1 Introduction

1.1 Chemical Product Engineering

Current globalization trends have resulted in a fierce competition between multinational companies for gaining more market share. Startup companies, on the other hand, also try to play in this game by offering differentiated or disruptive products that would potentially change the game and dynamics in each market segment. The main tool for technological companies to compete, however, remains their product offerings, and how they can serve the customers and address their needs. Any profitable market invites new entrants which creates competition. Companies try to accelerate their product development processes to launch more differentiated products to stay ahead of the game, while even reducing their costs. This is of course not a trivial task for scientists and engineers to take on. Furthermore, customers nowadays have been poised to see newer products and can quickly switch to other companies with better product offerings if the "newer" products are not commercialized quick enough, as the life cycle of the current products keeps becoming shorter. Brand loyalty does not exist as it used to be a few decades ago, and customers can quickly switch if they find a product with better features. An obvious example is the smartphone market, and that companies fiercely compete to introduce new products every year. Imagine one of the incumbents misses one product launch by a few months, and how catastrophic financial outcome they can encounter. In many cases, these new products are only simple modifications to existing technologies, but even these "small modifications" should carry enough value proposition to convince buyers among all choices they have. This competition is of course not limited to electronics market and is widespread in all industries, from cosmetics to pharmaceuticals and consumer to agriculture. In all these market segments, research and development teams work closely with their marketing counterparts to identify market needs and trends to stay ahead of the curve. There is no exaggeration to say that in the current market, innovation is like oxygen for the business, and without that any business will soon become irrelevant. Naturally, innovation can only be monetized if it is translated into a new product and capture revenue. This is why freshness index, i.e. the ratio of new products contributing to the revenue of the company over total revenue, is considered as a key success metric for most companies. A faster commercialization cannot be achieved without

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a lean and agile product development process, and therefore it is very important that companies spend their R&D dollars very wisely and try to avoid less efficient development methodologies.

Product design can have various interpretations, among them is the definition as the entire procedures required to deliver a product with defined properties that serve a specific need in society or industry based on inputs from various segments. For instance, inputs from the industry of how the product may serve and what specifications should be considered during the manufacturing process. Items that can be considered include environmental and regional regulations. An example of environmentally friendly product design is the manufacturing of a greenhouse ventilation system, where the house is designed to attenuate energy consumption and maintain required rate of fresh air exchange. In such a process of product design of a household air exchanger, various elements need to be considered including heat and humidity. In addition, material selection is a significant factor in the manufacturing of such a device to take into consideration environmental impacts such as energy conservation, corrosion, and exhaust gases, if any. The topic of product design has become even more important with the growing changes in industry and regulation to protect the environment. For example, the manufacturing process of synthetic textile fiber has been continuously developing since 1950. Starting wth a global production of less than 10 million mt in the 1950 and undergoing a 10-fold increase by 2017, the effective utilization of fibers in various applications was achieved through product design studies that were caried out on the development of various prototypes utilizing statistical software packages. In general, the process of product design encompasses the following steps: market needs, ideas, material selection, and finally manufacturing and process control and optimization.

Many of the products we touch and feel today have come out of a chemical plant one way or another. These products cannot be missed even in any quick visit to a grocery store. Consumer products (e.g. detergents), cosmetics, health care products (e.g. disinfectants, sanitizers), adhesives, pharmaceuticals, etc., are all examples of chemical products. Therefore, chemical product design (CPD) is a very important market segment and deserves enough attention in improving product development methodologies. Chemical product engineering is the science and art of creating chemical products, a much larger concept encompassing CPD. In other words, chemical product engineering can be seen as the general background of knowledge and practice supporting the concrete task of designing chemical products and their manufacturing processes.

1.2 Chemical Product Design

One of the crucial challenges facing modern corporations and industry is the growing competitive and dynamics market. A successful business requires continuous monitoring of consumers' needs and delivering valuable products at competitive prices and high quality, while addressing environmental regulations. Therefore, researchers from various fields of industry including but not limited to management, marketing, and engineering design always devote attention to development of new products and issues associated with the fabrication of the products such as environmental concerns. When designing a new product, different factors are usually combined such as strategic and technical effort. Here, strategic planning is required to deliver a successful launch of the product, while technical effort focuses on design, manufacturing, control, and process optimization aspects. Therefore, a growing number of researchers from different fields of engineering including chemical engineering have devoted attention to the area of efficient design of new products.

