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CURRENT APPROACHES ON CHEMICAL PRODUCT DESIGN: A STUDY OF OPPORTUNITIES IDENTIFICATION FOR INTEGRATED METHODOLOGIES

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ABSTRACT

Integrated methodologies for chemical product design have been proposed during the last decades as an alternative to reduce the time and resources invested in the early stages of product development. The objective of the present work is to classify the current strategies in this field, to identify research trends and key opportunities for integrative methodologies of design regarding formulated products. Based upon a comprehensive review from the classic to the most current literature, 157 significant references were selected from more than two thousand initial sources. It was found an increasing trend on the integration of modelling with experience support, product-process interactions, as well as multiscale and multidisciplinary approaches (consumer insight, business variables and sustainability assessment) using computer-based design tools. However, there are still only a limited number of systematic methodologies that integrate all these levels along with the available heuristic knowledge, allowing a quick and systematic design for consumer-oriented formulated products.

Keywords: chemical product design, formulated products, product-process design, multiscale

INTRODUCTION

The shift from commodities to high-value-added specialties and functional chemicals has been an increasing trend among the chemical manufacturers in recent years (Costa, Moggridge and Saraiva, 2006). Due to the growing worldwide competitiveness in this sector, today companies must be able to do a quick development of new and differentiated products without compromising quality or performance, as a key element for their success (Charpentier, 2010). Frequently, the decision of a product launch is taken far from the processing plant or the technical team, but in the marketing departments as a response to consumer trends. Then, in some particular sectors (e.g. personal care industry), the speed at which products are designed, developed and manufactured is the decisive point, even above the cost of production (Charpentier, 2009). Consequently, the need for rapid development of innovative chemical products becomes a major challenge for technical R&D departments (Cooper, 2013). Traditionally, chemical product design has been made following an experiment-based trial-and-error approach at different scales to get a set of candidate products that meet the targeted performance (Eden, 2003; Omidbakhsh *et al.*, 2012; Mattei, 2014; Zhang *et al.*,

2017). Then, based upon different criteria (e.g. economics, process constraints, consumer feedback, etc.), a specific product is selected to be manufactured and commercialized. Such series of stages results in a very resource-consuming activity in product design and development. This approach becomes particularly difficult when dealing with multiple-species products in which their components, processing variables, and even use conditions, among other factors, could play a major role in the product performance. Consequently, different systematic methodologies for these types of products have been proposed as an alternative to reduce the time spent in the early stages of development (Zhang, Babi and Gani, 2016).

With the aforementioned considerations, the present work aims to classify the most current contributions in the field of chemical product design. Particularly, it is intended to identify the key research opportunities for integrative methodologies, which involve mathematical modelling and experiment-based components, product-process interactions, multi-scale and multidisciplinary approaches (consumer perception, business variables and sustainability) at different levels. The classification of the different research approaches was done by reviewing scientific literature before 2018, from the classic works to the most recent publications on the field. Based on the reviewed material, a comprehensive description regarding integrated methodologies for chemical product design, focusing on their main contributions and their levels of integration for the case of formulated products is presented. This last feature distinguishes this study from previous reviews in the field or methodologies of chemical product design. As a starting point, in the first section, an overview of chemical product design research and the methodologies used in the current practice of chemical engineering along with a classification based on their type of integration are presented. Next, the applied searching methods for the various documents that supported the study are described. Then, the main results are presented and discussed. To conclude, a set of opportunities in the field of integrative methodologies for product design is identified for further research and development.

AN OVERVIEW ON CHEMICAL PRODUCT DESIGN

A chemical product can be defined as a system formed by different chemical substances, which is manufactured for one or more purposes (Cisternas, 2007). As there is a complex interaction of phenomena among the ingredients and during the manufacture of such systems (Schubert and Engel, 2004), the design procedure is in some cases, even a matter of art, relying mostly on the expertise of product developers. In this regard, the most recent paradigm of chemical engineering has focused on developing various methodologies to deal with product formulation and manufacture (Hill, 2009). This idea, named chemical product engineering, involves a backwards design methodology, from the identification of quality factors to the manufacture of marketable products (Costa, Moggridge and Saraiva, 2006). Chemical product design (CPD) is considered a facet of chemical product engineering and it is defined as the systematic framework of methodologies and tools whose aim is to provide faster and more efficient development of chemical products able to meet market demands (Costa, Moggridge and Saraiva, 2006). Despite a large amount of research in the field during the last decades, CPD has not yet developed into the foreseen third paradigm in chemical engineering. A major reason for that is the lack of understanding over the complex relationships between product manufacturing technologies and material properties, at the different levels of the chemical supply chain, and among the different types of chemicals (Charpentier, 2002; Picchioni and Broekhuis, 2012).

