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An integrated framework for designing formulated products☆

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ABSTRACT

Formulated products are created by mixing various ingredients together. They are commercially produced for drugs, cosmetics, cleaning agents, lubricants and many others. The design of formulated products is diverse and multidisciplinary in nature; physico-chemical properties, product microstructure, product quality, and all other related areas have to be considered integratively. Various types of data, methods and tools are needed to tackle formulated product design problems to achieve an optimal design. In this study, an integrated framework as well as the design steps are proposed for the design of all kinds of formulated products including liquids, solids, emulsions, etc. Strategies for the selection of different modelling methods such as rule-based methods, model-based methods, experiments and databases are also presented. A multi-layer knowledge library is proposed to store all the information needed in the design of formulated products. Case studies of battery electrolyte and laundry detergent are given to illustrate the design framework.

1. Introduction

Modern society needs all kinds of products to function. Zhang et al. (2016) considered a wide range of chemical-based products ranging from medicines to personal-care products. A subset of these chemical-based products consists of formulated products which are ubiquitous in daily life, for example pharmaceutical tablets and suspensions, cosmetic creams and gels, detergent powders and liquids, processed foods, paints, adhesives, lubricants and pesticide granules. Currently, there are a large number of organizations focusing on formulation technology and practice. For example, the Formulation Science and Technology Group (http://formulation.org.uk/) fosters the advancement of formulation science across scientific disciplines, and a point of focus for all industrialists and academics engaging in the practice of formulation science. Other organizations with an interest in formulated products include the French Chemical Society (SFC), Institute of Chemical Engineers (IChemE), Colloid and Surface Science Group of the Royal Society of Chemistry, and so on.

Chemical engineering has been expanding its focus from process-centered products such as chlorine and ammonia, to product centered products such as mosquito repellent sprays. Meanwhile, chemical product engineering has been introduced as the third paradigm in chemical engineering (Hill, 2009). Gani and Ng (2015) classified the chemical products into molecular products, formulated products, functional products, and devices. The design of formulated products involves aspects such as identification of product attributes, determination of product form, selection of ingredients, process design as well as economic analysis. It is necessary to develop a design framework for formulated products taking into consideration of all these related areas. Some researchers have already developed various frameworks and tools for chemical product design. Cheng et al. (2009) proposed a multidisciplinary hierarchical framework involving management, business and marketing, research and design, manufacturing, and finance and economics. Kalakul et al. (2015) developed VPPD-LAB (the Virtual Product-Process Design Laboratory) software for product-process design. It employs a template approach that follows product-specific steps in the framework for data, target property models, and calculation routines for product and process design. Fung et al. (2016) pointed out that the production of the B2C products focuses on product quality, ingredients, microstructure, process, cost and pricing model. Market and competitive analysis, government policies and regulations have to be explicitly considered in product design. All these considerations are accounted for in

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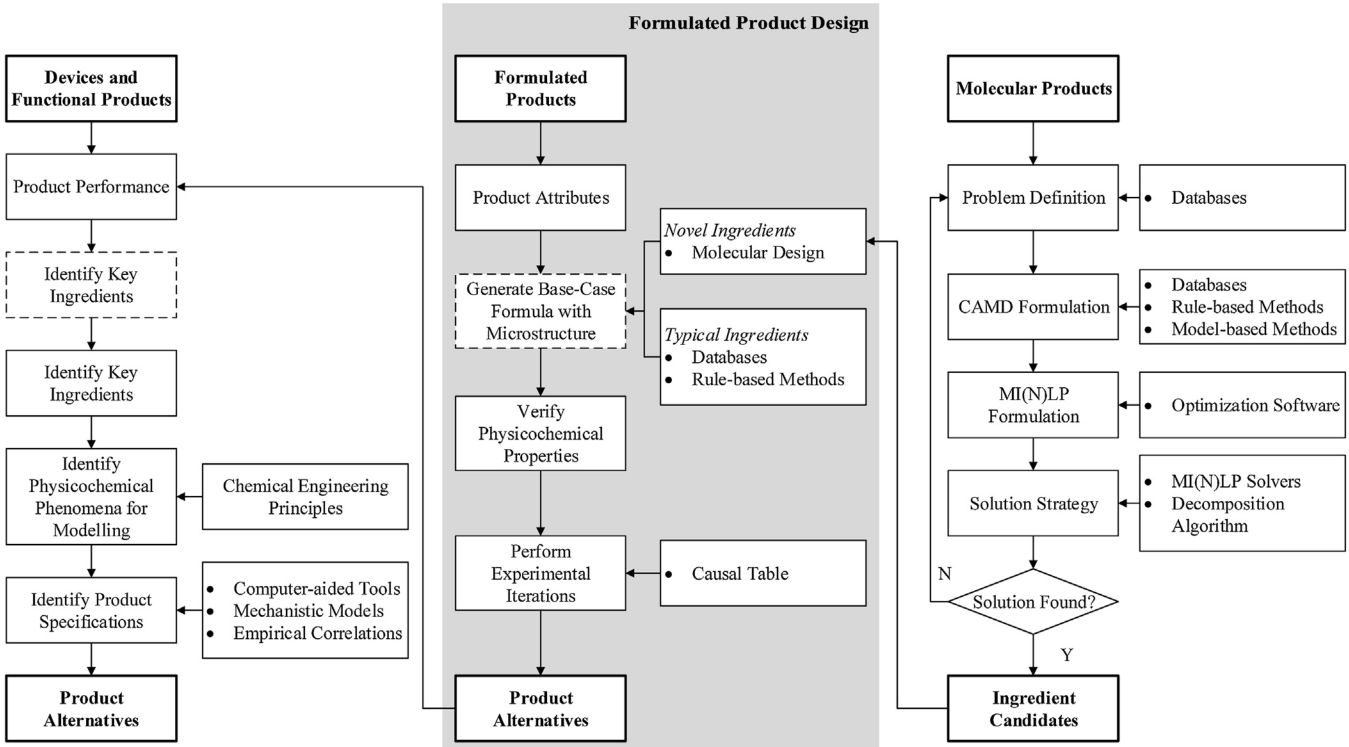

