Wibowo and Ng 2001);
- pharmaceuticals: rule-based and first principles (Fung and Ng 2003), and rule-based and neural networks (Guo et al. 2002).

5.3.2.5
Data Mining

Data mining is a term used for the group of techniques used in finding useful patterns in the datasets. A comprehensive survey of the methods is given by Hand et al. (2001). The approach consists of the analysis of huge data depositories in search for the useful correlations between material properties and its composition. A simple example of data mining application to rubber design is given by Chen et al. (2000). Beliaev and Kraslawski (2003) have applied a semantic analysis of the scientific literature to identify new products that can be synthesized from substrates (sucrose, glucose, fructose, fatty acids) with *Candida antarctica* lipase acting as a catalyst.

5.3.2.6 Semantic Networks

The application of the semantic networks to predict the qualitative properties of complex compounds as a function of their composition has been presented by Kiselyova (2000) for the design of inorganic materials. The results of predicting the crystal structure types at normal pressure and room temperature for compounds with given composition are presented.

5.4 Summary

Analysis of the literature shows that solving pure forward problems in product design is still in the trial phase. Exclusively predictive methods for product design are not yet in industrial use. Therefore, it seems the application of existing experience in product development is the main approach allowing the achievement, in a reasonable time, of good product design. However, the reuse of knowledge is mainly useful for incremental improvements of existing products. It is estimated that around 100 ideas are needed to generate a new product (Cussler and Wei 2003). The discoveries leading to the breakthrough innovations need new tools for the management of the existing knowledge, enabling the generation of new ideas. Tools like data mining and TRIZ still wait for broader application in product design.

A new subject will be the combination of CAPE tools and market analysis approach in the estimation of risk related with the rejection, by the consumers, of new chemical products (e.g., fears related with nanomaterials). The development of techniques for assessing the impact of new chemical products on the environment, health and safety as well as communication of those facts to society, is a new important role connected with their development.

A fascinating field of CAPE applications in product design is tangible and augments elements of chemical products, not only their structure-property behavior, but also the design of their dynamic behavior in the context of the product-related services or functions.

Keeping in mind the transition of product design from purely experimental towards computer-aided product design, the following challenges that face CAPE in the field of product development seem to be crucial:

- development and implementation of the approaches aimed at closing the gap between the phase of the data collection and generation of information;
- adaptation of the existing methods in process design to product development and possibility of reusing available software for new tasks;

- development of the methods aimed at the generation of product-related knowledge from the available information, and consequently creation of more generalized approaches for solving behavior-properties-composition (structure) problems at the level of project and business units.

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