Chemical products can be classified depending if their design is process-centered or product-centered (Gani and Ng, 2015). In the first group, we find most commodities and single-species products (small and large molecules), whereas in the second group there are mostly multiple-species products (formulated and functional products) and devices sold directly to the consumer. In particular, this research will consider the last group of products, focusing in formulated products, which are considered here as a mixture of one or more key ingredients responsible for the functionality of the product (active ingredients), and some supporting ingredients to enhance its performance (Wibowo and Ng, 2002), even if this definition could cover functional products as well. There are several approaches to solve a CPD problem depending on the type of product, but they all require the integration of several domains and disciplines, especially for consumer formulated products. In that respect, Cheng et al. (2009) developed a holistic approach for the case of a skin-care cream, involving five groups of job functions: Management, Sales & Marketing, Research & Design, Manufacturing and Finance & Economics. Smith and Ierapepritou (2010) were the first to discuss the different integration strategies in their review, supported by data involving chemical product manufacturers. They established a general framework for integrative product design with three main strategies to incorporate: Consumer influence, product/process, and business requirements. At the same time, three solution approaches for the design problem were proposed: Model-based, experience-based, and hybrid model/experience-based. Recently, Zhang et al. (2016) stated that hybrid systems (experience/model) should be employed to design product/process integrated solutions within a multiscale/multidisciplinary approach when designing a formulated product.

Taking into account the aforementioned, this study considers three main levels of integration, as they represent the identified strategies to effectively deal with the difficult task of formulated product design: experience/modelling, product/process and multiscale/multidisciplinary approaches.

Experience¹/Modelling integration

Experimentation in CPD is normally useful when the underlying physicochemical phenomena for the estimation of the target properties are not fully understood (or simply because the available mathematical models are not developed). Therefore, in this case, empirical knowledge and experience are needed to obtain the optimal formulations (Moulai Mostefa *et al.*, 2006; Ng, Gani and Dam-Johansen, 2007). On the other hand, when validated mathematical models for the estimation of all the target properties are available, a list of feasible candidates can be generated and tested by a model-based approach. Nevertheless, in most cases such mathematical models are available for just a fraction of the target end-use properties or only for some type of specific products, that's why a hybrid experience/modelling integrated approach is more suitable (Mattei, 2014; Zhang, Babi and Gani, 2016). By combining the two above-mentioned approaches, the weaknesses of the one are covered with the strengths of the other (Gani and Ng, 2015). Furthermore, the uncertainties of the mathematical-based approach are compensated by rule-based techniques or heuristics, while the number of experiments is reduced through the model predictions and only carried out for the most promising candidates, saving up resources and time (Arrieta-Escobar *et al.*, 2017).

¹ Experience is here understood as a combination of the empirical knowledge derived from direct observation of and participation in experiments

Product/Process integration

As it was mentioned before, most formulated products are usually complex systems with different ingredients that interact to provide several functions required by the customers (Abildskov and Kontogeorgis, 2004). These systems are very often characterized not only by the quantity of each ingredient but also by their microstructure; i.e. the relative spatial arrangement of each ingredient in the product (Bongers and Almeida-Rivera, 2009, 2012). In this sense, the microstructure is influenced by both the formulation and the process conditions. In some particular cases, the process could even determine both the product structure and its composition, for instance in the case of a crystalline solid (Bernardo, 2017). Bernardo and Saraiva (2005) illustrated how decisions regarding product formulation and microstructure interact with process design and operation, as well as how a decoupled sequential solution of product and process design problems may lead to suboptimal solutions.