Fig. 1. The workflow diagram for the design of molecular products, formulated products, and devices and functional products. Figure reproduced from Zhang et al. (2017).

the multi-scale and multi-disciplinary Grand Product Design (GPD) Model (Fung et al., 2016). Fig. 1 shows the design workflow diagram and relationship between formulated product design, molecular design, and the design of devices and functional products (Zhang et al., 2017). As can be seen, molecular design can be used to generate novel molecules that are not available in the existing database, but offer the properties needed in the formulated products.

Researchers have developed various methods and tools to systematically generate product alternatives to meet market and engineering requirements, and to quantitatively analyze those alternatives so as to select the best alternatives. As Fig. 1 shows, the ingredients of formulated products can be classified as typical ingredients and novel ingredients. For the design of typical ingredients, databases and rule-based methods are used. For example, Wibowo and Ng (2001) proposed heuristic design methods for creams and pastes. Fung and Ng (2003) proposed rules to select chemicals for specific product applications in the form of a database search and then verify them through a combination of models and experiments for pharmaceutical tablets and capsules. For novel ingredients, molecular design methods are used. Researchers have developed various methods for molecular design. They are classified into rule-based "generate and test" method and mathematical programming method.

Gani and Brignole (1983) proposed a rule-based synthesis-design method, called "generate and test" method to generate molecular structures by combining functional groups and use of functional groups based property estimation techniques for physical properties. The "generate and test" method was extended by Klein et al. (1992) to design solvent mixtures. Harper and Gani (2000) proposed a multi-step and multi-level approach of the "generate and test" method for chemical product design which includes problem formulation step incorporating a knowledge base for the identification and setup of the design criteria; candidate compounds generation step using a multi-level "generate and test" CAMD solution algorithm with a high level of molecular detail; a post solution step for result analysis and verification.

Many mathematical programming methods are also available for molecular design. Odele and Macchietto (1993) used mathematical programming for optimal solvent design. Venkatasubramanian et al. (1994) applied genetic algorithms to solve molecular and pharmaceutical product design problems. Later, the application of mathematical programming with group contribution method for property estimation methodology was expanded to polymer design (Vaidyanathan and El-Halwagi, 1994). Cignitti et al. (2015) presented a framework for computer-aided design of pure and mixed chemical based products. In their framework, the product needs and target properties are systematically converted into an MINLP problem, and sequentially solved through a decomposed optimization approach. Zhang et al. (2015) proposed a generic MILP/MINLP mathematical programming formulation, with the consideration of higher order groups for molecular structure representation and property estimation. Hostrup et al. (1999) presented the integration of solvent selection design with the design of separation processes involving azeotropes; the problem is formulated as MINLP and solved with decomposition method. Papadopoulos and Linke (2006) proposed the integration of solvent selection and process design problem, with the environmental impact taken into account. MacDowell et al. (2010) used an integrated approach for solvent selection and CO_2 capture process design.

Formulated product design has been an active area of research. Hill (2009) reviewed the heuristic methods of product-process design for formulated products, and cases such as soap bars, margarine and skin creams were presented. Conte et al. (2011, 2012) combined formulated product design with experiment-based product testing for insect repellent and hair spray products, and presented a systematic methodology for the design of formulated products. Since they focus on liquid formulated products, such as solvent mixtures, other forms of formulated products such as