Specialty chemical products include petrochemicals, pharmaceuticals, green chemicals, food products, household care consumables, and cosmetics. In different sectors, chemical products are undergoing continuous changes to meet the expectations of the consumers in addition to continuously stricter environmental requirements. The fabrication of a chemical product is a multistage process starting from synthesis, design, optimization, operation, and control. The successful execution of the previous steps would transform raw materials into valuable products. Furthermore, the design of a chemical product requires deep understanding of the properties of the materials and usage functions. Chemical products can be classified into six categories as follows: specialty chemicals, bioproducts, formulated products, devices, technology-based products, and virtual chemicals, where each category has a special identity. For example, specialty chemicals can be defined as pure compounds that are delivered in small quantities and may serve specific functions. Formulated products such as cosmetics and food represent a large market and can be defined as combined systems where various raw materials are blended together to deliver a multifunctional product with specific appearance and properties. Continued development in health care applications triggers the need to develop bioproducts that include biomaterials, tissue, and metabolic elements. Most of pharmaceutical drugs are now derived from biological sources rather than traditional synthetic chemicals. Moreover, products that cannot be classified as pure compounds, mixture, or fabricated biomaterials may include devices that carry out a physical or chemical transformation.

There have been major changes in the chemical industry during the last two decades. The dominance of commodity chemicals has been eroded by a newer emphasis on products such as specialty chemicals [1]. These chemicals include but are not limited to detergents, cosmetics, pharmaceutical drugs, fertilizers, adhesives, and many more. Today, there are many companies and industries that have focused on developing such products and are in fierce competition with each other for market share. Chemical process industries have always launched successful new products. However, the dynamic and demanding markets require companies to adopt a more systematic approach to bring the new product to the market faster and cheaper to guarantee competitiveness. Chemical Product Design and Engineering is becoming more important as a consequence of this change. While customer needs and product differentiation for competition purposes are significant drivers to faster develop products, global warming and climate change require newer products to have less environmental impact. Increased awareness by both people and governments, and media's increased attention to this important topic, has led governments to impose more stringent environmental regulations which puts even more pressure on companies to try to reduce waste and carbon footprint. It would be obvious for companies to try to optimize processes and product formulations to deliver the same performance using "less" chemicals in a faster time and using less resources. The million-dollar question to ask is how to achieve this, or simply how to do more with less? In this book, we are trying to answer this question partially and our focus will be on chemical and biological product mixtures.

In summary, the dynamic nature of the chemical and biochemical industries, intense competition for market share, and emergence of more strict environmental regulations require deployment of innovative product development methods to address increasing demands for faster, leaner, and optimized products.

1.3 Product Design and Computer-Aided Product Design

CPD can be defined as a systematic procedure or framework of methodologies and tools whose aim is to provide a more efficient and faster design of chemical products able to meet market demands. From the practical standpoint, Cussler and Moggridge [2] simply defined product design as a procedure consisting of four steps: (i) defining the needs, (ii) generating ideas to meet the needs, (iii) selecting the best ideas, and (iv) manufacturing the product. Generating ideas and selecting the best ideas are the most time-consuming steps. These two steps traditionally involved an exhaustive search by trial-and-error methods which often ended up with no significant results. One way to overcome this problem is by using computer-aided techniques to identify very quickly a set of promising candidates and select a subset of likely final products, from which the desired properties can be identified through experiments (Figure 1.1).

The first step in Figure 1.1 is the predesign, or problem formulation step. Steps 2 and 3 represent, respectively, two types of product design problems: molecular design and mixture/blend design. In the molecular design, the objective is to find a chemical product that exhibits certain functional properties. The invention of new fuel additives and solvents in organic synthesis are examples of this type of design. In the mixture/blend design, the objective is to find a recipe of chemical ingredients which give desirable final product properties. Examples of this type of design are the design of fuel blends and polymer blends, including polymer composites and additives. The associated computer-aided designs for the two CPDs are called computer-aided molecular design (CAMD) and computer-aided mixture/blend design (CAM^{b}D).