Multiscale/Multidisciplinary integration

Since the introduction of the triplet “molecular processes-product-process” engineering concept by Charpentier (2002), the term multiscale seems to be more than appropriate in CPD, as the design and manufacture of chemical products spans to a wide length and time scales, making necessary to consider different interactions and complexity levels to describe phenomena at the nano-, micro-, meso-, macro-, and mega-scale. This task is required to identify and model the relationships between the different levels and scales (Charpentier and McKenna, 2004). On the other hand, as the development of modern products requires different disciplines over a wide-scale range, multidisciplinary approaches have also been proposed in the last few years, especially when a specific desired attribute needs to be attained (Gani and Ng, 2015). In this sense, the product design framework should take into account not only the product structure and composition but also the manufacturing investments and costs, the associated supply chain, the marketing issues, such as the consumer behavior with respect to the product price, among other relevant factors that influence the product design (Bagajewicz, 2007). Multiscale and multidisciplinary integrative approaches are also being developed to address the increasing attention to environmental, safety and social requirements, to the transition towards sustainability, bringing the product design closer to the practice in the industry (Charpentier and McKenna, 2004; Edwards, 2006). Indeed, the modern industry is progressively adopting the principles of the “green chemistry” and “green engineering” (i.e. sustainability) in their designs to satisfy both the market requirements for specific end-use properties (nano- and micro-scales) and the social and environmental constraints of production processes and distribution networks (meso- and macro-scale) (Charpentier, 2016). Hence, the main trends regarding the incorporation of multiscale/multidisciplinary approaches in formulated product design can be roughly divided into four sublevels: Those considering the multiscale nature of the design procedure itself; the ones dealing with the consumer understanding using disciplines like marketing, psychology, etc.; those focused into business decision variables (economics, finances and management, etc.) and finally the ones considering the sustainability dimension.

In synthesis, this study considers three main levels of integration, as they represent the identified strategies to effectively deal with the difficult task of formulated product design: experience/modelling (EM), product/process (PP) and multiscale/multidisciplinary (MS/MD)

approaches. The last level could be additionally sorted in four sublevels: multiscale (MS); consumer insight (CO), business decision variables (BU), and sustainability dimension (SU), as shown in Figure 1.

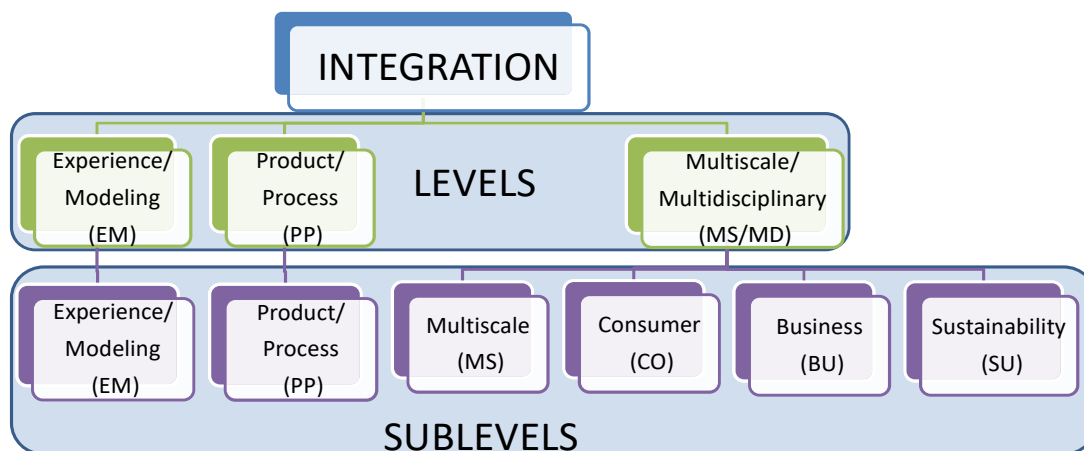


Figure 1: Levels and sublevels of integration in CPD methodologies

METHODS

To establish the scope and extent of literature to be covered and reviewed, a systematic procedure was adopted. The type of documents that were considered in the search (Web of Science and Scopus), included research and/or project reports, journal articles, book chapters, and dissertations in the chemical engineering field. The following search algorithm restricted to the title was used:

*(product) and (design * OR develop * OR formul * OR engineer *)*

Then, as the main interest of this paper was to select those documents, which could help to identify the major trends and main opportunities in the field of chemical product design, the list of documents was further restricted to those sources, which introduced a methodological approach that could be used as a framework to design chemical products, specifically using words of each of the levels and sublevels of integration mentioned in Figure 1. Finally, if there was a lack of information based on these criteria, the document was only considered for statistical purposes.

RESULTS AND DISCUSSION

More than 2500 documents were found with the aforementioned search algorithm (2085 in Scopus and 456 in Web of Science, with 429 common coincidences). Then, by applying further restrictions, the list was reduced to 200 relevant sources containing information on perspectives, methodologies and reviews about formulated chemical product design, as shown in Table 1.

Table 1: Type of selected contributions in CPD and their average publication year

Type of contribution	Perspective	Methodology	Review
Publications	35	157	8
Average publication year	2005.4	2009.7	2014.1

After analyzing the 157 documents on methodologies, it was found that the three levels are rather equally represented, as shown in Table 2. However, when considering the sublevels, some clearer trends can be distinguished. As it can be observed, BU and CO methodologies are the commonest in this category (73% and 64% of the MS/MD cases). On the other hand, the least represented sublevels in the MS/MD category of integrated methodologies in the CPD scene are SU and MS, accounting for only 18% and 14% of the documents, respectively. It is important to notice that these two sublevels are also the latest to be included for the first time in a methodology for CDP: 2006 for MS and 2008 for SU. As a matter of fact, MS integration is still regarded as one of the major challenges to be faced by the chemical process and product engineering (Charpentier, 2010). Compared to other dimensions, sustainability has only very late started to be taken into account in the field of CPD methodologies (2014.5 in average), despite the great importance it has for the chemical process industry (Grossmann, 2004).

Table 2: Documents by type of integration levels and sublevels

Integration level	EM	PP	MS/MD	Total
Number of publications	111	117	98	157
Average publication year	2009.9	2009.4	2010.7	2009.7
First publication year	1996	1996	1996	1996

Integration sublevel	EM	PP	MS	CO	BU	SU	Total
Number of publications	96	118	14	63	72	18	157
Average publication year	2009.9	2009.5	2011.6	2011.2	2010.5	2014.5	2009.7
First publication year	1998	1996	2006	2000	1996	2008	1996

As the main interest of this study is to classify the integrative methodologies to identify the key research opportunities for formulated products, the next step in the analysis was to investigate the comprehensiveness of the proposed methodologies. To do this, the number of different levels and sublevels of integration considered in each one of these 157 documents was counted. Table 3 contains the publications grouped by the number of integrated levels and sublevels, respectively². As it can be seen, 78% of the identified sources (122) incorporate at least two of the three levels proposed in this study, and almost a third of all (47) sources incorporate the three main levels of integration. When considering the sublevels, around half of the methodologies consider at least three sublevels (75), but only 5% of total sources (8) come up to five or more sublevels, including three very recently published articles, which deliver a methodology with all the six sublevels (Ng, 2015; Fung *et al.*, 2016; Zhang *et al.*, 2017).

² Arabic digits were chosen for the number of levels, while Roman ones for the number of sublevels.

Table 3: Methodologies by the number of combinations of integration levels and sublevels

Number of levels	1	2	3	Total
Number of publications	35	75	47	157
Average publication year	2008.9	2009.1	2011.3	2009.7
First publication year	1998	1996	2000	1996

Number of sublevels	I	II	III	IV	V	VI	Total
Number of publications	30	52	50	17	5	3	157
Average publication year	2008.1	2008.4	2010.8	2010.6	2014	2016	2009.7
First publication year	1998	1996	2001	2000	2009	2015	1996

Finally, in Figure 2, we present detailed information about the 28 specific combinations found on each level and sublevel, that enables the exploration of the opportunities in the CPD domain.