Chemical products are judged by consumers not from their technical specifications but rather by the functional and performance attributes which are usually described by a set of performance indices. These indices are determined by three factors: (i) the composition and physicochemical properties of materials that constitute the product; (ii) product structure, which is dependent on the manufacturing process; and (iii) product usage conditions. The relationship between performance

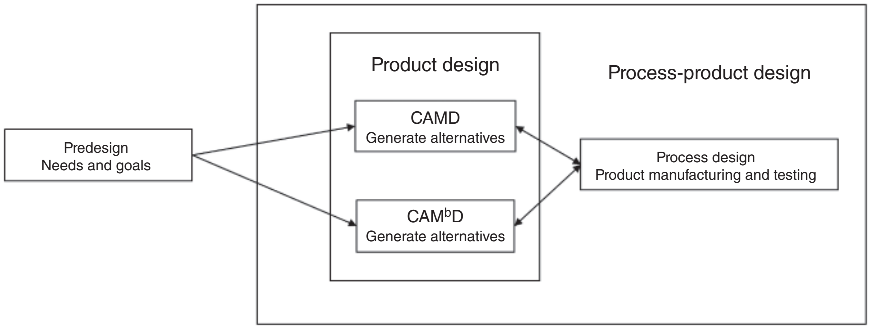

Figure 1.1 The design process for product design.

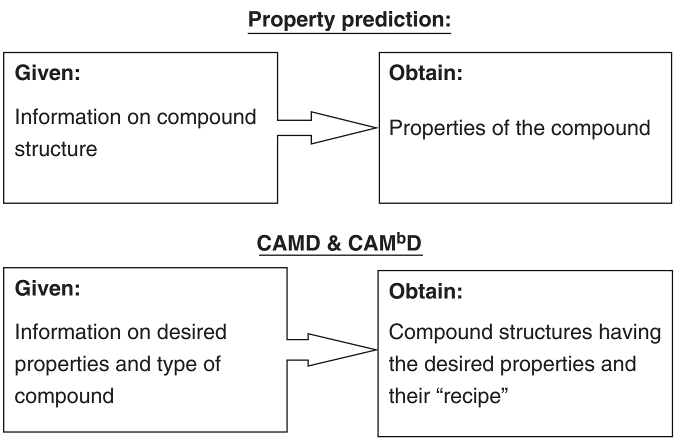

Figure 1.2 Chemical product design (CAMD, CAM^{b}D) are "reverse" of property prediction problems.

indices and product composition, product ingredients' properties, and product structure has been mathematically systematized through the concept of property function. In generic terms, the CPD can be defined as: given a set of desired (target) needs, determine a chemical product (molecule or mixture) that satisfies these needs. Based on this definition and the concept of property function, the CPD problem can be described as a "reverse property prediction," as illustrated in Figure 1.2, where the needs are defined through product properties [3].

A simple framework for CPD is illustrated in Figure 1.3. Different aspects of CPD are represented by methods for CAMD, CAM^{b}D, analysis, and model validation, while different calculation options are represented by tools of process simulation, pure component property estimation, mixture property estimation, and search engines for data retrieval from databases. Although the two-directional arrows in Figure 1.3 show the connection between two adjacent methods or tools, they are meant to indicate that all the tools and methods are connected to each other.

In any CPD problem, property functions and property models play important roles. While the framework is flexible enough to handle a large range of CPD

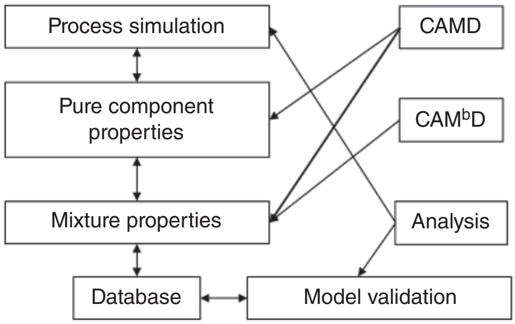

Figure 1.3 A simplified framework for computer-aided chemical product design.

problems, the currently available methods and tools can only solve a relatively small percentage of these problems. This is because the property models that are currently available are unable to predict the needed properties within an acceptable limit of uncertainty.

The framework, however, can give a great contribution to creating property models and database development in a systematic way. This will reduce time and effort in the early stages of the product design process and subsequently bring the product to the market cheaper and faster.

The remainder of this book is organized as follows: Chapter 2 surveys a variety of applications associated with CPD, while Chapter 3 covers tools commonly used to accelerate product development. Chapters 4–12 provide illustrative case studies related to CPD and formulation.

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