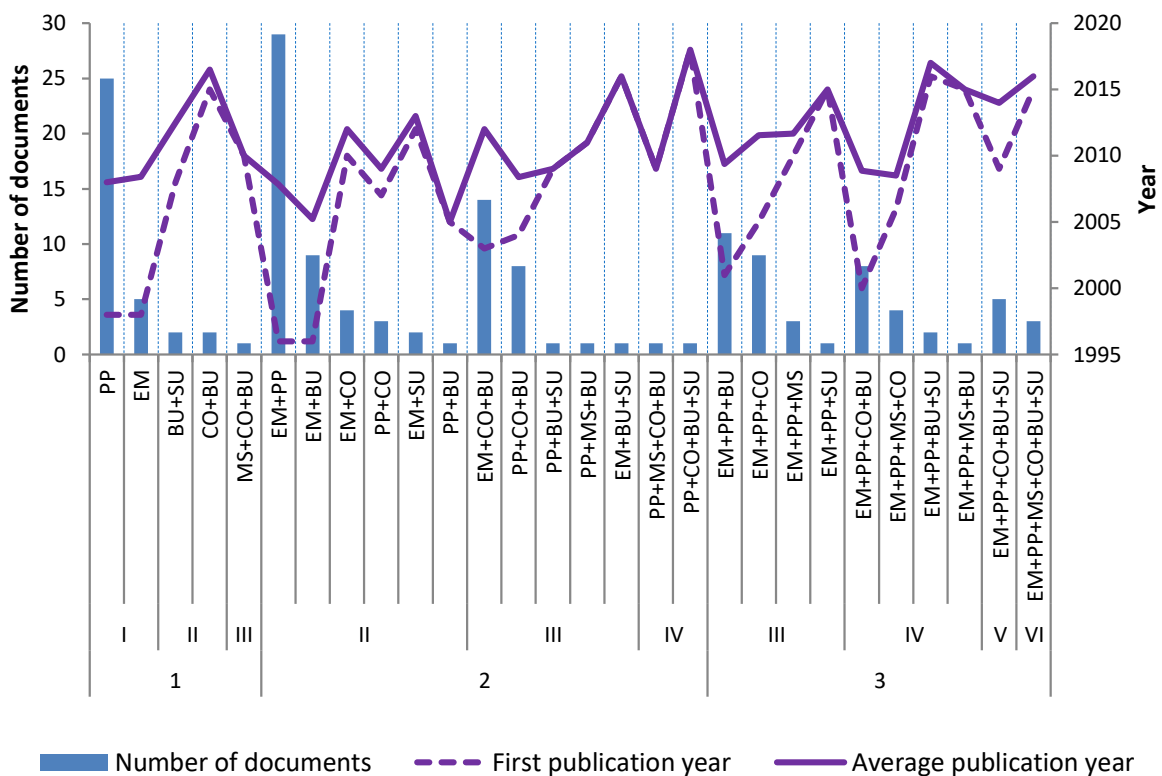


Figure 2: Detailed combinations of integration levels and sublevels

This figure could be considered as a picture of the current portfolio on CPD methodologies focused on formulated products, which could facilitate the integration of the existing strategies, to deliver new propositions on combinations that have no representation on the chart. At the same time, it could be

seen as a roadmap to understand historical trends, by looking at the difference between the first publication and the average publication year. Noteworthy is, in the case of fully integrated methodologies (3 levels for example), the complexity of incorporating the multiscale and/or sustainability dimensions is reflected on both the number of documents and the difference between the first and the average publication year for combinations without any of these sublevels and those considering them. This fact becomes more evident if we calculate the total number of missing combinations (35) and observe how many of them have not incorporated MS or SU sublevels: 71% and 66%, respectively. One of the main highlights of this analysis is that there is a large collection of available heuristic knowledge and property models for formulated products (Wibowo and Ng, 2001), which could be incorporated into a systematic methodology for its design (Arrieta-Escobar *et al.*, 2019).

CONCLUSION

From this study, it can be seen that systematic integrated approaches for formulated products are on the top of the current challenges in CPD. Nevertheless, only a few methodologies have proposed an integration covering the different levels and sublevels presented in this study. The classification made here could facilitate the task of creating new methodologies for formulated products. Considering the current state of the art of CPD, and in particular the opportunities regarding integrated methodologies for formulated product design, the research efforts should be concentrated in incorporating the consumer insight and some business decision variables along with hybrid experience/modelling tools to guide the product/process design of a well-known structured product. The inclusion of sustainability and/or multiscale dimensions in new fully integrated methodologies is also one of the main challenges for CPD.

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